specific criteria set jointly by the U.S. Department of Health and Human Services and the USEPA in order to become an NPL site.

RCRA Administrative Action Tracking System (RAATS): This database contains records based on enforcement actions issued under RCRA pertaining to major violators and includes administrative and civil actions brought by the EPA. For administration actions after September 30, 1995, data entry in the RAATS database was discontinued. The EPA will retain a copy of the database for historical records. It was necessary to terminate RAATS because a decrease in agency resources made is impossible to continue to update the information contained in the database.

RCRA Corrective Action Report (CORRACTS): The USEPA maintains this database of Resource Conservation and Recovery Act (RCRA) facilities that are undergoing "corrective action." A "corrective action order" is issued pursuant to RCRA Section 3008(h) when there has been a release of hazardous waste or constituents into the environment from a RCRA facility. Corrective actions may be required beyond the facility's boundary and can be required regardless of when the release occurred, even if it predated RCRA.

RCRA Registered Small or Large Generators of Hazardous Waste (GNRTR): The RCRA Large and Small Quantity Generators database is a compilation by the USEPA of facilities, which report generation, storage, transportation, treatment, or disposal of hazardous waste.

Resource Conservation and Recovery Information System (RCRIS): The RCRIS database includes selective information on sites that generate, transport, store, treat, and/or dispose of hazardous waste as defined by the Resource Conservation and Recovery Act (RCRA).

Records of Decision (ROD): ROD documents mandate a permanent remedy at an NPL (Superfund) site containing technical and health information to aid in the cleanup.

Superfund (CERCLA) Consent Decrees (CONSENT): These are major legal settlements that establish responsibility and standards for cleanup at NPL (Superfund) sites. They are released periodically by United States District Courts after settlement by parties to litigation matters.

Toxic Release Inventory System (TRIS): All facilities that manufacture, process, or import toxic chemicals in quantities in excess of 25,000 pounds per year are required to register with the USEPA under Section 313 of the Superfund Amendments and Reauthorization Act (SARA Title III) of 1986. Data contained in the Toxic Release Inventory (TRI) system covers approximately 20,000 sites and 75,000 chemical releases.

Toxic Substances Control Act (TSCA): This database identifies manufacturers and importers of chemical substances included on the TSCA Chemical Substance Inventory list. It includes data on the production volume of these substances by plant site.

3.2.2 State Sources State of California ASTM Records:

Aboveground Petroleum Storage Tank Facilities (AST): This is a database of registered aboveground storage tanks. It is maintained by the State Water Resources Control Board.

Annual Workplan Sites (AWP): California DTSC's Annual Workplan identifies known hazardous substance sites targeted for cleanup. The source of this database is the California Environmental Protection Agency.

CA Bond Expenditure Plan: (CA BOND EXP. PLAN): The Department of Health Services has developed a site-specific expenditure plan as the basis for an appropriation of Hazardous Substance Cleanup Bond Act funds.

Cal-Sites: This database contains both confirmed and potential hazardous substance release properties.

reported hazardous material incidents (accidental releases or spills).

California Facility Inventory Database (CA FID UST): The Facility Inventory Database (FID) contains a historical listing of active and inactive underground storage tank locations for the State Water Resource Control Board. Refer to local/county sources for current data.

CA UST: This database contains information gathered from the local regulatory agencies on active UST facilities

California Waste Discharge System (CA WDS): This database lists sites that have been issued waste discharge requirements.

"Cortese" California Hazardous Material Incident Report System (CORTESE): The California Environmental Protection Agency/Office of Emergency Information maintains this database. CORTESE sites are identified public drinking water wells with detectable levels of contamination, hazardous substance sites selected for remedial action, sites with known toxic material identified through the abandoned site assessment program sites with USTs having a reportable release and all solid waste disposal facilities from which there is know migration.

Cleaners: This is a list of dry-cleaning related facilities that have EPA ID numbers. These are facilities with certain SIC codes: power laundries, family and commercial; garment pressing and cleaners' agents; linen supply; coin-operated laundries and cleaning; dry-cleaning plants except rugs; carpet and upholster cleaning; industrial launderers; laundry and garment services.

Hazardous Waste Information System (HAZNET): The database contains notification of facility and manifest data. The data is extracted from the copies of hazardous waste manifests received each year by the DTSC. Data are from the manifests submitted without correction, and therefore many contain some invalid values for data elements such as generator ID, TSD ID, waste category, and disposal method.

Historical Underground Storage Tanks (HIST UST): This is a database of historical listings of underground storage tanks. Refer to local/county source for current data.

Leaking Underground Storage Tanks (LUST): This database is provided by the California Environmental Protection Agency.

Proposition 65 Records (Notify 65): This database contains facility notifications about any release that could impact drinking water and thereby expose the public to a potential health risks.

Solid Waste Information System SWL/LF (SWIS)): This database typically contains an inventory of solid waste disposal facilities or landfills. These may be active or inactive facilities or open dumps that failed to meet RCRA Section 4004 criteria for solid waste landfills or disposal sites.

Toxic Pits: This database identifies sites suspected of containing hazardous substances where cleanup has not yet been completed.

Underground Storage Tank (UST): This database contains information on active underground storage tanks facilities. The information is gathered from the local regulatory agencies.

Waste Management Unit Database (WMUDS/SWAT): The WMUDS is used by the State Water Resources Control Board staff and the Regional Water Quality Control Boards for program tracking and inventory of waste management units. WMUDS is composed of the following databases: Facility Information, Schedules Inspections Information. Waste Management Unit Information, SWAT Program Information, SWAT Report Summary Information, SWAT Report Summary Data, Chapter 15 Information, Chapter 15 Monitoring Parameters, TPCA Program Information, Closure Information, and Interested Parties Information.

3.2.3 Standard Environmental Record Searches

3.2.3.1 Subject Site

Available public records were reviewed. The lists, which were reviewed, identified two regulatory sites reported within the boundaries of the subject site (refer to Exhibit 4,

- **Propulsion Controls Engineering (1304 Sampson Street):** This property was listed within the San Diego County Hazardous Materials Management Division Database (San Diego Co. HMMD). The San Diego Co. HMMD database contains the business name, site address, business phone number, establishment permit number and type, and the business status. Additionally, the database provides inspection dates, violations received by the establishment, hazardous waste generated, the quantity, method of storage, treatment/disposal of waste and hauler, and information on USTs. This database also includes a unauthorized release list, which includes a summary of environmental contamination cases in San Diego County.

According to the EDR Database, the subject site maintains an active San Diego County HMMD permit. There is a small quantity generator on site, for which violations exist. Additionally, the site produces the following hazardous waste: asbestos-containing waste, other inorganic solid waste, waste oil and mixed oil, liquids with halogenated organic compounds, and unspecified organic liquid mixture with a reported disposal method of disposal, landfill, and recycler. Since no contamination was reported for the site, the potential for an environmental condition to exist on-site as a result of this business is considered to be low.

- **San Diego Gas & Electric Silvergate Power Plant (1348 Sampson Street)**: This property was listed within the Resource Conservation and Recovery Act Information–Small Quantity Generator (RCRA-SQG), Facility Index System/Facility Identification Initiative Program Summary Report (FINDS), AST, Historical Underground Storage Tank (HIST UST), and LUST databases. The RCRA-SQG database includes selective information on site which generate, transport, store, treat and/or dispose of quantity generators. SQGs generate between 100kg and 1,000kg of hazardous waste per month. The FINDS database contains both facility information and guidance to other sources that contain more detail. The AST database contains information on sites that maintain aboveground petroleum storage tank facilities. The HIST UST database is a historical listing of UST sites. The LUST database maintains information on leaking underground storage tank incident reports.

  According to the EDR Database the subject site maintains a small quantity generator, however no violations exist. There are five historical USTs reported for the subject site which were used to store diesel fuel and waste. One 21,459-gallon AST is present within the subject site as well. Diesel contamination occurred to soil only within the subject site. The case was closed on February 4, 1988. Additionally, the subject site has an inactive San Diego Co. HMMD permit. The potential for an environmental condition to occur on-site appears to be low due to the status of the subject site.

3.2.3.2 All Regulatory Listed Sites Within a One-Mile Radius of the Subject Site

The lists identified fifty-five listed regulatory properties located within a one-mile radius of the subject site. A potential REC on the subject site caused by these properties is considered to be high due to the groundwater flow direction towards the subject site, proximity of the subject site, and/or the status of the identified site. For the complete EDR lists, refer to Appendix A, *EDR Search*. Table 4, *Identified Sites Within a ½-Mile Radius of the Subject Site*, below, indicates the listed regulatory sites located within a one-mile radius of the subject site.

3.2.4 Additional Environmental Record Searches

No additional environmental records searches were performed during the preparation of this Assessment.

Table 4
IDENTIFIED SITES WITHIN A ½-MILE RADIUS OF THE SUBJECT SITE
(Were Identified in the Regulatory Database)

EDR Map ID#	Site Name/Address	Direction from Subject Site	Regulatory List	Site Status	Potential for an Environmental Condition on the Subject Site
A1	Propulsion Controls Engineering 1304 Sampson Street	**Subject Site**	San Diego Co. HMMD	Active San Diego County permit. Small quantity generator. Violations exist for all requirements. Asbestos-containing waste, other inorganic solid waste, waste oil and mixed oil, liquids with halogenated organic compounds, and unspecified organic liquid mixture. **Disposal Method: Disposal, Land Fill, Recycler.**	Low (No contamination reported)
B3-B7	Kelco, Division of Merck & Co., Inc. 2145 E. Belt Street	0.05-miles southwest of the subject site	LUST HIST UST FINDS Cortese TRIS EMI UST RCRA-SQG CERC-NFRAP	Waste oil contamination to soil only. Case closed on 8/15/1995. Diesel contamination to soil only. Preliminary site assessment underway. Ten HIST USTs on-site. Diesel contamination to soil only. Case closed on 3/26/1992. Kerosene contamination to soil only. Case closed on 9/28/1988. Unknown contamination to soil only. Remedial action underway. Unknown contamination to soil only. Case closed 8/20/1996. Diesel contamination to soil only. Case closed 8/21/1992. Unknown contamination, other groundwater and soil affected. Case closed 9/28/88. Gasoline contamination to soil only. Case closed February 10, 1997. Other inorganic solid waste. **Disposal Method: Disposal, Land Fill.** Small Quantity Generator – no violations found. CERCLIS-NFRAP list. Preliminary Assessment underway, however the site is not listed on the NPL.	**High** (Adjacent CERCLIS site)
C8	San Diego Gas & Electric Silvergate Power Plant	**Subject Site**	RCRA-SQG FINDS	Small Quantity Generator – no violations found.	**Moderate** (Material Threat)

	1348 Sampson Street		AST HIST UST LUST	Five historical USTs are reported for the subject site, used to store diesel fuel and waste. A 21,459 gallon AST is located on-site. Diesel contamination to soil only. Case Closed 2/4/1988. Inactive San Diego Co. HMMD permit.	
12	Solar Turbines 2201 Harbor Drive	0.07-miles east of the subject site	CA SLIC	Chrome 6, CR, MET, NOT substances released.	**Moderate** (Refer to site status)
D13	Chevron USA Inc. Bumble Bee Seafoods BP 2205 E. Belt	0.08-miles south of the subject site	RCRA-SQG FINDS HIST UST	Small Quantity Generator – no violations found. Three historical USTs reported on-site.	Low (No contamination reported)
15-16	Supervisor of Shipbuilding Conversion at Foot of Sampson Street, Sunship ·OFC	0.09-miles south of the subject site	FINDS HAZNET RCRA-LQG PADS Notify 65 HAZNET LUST Cortese RCRA-LQG UST San Diego Co. HMMD CERC-NFRAP EMI	Large Quantity Generator, no violations found. Detergent and soap, unspecified oil-containing waste, unspecified solvent mixture waste, other organic solids. **Disposal Method: Transfer Station, Recycler, Not Reported.** CERCLIS-NFRAP listed, preliminary site assessment underway. No on the NPL. Large Quantity Generator – violations exist. Contamination released from tank to soil only. Case closed 7/13/98. Asbestos-containing waste, aqueous solution, other inorganic solid waste. **Disposal Method: Disposal, Land Fill, Treatment, Tank, Not reported.** Inactive San Diego County HMMD permit.	**High** (Adjacent CERCLIS site)
E17-E19	Marine Barge Services, Inc. 2146 Main Street	0.13-miles northeast of the subject site	RCRA-SQG FINDS CERC-NFRAP	Small Quantity Generator. No violations found and violations found. Listed in CERCLIS-NFRAP database. Preliminary assessment underway. Not on the NPL.	**High** (Adjacent CERCLIS site)
E20-E23	SDG&E Tanks 801 and 802 2141 Main Street	0.13-miles northeast of the subject site	RCRA-SQG FINDS LUST HIST UST Cortese San Diego Co.	Small Quantity Generator – no violations found. Contamination to soil and other groundwater. Case closed 10/13/1994. Tanks on-site used for Inactive San Diego County HMMD permit.	Low (Refer to site status)
F24-F26	Cleaning Dynamics/Pacific Treatment Corp. 2190 Main Street	0.14-miles northeast of the subject site	REF HAZNET LUST	Preliminary assessment done. Recommended to check for the evidence of contamination. Submit to	**HIGH** (Adjacent CERCLIS site)

			Cortese RCRIS-SQG FINDS RCRA-TSDF CORRACTS CERC-NFRAP Tx. Ind. Haz. Waste	EPA. Large industrial cleaning yard with evidence of hazardous materials. Site closure plan approved on 9/17/1991. Undergoing closure oversight. Facility to submit workplan for arsenic contamination removal and HRA in 94/95. According to AWP, closure to be completed by 94/95 FY. Recommended NFA for Site Mitigation Branch. Contamination, other groundwater affected. Remedial action underway. Aqueous solution. **Disposal Method: Recycler.** Listed on CERCLIS-NFRAP, preliminary assessment. Not listed on NPL. Facility was assigned a low corrective action priority. RCRA info – violations exist. Diesel contamination, other groundwater affected. Remedial action underway.	
F27	Southwest Marine Inc. 2201-2399 Main Street	0.14-miles northeast of the subject site	LUST Cortese	Unknown contamination released to soil only. Case closed 11/3/98.	Low (Refer to site status)

G28-G35	Continental Maritime of San Diego 1995 Bayfront Street	0.16-miles northwest of the subject site	FINDS HAZNET RCRIS-LQG LUST CHMIRS RCRA-LQG CERC-NFRAP RCRA-SQG Cortese San Diego Co. HMMD HIST UST	Large Quantity Generator – no violations found. Other inorganic solids, off-specification, aged, or surplus inorganics, adhesives, oxygenated solvents. **Disposal Method: Recycler, Transfer Station.** Diesel contamination, other groundwater affected. Case closed 2/24/1997. Listed in CERCLIS-NFRAP. Preliminary assessment. Not listed on NPL. Large Quantity Generator – violations exist. Regular gasoline released to soil only. Leak being confirmed. Case 9UT138: Diesel contamination, soil and other groundwater affected. Case closed 5/25/1989. Case 9UT2467: Unknown contamination. Drinking water aquifer affected. Case closed 2/24/97. Case 9UT2996: Diesel contamination, other groundwater affected. Preliminary site assessment underway. Transmission fluid released to San Diego Bay trough outfall of storm drain. Spill has been contained. Some residual staining remains on the ground. Small Quantity Generator – no violations found. Hydraulic fluid released. No cleanup underway. Inactive San Diego Co. HMMD permit. Small Quantity Generator – no violations found. Four USTs used to store diesel, premium, and regular fuel.	**High** (Adjacent CERCLIS site and groundwater contamination)
H36	CP Kelco 2025 E. Harbor Drive	0.17-miles northwest of the subject site	FINDS RCRA-LQG LUST San Diego Co. HMMD	Large Quantity Generator. Violations exist. Unleaded gasoline released to soil only. Remedial action underway. Diesel contamination to soil only. Case closed 12/31/2001. San Diego HMMD Permit: Hazardous materials stored on-site and USTs present on-	**Moderate** (Refer to site status)
I39-I45	Atlantic Richfield Co. San Diego Term. 2295 E. Harbor Drive	0.19-miles southeast of the subject site	FINDS RCRA-LQG LUST Cortese UST	Large quantity generator – no violations found. Case 9UT3030: Unknown contamination to soil and other groundwater. Preliminary site assessment	**Moderate** (Refer to site status)

			TRIS San Diego Co. HMMD EMI HIST UST	underway. Case 9UT3218: Unknown contamination, other groundwater and soil affected. Preliminary site assessment underway. Case 9UT2279: Unknown contamination, other groundwater affected. Preliminary site assessment underway. MTBE detected. Case 9UT3986: Unleaded gasoline contamination, other groundwater and soil affected. Preliminary site assessment underway. Case 9UT19: Unknown contamination. Other groundwater affected. MTBE detected on-site. Case closed 4/20/1987. Active San Diego HMMD permit – Hazardous materials, USTs, and waste streams reported. One HIST UST reported on-site.	
46	Chevron Pipeline Rupture Belt Street/Sicard Street	0.19-miles southeast of the subject site	CA SLIC	State SLIC site.	**High** (Refer to site status)
J47-J48	Carlson and Beauloye 2141 Newton Avenue	0.20-miles northeast of the subject site	LUST Cortese RCRA-SQG FINDS HAZNET San Diego Co. HMMD EMI	Case 9UT1576: Chromic acid released to soil only. Case closed 12/9/1992. Small Quantity Generator – violations exist. Unspecified oil-containing waste, other inorganic solid waste, metal sludge. **Disposal Method: Recycler, Not Reported, Transfer Station.** Active San Diego County HMMD: Hazardous materials on-site, USTs, and waste streams. Located within the San Digeo County APCD.	Low (Refer to site status)
K49-K50	Master Plating 2109 Newton Avenue	0.20-miles northeast of the subject site	RCRA-SQG FINDS San Diego Co. HMMD CERCLIS HAZNET	Small Quantity Generator – violations exist. Inactive San Diego Co. HMMD permit. Non-NPL status: Removal only site (no site assessment work needed). Other inorganic solid waste, other organic solids. **Disposal Method: Transfer Station.**	Low (Refer to site status)
51	Southbay Sandblasting and Tank Clean 1995 Bayfront Street, Pier 1, 2, 3	0.20-miles northwest of the subject site	FINDS RCRA-LQG	Large Quantity Generator – no violations found.	Low (No contamination reported)

L52- L54	Willig Freight Lines 2286 Main Street	0.21-miles east of the subject site	HIST UST LUST Cortese San Diego Co. HMMD	One UST located on-site used to store diesel fuel. Unknown contamination to soil only. Case closed 7/25/1991. Case 9UT880: Diesel contamination to soil only. Case closed 5/27/1988. Inactive San Diego Co. HMMD permit. Violations of HMMD permit exist.	Low (Refer to site status)
M55	Performance Contracting, Inc. 2015 Main Street	0.21-miles north of the subject site	RCRA-SQG FINDS	Conditionally exempt small quantity generator. No violations exist.	Low (No contamination reported)
L56- L59	San Diego Express Inc. 2304 Main Street	0.21-miles east of the subject site	RCRA-SQG LUST San Diego Co. HMMD HIST UST Cortese FINDS	Small Quantity Generator. No violations exist. Case 9UT2130: unknown contamination released to soil only. Case closed 6/20/1996. Inactive San Diego Co. HMMD. Three historical USTs on-site.	Low (Refer to site status)
M60- M62	P&L Knepp Trucking 2001 Main Street	0.23-miles north of the subject site	LUST Cortese San Diego Co. HMMD HIST UST	Case 9UT862: Unknown contamination, other groundwater affected. Case closed 6/16/94. Inactive San Diego Co. HMMD Permit. Two historic USTs on-site used to store diesel and unleaded fuel.	Low (Refer to site status)
N63- N66	Chevron Bulk Terminal 2351 E. Harbor Drive	0.23-miles southeast of the subject site	LUST HAZNET RCRA-LQG HIST UST UST Cortese EMI	Unleaded gasoline contamination, other groundwater affected. Remedial action (cleanup) underway. Large quantity generator. Violations exist. Case 9UT0015: unknown contamination, other groundwater affected. Remedial action underway. Aqueous solution, off-specification, aged, or surplus organics, waste oil and mixed oil, contaminated soil from site clean-ups, oil/water separation sludge. **Disposal Method: Recycler, Disposal, Land Fill, Transfer Station.** Six historic USTs used for waste and waste oil. Unleaded gasoline contamination to soil only. Case closed 12/5/2001.	**Moderate** (Refer to site status)
[illegible]	2043 Newton Avenue	north of the subject site	Cortese	Unleaded gasoline released to soil only. Case closed 4/26/2001.	(Refer to site status)

Note: Map ID numbers match the site numbers indicated on the map of sites within one-mile radius contained within Appendix A, *EDR Search.*

POTENTIAL FOR ENVIRONMENTAL CONDITION KEY:

Low Potential=Potential to create environmental conditions on subject site is considered to be low for one or several factors including, but not limited to, the following:

> direction of groundwater flow is away from the subject site (down gradient); remedial action is underway or completed at off-site location; distance from subject site is considered great enough to not allow the creation of a potential environmental condition; only soil was affected by the occurrence; and/or reporting agency has determined no further action is necessary.

Moderate Potential=Potential to create environmental condition on subject site is considered to be moderate and further investigation may be necessary due to one or several factors including, but not limited to, the following:

> occurrence reported but remedial status unknown; unable to confirm remedial action completed; proximity to subject site; groundwater flow is towards the subject site (up gradient).

High Potential= Potential to create environmental condition on subject site is considered to be high and further investigation necessary due to one or several factors including the following:

> occurrence noted on-site and status if remedial action unknown; occurrence affected groundwater and is located up gradient from subject site.

4.0
POTENTIAL AREAS OF ENVIRONMENTAL CONCERN

The following section documents the result of the visual site inspection conducted by RBF on February 1, 2005 and February 24, 2005 and identifies potential areas in which an environmental condition could arise. Refer to both on and off-site photographs taken on February 1, 2005 and February 24, 2005 at the end of this section as a general visual reference. For information regarding results of the historical and governmental records searches, refer to Section 3.0, HISTORICAL AND REGULATORY INFORMATION SEARCHES.

4.1 ON-SITE OBSERVATIONS

4.1.1 Methodology and Limiting Conditions

The objective of the site reconnaissance is to obtain information indicating the likelihood of identifying RECs, including hazardous substances and petroleum products in connection with the property (including soils, surface water, and groundwater). During the February 1, 2005 and February 25, 2005 site inspections, RBF performed a visual observation of readily accessible areas of the subject site and immediately adjoining properties.

4.1.2 Description of On-Site Structures and/or Uses

The main plant structure contains four generating units, numbered 1, 2, 3, and 4. The building structure in **Area 1** is approximately 490 feet long by 125 feet wide and consists of six floors, a mezzanine, and a basement. The basement is located approximately 16 feet below street level. The building houses six boilers and four steam turbine-driven generating units.

The switchyard (**Area 2**) which also contains substation equipment is a group of exposed steel framed structures with a complex wiring system located north of **Area 1**. **Area 2** previously acted as a switchyard for the active power plant. Today the area is an active San Diego Gas & Electric substation. Several underground storage tanks, and associated electrically driven pumps used to store fuel oil are located under the substation. Four aboveground control houses are located in **Area 2**.

Area 3 consists of a parking lot and a miscellaneous equipment storage area. The property is approximately 40 feet wide and is rented by Kelco, Inc.

Area 4 is owned and operated by Propulsion Controls Engineering. The property consists of one structure and a parking lot/maintenance yard located to the west and south of the structures.

Table 4
Summary of Site Reconnaissance

Feature and Description	Observed	Not Observed
Structures	X	
Evidence of past uses	X	
Hazardous substances and/or petroleum products	X	
Aboveground storage tanks (ASTs)	X	
Underground storage tanks (USTs) or evidence of USTs	X	
Undocumented pipe(s)		X
Strong, pungent, or noxious odors		X
Pools of liquid likely to be hazardous materials or petroleum products	X	
Drums	X	
Unidentified substance containers	X	
Miscellaneous debris	X	
Dirt piles		X
Potential polychlorinated biphenyl (PCB)-containing equipment	X	
Subsurface hydraulic equipment	X	
Heating/ventilation/air conditioning (HVAC)	X	
Stains or corrosion on floors, walls, or ceilings	X	
Floor drains and sumps	X	
Pits, ponds, or lagoons	X	
Stained soil and/or pavement	X	
Stressed vegetation		X
Waste or wastewater discharges to surface waters on subject site, including stromwater		X
Wells (agriculturally related)		X
Septic Systems		X

4.1.3 Asbestos Containing Material

Asbestos is a strong, incombustible, and corrosion resistant material which was used in many commercial products since prior to the 1940's and up until the early 1970's. If inhaled, asbestos fibers can result in serious health problems. ACMs are building materials containing more than one percent (1%) asbestos (some state and regional regulators impose a one tenth of one percent (0.1%) threshold). Based on the year the existing structure was constructed, prior to 1978, the potential for ACMs to be found on-site is considered likely.

4.1.4 Lead-Based Paints

Until 1978, when the U.S. Consumer Product Safety Commission (CPSC) phased out the sale and distribution of residential paint containing lead, may homes were treated with paint containing some amount of lead. It is estimated that over 80 percent of all housing built prior to 1978 contains some LBP. The mere presence of lead in paint may not constitute a material to be considered hazardous. In fact, if in good condition (no flaking or pealing), most intact LBP is not considered to be a hazardous material. In poor condition LBPs can create a potential health hazard for building occupants, especially children. Based on the year the existing structure was constructed, prior to 1978, the potential for LBPs to be found on-site is considered likely.

No indication of on-site solid waste disposal practices (i.e., landfills) was apparent during the February 1, 2005 and February 25, 2005 site inspections. Although no land-filling operations were noted, miscellaneous debris (e.g., equipment, drums) was observed throughout **Area 3**. RBF could not visually observe the ground surface conditions under the debris.

4.1.6 Utilities

Area 2 of the subject site consisted of an active electrical substation. Initiating at the subject station were numerous power lines. These lines traversed the surrounding properties. Patches of staining were noted within the substation area during the February 1, 2005 and February 25, 2005 site inspections. However, no staining with respect to the properties to the north was noted on the surrounding properties.

4.1.7 Polychlorinated Biphenyls (PCBs)

PCBs are ubiquitous in the environment and are stable even at high temperatures. PCBs have been widely used in transformer fluids and dielectrics. Due to health impacts, the Environmental Protection Agency (EPA) banned some uses of PCBs in 1977 and most production in 1979. However, many transformers and other materials (e.g., capacitors and hydraulic fluids) still contain PCBs. Such items made after 1979 are required to be properly labeled/marked and specific records maintained.

Several transformers were noted on-site in **Area 2** during the February 1, 2005 and February 25, 2005 site inspections. No evidence of di-electric fluid or staining associated with the transformers was noted on-site during the February 1, 2005 and February 24, 2005 field reconnaissance. Additionally, fluorescent lamps and lightbulbs were noted within the subject site. Fluorescent lamp ballasts typically contain capacitors, and therefore, may contain PCBs. Capacitors are generally provided with a nameplate, power rating, serial number, test number, and type number. Generally, capacitors in service before 1978 are likely to contain PCBs.

4.1.8 Chemical Storage Tanks

During the February 1, 2005 and February 25, 2005 site inspections the subject site was inspected for fill pipes, vent pipes, areas of abnormal or heavy staining, manways, manholes, access covers, concrete pads not homogenous with surrounding surfaces, concrete build-up areas potentially indicating pump islands, abandoned pumping equipment, or fuel pumps. Several manholes were noted within Area 2 during the February 1, 2005 and February 25, 2005 site inspections. It was indicated by SDG&E staff that USTs were located below the manholes. Additionally, within the interior of the structure in Area 1, several structures and containers were labeled as containing chemicals. SDG&E staff indicated that all on-site USTs have been emptied. According to an interview, chemicals are stored within **Area 4** of the subject site as well.

4.1.9 Undocumented Pipes

No undocumented pipes were noted during the February 1, 2005 and February 25, 2005 site inspections.

4.1.10 Aboveground Storage Tanks

inspected for fill pipes, vent pipes, areas of abnormal or heavy staining, manways, manholes, access covers, concrete pads not homogenous with surrounding surfaces, concrete build-up areas potentially indicating pump islands, abandoned pumping equipment, or fuel pumps. Several ASTs were noted within **Area 1** of the subject site.

The specific use of these ASTs remains undefined, however several were labeled as historically containing chemicals.

4.1.11 Spills

Surficial staining was noted throughout the subject site. In **Area 1** staining was noted within the on-site structure near the generators. In **Area 2** staining was noted at the base of several of the on-site structures. This staining was noted as being heavy and dark. The staining within **Area 3** and **Area 4** consists of staining associated with automobiles. Access to the ground surface underneath the stockpiled equipment and debris was not available during the February 1, 2005 and February 25, 2005 site inspections.

4.1.12 Wells

No wells were noted within the subject site during the February 1, 2005 and February 25, 2005 site inspections. However, equipment that was utilized to bring water into and expel water from the power plant were noted within **Area 1**.

4.1.13 Pits, Ponds, Lagoons

No evidence of pits, ponds, or lagoons was observed within the subject site during the February 1, 2005 and February 25, 2005 site inspections. However, open water was noted within the western portion of **Area 1**. The previous Phase I and II ESAs indicate that a settling pond was historically located on-site and had been buried. Mr. Carr of PCE indicated that his property has its own on-site stormwater drainage system.

4.1.14 Septic Systems

Residential septic systems are possible receivers of household waste and can be the source for soil and groundwater contamination. Active and abandoned residential structures not connected to the city sewer are likely to have septic systems. No visible evidence of septic tanks or cesspools was observed on-site during the February 1, 2005 and February 25, 2005 site inspections.

4.1.15 Miscellaneous Observations

Numerous gauges were noted within the interior of the on-site structures. Due to the year the structures were constructed and the equipment utilized, it is likely that mercury is present within the gauges.

4.2 OFF-SITE OBSERVATIONS

As previously stated in Section 2.0, *Physical Setting*, an adjoining property is considered any real property or properties that the border of which is contiguous or partially contiguous with that of the subject site, or that would be contiguous or partially contiguous with that of the subject site but for a street, road, or other public thoroughfare separating them. An adjacent property is any real property located within 0.25 miles of

adjoining properties were conducted on February 1, 2005 and February 24, 2005 as part of this Assessment and are described below.

4.2.1 Utilities

Typical utilities (power lines) were noted along adjoining roadways and within adjacent properties during the February 1, 2005 and February 25, 2005 site inspections.

4.2.2 Tanks

No evidence of ATSs and USTs were visible within the adjoining properties during the February 1, 2005 and February 25, 2005 site inspections. However, it is anticipated that USTs and ASTs are present within the surrounding properties based on the industrial usage of the area.

4.2.3 Hazardous Materials

During a preliminary observation of accessible adjoining properties on February 1, 2005 and February 24, 2005, no visible or physical evidence was observed to suggest that a surface release of petroleum based material has recently occurred. No unusual or suspicious materials handling or storage practices were observed with respect to adjacent properties.

4.2.4 Railroad Tracks

Several railroad tracks are present to the north and south of the subject site.

Exhibit 5a, *On-Site Photographs*

Exhibit 5b, On-Site Photographs

Exhibit 5c, On-Site Photographs

Exhibit 5d, On-Site Photographs

Exhibit 6, Off-Site Photographs

5.0
FINDINGS, OPINIONS, AND RECOMMENDATIONS

RBF has performed a Phase I Environmental Site Assessment in conformance with the Scope-of-Services and limitations of ASTM Standard Practice E 1527-00 within parcels 538-700-01, 02, and portions of 05 and 06 located within the City of San Diego, County of San Diego; also known as the subject site within this Assessment. Any exceptions to, or deletions from, this practice are described in Section 1.0, INTRODUCTION, of this report. This Assessment has revealed the following in connection with the subject site.

5.1 FINDINGS

5.1.1 Site Conditions

Evidence of RECs within the boundary of the subject site were observed during the February 1, 2005 and February 25, 2005 site inspections, and consist of the following:

- The subject site consists of industrial-type uses. The majority of the subject site is situated on concrete or asphalt foundations. Typically, chemicals from on-site uses and maintenance operations include oil and grease, solvents, and gasoline. The use of the subject site as a power plant and substation is considered to pose a potential REC.
- Cracked and peeling paint was noticed throughout the power plant, especially on the ceiling. Based on the year the structure was constructed, it is likely that lead based paints are present within the wall and ceiling paint.
- Hundreds of 55-gallon drums were stockpiled within **Area 3** of the subject site. The contents and specific use of the drums remains undefined.
- Stockpiled equipment was noted through **Area 3**. The equipment was located on wood pallets. However, the ground surface underneath the equipment could not examined.
- Surficial staining was noted throughout the subject site. Within **Area 1** the staining was noted on floor tiles and appeared to consist of diesel or fuel. Within **Area 2**, the staining was noted at the base of the substation infrastructure. In **Areas 3** and **4** the staining was noted on the ground surface and appeared to be typical staining of parking lots. This staining appeared to consist of grease or fuel and was located on concrete, rocks, and dirt. The on-site stained surfaces are considered to be a potential REC since the extent of contamination remains undefined.
- It was noted that the subject site has hydraulic lifts on-site. Due to health impacts, the Environmental Protection Agency (EPA) banned some uses of PCBs in 1977 and most production/use in 1979. However, many hydraulic lifts [illegible] is the potential for subsurface leakages of hydraulic fluids from the lift's piston. RBF could not confirm the actual presence of PCBs associated with on-site lifts during the course of this ESA.

- Fluorescent lighting was noted within the on-site structure during the February 1, 2005 and February 25, 2005 site inspections. It should be noted that some fluorescent lamp ballasts contain capacitors, and therefore, may contain PCBs.

- **Area 2** of the subject site consists of the electrical substation. High voltage power lines and several transformers were noted within this area. Due to the age of the structures, it is likely that PCBs are present within the power lines and transformers.

- Several manholes were noted within **Area 2** of the subject site. It was indicated by SDG&E staff that underground storage tanks (USTs) are present below the manholes. It was also indicated that these USTs were used to store fuel oil. Several additional USTs were identified within the power plant structure. It was indicated that all tanks on-site are empty.

- Aboveground storage tanks (ASTs) were observed to occur within **Area 1** and **4** of the subject site.

- Railroad tracks are present within the subject site. The subject site was historically utilized as a lumberyard, and SDG&E staff noted that these tracks were utilized for transport. Due to the historical use of portions of the subject site as a railroad ROW and the known past practices of railroad companies to use diesel fuel as a method to control weeds, and the use of creosote to seal the wood railroad ties, the potential exists for soils within the railroad ROW to be contaminated.

- Numerous gauges are present within **Area 1** and **Area 2** of the subject site. Based on the year the structure was constructed, it is likely that mercury is present within the gauges.

5.1.2 Public Records

Available public records were reviewed. The lists, which were reviewed, identified two regulatory sites reported within the boundaries of the subject site (refer to Exhibit 4, *Overview Map*). The subject site was listed as the following:

- **Propulsion Controls Engineering (1304 Sampson Street)**: This property was listed within the San Diego County Hazardous Materials Management Division Database (San Diego Co. HMMD). The San Diego Co. HMMD database contains the business name, site address, business phone number, establishment permit number and type, and the business status. Additionally, the database provides inspection dates, violations received by the establishment, hazardous waste generated, the quantity, method of storage, treatment/disposal of waste and hauler, and information on USTs. This database also includes a unauthorized release list, which includes a summary of environmental contamination cases in San Diego County.

  According to the EDR Database, the subject site maintains an active San Diego County HMMD permit. There is a small quantity generator on site, for

  waste: asbestos-containing waste, other inorganic solid waste, waste oil and mixed oil, liquids with halogenated organic compounds, and unspecified organic liquid mixture with a reported disposal method of disposal, landfill, and recycler. The potential for an environmental condition to exist on-site as a result of PCE is considered to be low since no contamination was reported.

- **San Diego Gas & Electric Silvergate Power Plant (1348 Sampson Street):** This property was listed within the RCRA-SQG, FINDS, AST, HIST UST, and LUST databases. The RCRA-SQG database includes selective information on properties that generate, transport, store, treat and/or dispose of quantity generators. SQGs generate between 100kg and 1,000kg of hazardous waste per month. The FINDS database contains both facility information and guidance to other sources that contain more detail. The AST database contains information on sites that maintain aboveground petroleum storage tank facilities. The HIST UST database is a historical listing of UST sites. The LUST database maintains information on leaking underground storage tank incident reports.

  According to the EDR Database the subject site maintains a small quantity generator, however no violations exist. There are five historical USTs reported for the subject site which were used to store diesel fuel and waste. One 21,459-gallon AST is present within the subject site as well. Diesel contamination occurred to soil only within the subject site. The case was closed on February 4, 1988. Additionally, the subject site has an inactive San Diego Co. HMMD permit. The potential for an environmental condition to occur on-site appears to be low due to the status of the subject site.

The lists identified fifty-five listed regulatory properties located within a one-mile radius of the subject site. A potential REC on the subject site caused by these properties is considered to be high due to the groundwater flow direction towards the subject site, proximity of the subject site, and/or the status of the identified site. For the complete EDR lists, refer to Appendix A, *EDR Search.*

5.1.3 Historic Recognized Environmental Condition(s)

No HRECs have been noted within the boundaries of the subject site.

5.1.4 Historical Use(s) Information

Based upon the site inspection, review of available historical aerial photographs, and interview, the subject site has consisted of the Sivergate Substation since 1948. Prior to 1948 the subject site consisted of a lumberyard. Therefore, the potential that adverse environmental conditions were created by historic activities on-site is considered to be low.

5.1.5 Other Potential Sources of Hazardous Material

The presence of hazardous materials on the subject site that may have been generated from adjacent properties was not visually or physically evident.

5.2 CONSULTANT'S OPINION/RECOMMENDATION

The following opinions are based upon review of reasonable ascertainable referenced material available to RBF during the preparation of this Assessment, which included historical aerial photographs, historical topographic maps, regulatory databases,

5.3 FORMAL RECOMMENDATIONS

Based on the records and other data reviewed during the preparation of this Phase I Environmental Site Assessment, in accordance with ASTM Standard Practice E 1527-00 and the scope-of-services, and subject to the limitations thereof, the following measures are recommended:

All miscellaneous equipment, materials, wood pallets, 55-gallon drums, and miscellaneous stockpiled debris should be removed off-site and properly disposed of at an approved landfill facility. Once removed, a visual inspection of the areas beneath the removed materials should be performed. Any stained soils observed underneath the removed materials should be sampled. Results of the sampling (if necessary) would indicate the level of remediation efforts that may be required.

All floors within the interior of individual on-site structures within the subject site should be visually inspected prior to demolition or renovation activities. Should hazardous materials be encountered with any on-site structure, the materials should be tested and properly disposed of in accordance with State and Federal regulatory requirements. Any stained soils or surfaces underneath the removed materials should be sampled. Results of the sampling would indicate the appropriate level of remediation efforts that may be required.

Due to the visible evidence of surficial staining of potential oil/petroleum products located throughout the subject site, any stained concrete and soils should be excavated and removed to determine the exact vertical extent of the contamination. If during soil/concrete removal, staining (evidence of petroleum products) appears to continue below the ground surface, sampling should be performed to characterized the extent of contamination and identify appropriate remedial measures.

5.3.1 Asbestos Containing Materials

The National Emission Standards for Hazardous Air Pollutants (NESHAP) mandates that building owners conduct an asbestos survey to determine the presence of ACMs prior to the commencement of any remedial work, including demolition. Based on the year the on-site structures were built (prior to 1978) and according to the Phase I and Phase II ESAs conducted by IT Corporation, ACMs were identified and located on all floors of the power plant building, the administration building, and on all three roof levels of Silvergate. The majority of ACMs present within the subject site exist within the pipe insulation, boiler insulation, fire brick, roofing material, and other materials. Prior to demolition work, it is recommended that areas be sampled as part of an asbestos survey.

Some of the identified friable ACMs are damaged and debris is present on or around some boilers and pipes. Any demolition of the existing buildings must comply with State law, which requires a contractor, where there is asbestos-related work involving 100 square feet of more of ACMs, to be certified and that certain procedures regarding the removal of asbestos be followed. Workers should be notified of the presence of ACMs [illegible] implemented to prevent further damage of the ACMs.

5.3.2 Lead Based Paints

Based on the year the on-site structures were built (prior to 1978) and samples taken and analyzed in the previous Phase I and II ESAs, LBP is present on-site.

If during demolition and decommissioning activities of the structures, paint is separated from the building material (e.g., chemically or physically), the paint waste should be evaluated independently from the building material to determine its proper management. According to the Department of Substances Control, if paint is not removed from the building material during demolition (and is not chipping or peeling), the material could be disposed of as construction debris (a non-hazardous waste). It is recommended that the landfill operator be contacted in advance to determine any specific requirements they may have regarding the disposal or lead-based paint materials.

5.3.3 Underground Storage Tanks

Several USTs have historically been present within the boundaries of the subject site. The specific location of the documented USTs should be determined. Once found, the USTs should be removed and properly disposed of at an approved landfill facility. Once the USTs are removed, a visual inspection of the areas beneath and around the removed USTs should be performed. Any stained soils observed underneath the USTs should be sampled. Results of the sampling (if necessary) would indicate the level of remediation efforts that may be required.

5.3.4 Aboveground Storage Tank

According to the current on-site tenant interview, one 21,495 gallon AST is located on-site. However, several additional ASTs were noted during the site inspection. The specific location of all the on-site ASTs should be determined. If present, the ASTs should be removed and properly disposed of at an approved landfill facility. Once the ASTs are removed, a visual inspection of the areas beneath and around the removed ASTs should be performed. Any stained soils observed underneath the ASTs should be sampled. Results of the sampling (if necessary) would indicate the level of remediation efforts that may be required.

5.3.5 Polychlorinated Biphenyls

According to the Phase I ESA, Phase II ESA, and the February 1, 2005 and February 25, 2005 site inspections, PCBs are present within the subject site. The PCBs are present within the on-site transformers at a concentration of 50 ppm, the fluorescent light fixtures that likely contain PCBs in the light ballasts, hydraulic equipment, and other PCB containing articles and equipment.

Any potential PCB containing equipment to be removed/relocated should be conducted under the purview of the local utility purveyor to identify proper handling procedures regarding potential PCBs.

5.3.6 Railroad

Active and inactive railroad beds frequently have concentrations of petroleum products and lead elevated above natural background conditions. Petroleum product concentrations and lead concentrations are derived from drippings from rail vehicles and flaked paint, respectively. Wooden railroad ties may contain preservatives (i.e., creosote), some of which may contain hazardous constituents. Track switch locations often have elevated levels of petroleum hydrocarbons. Inorganic and organic herbicides, along with diesel fuel, may have been used for vegetation control.

Due to the historic railroad that traverses the subject site, and the portion of the track that has been paved over, the presence of gasoline, diesel, and/or creosote underneath the concrete and surrounding the railroad is likely. Any removal/relocation of railway during site decommissioning, demolition, or construction should be conducted under the purview of the local regulatory agency to identify proper handling procedures. Once the railroad tracks are removed, a visual inspection of the areas beneath and around the removed tracks should be performed. Any stained soils observed underneath the tracks should be sampled. Results of the sampling (if necessary) would indicate the level of remediation efforts that may be required.

5.3.7 Mercury

Due to the age of the on-site structure, the presence of mercury within the on-site gauges is likely. Any removal/relocation of gauges during site demolition/decommissioning should be conducted under the purview of the local regulatory agency to identify proper handling procedures. Additionally, removed gauges should be disposed of at an appropriate permitted landfill location.

5.3.8 Construction Activities

If unknown wastes or suspect materials are discovered during construction by the contractor, which he/she believes may involve hazardous waste/materials, the contract shall:

- Immediately stop work in the vicinity of the suspected contaminant, removing workers and the public from the area;
- Notify the Project Engineer of the implementing Agency;
- Secure the areas as directed by the Project Engineer; and
- Notify the implementing agency's Hazardous Waste/Materials Coordinator.

6.0

REFERENCES

Date	Approximate Scale	Reference #
1953	1"=555'	1352610.12
1963	1"=555'	1352610.12
1974	1"=600'	1352610.12
1989	1"=666'	1352610.12
1994	1"=666'	1352610.12
2002	1"=666'	1352610.12

Note: 1953-2002 Historical Aerial Photographs provided by Environmental Data Resources, Inc.

Building Department Records, City of San Diego, February 1, 2005.

California Department of Oil, Gas, and Geothermal Resources (DOGGR), Wildcat Map #W1-1, Los Angeles and Kern Counties, dated February 6, 1999.

Chain of Title Report, PDS Enterprises, January 6, 2005.

Database Search/GeoCheck, Environmental Data Resources, Inc., January 3, 2005.

EPA Map of Radon Zones, U.S. EPA, 1993.

File Review, County of San Diego Department of Environmental Health, February 24, 2005.

Interview, City of San Diego-Building Department, February 24, 2005.

Site Inspections, conducted on February 1, 2005 and February 24, 2005.

Thomas Brothers Map, Orange and Los Angeles Counties, 2005.

USGS Topographic Quadrangle, Point Loma, California Quadrangle, dated 1974.

USGS Historical Topographic Quadrangles, San Diego and Point Loma, California Quadrangles, 1917 through 1974.

City of San Diego Zoning Map, October 1998.

TN &A
T N & Associates, Inc.
Engineering and Science

Memorandum

Date: December 21, 2006

To: Ken Rowland, SDG&E

From: Mary Londquist

Copy: Tom Mulder

Subject: **Silver Gate Power Plant – Basement Trench System Sediment Sampling**

On November 28, 2006, T N & Associates (TN&A) collected sediment samples from the basement trench system of the San Diego Gas and Electric (SDG&E) Silver Gate Power Plant. Sediments were sampled and analyzed to determine their chemical waste characteristics. Four composite samples (Generating Unit 1, Unit 2, Unit 3, and Unit 4), each composed of eight grab samples, were collected from the basement trench system. Composite sample Unit 1 was composed of samples 1A through 1H, composite sample Unit 2 was composed of 2A though 2H, composite sample Unit 3 was composed of 3A though 3H, and composite sample Unit 4 was composed of 4A though 4H. The grab sample locations are presented in the attached sketches.

Composite samples were collected by removing the metal grating covering the trenches, collecting a grab sample of sediment with a large stainless steel spoon, placing the sediment into a stainless steel bowl. Once a grab sample was collected from each of the eight locations, the resulting material was mixed together and placed into 8-ounce glass jars.

Samples were submitted to SDG&E's environmental laboratory under chain-of-custody documentation for analysis. All samples were analyzed for total petroleum hydrocarbons as gasoline and diesel, (by EPA Method 8015M), volatile organic compounds (by EPA Method 8260B), polychlorinated biphenyl aroclors (by EPA Method 8082), TTLC metals (by EPA Methods 7471A and 6010B), and semivolatile organic compounds (by EPA Method 8270). Selected samples with relatively higher metal concentrations were further analyzed to determine waste characteristics using Soluble Threshold Limit Concentration (STLC) and Toxicity Characteristic Leaching Procedure (TCLP) methods. Laboratory analytical results and chain-of-custody documentation are attached.

Should you require additional assistance or further information, please do not hesitate to call.

[illegible]
DEC 29 2006
[illegible]

2247 San Diego Avenue, Suite 238
San Diego, CA 92110

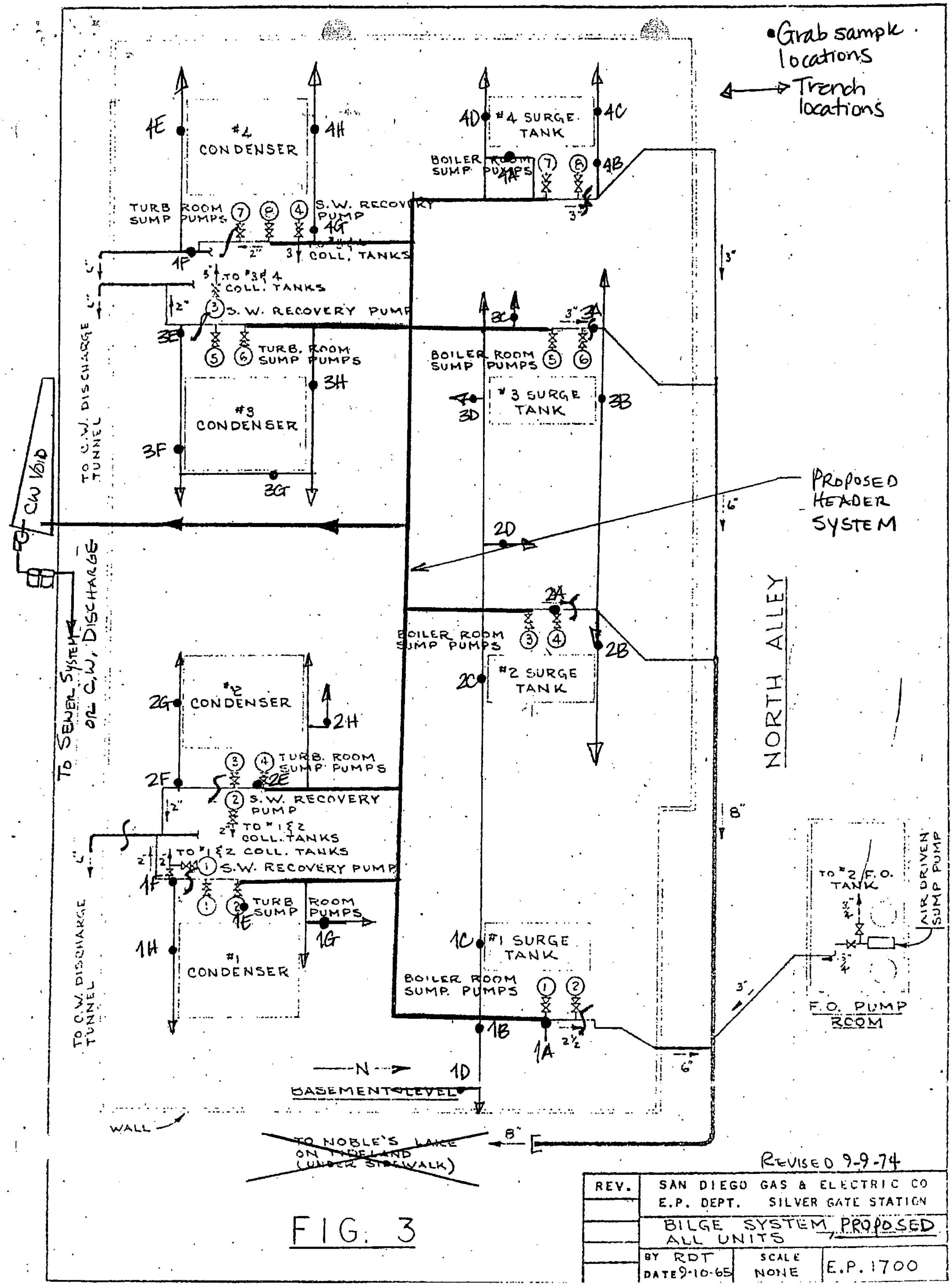
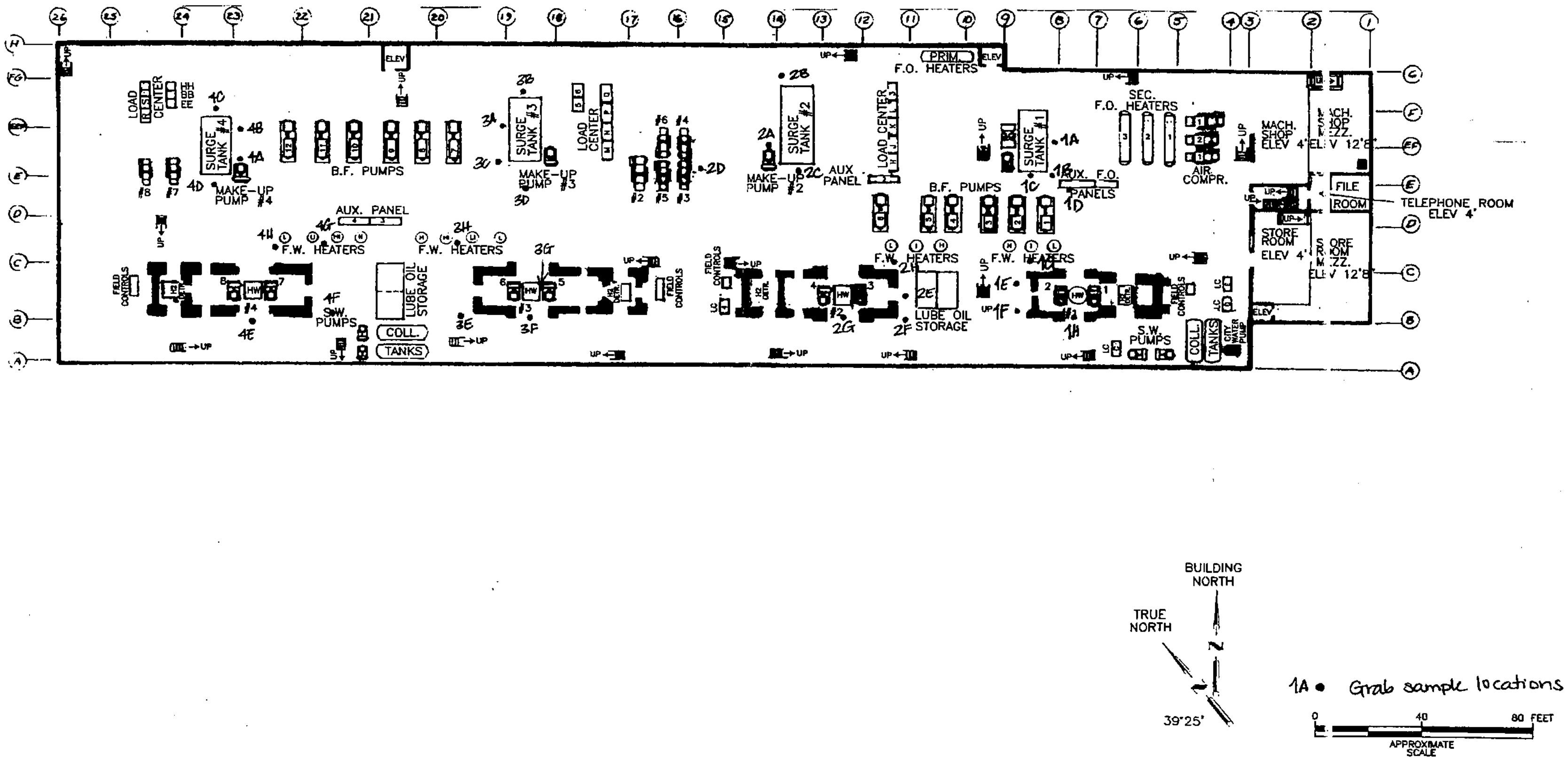


FIG. 3

REV.	SAN DIEGO GAS & ELECTRIC CO E.P. DEPT. SILVER GATE STATION		
	BILGE SYSTEM, PROPOSED ALL UNITS		
	BY RDT DATE 9-10-65	SCALE NONE	E.P. 1700

DRAWN BY	DP	CHECKED BY			FILE NAME	BASEMENT
	8/28/03	APPROVED BY			PROJECT NUMBER	SDG-01-T002.211



NOTE: THIS FIGURE WAS MADE FROM A SCAN OF THE FOLLOWING DRAWING:

PLAN OF S.G. BASEMENT (ELEV. 4') & ADMIN. BLDG. MEZZANINE (ELEV. 12'8"). DRAWING NO. EP-642, LAST REVISED OCTOBER 1, 1982 (BASED ON DRAWING NO. EP 020.1, DATED NOVEMBER 16, 1954, BY SDG&E ELEC. PROD. DEPT.)

ENV AMERICA
ENVIRONMENTAL ENGINEERING, CONSULTING & CONSTRUCTION

FIGURE

PLAN VIEW OF BASEMENT

SAN DIEGO GAS & ELECTRIC COMPANY
SILVERGATE POWER PLANT
1348 SAMPSON STREET
SAN DIEGO, CALIFORNIA

SDGE
A Sempra Energy utility

ENVIRONMENTAL ANALYSIS LABORATORY

19 December 2006

Ken Rowland - GT16G2
SDG&E - Site Assessment and Mitigation
555 W. 5th Street
Los Angeles, CA 90013-1036

RE: Silver Gate 138 kV - Substation Demo (Trenches)

Enclosed are the results of analyses for samples received by the laboratory on 11/29/06 13:46. If you have any questions concerning this report, please feel free to contact me.

Sincerely,

12/19/06
Authorized Signature

Randal L. Calentine
Environmental Laboratory
Team Leader
Name / Title

San Diego Gas & Electric
ELAP Certificate No. 1289

The results in this report apply to the samples analyzed in accordance with the chain of custody document. This analytical report must be reproduced in its entirety.

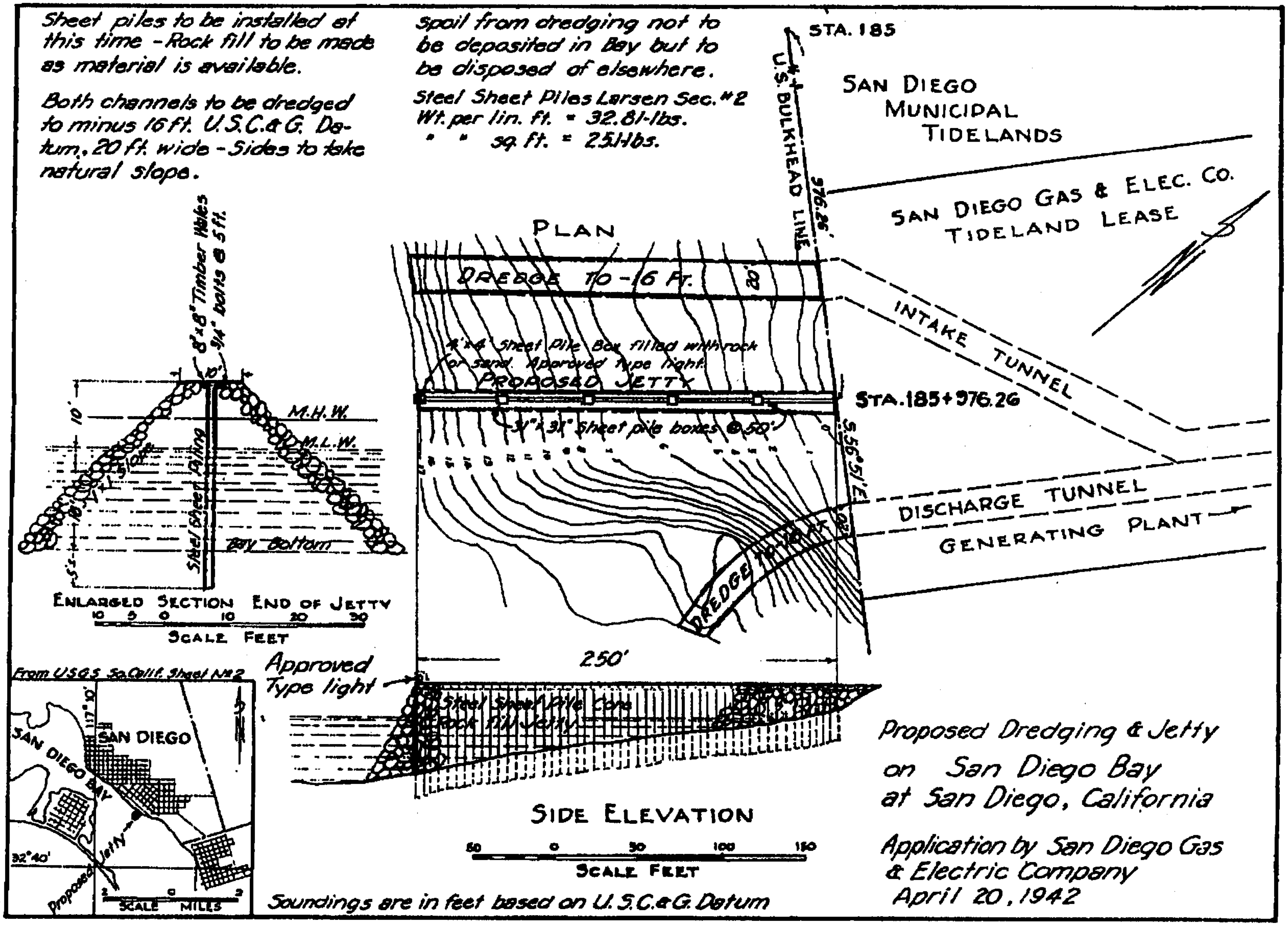
ANALYTICAL REPORT FOR SAMPLES

Sample ID	Laboratory ID	Matrix	Date Sampled	Date Received
Unit 1	0611205-01	Solid	11/28/06 11:30	11/29/06 13:46
Unit 2	0611205-02	Solid	11/28/06 13:05	11/29/06 13:46
Unit 3	0611205-03	Solid	11/28/06 14:50	11/29/06 13:46
Unit 4	0611205-04	Solid	11/28/06 16:05	11/29/06 13:46

cc: BMontgomery@SempraUtilities.com
mlondquist@tnainc.com
tmulder@tnainc.com

Tom Mulder
TN and Associates, Inc.
2247 San Diego Ave
Suite 238
San Diego, CA 92110

Note: This Re-issued report of Dec. 19, 2006 includes STLC and TCLP extraction data for certain metals.



Sheet piles to be installed at this time - Rock fill to be made as material is available.

Both channels to be dredged to minus 16 ft. U.S.C.&G. Datum, 20 ft. wide - Sides to take natural slope.

Spoil from dredging not to be deposited in Bay but to be disposed of elsewhere.

Steel Sheet Piles Larsen Sec. #2
Wt. per lin. ft. = 32.81-lbs.
" " sq. ft. = 25.1-lbs.

Soundings are in feet based on U.S.C.&G. Datum

Proposed Dredging & Jetty
on San Diego Bay
at San Diego, California

Application by San Diego Gas
& Electric Company
April 20, 1942

SOLID WASTE MANAGEMENT UNIT INFORMATION DATA SHEET

Instructions: Complete the following questions in detail for EACH SWMU identified in the Summary Chart, Section VI. If the SWMU is identified as a Process System the SOLID WASTE MANAGEMENT UNIT DATA SHEET FOR PROCESS SYSTEMS (attached) should be completed in place of this data sheet. All other SWMUs should be identified with this form.

For Example: If a facility has 2 furnaces and 3 boilers, then a total of 5 Solid Waste Management Unit Information Data Sheets should be completed; one data sheet for each furnace and one data sheet for each boiler.

1. Facility name:

Silvergate Power Plant

2. Identify the type of SWMU as listed in the Summary Chart (i.e., trenches):

Substation

3. Is the SWMU still in operation? YES [✓ NO]

4. How much hazardous materials/waste does the SWMU process/handle per month (i.e., 1,000 gallons per month)?

There is no throughput of transformer coolant oil. The coolant oil historically contained PCBs.

5. Indicate the maximum capacity (i.e., gallons, cubic feet) and dimensions (i.e., 10 feet height x 10 feet width x 20 feet length). *Total capacity: 24,000 gallons of coolant oil. Each transformer contains approximately 6,000 gallons, each circuit breaker contains approximately 600 gallons. Size of transformer 20' x 12' x 25'. Size of each circuit breaker 8' x 2' x 2'*

6. Indicate age of SWMU (years). 50

Maximum life expectancy of SWMU (years). 70

7. What is the purpose of the SWMU? (Check one)

___ Storage
✓ Other: Voltage control
___ Process

8. Is the SWMU showing excessive signs of wear or weathering? If YES, then explain. YES [✓ NO]

9. Does the SWMU have any leaks, cracks, or holes? [✓ YES] NO

SOLID WASTE MANAGEMENT UNIT
INFORMATION DATA SHEET

10. Is the SWMU protected from erosion and corrosion? [✓ YES] NO

11. Describe the general inspection and/or maintenance program for the SWMU. Indicate the frequency and record keeping policy used (i.e., visual, two times a month).

Monthly during maintenance

12. Has there been any analytical testing of the area around the SWMU? If YES, then indicate the sample type (i.e., vapor, liquid, or soil), date, and the constituents analyzed. YES [✓ NO]

13. Does the SWMU have an environmental permit? If YES, then indicate the agency issuing the permit, permit number, and expiration date. Attach a copy of the permit from agencies other than the Department. YES [✓ NO]

14. Is the SWMU currently under a compliance order from a federal, state, or local regulatory agency? If YES, list of date and agency issuing the order and attach a copy of the order from agencies other than the Department. YES [✓ NO]

15. List any environmental reports or studies performed on the SWMU and attach a copy of the reports not submitted to the Department.

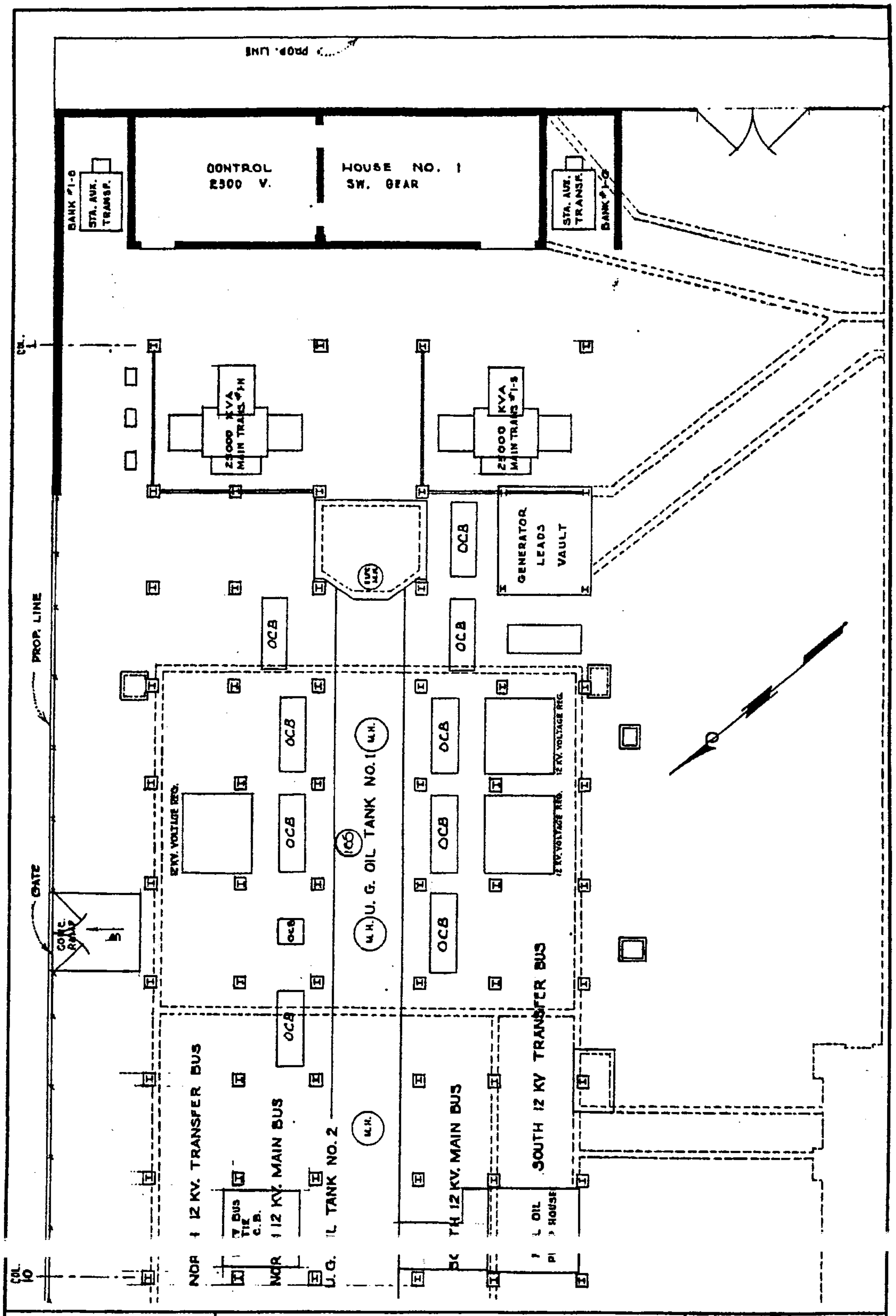
None

16. List any current and past environmental problems with the SWMU (i.e., spills, unauthorized releases, and/or stains?). Include the data, material involved, regulatory agency notified, and cleanup method. *Stains caused by minor leaks over time. Stains are due to coolant oil. Stains are visible on concrete pads and in secondary containment of several of the transformers. Stains are visible by N and S pot heads on ground and equipment. Since the coolant oil has historically contained PCBs, the stains may possibly contain PCBs.*

17. If the SWMU has had a release, complete the attached RELEASE INFORMATION DATA SHEET for each release

Name of Preparer:

Title of Preparer: Date:



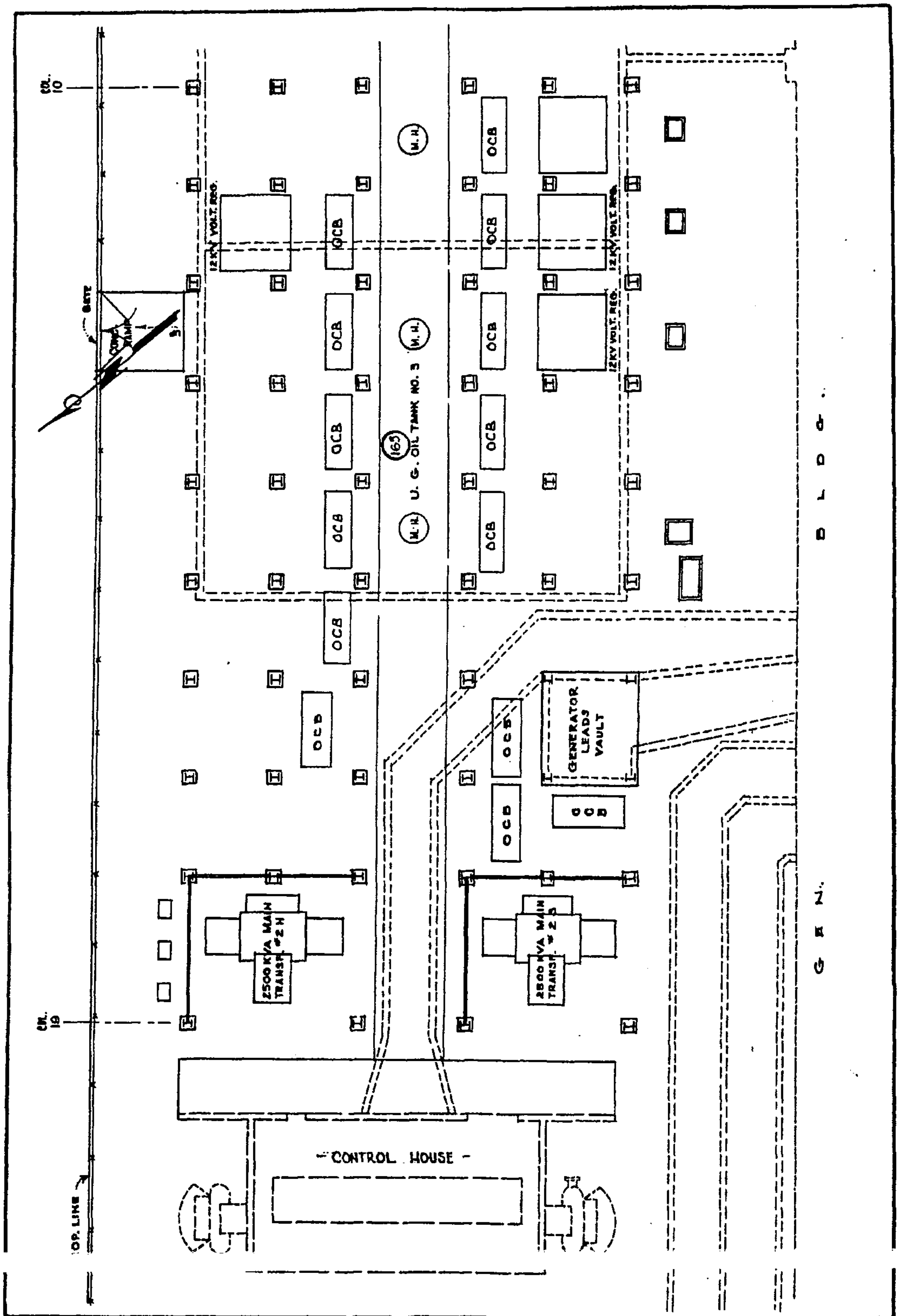
DWG. P-7186	DATE 1-1-55		
1	6-1-65 LA	5	
2	7-8-74 KS	6	
3		7	
4		8	

PROPERTY ATLAS · SAN DIEGO GAS & ELECTRIC COMPANY

SAMPSON SUBSTATION
12 KV. SWITCH & BUS STRUCTURE

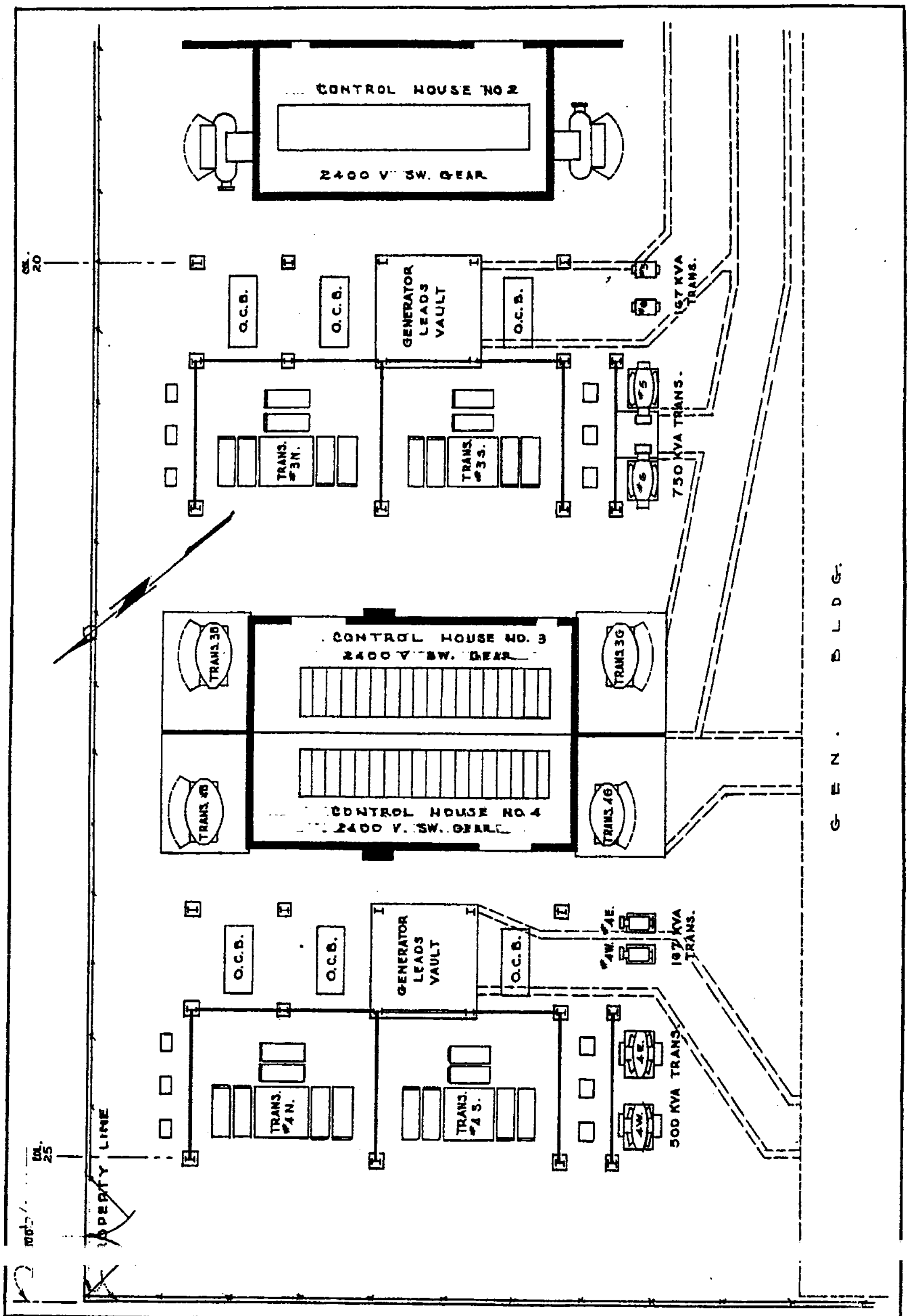
SCALE	SHEET
1" = 16'	P2-5

V1-2.3-3



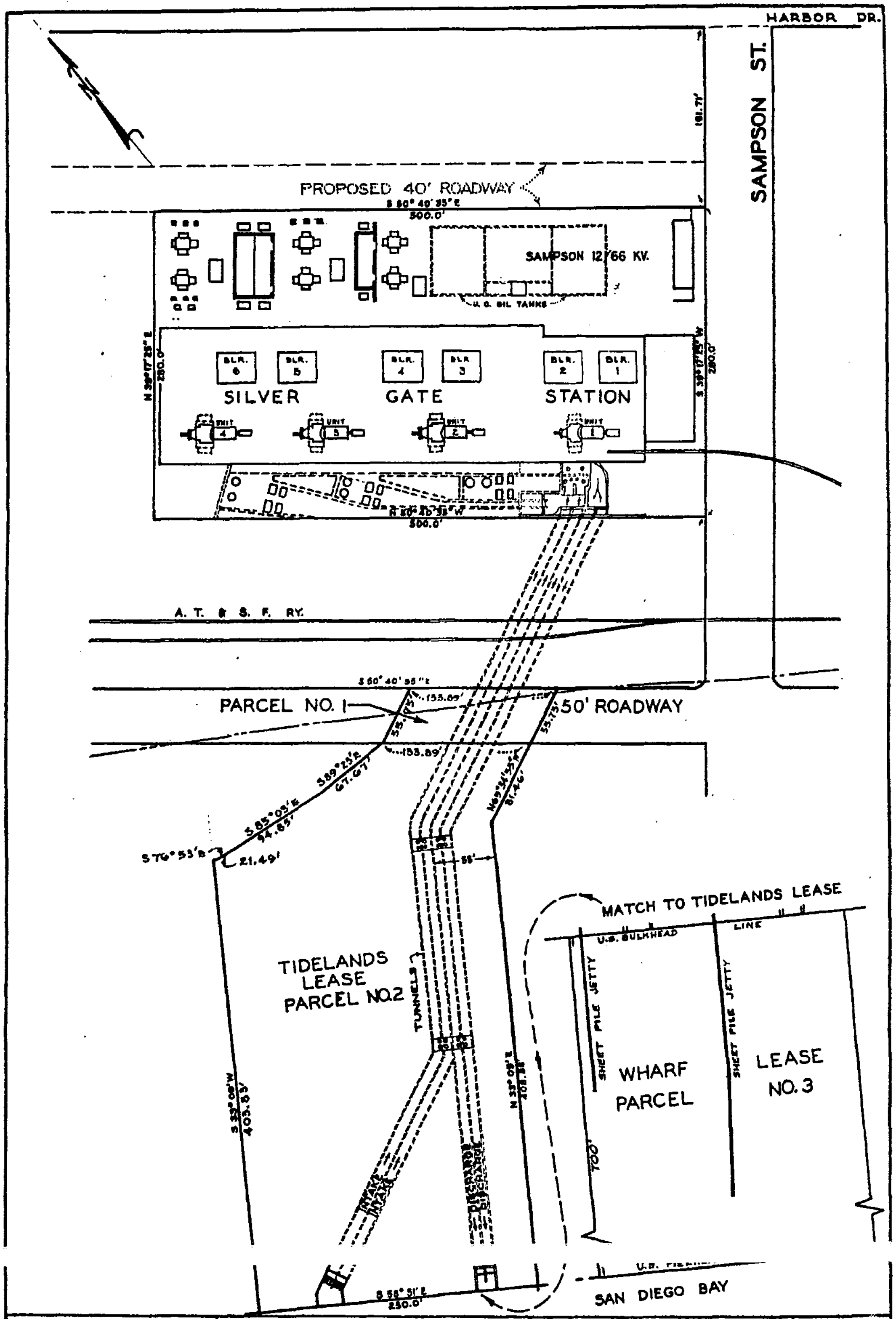
DWG.P-7187 DATE 1-2-55				PROPERTY ATLAS · SAN DIEGO GAS & ELECTRIC COMPANY	SCALE	SHEET
1	6-1-65 LA	5		SAMPSON SUBSTATION 12 KV SWITCH & BUS STRUCTURE	1"=16'	P2-6
2		6				
3		7				
4		8				

VI-2.3-4



DWG. P-7188 DATE 12-31-55				PROPERTY ATLAS - SAN DIEGO GAS & ELECTRIC COMPANY	SCALE	SHEET
1	6-1-65 LA	5		SAMPSON SUBSTATION 12 KV. SWITCH & BUS STRUCTURE	1"=16'	P2-7
2		6				
3		7				
4		8				

VI -2.3-5



DWG. P-4409 DATE 1-19-42				PROPERTY ATLAS · SAN DIEGO GAS & ELECTRIC COMPANY	SCALE	SHEET
1	8-3-48	5		SILVER GATE POWER PLANT SAMPSON SUBSTATION & TIDELANDS LEASE PLOT PLAN	1"=100'	P2-4
2	3-29-56.	6				
3	4-4-63	7				
4	6-1-65 LA	8				

VI-2.36

CROSBY & OVERTON
Environmental Management Inc.
11791 Monarch Street • Garden Grove, California 92641
(714) 893-2468

PREPARED FOR: MIKE CARROLL
SAN DIEGO GAS AND ELECTRIC
110 W. "A" STREET, SUITE 850
SAN DIEGO, CA 92101

SITE ASSESSMENT AND HYDROCARBON MITIGATION AT THE SILVER GATE POWER PLANT

SAN DIEGO, CALIFORNIA

PREPARED BY: CROSBY & OVERTON ENVIRONMENTAL
MANAGEMENT, INC.
11791 MONARCH STREET
GARDEN GROVE, CA 92641

NOVEMBER 10, 1987

WRITTEN BY:	REVIEWED BY:
John Hubbard	Thomas J. Twillie
JOHN HUBBARD GEOLOGIST	THOMAS J. TWILLIE OPERATIONS MANAGER

TABLE OF CONTENTS

FIGURES

APPENDICES

Site Background Information

The Silver Gate Power Plant is located at 1348 Sampson St., just south of downtown San Diego (Figure 1). Located north of the power plant are three underground concrete and steel-lined fuel oil tanks.

In the latter part of 1986, Woodward-Clyde Consultants were retained by San Diego Gas & Electric (SDG&E) to assess the underground tanks and to initiate a site assessment. In a report dated November 18, 1986, the following conditions were noted for the Silver Gate facility:

- Although visual inspection of tanks revealed no evidence of defects (eg. leaks), it was suggested that contaminated soil encountered subsurface and adjacent to the tanks may be attributed to underground tank leakage.
- Contaminated soil was encountered in two (2) boreholes located adjacent to the underground tanks. Laboratory values for TEH upwards of 7,700 ppm were recorded. The contamination plume was not defined in three dimensions.
- The boreholes referred to above were converted to groundwater monitoring wells and water samples were collected and analyzed for TEH. Laboratory results revealed non-detectable (ND) levels of TEH for both water samples. It was reported that groundwater exists approximately nineteen (19) feet below grade.

Upon review of the assessment report referenced above, the Department of Health Services (DHS) set a soil clean-up level of 1,000 ppm (TEH). The study by Woodward-Clyde revealed no evidence that hydrocarbon contamination had impacted groundwater.

Site Assessment Activities (Phase I)

On February 25, 1987 C&O EMI was retained by SDG&E to attempt to define the limits of the >1,000 ppm hydrocarbon contamination plume by excavating contaminated soil with a backhoe in a area as designated by SDG&E (Figure 2).

On March 4, 1987 fieldwork at the Silver Gate Power Plant began. Excavated contaminated soil was stockpiled on 6-mil plastic next to the excavation trench.

Soils closest to MW-2 were excavated first. Approximately 2.5 feet below grade a fuel oil line approximately eight (8) inches in diameter and trending roughly east-west was unearthed. As the excavation continued along the alignment of the fuel oil pipeline it took-on the shape of a trench (Figure 2).

As a result of impending stress on the fuel oil pipe with ongoing soil excavation, SDG&E decided to curtail further excavation until a means of supporting the pipeline at an isolation valve could be designed and installed.

The final areal dimensions of the trench were 3' x 18'. The east end of the trench was five (5) feet deep and the west end thirteen (13) feet deep. Upon inspection of the sidewalls and floor, it appeared that hydrocarbon contamination increased to the west. Considerable contamination was also noted in soil directly under the pipeline isolation valve (Figure 2).

Five soil samples were collected from strategic locations along the trench sidewalls and the floor and analyzed for TPH (EPA Method 8015 modified) at West Coast Analytical Services in Santa Fe Springs. All soil samples were contained in glass vessels with teflon lined caps and immediately chilled in a "cooler" with ice. Proper chain of custody protocol was adhered to.

Need Lab Data

Laboratory results indicated that the >1,000 ppm contamination plume was defined in the direction parallel to the fuel oil pipe (roughly east-west). A sample from the western sidewall of the trench showed 530 ppm and a sample from the eastern sidewall contained ND levels of TPH. A bottom sample taken at a depth of fourteen (14) feet showed 2,800 ppm. Sample locations for Phase I are not portrayed in Figure 2 as it is inconclusive (eg. the lateral and vertical extent of the contamination plume was not defined).

On March 5, 1987 the trench was lined with 6-mil plastic and backfilled with the excavated soil.

Site Mitigation Activities (Phase II)

On August 25, 1987 fieldwork at the Silver Gate Power Plant resumed. Initially excavation occurred in soils adjacent to the underground tank and fuel oil line. As the excavation proceeded it appeared that the sources of hydrocarbon contamination were the pipeline isolation valve and adjacent flow measuring station located on the fuel oil pipeline.

Present at the site during this phase of the work was the State Certified Chemical Research Mobile Laboratory. This permitted a short turn-around time for laboratory data which expedited and aided in monitoring the process of excavating the hydrocarbon contamination plume as defined by the DHS (eg > 1,000 ppm, TPH).

A total of twenty-five (25) soil samples were collected and analyzed for TPH (EPA Method 8015 modified). Six of these were "retests". When a sample was analyzed and recorded a TPH value >1,000 ppm, a second sample was collected at the same location but at a lower depth and analyzed. This process was repeated until a sample showed <1,000 ppm TPH, at which point the vertical extent of the contamination was defined for that particular sample location. Retests are designated in the laboratory data by a letter (eg. A, B or C) following the sample number (Appendix A).

Sample 18 was taken directly under the tank fill valve and showed 2,500 ppm TPH (Figure 2). Further excavation in this area, in order to retest, was inhibited due to poor accessibility by the backhoe. Vickie Church (County of San Diego Department of Health Services) was notified and upon inspecting the area in question, waived any requirement for soil removal. Sample 17, collected 3 feet west of Sample 18, showed 110 ppm.

Further testi
in area
waived du
to
inaccessib
+
safety
concer
VC

manifests reflect 210 yds

The mitigation plan required the removal of 150 yards of contaminated soil. The contaminated soil was manifested, transported and disposed of by International Technology (IT) at the TSDF in Imperial Valley (Westmoreland).

Groundwater

The deepest part of the excavation pit was seventeen (17) feet below grade. Groundwater is thought to exist approximately 20 feet below grade and was not encountered during the course of this investigation.

Conclusions

1. Fuel oil had leaked from a pipeline at the Silver Gate Power Plant and impacted surrounding soils.

2. Soils showing hydrocarbon contamination >1,000 ppm were excavated and disposed of pursuant to the County of San Diego Department of Health Services guidelines.

3. The maximum depth of contamination permeation is seventeen (17) feet. Groundwater is thought to exist approximately twenty (20) feet below grade.

4. The excavation pit was backfilled with pea gravel and degenerated granite and compacted to 90% maximum.

5. Evidence indicates that the underground fuel oil tanks were not the source of the contamination.

6. SDG&E to enclose the pipeline isolation valve and flow measuring station to prevent further soil contamination.

FIGURE 1. SITE LOCATION MAP

CROSBY AND OVERTON
Environmental Management, Inc.
11791 Monarch Street
Garden Grove, California 92641

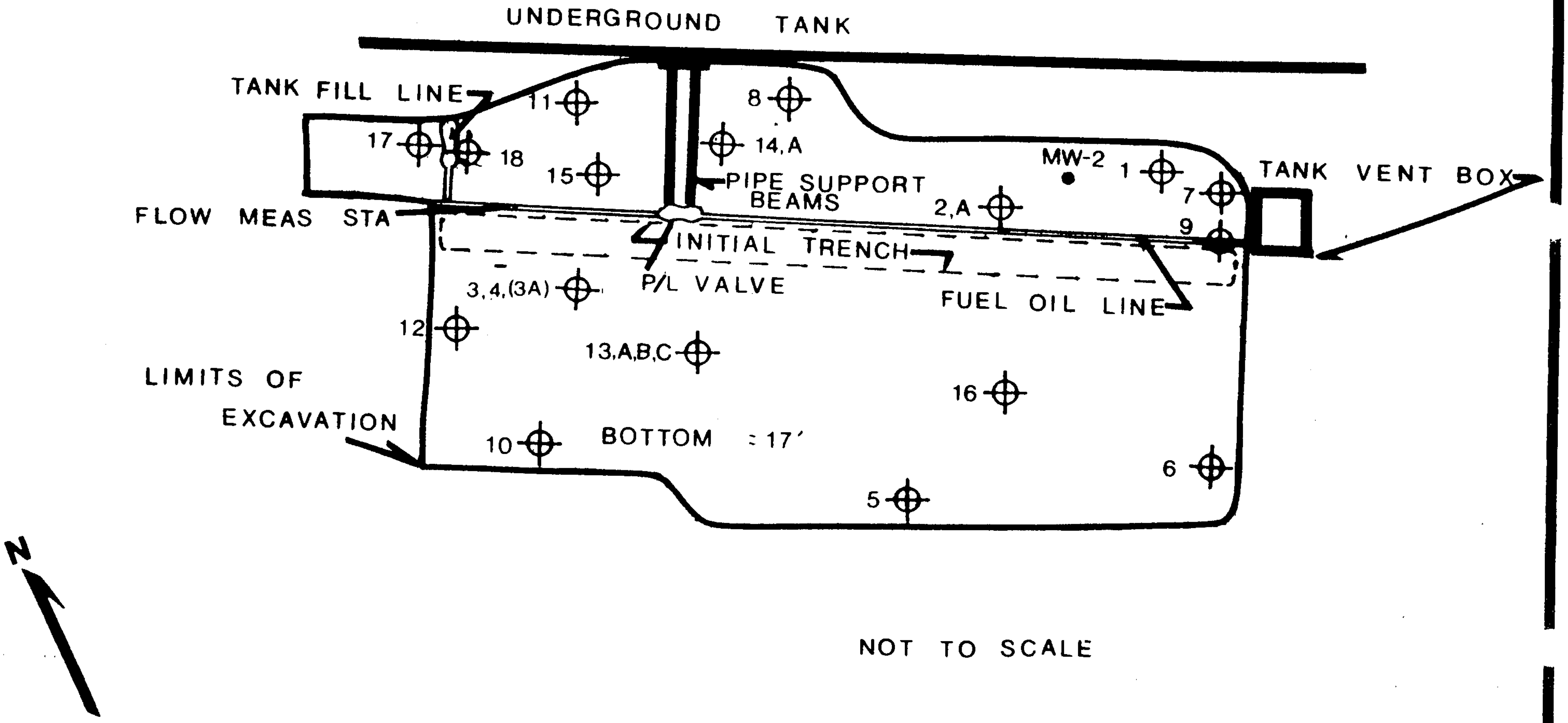


FIGURE 2. EXCAVATION PIT AND SAMPLING LOCATIONS.

CROSBY AND OVERTON
Environmental Management, Inc.
11791 Monarch Street
Garden Grove, California 92641

SDG&E SILVER GATE
POWER PLANT

98804

See photos...
need to get full-size
co.

SDGE

A Sempra Energy utility®

SAN DIEGO GAS & ELECTRIC

ONSITE HYDROLOGY/DRAINAGE STUDY

SILVERGATE 230/69kV SUBSTATION
1348 SAMPSON STREET
SAN DIEGO, CA 92113

PREPARED BY:
SAN DIEGO GAS & ELECTRIC
CIVIL / STRUCTURAL ENGINEERING
8316 CENTURY PARK CT.; CP52G
SAN DIEGO, CA 92123

Tyler Lonsdale
BY: TYLER W. LONSDALE

3/14/06
DATE:

Craig Riker
APPROVED BY: CRAIG H. RIKER
R.C.E. # 32108

3-14-06
DATE:

TABLE OF CONTENTS

SECTION **PAGE**

Appendices

Figures

1.0 Introduction & Objective

San Diego Gas & Electric (SDG&E) is proposing to build the Silvergate 230/69kV Substation located at 1348 Sampson Street San Diego, CA 92113. The existing SDG&E owned Silvergate Power Plant and facilities occupy approximately 3.2 acres of the proposed 5.07 acres of substation development. The proposed development includes the new substation, perimeter security wall, retaining walls, driveways, sidewalks, and underground storm drain facilities. Approximately 3.0 acres of the proposed site currently drains by means of surface sheet flow to Sampson Street. The remaining 2.07 acres drain through the existing cooling water tunnels to the San Diego Bay. The cooling water tunnels will be decommissioned and sealed during the removal of the existing power plant. The drainage of the 2.07 acres will be redirected to the existing storm drain system on Sampson Street. Please refer to the Figures 4 and 5 for the existing and proposed site plans.

According to the City of San Diego Drawing Numbers 24356 2 D and 2682 L, a 30" RCP storm drain exists on the East side of Sampson Street. Prior to the intersection of Sampson Street and Belt Street, a 24" RCP lateral storm drain ties into the 30" RCP. The 24" lateral is tied to a catch basin just outside the southeast corner of the SDG&E owned property. Shortly after the intersection of the 24" RCP with the 30" RCP the storm drain is increased to a 42" storm drain.

The objective of this study is to show that the 24" RCP storm drain will be able to convey the additional drainage resulting from the proposed site. This will be accomplished by calculating and comparing the following items:

- The peak discharge (cfs), that flows to Sampson Street, of existing site (approx. 3 acres) analyzed by the Rational Method for a 6 hour 100 year flood.
- The peak discharge (cfs) of the proposed site, that flows to Sampson Street, analyzed by the Rational Method for a 6 hour 100 year flood.

2.0 References

1. San Diego County Hydrology Manual June 2003
2. Hydraulic Engineering, Roberson, Cassidy, Chadhry 1998
3. Evaluation of Rational Method "C" Values, Joe Hill June 2002
4. Initial Time of Concentration Analysis of Parameters Joe Hill June 2002
5. Water Group 445 Sampson Street – 8" Pipe Belt St. to Harbor Drive, As-Built 21547 5 D 2/27/85
6. San Diego County Drainage Design Manual July 2005
7. City of San Diego Drawings 2682 – L
8. City of San Diego Drainage Design Manual, March 1989/April 1984

3.0 Brief Summary

The calculations show that the amount of peak discharge 9.93 (cfs) generated from the proposed site is less than the peak discharge 12.47 (cfs) currently flowing into the 24" RCP storm drain on Sampson Street. The overall watershed area is increased by approximately 2 acres yet the run off coefficient is reduced as the majority of the site is covered with Class II Aggregate Base ($C \approx 0.57$). Therefore, the permeable surface area is increased reducing the peak discharge as shown in the calculations.

4.0 Declaration of Responsible Charge

DECLARATION OF RESPONSIBLE CHARGE

I, HERBY DECLARE THAT I AM THE CIVIL ENGINEER OF WORK FOR THIS PROJECT, THAT I HAVE EXERCISED RESPONSIBLE CHARGE OVER THE DESIGN OF THE PROJECT AS DEFINED IN SECTION 6703 OF THE BUSINESS AND PROFESSIONS CODE, AND THAT THE DESIGN IS CONSISTENT WITH CURRENT STANDARDS.

I UNDERSTAND THAT THE CHECK OF THE PROJECT DRAWINGS AND SPECIFICATIONS BY THE CITY OF SAN DIEGO IS CONFINED TO A REVIEW ONLY AND DOES NOT RELIEVE ME, AS ENGINEER OF WORK, OF MY RESPONSIBILITIES FOR PROJECT DESIGN.

Craig Riker — 3-14-06

CRAIG HALL RIKER
R.C.E. # 32108
EXP. DECEMBER 31, 2006

DATE

REGISTERED PROFESSIONAL ENGINEER
CRAIG HALL RIKER
No. 32108
12-31-06
CIVIL
STATE OF CALIFORNIA

5.0 Watershed Boundary

5.1 Existing Conditions

As shown in the aerial photograph Figure 3, the existing SDG&E owned property contains the decommissioned Silvergate Power Plant. The roof and cooling water deck (south-west of the power house) currently drain into the cooling water tunnels. The SDG&E owned property north-east of the power house currently drains to a storm drain on Sampson Street. The parcel within the bounds of the proposed site, owned by Kelco and the adjacent parcel owned by PCE (Propulsion Control Engineering) drain to the storm drain on Sampson Street. Figure 4 of the existing site plan shows the elevations of the watershed area. The site drains to the west side of Sampson Street where the runoff flows to a curb inlet and catch basin (prior to the intersection of the railroad tracks on Sampson Street). From the catch basing and curb inlet a 24" storm drain connects to the 30" RCP storm drain on the east side of Sampson Street (as shown on the City of San Diego drawing # 24356-2-D). Ground surface elevations range from approximately 25 feet above Mean Sea Level (MSL) at the northeast property line, to approximately 15 feet above MSL at the south corner (as shown in Figure 1).

5.2 Proposed Conditions

The proposed improvements consist of altering approximately 5 acres of existing industrial land to produce a relatively level substation pad maintaining an approximate of 1% slope for positive drainage. The finished grades are shown on Figure 5. Surface runoff in the new substation will sheet flow into the driveway surfaces. The center of the driveways will contain concrete swales, which will capture the flow and transport it to the catch basins and storm drain system along the southwest side of the property. The proposed storm drain system on our property will connect to the 24" storm drain on west side of Sampson Street. The proposed grading and drainage plan is shown in Figure 5. Prior to running off site, all storm water will filtered per the City of San Diego Municipal Code Land Development Manual and the Storm Water Standards.

6.0 Drainage Analysis

The watershed hydrology calculations are described in the following section. See Figures 3 to 5 for the watershed area and conceptual grading and drainage design.

6.1 Hydrology and Hydrology Calculations

The hydrology calculations for this study were completed per the San Diego County Hydrology Manual dated June 2003. According to the manual, the Rational Method (RM) can be utilized for watersheds less than 1 square mile in area for any storm frequency.

The RM formula estimates the peak rate of runoff at any location in a watershed as a function of the drainage area (A), runoff coefficient (C), and rainfall intensity (I) for a duration equal to the time of concentration (Tc), which is the time required for water to flow from the most remote point of the basin to the location being analyzed. The formula is expressed as follows:

$$Q = C\,I\,A$$

Where:
Q = peak discharge, in cubic feet per second (cfs)
C = runoff coefficient, proportion of the rainfall that runs off the surface (no units)
I = average rainfall intensity for a duration equal to the Tc for the area, in inches per hour
A = drainage area contributing to the design location, in acres

Runoff Coefficient, C:

Table 1 in Appendix C lists the estimated runoff coefficients for urban areas. Soil type "D" was used in this analysis for developing the appropriate C value for design. The runoff coefficients used in this study consist of the following:

- Paved Areas: C = 0.90
- Substation Class II Surface: C = 0.57

Rainfall Intensity, I:

The rainfall intensity (I) is the rainfall in inches per hour (in/hr) for a duration equal to the Tc for a selected storm frequency. Per SDG&E standards, all substation drainage is designed to convey 100 year storm flows. The rainfall intensities for the study were calculated using the following equation:

$$I = 7.44\,P6\,D^{-0.645}$$

$$I = 7.44\ P6\ D^{-0.645}$$

Where:
P6 = adjusted 6-hour storm rainfall amount
D = duration in minutes (Tc)

Time of Concentration, Tc:

The Time of Concentration (Tc) is the time required for runoff to flow from the most remote part of the drainage area to the point of interest. Urban overland flow methods are used to determine the initial times of concentration (Ti). Pipe and open channel flows are added to the initial times where applicable (Tt).

Time of Concentration: $Tc = Ti + Tt$

Drainage Basin Area, A:

For both the existing and proposed drainage calculations, the site was divided into sub-areas based on varying site characteristics. The drainage basin areas, in acres, are shown on Figure 4 & 5.

SEE APPENDIX B FOR ALL HYDROLOGY CALCULATIONS

7.0 Results and Conclusions:

Results of the hydrology calculations indicate the peak discharge and drainage characteristics of the site are enhanced by the proposed construction. The proposed conditions will yield an approximate 20% reduction in peak discharge introduced to the existing storm drain on Sampson Street during a 100-year storm event.

The peak discharge introduced into the Sampson Street storm drain system for a 100 year storm event is 12.47 cfs and the peak discharge for the same storm event for the proposed development is 9.93 cfs. The 20% decrease in the peak discharge is mostly due to the removal of the existing pavement and impermeable surfaces and replacing it with the substation Class II aggregate base ($C \approx 0.57$). Hydraulic calculations and design details will be completed for the grading plan submittal in accordance with the City of San Diego's Drainage Design Manual.

APPENDIX B – RATIONAL METHOD CALCULATIONS

Project: Silvergate 230/69kV Substation	Page ____ of ____
Subject: Hydrology Calculations (Existing Site)	Computed By: TWL Date_____ Checked By:___Date_____

APPENDIX B

Existing Site Hydrology, captured by Sampson Street storm drain (approx. 3 acres) See Figure 4

***All Calculations are based on a preliminary grading plan.**

Rational Method: $Q = CiA$

Existing Site Dimensions (area):

From Figure 4

Overland flow length: $L_o := 560 \cdot ft$

Gutter Flow Length: $L_g := 145\ ft$

Total Area:

$A_t := 129373.2 \cdot ft^2$ $A_t = 2.97\,acre$

Area 1:

Class II Base Area:

$A_{CII} := 14260 \cdot ft^2$ (from exhibit 2)

$A_{CII} = 0.327\,acre$

Asphalt Concrete and Impermeable Area:

$A_{ac} := A_t - A_{CII}$

$A_{ac} = 2.643\,acre$

Run off Coefficient:

$C_1 := 0.57$ (Class II Aggregate Base)

$C_2 := 0.90$ (AC & Concrete Paving)

$$C_t := C_1 \cdot \left(\frac{A_{CII}}{A_t}\right) + C_2 \cdot \left(\frac{A_{ac}}{A_t}\right)$$

$C_t = 0.864$

Intensity - (assumed Limited Industrial Table 3-2 SDCHM) SEE FIGURE 1, APPENDIX C

Project: Silvergate 230/69kV Substation	Page ____ of ____
Subject: Hydrology Calculations (Existing Site)	Computed By: TWL Date_____
	Checked By:___Date_____

Overland Flow:

$t_{i1} := 3.1$ min $\quad L_{max} := 70 \cdot ft$

remaining length: $\quad L_1 := L_o - L_{max} \quad L_1 = 490\ ft$ in miles = 0.093 miles

Use Kirpich formula:

$$t_{i2} := \left[\frac{\left[11.9 \cdot (L_1)^3 \right]}{\Delta E} \right]^{0.385}$$

where L1 is in miles

$\Delta E := 11.2 \cdot ft$

$t_{i2} := 3.94$ min

$t_i := t_{i1} + t_{i2} \qquad t_i = 7.04$ min

Gutter Flow: (Per Figure 3-6 SDCHM) SEE FIGURE 2, APPENDIX C

From Figure 3 - 6

Assume Q = 12.5 cfs $\quad$ s = 2% $\quad v := 255 \dfrac{ft}{min}$

$$t_t := \frac{L_g}{v} \qquad t_t = 0.569$$

$t_c := t_i + t_t \qquad t_c = 7.609$ min

$P_6 := 2.4$ in 100 yr 6 hour event (from rainfall Isopluvial Map)

$P_{24} := 3.9$ in 100 yr 24 hour event (from rainfall Isopluvial Map)

(FIGURE 3-1, SDCHM) SEE FIGURE 3, APPENDIX C

$$P_6 := \text{if}\left[0.45 < \left(\frac{P_6}{P_{24}} \right) < 0.65, P_6, \text{"NO GOOD"} \right] \qquad P_6 = 2.4 \text{ in}$$

$$i := 7.44 \cdot P_6 \cdot (t_c)^{-0.645} \cdot \frac{in}{hr} \qquad i = 4.823 \frac{in}{hr}$$

Peak Discharge (cfs)

$Q := C_t \cdot i \cdot A_t \qquad Q = 12.475 \dfrac{ft^3}{s}$ $\quad$ Assumed Q = 12.5cfs for Tt O.K.

Project: Silvergate 230/69kV Substation **Subject:** Hydrology Calculations (Proposed Site)	Page ____ of ____ Computed By: TWL Date_____ Checked By: ___ Date_____

Proposed Site Hydrology, captured by Sampson Street storm drain (approx. 5 acres composed of 4 watershed areas) See Figure 5

***All Calculations are based on a preliminary grading plan.**

Area 1

Rational Method: $Q = CiA$

Existing Site Dimensions (area):

From Figure 5

Overland flow length: $L_o := 180 \cdot ft$

Gutter Flow Length: $L_g := 230\ ft$

Storm Drain Flow: $L_{sd} := 425\ ft$

Total Area:

$A_t := 1.25 \cdot acre$

Area 1:

Class II Base Area:

$A_{CII} := 29600 \cdot ft^2$ (from figure 5)

$A_{CII} = 0.68\ acre$

Area foundation:

$A_{fd} := 1850 \cdot ft^2$

$A_{fd} = 0.042\ acre$

Asphalt Concrete and Impermeable Area:

$A_{ac} := A_t - A_{CII} - A_{fd}$

$A_{ac} = 0.528\ acre$

Run off Coefficient:

$C_1 := 0.57$ (Class II Aggregate Base)

$C_2 := 0.90$ (AC & Concrete Paving)

$C_3 := C_2$

$$C_t := C_1 \cdot \left(\frac{A_{CII}}{A_t}\right) + C_2 \cdot \left(\frac{A_{ac}}{A_t}\right) + C_3 \cdot \left(\frac{A_{fd}}{A_t}\right)$$

$C_t = 0.721$

Intensity - (assumed Limited Industrial Table 3-2 SDCHM) SEE FIGURE 1, APPENDIX C

Overland Flow:

$t_{i1} := 7.9$ min $\quad L_{max} := 65 \cdot ft$

remaining length: $L_1 := L_o - L_{max} \quad L_1 = 115\,ft$ in miles = 0.022 miles

Use Kirpich formula:

$$t_{i2} := \left[\frac{\left[11.9 \cdot (L_1)^3\right]}{\Delta E}\right]^{0.385}$$

where L1 is in miles

$\Delta E := 1.8 \cdot ft$

$t_{i2} := 1.5$ min

$t_i := t_{i1} + t_{i2} \qquad t_i = 9.4$ min

Gutter Flow: (Per Figure 3-6, SDCHM) SEE FIGURE 2, APPENDIX C

From Figure 3 - 6

Assume Q = 2.25 cfs $\quad$ s = 1% assumed avg. $\quad v := 138\ \frac{ft}{min}$

$t_{t1} := \frac{L_g}{v} \qquad t_{t1} = 1.667$

Pipe Flow: Assume Q = 2.25 cfs and diameter of the storm drain = 30 in

Q = VA

$A_{sd} := \left(\frac{\pi}{4}\right) \cdot 2.5^2 \qquad A_{sd} = 4.909\ ft^2$

$v_1 := \left(\frac{2.25}{A_{sd}}\right) \cdot 60 \qquad v_1 = 27.502\ \frac{ft}{min}$

$t_{t2} := \frac{L_{sd}}{v_1} \qquad t_{t2} = 15.453$ min

$t_c := t_i + t_{t1} + t_{t2} \qquad t_c = 26.52$ min

$P_6 := 2.4$ in 100 yr 6 hour event (from rainfall Isopluvial Map)

$P_{24} := 3.9$ in 100 yr 24 hour event (from rainfall Isopluvial Map)

Project: Silvergate 230/69kV Substation	Page ____ of ____
Subject: Hydrology Calculations (Proposed Site)	Computed By: TWL Date_____ Checked By:___Date_____

(FIGURE 3-1, SDCHM) SEE FIGURE 3, APPENDIX C

$$P_6 := \text{if}\left[0.45 < \left(\frac{P_6}{P_{24}}\right) < 0.65, P_6, \text{"NO GOOD"}\right] \qquad P_6 = 2.4 \ \text{in}$$

$$i := 7.44 \cdot P_6 \cdot (t_c)^{-0.645} \cdot \frac{\text{in}}{\text{hr}} \qquad i = 2.156 \frac{\text{in}}{\text{hr}}$$

Peak Discharge (cfs)

$$Q_1 := C_t \cdot i \cdot A_t \qquad Q_1 = 1.958 \frac{\text{ft}^3}{\text{s}}$$

Assumed Q = 2.25cfs for Tt O.K.

Area 2

Rational Method: Q = CiA

Existing Site Dimensions (area):

From Figure 5

Overland flow length: $L_o := 120 \cdot ft$

Gutter Flow Length: $L_g := 485\ ft$

Storm Drain Flow: $L_{sd} := 425\ ft$

Total Area:

$A_t := 2.47 \cdot acre$

Area 1:

Class II Base Area:

$A_{CII} := 65335 \cdot ft^2$ (from figure 5)

$A_{CII} = 1.5\, acre$

Area foundation:

$A_{fd} := 13065 \cdot ft^2$

$A_{fd} = 0.3\, acre$

Asphalt Concrete and Impermeable Area:

$A_{ac} := A_t - A_{CII} - A_{fd}$

$A_{ac} = 0.67\, acre$

Run off Coefficient:

$C_1 := 0.57$ (Class II Aggregate Base)

$C_2 := 0.90$ (AC & Concrete Paving)

$C_3 := C_2$

$$C_t := C_1 \cdot \left(\frac{A_{CII}}{A_t}\right) + C_2 \cdot \left(\frac{A_{ac}}{A_t}\right) + C_3 \cdot \left(\frac{A_{fd}}{A_t}\right)$$

$C_t = 0.7$

Project: Silvergate 230/69kV Substation
Subject: Hydrology Calculations (Proposed Site)

Page ____ of ____
Computed By: TWL Date______
Checked By:___ Date______

Intensity - (assumed Limited Industrial Table 3-2 SDCHM) SEE FIGURE 1, APPENDIX C

Overland Flow:

$t_{i1} := 7.9$ min $\quad L_{max} := 65\cdot ft$

remaining length: $L_1 := L_o - L_{max}$ $\quad L_1 = 55\,ft$ $\quad$ in miles = 0.010 miles

Use Kirpich formula:

$$t_{i2} := \left[\frac{\left[11.9\cdot\left(L_1\right)^3\right]}{\Delta E}\right]^{0.385}$$

where L1 is in miles

$\Delta E := 1.2\cdot ft$

$t_{i2} := 0.75$ min

$t_i := t_{i1} + t_{i2}$ $\quad t_i = 8.65$ min

Gutter Flow: (Per Figure 3-6 SDCHM) SEE FIGURE 2, APPENDIX C

From Figure 3 - 6

Assume Q = 4.5 cfs $\quad$ s = 1% $\quad$ assumed avg. $\quad$ $v := 156\ \dfrac{ft}{min}$

$t_{t1} := \dfrac{L_g}{v}$ $\quad t_{t1} = 3.109$

Pipe Flow: $\quad$ Assume Q = 4.5 cfs and diameter of the storm drain = 30 in

Q = VA

$A_{sd} := \left(\dfrac{\pi}{4}\right)\cdot 2.5^2$ $\quad A_{sd} = 4.909\ ft^2$

$v_1 := \left(\dfrac{4.5}{A_{sd}}\right)\cdot 60$ $\quad v_1 = 55.004\ \dfrac{ft}{min}$

$t_{t2} := \dfrac{L_{sd}}{v_1}$ $\quad t_{t2} = 7.727$ min

$t_c := t_i + t_{t1} + t_{t2}$ $\quad t_c = 19.486$ min

$P_6 := 2.4$ in $\quad$ 100 yr 6 hour event (from rainfall Isopluvial Map)

$P_{24} := 3.9$ in $\quad$ 100 yr 24 hour event (from rainfall Isopluvial Map)

Project: Silvergate 230/69kV Substation	Page ____ of ____
Subject: Hydrology Calculations (Proposed Site)	Computed By: TWL Date_____ Checked By:___ Date_____

(FIGURE 3-1, SDCHM) SEE FIGURE 3, APPENDIX C

$$P_6 := \text{if}\left[0.45 < \left(\frac{P_6}{P_{24}}\right) < 0.65, P_6, \text{"NO GOOD"}\right] \qquad P_6 = 2.4 \text{ in}$$

$$i := 7.44 \cdot P_6 \cdot (t_c)^{-0.645} \cdot \frac{\text{in}}{\text{hr}} \qquad i = 2.63 \frac{\text{in}}{\text{hr}}$$

Peak Discharge (cfs)

$$Q_2 := C_t \cdot i \cdot A_t \qquad Q_2 = 4.582 \frac{\text{ft}^3}{\text{s}}$$

Assumed Q = 4.5 cfs for Tt O.K.

Project: Silvergate 230/69kV Substation
Subject: Hydrology Calculations (Proposed Site)

Page ____ of ____
Computed By: TWL Date______
Checked By:___ Date______

Area 3

Rational Method: $Q = CiA$

Existing Site Dimensions (area):

From Figure 5

Overland flow length: $L_0 := 155 \cdot ft$

Gutter Flow Length: $L_g := 275\ ft$

Storm Drain Flow: $L_{sd} := 75\ ft$

Total Area:

$A_t := 1.08 \cdot acre$

Area 1:

Class II Base Area:

$A_{CII} := 22845 \cdot ft^2$ (from figure 5)

$A_{CII} = 0.524\,acre$

Area foundation:

$A_{fd} := 4355 \cdot ft^2$

$A_{fd} = 0.1\,acre$

Asphalt Concrete and Impermeable Area:

$A_{ac} := A_t - A_{CII} - A_{fd}$

$A_{ac} = 0.456\,acre$

Run off Coefficient:

$C_1 := 0.57$ (Class II Aggregate Base)

$C_2 := 0.90$ (AC & Concrete Paving)

$C_3 := C_2$

$$C_t := C_1 \cdot \left(\frac{A_{CII}}{A_t}\right) + C_2 \cdot \left(\frac{A_{ac}}{A_t}\right) + C_3 \cdot \left(\frac{A_{fd}}{A_t}\right)$$

$C_t = 0.74$

Project: Silvergate 230/69kV Substation
Subject: Hydrology Calculations (Proposed Site)

Page ____ of ____
Computed By: TWL Date_____
Checked By: ___ Date_____

Intensity - (assumed Limited Industrial Table 3-2 SDCHM) SEE FIGURE 1, APPENDIX C

Overland Flow:

$t_{i1} := 7.9$ min $\quad L_{max} := 65 \cdot ft$

remaining length: $\quad L_1 := L_o - L_{max} \qquad L_1 = 90\,ft$ $\quad$ in miles = 0.017 miles

Use Kirpich formula:

$$t_{i2} := \left[\frac{\left[11.9 \cdot \left(L_1\right)^3\right]}{\Delta E}\right]^{0.385}$$

where L1 is in miles

$\Delta E := 1.55 \cdot ft$

$t_{i2} := 1.2$ min

$t_i := t_{i1} + t_{i2} \qquad t_i = 9.1$ min

Gutter Flow: (Per Figure 3-6, SDCHM) SEE FIGURE 2, APPENDIX C

From Figure 3 - 6

Assume Q = 2.75 cfs $\quad$ s = 1% $\quad$ assumed avg. $\qquad v := 144 \, \frac{ft}{min}$

$t_{t1} := \frac{L_g}{v} \qquad t_{t1} = 1.91$

Pipe Flow: $\qquad$ Assume Q = 2.75 cfs and diameter of the storm drain = 30 in

Q = VA

$A_{sd} := \left(\frac{\pi}{4}\right) \cdot 2.5^2 \qquad A_{sd} = 4.909 \; ft^2$

$v_1 := \left(\frac{2.75}{A_{sd}}\right) \cdot 60 \qquad v_1 = 33.614 \, \frac{ft}{min}$

$t_{t2} := \frac{L_{sd}}{v_1} \qquad t_{t2} = 2.231$ min

$t_c := t_i + t_{t1} + t_{t2} \qquad t_c = 13.241$ min

$P_6 := 2.4$ in $\quad$ 100 yr 6 hour event (from rainfall Isopluvial Map)

$P_{24} := 3.9$ in $\quad$ 100 yr 24 hour event (from rainfall Isopluvial Map)

Project: Silvergate 230/69kV Substation
Subject: Hydrology Calculations (Proposed Site)

Page ____ of ____
Computed By: TWL Date_____
Checked By:___ Date_____

(FIGURE 3-1, SDCHM) SEE FIGURE 3, APPENDIX C

$$P_6 := \text{if}\left[0.45 < \left(\frac{P_6}{P_{24}}\right) < 0.65, P_6, \text{"NO GOOD"}\right] \qquad P_6 = 2.4 \text{ in}$$

$$i := 7.44 \cdot P_6 \cdot (t_c)^{-0.645} \cdot \frac{in}{hr} \qquad i = 3.374 \frac{in}{hr}$$

Peak Discharge (cfs)

$$Q_3 := C_t \cdot i \cdot A_t \qquad Q_3 = 2.718 \frac{ft^3}{s}$$

Assumed Q = 2.75 cfs for Tt O.K.

Project: Silvergate 230/69kV Substation
Subject: Hydrology Calculations (Proposed Site)

Page ___ of ___
Computed By: TWL Date_____
Checked By:___ Date_____

Area 4

Rational Method: Q = CiA

Existing Site Dimensions (area):

From Figure 5

Gutter Flow Length: $L_g := 420\ \text{ft}$

Total Area:

$A_t := 0.10 \cdot \text{acre}$

Area 1: (conservatively assume the landscape area and driveways have a runoff coefficient equivalent to Class II Base.)

Class II Base Area:

$A_{CII} := A_t$ (from figure 5)

$A_{CII} = 0.1\ \text{acre}$

Run off Coefficient:

$C_1 := 0.57$ (Class II Aggregate Base)

$C_t := C_1$

$C_t = 0.57$

Gutter Flow: (Per Figure 3-6, SDCHM) SEE FIGURE 2, APPENDIX C

Assume all Area 4 drains into the curb and has gutter flow.

From Figure 3 - 6

Assume Q = 0.75 cfs s = 3% assumed avg. $v := 216\ \frac{\text{ft}}{\text{min}}$

$t_{t1} := \frac{L_g}{v}$ $t_{t1} = 1.944$

$t_c := t_{t1}$ $t_c = 1.944\ \text{min}$

$P_6 := 2.4\ \text{in}$ 100 yr 6 hour event (from rainfall Isopluvial Map)

$P_{24} := 3.9 \text{ in}$ 100 yr 24 hour event (from rainfall Isopluvial Map)

(FIGURE 3-1, SDCHM) SEE FIGURE 3, APPENDIX C

$$P_6 := \text{if}\left[0.45 < \left(\frac{P_6}{P_{24}}\right) < 0.65, P_6, \text{"NO GOOD"}\right] \qquad P_6 = 2.4 \text{ in}$$

$$i := 7.44 \cdot P_6 \cdot (t_c)^{-0.645} \cdot \frac{\text{in}}{\text{hr}} \qquad i = 11.628 \frac{\text{in}}{\text{hr}}$$

Peak Discharge (cfs)

$$Q_4 := C_t \cdot i \cdot A_t \qquad Q_4 = 0.668 \frac{\text{ft}^3}{\text{s}}$$

Assumed Q = 0.75 cfs for Tt O.K.

Proposed Total Peak Discharge (cfs):

$$Q_{peak} := Q_1 + Q_2 + Q_3 + Q_4$$

$$Q_{peak} = 9.927 \frac{(\text{ft}^3)}{\text{s}}$$

APPENDIX C – RATIONAL METHOD SUPPORTING TABLES AND FIGURES

Project: Silvergate 230/69kV Substation
Subject: Hydrology Calculations (Proposed Site)

Page ____ of ____
Computed By: TWL Date ____
Checked By: ____ Date ____

FIGURE # 1 APPENDIX C

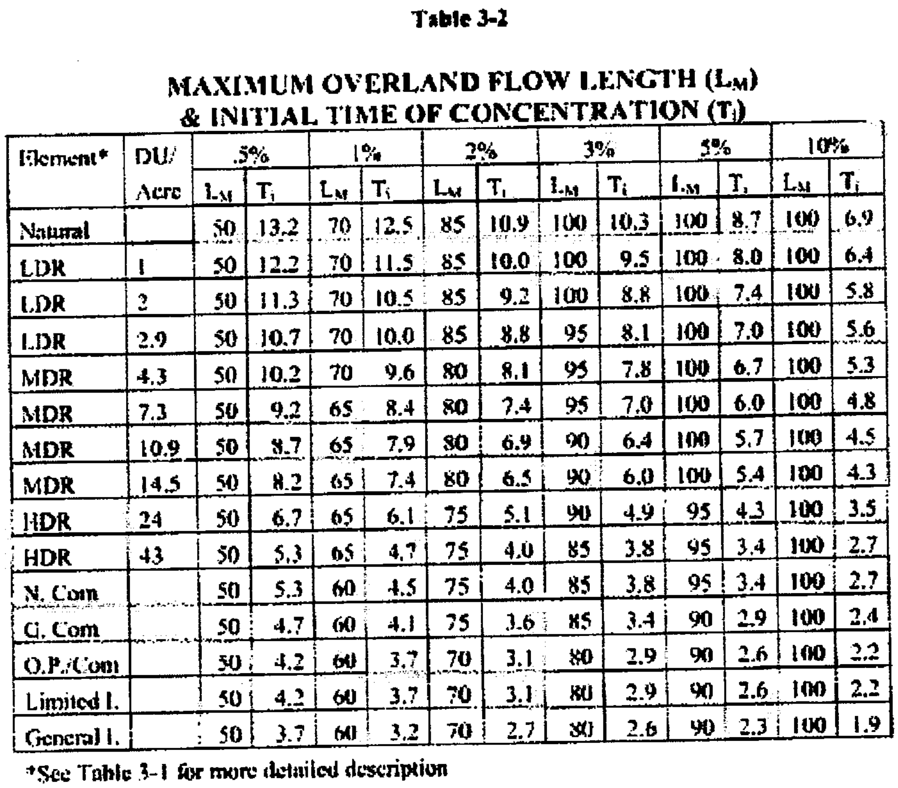


Table 3-2

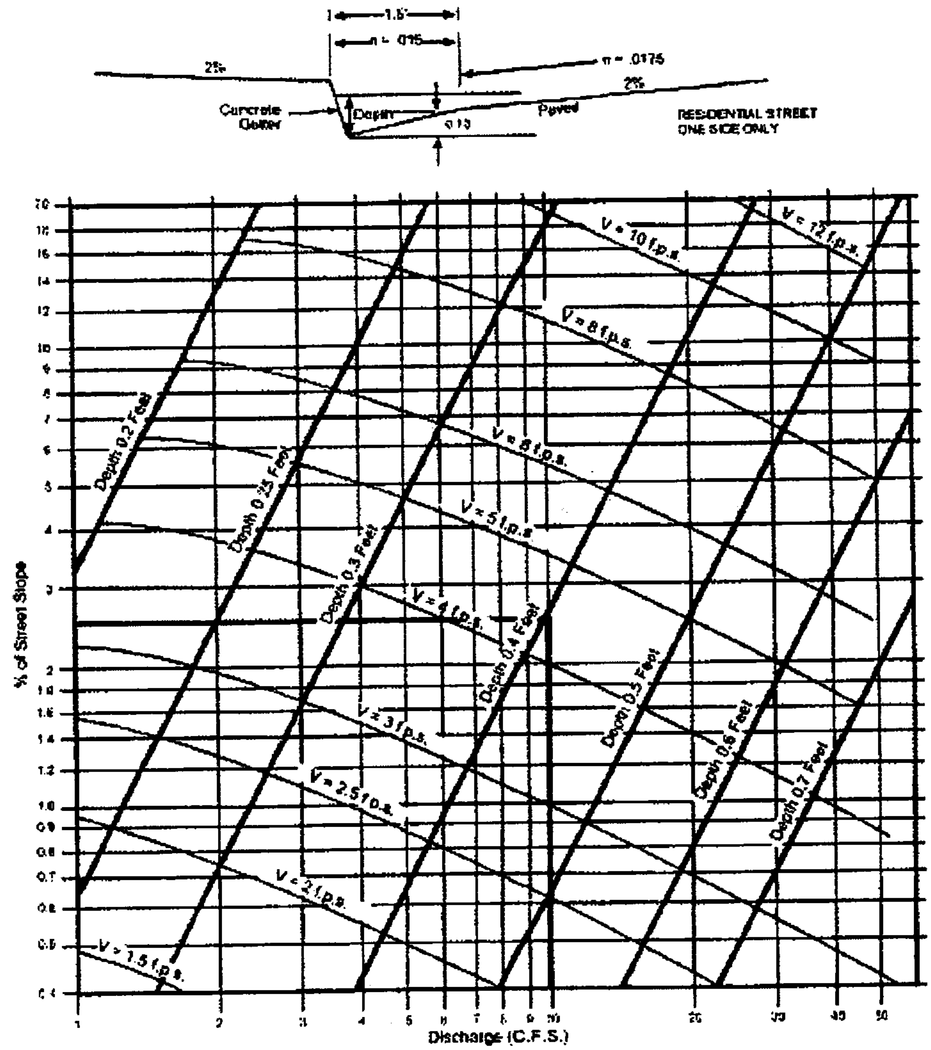
**MAXIMUM OVERLAND FLOW LENGTH (L_M)
& INITIAL TIME OF CONCENTRATION (T_i)**

Element*	DU/ Acre	.5%		1%		2%		3%		5%		10%	
		L_M	T_i	L_M	T_i	L_M	T_i	L_M	T_i	L_M	T_i	L_M	T_i
Natural		50	13.2	70	12.5	85	10.9	100	10.3	100	8.7	100	6.9
LDR	1	50	12.2	70	11.5	85	10.0	100	9.5	100	8.0	100	6.4
LDR	2	50	11.3	70	10.5	85	9.2	100	8.8	100	7.4	100	5.8
LDR	2.9	50	10.7	70	10.0	85	8.8	95	8.1	100	7.0	100	5.6
MDR	4.3	50	10.2	70	9.6	80	8.1	95	7.8	100	6.7	100	5.3
MDR	7.3	50	9.2	65	8.4	80	7.4	95	7.0	100	6.0	100	4.8
MDR	10.9	50	8.7	65	7.9	80	6.9	90	6.4	100	5.7	100	4.5
MDR	14.5	50	8.2	65	7.4	80	6.5	90	6.0	100	5.4	100	4.3
HDR	24	50	6.7	65	6.1	75	5.1	90	4.9	95	4.3	100	3.5
HDR	43	50	5.3	65	4.7	75	4.0	85	3.8	95	3.4	100	2.7
N. Com		50	5.3	60	4.5	75	4.0	85	3.8	95	3.4	100	2.7
G. Com		50	4.7	60	4.1	75	3.6	85	3.4	90	2.9	100	2.4
O.P./Com		50	4.2	60	3.7	70	3.1	80	2.9	90	2.6	100	2.2
Limited I.		50	4.2	60	3.7	70	3.1	80	2.9	90	2.6	100	2.2
General I.		50	3.7	60	3.2	70	2.7	80	2.6	90	2.3	100	1.9

*See Table 3-1 for more detailed description

*source: San Diego County Hydrology Manual, June 2003

FIGURE # 2 APPENDIX C



EXAMPLE:
Given: Q = 10 S = 2.5%
Chart gives: Depth = 0.4, Velocity = 4.4 f.p.s.

SOURCE: San Diego County Department of Special District Services Design Manual

FIGURE **3-6**

Gutter and Roadway Discharge - Velocity Chart

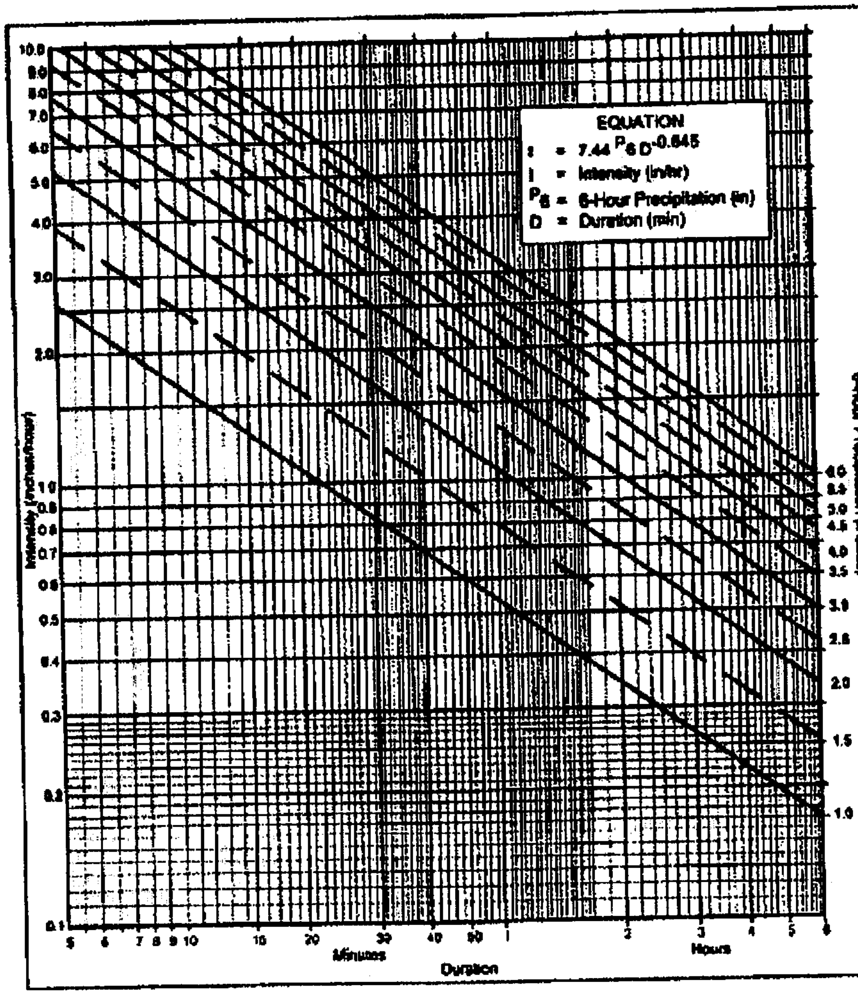
*source: San Diego County Hydrology Manual, June 2003

Project: Silvergate 230/69kV
Substation
Subject: Hydrology Calculations
(Proposed Site)

Page ____ of ____
Computed By: TWL Date______
Checked By:____Date______

FIGURE # 3 APPENDIX C

*source: San Diego County Hydrology Manual, June 2003



$I = 7.44\ P_6\ D^{-0.645}$
I = Intensity (in/hr)
P_6 = 6-Hour Precipitation (in)
D = Duration (min)

Directions for Application:

(1) From precipitation maps determine 6 hr and 24 hr amounts for the selected frequency. These maps are included in the County Hydrology Manual (10, 50, and 100 yr maps included in the Design and Procedure Manual).

(2) Adjust 6 hr precipitation (if necessary) so that it is within the range of 45% to 65% of the 24 hr precipitation (not applicable to Desert).

(3) Plot 6 hr precipitation on the right side of the chart.

(4) Draw a line through the point parallel to the plotted lines.

(5) This line is the intensity-duration curve for the location being analyzed.

Application Form:

(a) Selected frequency ______ year

(b) P_6 = ______ in., P_{24} = ______, $\frac{P_6}{P_{24}}$ = ______ %$^{(2)}$

(c) Adjusted $P_6^{(2)}$ = ______ in.

(d) t_x = ______ min.

(e) I = ______ in./hr.

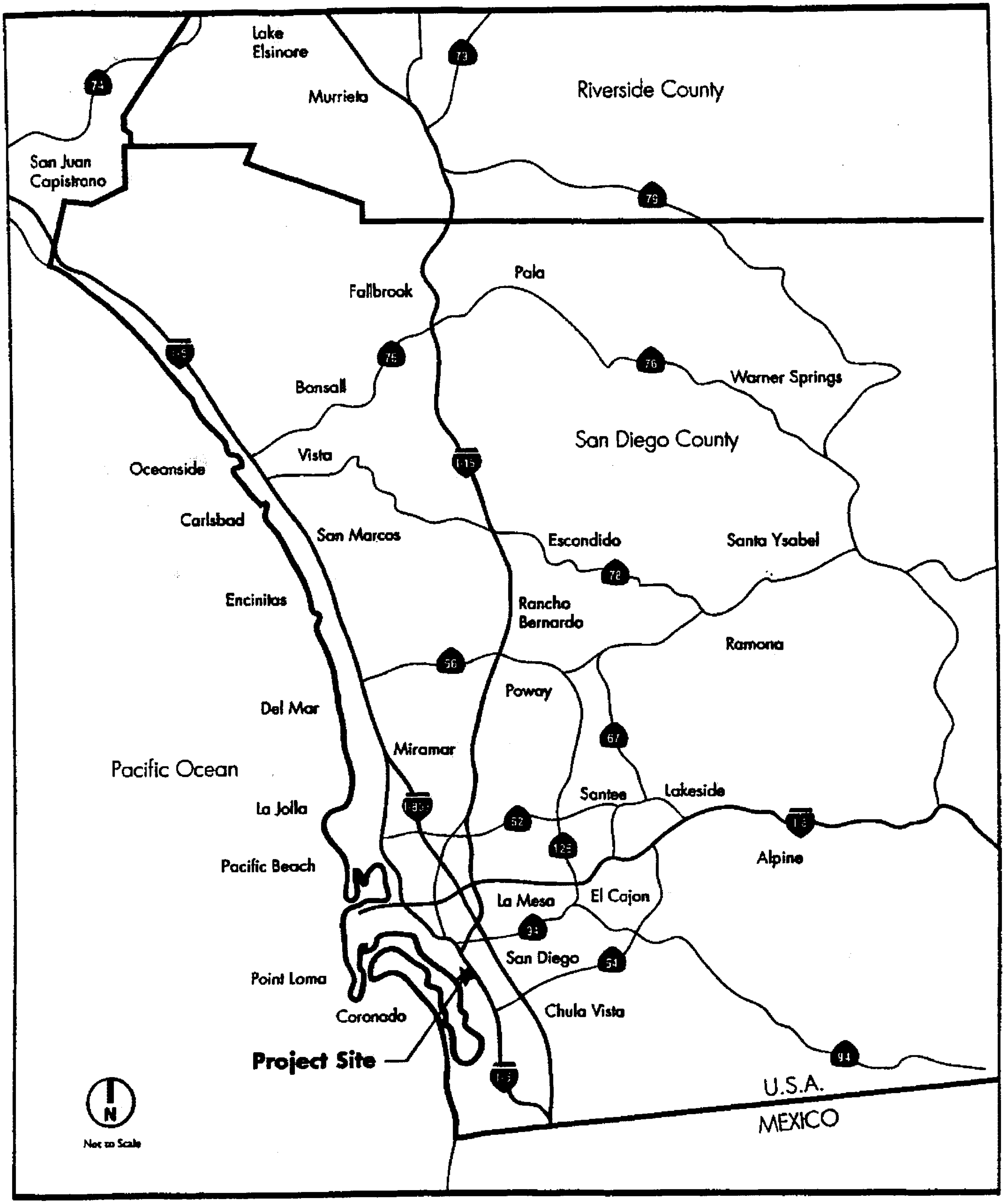
Note: This chart replaces the Intensity-Duration-Frequency curves used since 1965.

P6 Duration	1	1.5	2	2.5	3	3.5	4	4.5	5	5.5	6
5	2.63	3.95	5.27	6.59	7.90	9.22	10.54	11.86	13.17	14.49	15.81
7	2.12	3.18	4.24	5.30	6.36	7.42	8.48	9.54	10.60	11.66	12.72
10	1.68	2.53	3.37	4.21	5.05	5.90	6.74	7.58	8.42	9.27	10.11
15	1.30	1.95	2.59	3.24	3.89	4.54	5.19	5.84	6.49	7.13	7.78
20	1.08	1.62	2.15	2.69	3.23	3.77	4.31	4.85	5.39	5.93	6.46
25	0.93	1.40	1.87	2.33	2.80	3.27	3.73	4.20	4.67	5.13	5.60
30	0.83	1.24	1.66	2.07	2.49	2.90	3.32	3.73	4.15	4.56	4.98
40	0.69	1.03	1.38	1.72	2.07	2.41	2.76	3.10	3.45	3.79	4.13
50	0.60	0.90	1.19	1.49	1.79	2.09	2.39	2.69	2.98	3.28	3.58
60	0.53	0.80	1.06	1.33	1.59	1.86	2.12	2.39	2.65	2.92	3.18
90	0.41	0.61	0.82	1.02	1.23	1.43	1.63	1.84	2.04	2.25	2.45
120	0.34	0.51	0.68	0.85	1.02	1.19	1.36	1.53	1.70	1.87	2.04
150	0.29	0.44	0.59	0.73	0.88	1.03	1.18	1.32	1.47	1.62	1.76
180	0.26	0.39	0.52	0.65	0.78	0.91	1.04	1.18	1.31	1.44	1.57
240	0.22	0.33	0.43	0.54	0.65	0.76	0.87	0.98	1.08	1.19	1.30
300	0.19	0.28	0.38	0.47	0.56	0.66	0.75	0.85	0.94	1.03	1.13
360	0.17	0.25	0.33	0.42	0.50	0.58	0.67	0.75	0.84	0.92	1.00

Intensity-Duration Design Chart - Template

FIGURE
3-1

FIGURE 1 – PROJECT LOCATION



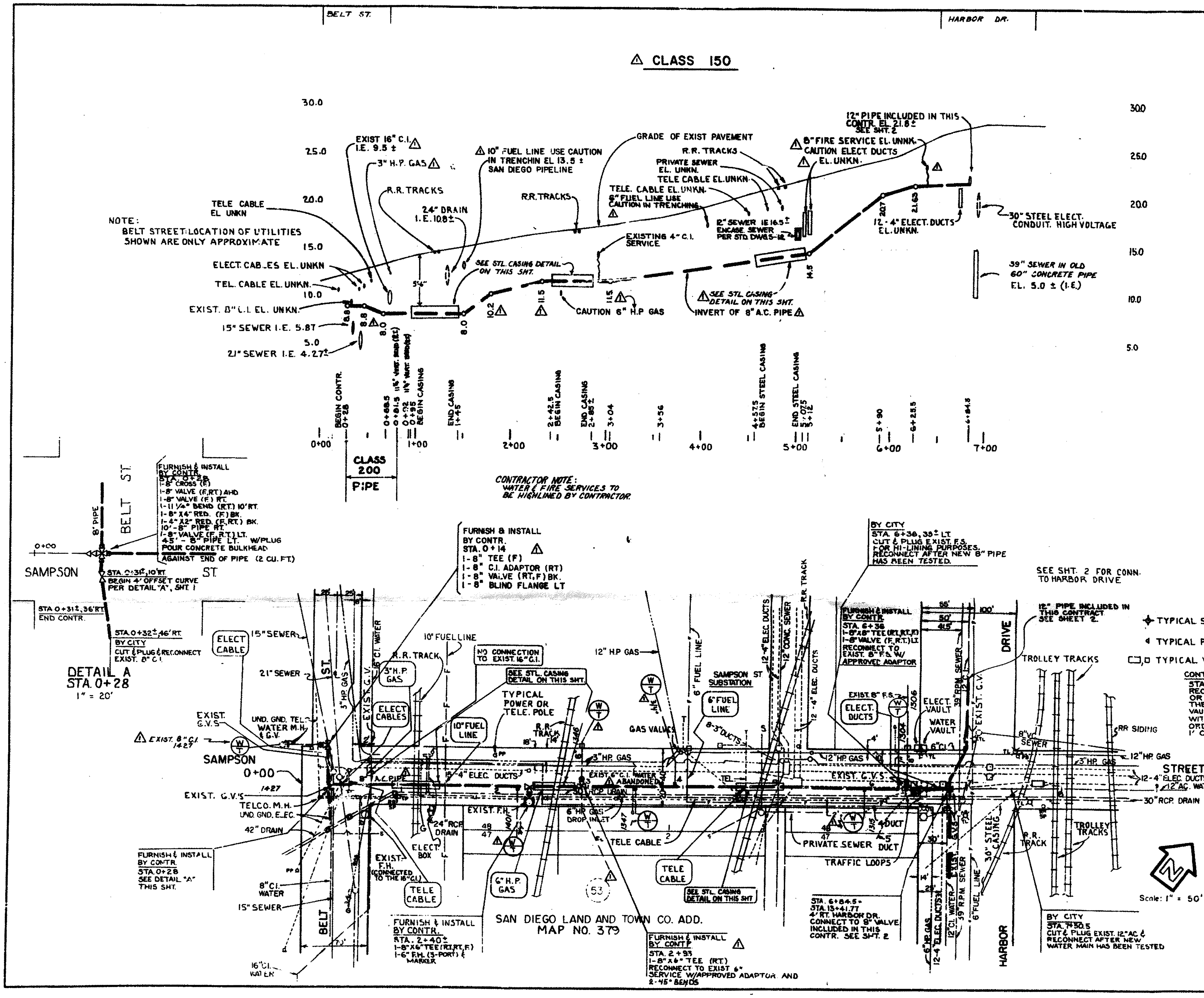
RBF CONSULTING

Regional Map

SDG&E Silvergate Transmission Substation

Figure 1

SOURCE: SDG&E'S PEA DOCUMENT MARCH 30, 2005



REFERENCES:
WATER, SEWER & DRAINAGE 100' SCALE 192-1725 194-1725
GAS BOOK 10 PAGES 548A, 547, 547A
WATER: 2682-L 11558-15-D
SEWER: 18366-7-D 12333-D
OIL PIPELINES GAS BOOK 10 PAGE 548A
ELECT. 15169-1-D S.D.G.&E. S-5869 S.D.G.&E. A-4650
DRAIN 6802-L 14011-5-D 2682-L

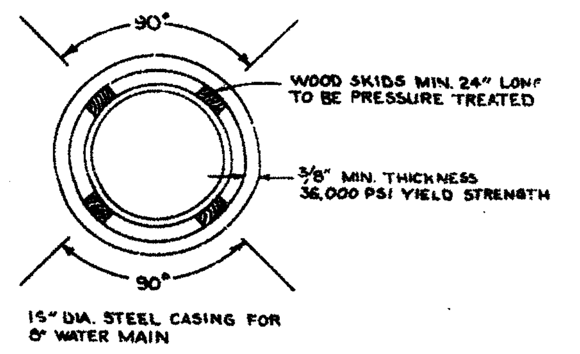
FIELD NOTES: BURRIS 9-15-83 192, 194-1725 148171

BENCH MARK: (MEAN SEA LEVEL DATUM)
W.B.P. SAMPSON ST. & NEWTON AVE.
ELEV. 43.016

RETIREMENT:

660	LIN./FT.	6" C.I.	1988
80	LIN./FT.	8" C.I.	UNKNOWN
FIRE	HYDRANT	1	UNKNOWN

STEEL CASING DETAIL



15" DIA. STEEL CASING FOR 8" WATER MAIN

CONTRACTOR NOTE
STA. 6+47, 4' RT.
RECORDS INDICATE THAT LITTLE OR NO CLEARANCE EXISTS BETWEEN THE EXIST. 12" C.I. & THE S.D.G.&E. VAULT. IF NECESSARY, PULL PIPE JOINTS WITHIN 10'-20' OF THE VAULT IN ORDER TO PROVIDE A MINIMUM 1' CLEARANCE.

△2 NOTE: NO CITY CONNECTION SHEET AVAILABLE

SAMPSON ST.

WATER GROUP 445
SAMPSON STREET----- 8" PIPE
BELT ST. TO HARBOR DR.

CITY OF SAN DIEGO, CALIFORNIA
UTILITIES DEPARTMENT
SHEET 5 OF 15 SHEETS

E.W.O. 148171
U.W.O. 17121

E E Clay
UTILITIES DIRECTOR DATE

Mike Mill 2-27-85
ENGINEERING SUPERINTENDENT

2-27-85
DESIGN ENGINEER

DESCRIPTION	BY	APPROVED	FILMED
ORIGINAL	JS/HF	R. Budd	
△1 AS-BUILT	AA/EB		
△2 CITY FORCE	AA/EB		

CONTROL CERTIFICATION

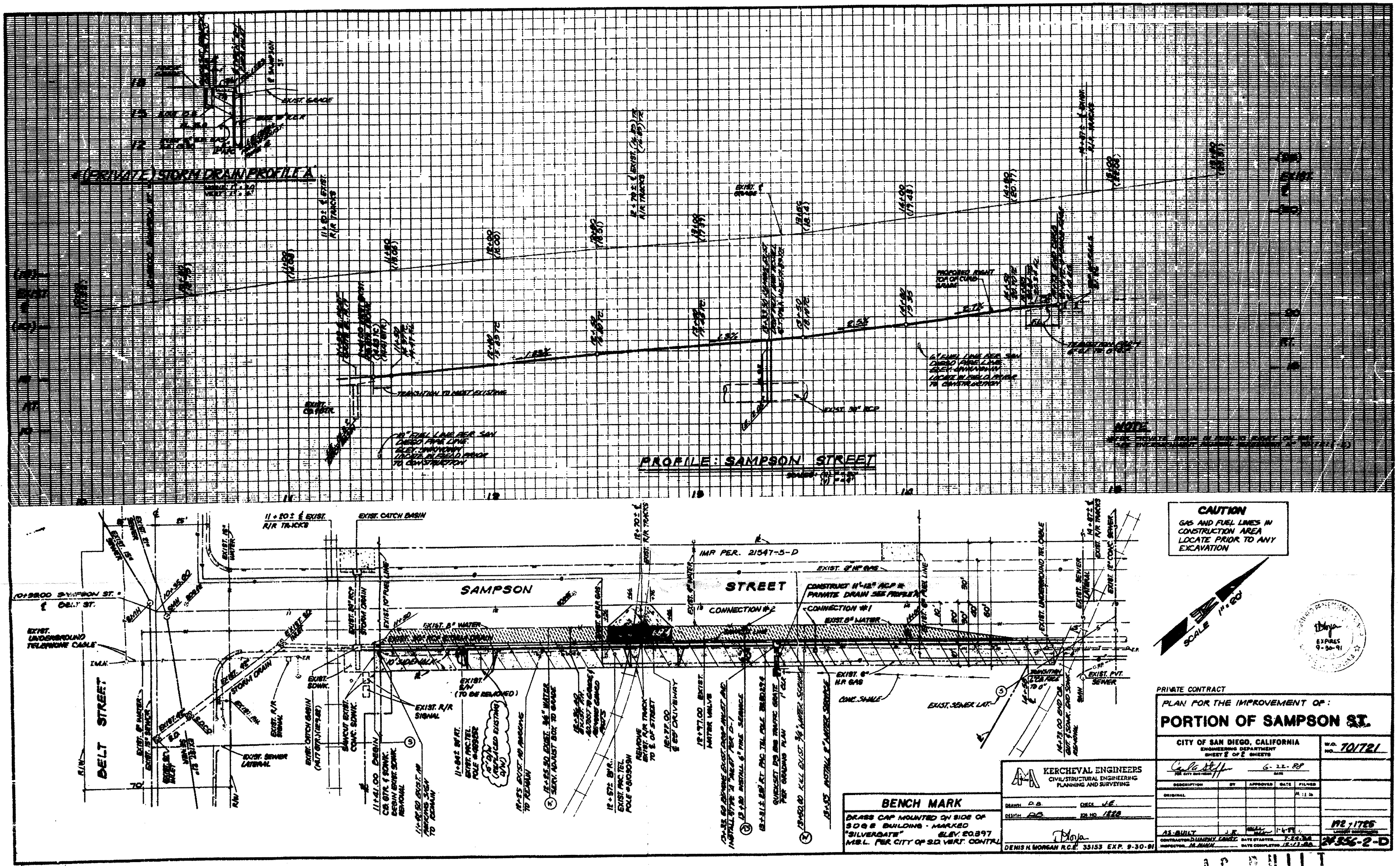
CONSTRUCTION RECORD
CONTRACTOR: CAMERON BRO. DATE STARTED 10-14-85
INSPECTOR: KEVIN ESTRADA DATE COMPLETED 6-5-86
CONNECTIONS BY: CITY FORCES

192 - 1722
LAMBERT COORDINATES

21547-5-D

AS-BUILT

0 1 2 3 4 IN.



CAUTION

GAS AND FUEL LINES IN CONSTRUCTION AREA LOCATE PRIOR TO ANY EXCAVATION

EXPIRES 9-30-91

PRIVATE CONTRACT

PLAN FOR THE IMPROVEMENT OF :

PORTION OF SAMPSON ST.

CITY OF SAN DIEGO, CALIFORNIA
ENGINEERING DEPARTMENT
SHEET 2 OF 2 SHEETS

W.O. NO. 701721

FOR CITY ENGINEER 6-22-88 DATE

DESCRIPTION	BY	APPROVED	DATE	FILMED
ORIGINAL				
AS-BUILT	J.R.		1-4-89	

CONTRACTOR D.LUNDY CONST. DATE STARTED 7-24-88
INSPECTOR M. NUNN DATE COMPLETED 12-13-88

192-1725

LAMBERT COORDINATES

24356-2-D

KERCHEVAL ENGINEERS
CIVIL/STRUCTURAL ENGINEERING
PLANNING AND SURVEYING

DRAWN D.B. CHECK J.E.
DESIGN D.B. JOB NO 1228

DMorgan
DENIS H. MORGAN R.C.E. 35153 EXP. 9-30-91

BENCH MARK

BRASS CAP MOUNTED ON SIDE OF SDG&E BUILDING - MARKED "SILVERGATE" ELEV. 20.897 M.S.L. PER CITY OF S.D. VERT. CONTROL

AS BUILT

City of San Diego
Storm Water Pollution Prevention Program
1970 B Street, MS 27A
San Diego, CA 92102

October 25, 2005

Attn: Chris Zirkle

Subject: Notice of Violation, October 14, 2005

Dear Mr. Zirkle:

This letter is written in response to your letter to SDG&E, dated October 14, 2005. The letter was notification of an unauthorized discharge to the municipal storm drain system in the area of our Silver Gate Power Plant.

Because we have limited knowledge of the storm drain system in the vicinity of Silver Gate, and also have no knowledge of how storm water runoff from Silver Gate may be collected in the storm drains, we can reach no conclusion if the contaminants found are the responsibility of SDG&E. In an effort to be cooperative with the City, and to assist with resolving this issue, SDG&E has elected to take the following steps:

1. On Monday, October 24, an SDG&E contractor removed the sediment from the catch basin and adjoining pipes. The material was drummed and prepared for appropriate disposal.

2. Over the next several weeks, we will attempt to determine the routing of the six inch and twelve inch laterals which discharge to the catch basin. We will also evaluate how the Silver Gate systems may connect to the storm water system, if in fact they do.

3. We will review the systems at Silver Gate to determine of a source of PCBs and PAHs may be present.

We met with Ruth Kolb of your department on Thursday, October 20. She was very helpful at helping us understand this issue. We look forward to working with you and your staff to reolve this problem.

Sincerely,

Ken Rowland

City of San Diego
Storm Water Pollution Prevention Program
1970 B Street, MS 27A
San Diego, CA 92102

December 1, 2005

Attn: Chris Zirkle

Subject: Notice of Violation, October 14, 2005

Dear Mr. Zirkle:

This letter is written as further response to your letter to SDG&E, dated October 14, 2005, and will also serve as our monthly status update pursuant to your letter of November 8, 2005.

We have determined that the six inch line which enters the interceptor at Sampson and the railroad tracks originates at the Silver Gate turbine room roof. Rainfall drainage from the turbine room roof and the Unit #1 roof proceeds underground from the southeast corner of the power house to the interceptor.

We know of no source of PCBs which would be on the roof of the power house. We therefore will begin sampling areas in and around the Silver Gate facility to determine if the PCBs have some source other than the lines which enter the interceptor.

We also determined that the twelve inch line which terminates in the interceptor is blocked with dirt and debris approximately ten feet from the outlet. Is doesn't appear that the twelve inch line will transmit stormwater anymore.

To reduce the amount of debris and trash which may enter the storm drain, we have undertaken to remove all rubbish from the front of the power house building. We will work to maintain good housekeeping in the area of the power plant to continue to reduce the impact to the Bay.

If you have any questions or comments, please don't hesitate to contact me at 213-220-1405.

Sincerely,

Ken Rowland
Senior Project Manager

City of San Diego
Storm Water Pollution Prevention Program
1970 B Street, MS 27A
San Diego, CA 92102

January 10, 2006

Attn: Chris Zirkle

Subject: Notice of Violation, October 14, 2005

Dear Mr. Zirkle:

This letter is written as our continuing response to your letter to SDG&E, dated October 14, 2005, and will also serve as our monthly status update pursuant to your letter of November 8, 2005.

We have collected a number of samples which represent the sediment from the street and driveway areas around the Silver Gate Power Plant. The samples were collected from areas in front of and up gradient of the Power House. These samples are being analyzed for PCBs and we hope to have all data available in a report by the end of the first week in February.

We have also examined the rooftop of the turbine room at the Power Plant to determine if there could be any source of PCBs at which could enter the 6-inch drain leading to the interceptor. We have sampled loose material on the roof and will include that data in the above mentioned report. We will continue to evaluate potential sources of contaminants into the storm water system.

If you have any questions or comments, please don't hesitate to contact me at 213-220-1405.

Sincerely,

Ken Rowland
Senior Project Manager

March 16, 2006

City of San Diego
Storm Water Pollution Prevention Program
1970 B Street, MS 27A
San Diego, CA 92102

Attn: Chris Zirkle

Subject: Notice of Violation, October 14, 2005

Dear Mr. Zirkle:

Attached are three copies of a report summarizing findings of our investigation related to the Notice of Violation issued on October 14, 2005. The investigation was designed to resolve concerns about the source of contaminants found in a storm drain catch basin near the intersection of Sampson and Belt Streets.

We have collected a number of samples which represent the sediment from the street and driveway areas around the Silver Gate Power Plant. The samples were collected from areas in front of and up gradient of the Power House. These samples were found to contain PCBs, PAHs, and metals in various concentrations. Because of the variety of locations, there are likely a variety of sources for the contaminants.

We will now begin to formulate corrective actions for those potential sources which we have identified. In addition, we will continue expand our sampling to attempt to determine whether other sources distinct from Silver Gate can be identified.

Please review the attached information. If you have any questions or comments, please don't hesitate to contact me at 213-220-1405.

Sincerely,

Ken Rowland
Senior Project Manager

Freshwater Contamination (Proceedings of Rabat Symposium S4, April-May 1997).
IAHS Publ. no. 243, 1997

Pollutant and organic matter content in sediment particle size fractions

MARCELL SCHORER
Department of Hydrology, University of Trier, D-54286 Trier, Germany

Abstract In a partly urbanized catchment to the south of Trier, Germany, selected sediment samples were separated into different size fractions ranging from <2 μm to 200 μm. Each sample fraction was analysed for heavy metals, polychlorinated biphenyls (PCB), polycyclic aromatic hydrocarbons (PAH) and organic carbon. The results show a linear correlation between heavy metal content and particle size. The organic content of the samples does not play an important role in heavy metal adsorption. In contrast, the organic micropollutants (PAHs and PCBs) do not correlate with the particle size distributions but with the content of the organic material. The maximum concentrations of organic micropollutants and organic carbon are not associated with the clay fraction but are bimodally distributed. The bimodal distribution can be explained by the presence of two types of organic material in the sediment.

INTRODUCTION

River sediments are a major potential sink for hydrophobic pollutants in the aquatic environment (Karickhoff *et al.*, 1979; Means *et al.*, 1980; Voice & Weber, 1983). The organic matter content of river sediment has been shown to be an important factor determining the extent of sorption (Means *et al.*, 1980; Baughman & Paris, 1981; Karickhoff, 1981; Calmano & Förstner, 1996). In the literature, the occurrence of organic pollutants in river sediments has been correlated with the abundance of clay. It has been assumed that the efficacy of inorganic exchange sites of the clay and its associated organic matter are responsible for the amount and the behaviour of the sorbed substances (Karickhoff & Brown, 1978).

Only a few studies discuss the behaviour of organic micropollutants and the influence of different grain size fractions. Even within these studies, the lack of standardization in particle fractionation methods aggravates the comparison and generalization of acquired data (Karickhoff *et al.*, 1979; Readman *et al.*, 1984; Umlauf & Bierl, 1987; Evans *et al.*, 1990). Since sediments are potential sinks and sources of contaminants in the aquatic environment it is of overriding importance to determine the partition of pollutants to different particle size fractions, because different particle sizes exhibit different remobilization and transport processes.

In the present investigation, sediment size classes ranging from <2 μm to 200 μm were examined with the aim of determining the relationships between the organic material, clay content, and the individual and total PAH, PCB and heavy metal content in each particle size fraction.

MATERIAL AND METHODS

Study area

The study area, which comprises the 39 km^2 drainage basin of the Olewiger Bach, is located to the south of Trier in the western part of Germany. Devonian shales of the Hunsrück Mountains with quartz and diabase veins dominate the geology. Pleistocene terraces of the River Mosel overlie the solid geology in the northern part of the drainage basin. Land use is predominantly agriculture with grassland and arable farming. Settlement covers about 10% of the area. Runoff from several roads, effluents from small industries and untreated waste water from solitary farms influence river water quality.

Sediment sampling

Freshwater surface sediments from two sites were sampled weekly from August 1993 to December 1995. For sediment sampling, several concrete slabs (each 0.1 m^2 in area) were placed into the river at the sampling sites. Care was taken to keep the slab surface even with the river sediment. For a better understanding of the highly dynamic process of pollutant enrichment in sediments, it is necessary to sample frequently (Schorer *et al.*, 1994; Schorer *et al.*, 1995; Symader *et al.*, 1994), and therefore material was collected on a weekly basis. Interactions with the underlying bed were prevented by the complete removal of the sediments from the slabs. Biogeochemical changes following deposition were minimized.

The sediments were placed directly into solvent-washed, 2 l glass bottles with glass cutting lids. Fresh samples were wet sieved (200 μm and 63 μm) within 2 h. The fraction smaller 63 μm was centrifuged to separate the sediment particles from the aqueous phase, and the 63-200 and <63 μm fractions were freeze dried.

Particle size fractionation

Selected sediment samples were separated into the following size fractions: <2 μm (clay), 2-6.3 μm (fine silt), 6.3-12.5 μm (finer middle silt), 12.5-20 μm (coarser middle silt), 20-63 μm (coarse silt) and 63-200 μm (fine sand). The 63-200 μm fraction was wet sieved and the different particle sizes <63 μm were obtained using an elutriation system (Muller & Tisue, 1977; Umlauf & Bierl, 1987). The sedimentological and soil science literature abounds with particle size separation techniques, including wet and dry sieving, normal and centrifugally accelerated sedimentation in several media, filtration, ultrafiltration and elutriation. The choice of method depends on the demands of the particular case. Sieving cannot separate particles of <20 μm, and centrifugation requires special equipment. Elutriation procedures seem to avoid these difficulties.

Elutriation involves suspending the sample in an upward water flow. Particles that settle at velocities greater than the upward velocity remain in the separation chamber; those that settle at lower velocities are carried out upward to the next separation chamber. The separation apparatus consists of a magnetic stirrer to keep the initial sample in suspension. A peristaltic pump, which can be set at different speeds and is linked to separation cylinders of varying sizes, provides the required upward velocities. The settling velocities for each particle size fraction can be calculated using Stoke's law. Since the settling behaviour of a particle is a function of its density, shape and other hydrodynamic parameters, an examination of the fractionation efficiency can be determined. For referencing, the grain size distribution of a small part of each fraction was determined using a laser particle analyser (CIS, Fa. GALAIS/LOT).

Samples were dispersed in 0.001 M $Na_4P_2O_7$ and stirred for 1 h. After flushing the separation tubes with water, the peristaltic pump was activated. The separation is finished, when the cylinders become clear (after about 30 h). The isolated fractions in the cylinders are flushed through a valve at the bottom of the separation tubes and the finest fraction is centrifuged using a continuous flow centrifuge. All fractions were freeze dried and weighed.

Analyses

Each fraction of the sediment samples was investigated for selected heavy metals (Pb, Cu, Zn, Fe, Mn), polychlorinated biphenyls (PCBs), polycyclic aromatic hydrocarbons (PAHs) and organic carbon content. Heavy metals were analysed with an atomic absorption spectrometer (AAS), after decomposition under pressure with concentrated nitric acid. Nitrogen and organic carbon were determined with an element analyser. For the analysis of PAHs and PCBs, the samples were spiked with internal standards and were solvent extracted using Aceton/Hexan 1:1 in a Soxhlet system for 8 h. After rotary evaporation almost to dryness, the solvent extracts were purified by column chromatography. Identification and quantification were achieved by gas chromatography/mass spectrometry operating in the selected-ion-monitoring mode.

RESULTS AND DISCUSSION

Selected river sediments that have been taken weekly from August 1993 to December 1995 from two sampling sites were fractionated. Table 1 presents the percentage organic carbon content in each size fraction. Many previous field studies suggest that the organic matter content of river sediment increases with decreasing particle size (Evans *et al.*, 1990). In the present study, highest organic matter contents were not found in the clay fraction, but in a bimodal distribution showing peaks in the fine silt and fine sand fractions. This bimodal distribution of organic carbon can be explained by the presence of different types of organic material in the sediment, which is reflected in its C/N ratio. The organic material associated with different size fractions of the sediment in the Olewiger Bach has different origins. Condensed humic substances form coatings and complexes with particles in smaller fractions, while organic material in the larger fractions comprises flocs of algae and small

Table 1 Organic carbon (%) and PAH and PCB concentrations (µg kg^{-1}) in size fractions of selected sediment samples.

Sample	Parameter	<2 µm	2-6.3 µm	6.3-12.5 µm	12.5-20µm	20-63 µm	63-200 µm
IR 06	Org. C	3.3	4.2	3.6	3.2	1.9	4.1
	C/N	6.2	9.0	10.7	11.6	10.0	12.0
	ΣPCB	20.7	38.8	31.8	31.3	30.7	67.0
	ΣPAH	1562.0	2458.5	2964.3	3736.6	2246.5	3349.0
IR 26	Org. C	1.8	2.6	2.4	2.5	1.7	4.6
	C/N	6.0	8.0	8.8	9.1	8.1	11.6
	ΣPCB	8.2	22.5	21.3	22.0	17.7	44.4
	ΣPAH	2781.9	2934.8	2790.0	2944.1	1853.9	3105.4
IR 27	Org. C	1.8	2.7	2.7	2.4	1.6	4.2
	C/N	5.4	8.4	9.8	9.8	8.7	11.8
	ΣPCB	12.4	23.1	21.3	19.5	19.6	52.5
	ΣPAH	1959.5	2018.4	2117.0	2133.9	1408.2	3487.5
IR 28	Org. C	1.8	2.2	1.9	1.8	0.7	1.4
	C/N	5.8	8.4	9.0	9.8	7.9	8.6
	ΣPCB	4.9	11.7	10.2	10.4	5.3	13.6
	ΣPAH	1180.7	1268.5	1318.2	1393.7	667.0	1222.4
IR 29	Org. C	2.0	2.6	2.2	2.0	0.9	2.2
	C/N	6.2	8.6	9.3	9.4	8.2	10.8
	ΣPCB	4.4	17.8	14.9	9.9	8.4	27.6
	ΣPAH	1171.9	1331.1	1404.0	1598.3	870.4	2299.2
IR 30	Org. C	2.2	3.0	2.8	2.7	1.3	4.0
	C/N	5.9	8.5	9.9	10.8	8.7	11.5
	ΣPCB	3.4	21.3	18.2	17.3	14.6	51.8
	ΣPAH	1724.3	1889.7	1883.8	1972.0	1271.1	3219.2
IR 39	Org. C	3.1	4.0	3.3	2.7	1.1	5.2
	C/N	6.4	9.1	10.7	11.7	10.4	12.5
	ΣPCB	10.1	35.2	25.1	23.6	21.0	84.5
	ΣPAH	1442.1	2005.7	2374.7	2757.1	1622.1	3836.1
KG 06	Org. C	3.9	4.7	4.5	4.7	3.2	7.0
	C/N	5.6	8.9	10.1	10.5	9.9	12.9
	ΣPCB	35.0	40.2	37.5	39.1	33.1	84.4
	ΣPAH	3255.6	4235.4	4329.7	4642.0	2868.5	6040.8
KG 12	Org. C	3.6	4.0	3.8	3.2	1.8	3.3
	C/N	5.8	8.7	9.8	10.0	9.3	12.8
	ΣPCB	14.9	22.0	19.5	17.4	12.2	36.0
	ΣPAH	1962.8	2143.1	2214.5	2278.4	1162.9	3449.4
KG 39	Org. C	4.0	4.3	4.0	2.9	1.1	4.4
	C/N	6.3	9.4	11.8	12.7	10.8	13.7
	ΣPCB	27.7	37.3	33.3	29.7	25.5	128.3
	ΣPAH	2103.5	2809.3	3972.0	4031.1	1915.4	6331.6
KG 41	Org. C	4.0	4.9	4.7	4.1	1.9	7.5
	C/N	6.6	9.4	10.9	11.7	11.4	14.2
	ΣPCB	20.1	33.5	30.6	30.7	21.0	79.8
	ΣPAH	2164.4	2695.4	2836.2	3127.8	1810.3	5276.5

pieces of degraded plant material. Sorption behaviour is known to differ according to the origin and composition of the organic material (Chen *et al.*, 1995; Flemming *et al.*, 1996).

Figure 1 plots the heavy metal content in the different particle sizes for selected samples. Heavy metals are more adsorbed by the smaller particles, especially clay, than by the coarser fractions. The organic content of the samples plays a minor role in heavy metal adsorption. In contrast to the organic content, the heavy metal content decreases continuously from the clay to the coarse silt fraction. In the fine sand fraction, however, there is a weak, but unexpected, increase in heavy metals which is an artefact of the fractionation techniques used in this study. Wet sieving without dispersion for the 63-200 μm fraction does not remove all <63 μm inorganic particles from the fine sand fraction, and these aggregate to flocs of >63 μm with

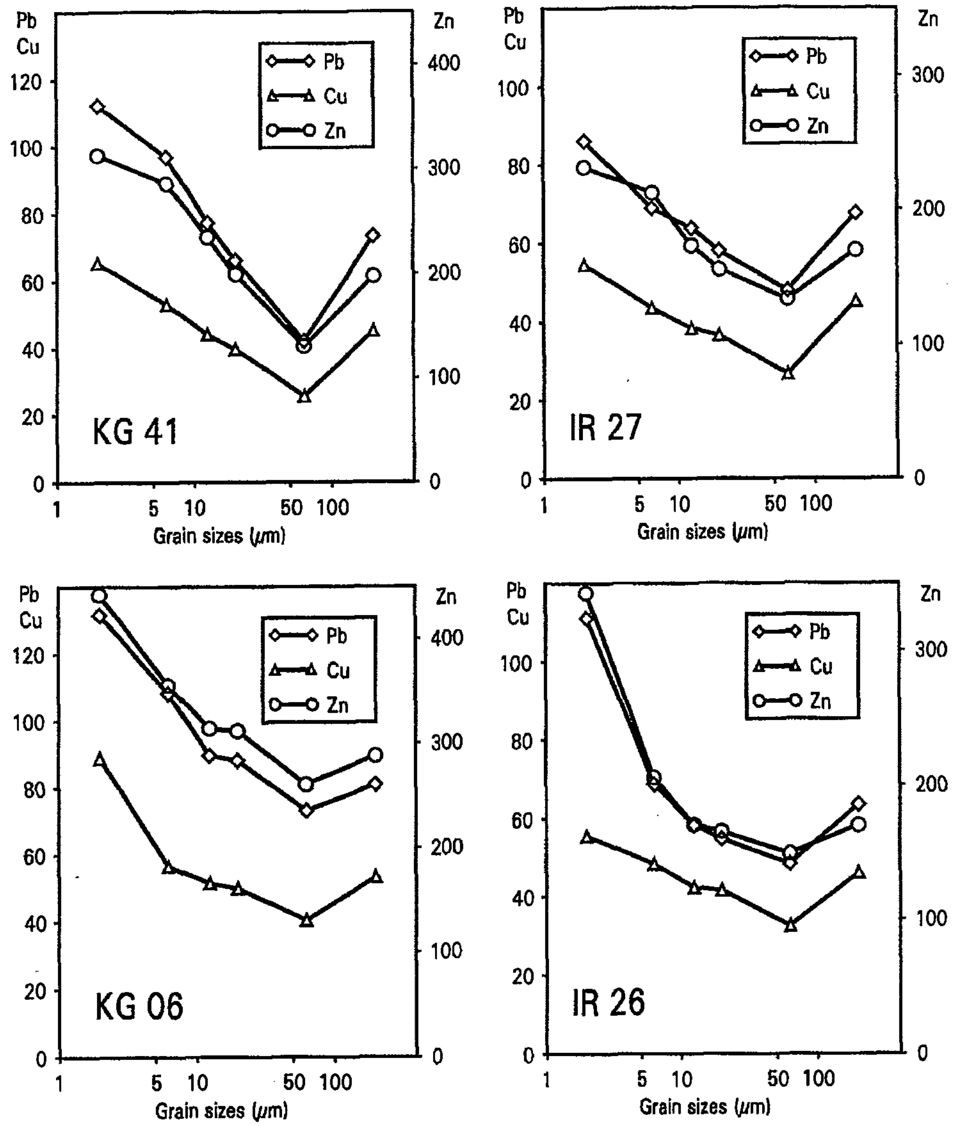


Fig. 1 Heavy metal content (mg kg^{-1}) of sediment size fractions for selected samples.

organic material. This aggregated fine inorganic material is responsible for the increase in heavy metal content associated with the fine sand fraction. Dispersion and particle size analysis of the latter revealed a significant portion of <63 μm particles.

The behaviour of total PAH and PCB contents, however, is different to that of the heavy metals. They show no correlation with the particle size distributions but are correlated with the abundance of organic material. Maximum contents of the organic pollutants and organic carbon are not found in the clay fraction but are bimodally distributed (Table 1). The PAH and PCB loadings do not vary in a simple way with particle size. For example, the PCB content of sample IR06 increases from the clay to fine silt fraction, decreases as the fractions coarsen to coarse silt, but increases again in the fine sand fraction (Table 1). The PAH content of sample IR06, however, increases from the clay to the coarse middle silt fraction, decreases to the coarse silt fraction but increases again in the fine sand fraction. In general, the PCB content (sum of the congeners 28, 52, 101, 138, 153 and 180) follows the organic carbon content so that PCBs are bimodally distributed with maxima in the fine silt and in the fine sand fraction. The number of possible sorption sites, in contrast to qualitative aspects of the organic material, seems to be decisive for the sorption of PCB. In comparison, the total PAH content (sum of the 16 PAHs of the US-EPA priority pollutants list without Naphthalene and with Benzo(e)pyren) demonstrate a different sorption behaviour. They are also bimodally distributed, but the first maximum occurs in the coarser middle silt fraction, in contrast to the fine silt fraction for PCBs. It is clear from Table 1, that the total PAH content and the C/N ratio is similarly distributed between the different size fractions. Like the PAHs, the C/N ratio increases from clay to the coarser middle silt fraction, decreases to the coarse silt fraction, and increases again in the fine sand fraction. It is not the highly condensed organic substances with an enriched aromatic fraction forming coatings and films on clay (Schmitt *et al.*, 1996) and characterized by low C/N values that adsorb the highest PAH content, but rather the less decomposed organic matter with high C/N values, such as fragmentary plant material. Other studies of PAHs and sediments have found two general types of organic material with different affinities to PAHs in different particle size fractions (Evans *et al.*, 1990). In the present investigation, the chemical composition and structure, and not the quantity of the organic material in sediments, are the decisive factors affecting sorption of PAHs. The distribution of PAHs and PCBs in the different grain sizes suggests that the time of adsorption of the pollutants onto particles is a leading factor. The PAHs represent a later period of adsorption, since they are adsorbed on growing organic material such as biofilms and flocs with incorporated plant material. The PCB congeners, however, are adsorbed a long time before the PAHs are adsorbed onto the sediment particles. They are associated with highly condensed organic material, which is distributed regularly in all fractions.

Figure 2 demonstrates the relationship between selected individual PAH and PCB compounds and organic carbon. Results from all samples collected from one sampling site (Irsch) were used to construct the graphs. Regression analyses (Table 2) show a highly significant linear relationship between individual PAHs and PCBs and organic carbon. The individual PCB congeners, such as PCB 138, show a stronger correlation with organic carbon than the individual PAHs (Phen, Flua, Chry, I(cd)P, B(ghi)P). For individual PAHs, it is noticeable that the scatter in the

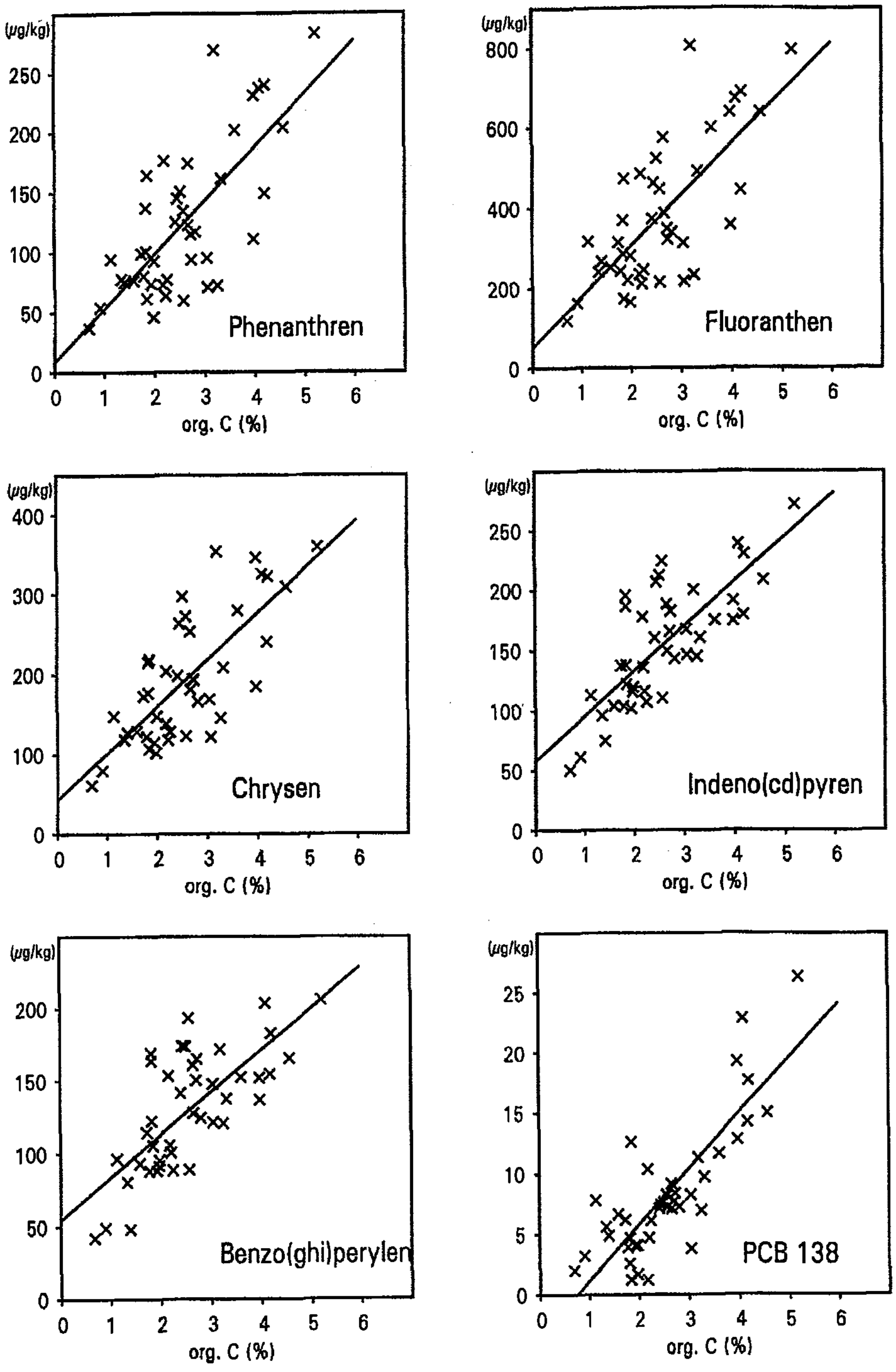


Fig. 2 Relationship between selected individual PAHs and PCBs and organic carbon from the sampling site of Irsch.

relationship with organic carbon decreases with increasing molecular weight (from Phenanthren to Benzo(ghi)perylen). The hydrophobicity, which increases with molecular weight, seems to be responsible for the stronger sorption on the organic matter of the sediment size fractions. The slope of each regression line however is

Table 2 Regression relationships between selected PAHs and PCBs and organic carbon at the sampling site of Irsch.

Pollutant	Regression equation	Correlation coefficient	Significance (%)
Phenanthren	$y = 44.86x + 8.82$	0.77	<0.1
Fluoranthen	$y = 126.9x + 52.38$	0.77	<0.1
Chrysen	$y = 58.47x + 42.94$	0.79	<0.1
Indeno(cd)pyren	$y = 37.35x + 58.21$	0.81	<0.1
Benzo(ghi)perylen	$y = 29.12x + 54.65$	0.79	<0.1
PCB 138	$y = 4.43x - 3.07$	0.85	<0.1

not dependent on the binding capacity of the organic matter. The supply or the absolute amount of each pollutant in the environment is responsible for the slope of the regression lines. Thus, the organic pollutant compounds with low regression slopes (I(cd)P, B(ghi)P) are present generally in low concentrations, while other pollutants with steeper regression slopes (Flua) occur in higher concentrations.

CONCLUSIONS

- The organic material content in the different particle size fractions is bimodally distributed with maxima in the fine silt and fine sand fractions reflecting two types of organic material.
- Heavy metals increase with decreasing particle size, due to the higher number of inorganic exchange sites in the clay fraction.
- The PCB content of the particle fractions is bimodally distributed and correlated with the organic carbon distribution.
- PAHs show a comparable affinity to the organic material, but the chemical composition and structure of the organic material plays a leading role in the sorption process. The chemical and biological alteration of organic material and humic substances can change the adsorption properties significantly (Abbt-Braun & Frimmel, 1996).
- There is a positive linear relationship between individual PCBs and PAHs and organic carbon. The particle size distribution plays a minor role for the adsorption of organic micropollutants.
- The partition of pollutants to different size fractions is of overriding importance, because sediments could be a source for contaminants. On the one hand changing hydrodynamic conditions (e.g. flood waves) can mobilize and transport variable particle sizes from the sediment. Therefore, an enrichment of individual contaminants must be expected through this sorting of the particles. On the other hand, a resuspension of particle sizes with high pollutant contents into the water column can lead to an increased bioavailability.

REFERENCES

Abbt-Braun, G. & Frimmel, F. H. (1996) Interaction of pesticides with river sediments and characterization of organic matter of the sediments. In: *Sediments and Toxic Substances* (ed. by W. Calmano), 51-89. Springer, Berlin.

Baughman, G. L. & Paris, D. F. (1981) Microbial bioconcentration of organic pollutants from aquatic systems — a critical review. *Critical Reviews in Microbiology* **8**, 205-228.

Calmano, W. & Förstner, U. (1996) *Sediments and Toxic Substances*. Springer, Berlin.

Chen, J. H., Lion, L. W., Ghiorse, W. & Shuler, M. (1995) Mobilization of adsorbed cadmium and lead in aquifer material by bacterial extracellular polymers. *Wat. Res.* **29**, 421-430.

Evans, K. M., Gill, R. A. & Robotham, P. W. J. (1990) The PAH and organic content of sediment particle size fractions. *Water, Air, and Soil Pollution* **51**, 13-31.

Flemming, H.-C., Schmitt, J. & Marshall, K. C. (1996) Sorption properties of biofilms. In: *Sediments and Toxic Substances* (ed. by W. Calmano), 115-157. Springer, Berlin.

Karickhoff, S. W. & Brown, D. S. (1978) Paraquat sorption as a function of particle size in natural sediments. *J. Environ. Qual.* 7, 246-252.

Karickhoff, S. W., Brown, D. S. & Scott, T. A. (1979) Sorption of hydrophobic pollutants on natural sediments. *Wat. Res.* **13**, 241-248.

Karickhoff, S. W. (1981) Semi-empirical estimation of sorption of hydrophobic pollutants on natural sediments and soils. *Chemosphere* **10**, 833-846.

Means, J. C., Wood, S. G., Hassett, J. J. & Banwart, W. L. (1980) Sorption of polynuclear aromatic hydrocarbons by sediments and soils. *Environ. Sci. & Technol.* **14**, 1524-1528.

Muller, R. N. & Tisue, G. T. (1977) Preparative-scale size fractionation of soils and sediments and an application to studies of Plutonium geochemistry. *J. Soil Sci.* **124**, 191-198.

Readman, J. W., Mantoura, R. F. C. & Rhead, M. M (1984) The physico-chemical speciation of PAH in aquatic systems. *Fresenius Z. Anal. Chem.* **319**, 126-131.

Schmitt, J., Gu, B., Schorer, M., Flemming, H.-C. & McCarthy, J. J. (1996) The role of natural organic matter as a coating on iron oxide and quartz. *Arch. Hydrobiol. Spec. Issues Advanc. Limnol.* **47**, 315-322.

Schorer, M., Bierl, R. & Symader, W. (1994) Zeitliche Veränderung von Schadstoffgehalten in Flußsedimenten (Temporal variations of pollutant contents in river sediments) (in German with an English summary). *Vom Wasser* **83**, 117-126.

Schorer, M., Symader, W., Nagel, N. & Udelhoven, T. (1995) Zeitliche Dynamik von Schadstoffen in mobilen Flußsedimenten (Temporal dynamic of pollutants in mobile river sediments). *Short Communications of the German Water Chemistry Conference 1995*, 15.

Symader, W., Schorer, M. & Bierl, R. (1994) Temporal variations of pollutants in channel sediments. In: *Variability of Stream Erosion and Sediment Transport* (ed. by L. J. Olive, R. J. Loughran & J. A. Kesby) (Proc. Canberra Symp., December 1994), 491-498. IAHS Publ. no. 224.

Umlauf, G. & Bierl, R. (1987) Distribution of organic micropollutants in different size fractions of sediment and suspended solid particles of the river Rotmain. *Z. Wasser-Abwasser-Forsch.* **20**, 203-209.

Voice, T. C. & Weber, W. J. (1983) Sorption of hydrophobic compounds by sediments, soils and suspended solids. *Wat. Res.* **17**, 1433-1441.

PAH AND PCB DISTRIBUTION IN SEDIMENT FRACTIONS AND SORPTIVE PHASES

A Dissertation

Submitted to the Graduate Faculty of the
Louisiana State University and
Agricultural and Mechanical College
in partial fulfillment of the
requirements of the degree of
Doctor of Philosophy

In

The Department of Civil and Environmental Engineering

By
Trudy J. Estes
B.S., Colorado State University, 1992
M.S., Mississippi State University, 1996
May, 2005

CHAPTER 6

FRACTIONATION STUDY OF NATURAL SEDIMENTS FOR DETERMINING PAH AND PCB DISTRIBUTION – PART 2: PCBS

INTRODUCTION

The fate of contaminants mobilized from sediment during dredging and disposal is of concern in Section 404 (Clean Water Act) evaluations (USEPA/USACE 2004). To demonstrate compliance with water quality standards and assess the need for mixing zones or mitigation measures, the magnitude of contaminant release resulting from a dredging action is evaluated for applicable contaminant exposure pathways (USEPA/USACE 1991, 1998; USACE 2003). Additionally, because disposal space for dredged material is becoming more limited in some areas of the United States, alternative management practices are increasingly being considered (Great Lakes Commission 2004; Price et al. 1997). Separation of relatively clean fractions of the sediment for beneficial use reduces the amount of dredged material requiring confined disposal (Olin-Estes and Palermo 2001).

In both cases, contaminant partitioning and distribution are central to alternatives analysis (USEPA/USACE 1991, 1998; USACE 2003). Effluent quality, for example, is based upon evaluation of contaminant solubility under two boundary conditions: 1) mixing of sediment pore water and the overlying carrier water, and 2) equilibrium between sediment, pore water and carrier water. Equilibrium calculations require knowledge of the partitioning behavior of the contaminants of concern. Theoretical partitioning coefficients may be developed based on site specific sediment and contaminant properties (Hansen et al. 1999; Brannon et al. 1998; Chiou, McGroddy and Kile 1998; DiToro et al. 1991; Pardue et al. 1993), values may be obtained from published references, or an observed coefficient may be calculated from sediment and pore water data (EPA 1999). Disparity of theoretical and observed partitioning coefficients may be as much as an order of magnitude or more, however (Kan et al. 1998). These differences are usually resolved and representative values selected by taking into account other available information, such as the results of an elutriate test (Palermo 1986). Alternatively, the most conservative values are selected for the analysis. Fractionation studies may be also conducted to evaluate the association of contaminants with specific size or density fractions of sediments, to assess the feasibility of separation for contaminant reduction or to assess the suitability of material for beneficial use (Olin-Estes and Palermo 2001; Olin et al. 1999).

PCBs are hydrophobic organic compounds commonly found in sediments of navigation waterways (National Research Council 1997; USEPA 1993). PCBs are chlorinated, aromatic compounds that were produced for use as dielectric fluids in capacitors and transformers and as industrial fluids in various systems (Hutzinger et al. 1983). There are 209 congeners, of which approximately 150 congeners are found in the environment (Hansen et al. 1999). PCBs are highly lipophilic with low solubility in water, with solubility decreasing with increasing degree of chlorination. PCBs of higher molecular weight tend to be associated with mineral and organic particulates in the environment, with organic sorption dominating (Girvin and Scott 1997; Karichoff 1984). The presence of high levels of dissolved organic carbon may increase the apparent solubility of PCBs (Brannon et al. 1998; Hwang et al. 1998), although aromaticity of the DOC may be important, as was shown for PAHs, which have lower affinity for aliphatic (non-aromatic) carbon (Hwang and Cutright 2004).

The major objectives of this research effort were to ascertain the distribution trends of PCBs in three natural sediments and to evaluate the potential usefulness of fractionation studies to treatability and fate and effects evaluations. Fractionation studies offer a vehicle to evaluate the association of contaminants with specific phases of sediments and to establish correlations to those phases from which more global partitioning coefficients might be derived. This research effort was developed to meet the dual objectives of developing simple bench scale testing methods for separation feasibility evaluations and laying a foundation for improved understanding of the target phases important to contaminant reduction.

MATERIALS AND METHODS

Sediments and Analytes. Materials employed in the separation study included one freshwater and two marine sediments. The freshwater sediment was obtained at the offloading point to the confined disposal facility (CDF) for Calumet River. The marine sediments were taken directly from the harbor in New York and New Bedford. Sediments were packaged in 5-gallon HDPE buckets and maintained at 4°C during transport and while in storage.

Sediments were homogenized in a large stainless steel mixer when received at the laboratory. Aliquots of homogenized sediment were tested to determine specific gravity of solids (MD0302), moisture content, grain size distribution (ASTM D422), classification (ASTM D2488), fraction organic carbon (ASTM D2974), cation exchange capacity (CEC) (SW-846 Method 9080/9081), pH (SW-846 Method 9040B), and fraction expandable clay (x-ray diffraction). Soot analysis was conducted using the procedure reported in Gustafsson et al. (1997), which is essentially a modification of the acidification and combustion procedure used for TOC determination (SW-846 9060). Samples were also analyzed in duplicate for selected analytes, using SW-846 methods. These samples were packaged in amber glass jars with Teflon® lids and maintained at 4°C without preservatives, prior to analysis. Samples were analyzed for 70 different PCB congeners. Congeners representative of each homolog group, found in common aroclors, and that typically can be resolved without co-elution, were selected. Sediments were also analyzed for oil and grease (O&G), and total organic carbon (TOC).

Samples of pore water were obtained by centrifuging homogenized sediment. Pore water was analyzed for the same constituents as the sediments, as well as dissolved organic carbon (DOC). Due to volume limitations, only PCBs were analyzed in duplicate in the pore water.

Density Separations. A solution of non-toxic, water-soluble sodium polytungstate was used for the density separations. The heavy media was made up to give a solution density of 2.0 g/cm^3 when mixed with the sediment, adjusting for expected dilution from pore water in the sediment sample. In order to prevent formation of a calcium precipitate in the media, calcium ions were removed from the sediment by saturating the sediment with a 1N Sodium Acetate solution at a 6:1 water:sediment ratio. This was tumbled overnight and centrifuged, and supernatant decanted. The procedure was repeated once with sodium acetate and again with distilled, de-ionized water (DDI) to remove the sodium acetate.

Samples of pretreated bulk sediment were placed in 250-ml Nalgene® centrifuge bottles with the solution of sodium polytungstate. Samples were sonicated briefly in a water bath to encourage separation of the different density materials and then centrifuged until a clear separation of phases occurred. The light (organic) fraction was decanted onto a microfiltration apparatus and rinsed with DDI water to remove residual heavy media. Initially, filters used were Whatman GF/F Glass Microfibre Filters (0.7-µm). Because solids were difficult to remove from these filters, Lida 0.45-µm nylon filter membranes were later substituted. Filtration through the nylon filters was slower, but removal of solids from the filters was less problematic. The heavy (mineral) fraction was recombined with additional sodium polytungstate and the procedure repeated until no further organic phase could be separated from the mineral phase. The heavy fraction was then recombined with DDI water, sonicated, centrifuged and decanted through a microfiltration apparatus to remove residual heavy media. Samples from each density fraction were analyzed on the Coulter LS 100 particle size analyzer (Beckman Coulter, Inc., USA) to determine particle size distribution.

The density separation was performed once per sediment. Wet solids were collected from the microfiltration apparatus and placed in amber glass jars with Teflon-lined lids for chemical and physical analysis. No preservatives were added. Samples were maintained in storage at 4°C. Replicate samples were obtained from the mineral fraction where sufficient material was available. Material volume was insufficient for replicates from the organic fraction.

Size Separations. Size separation of homogenized sediment was accomplished in three stages. A specified amount of wet sediment, sufficient to produce adequate quantities of each fraction, was weighed out and wet sieved through a 4.75-mm sieve and a 200-mesh (75-µm) sieve. Material retained on the coarse sieve was classified as oversize and was not tested. Material retained on the fine sieve was classified as sand. Slurry passing the 200-mesh sieve was diluted to approximately 15 percent solids by weight and processed through a 2-inch Mozely hydrocyclone. Underflow was designated as the operationally defined silt fraction; overflow was designated as the operationally defined clay fraction. Both silt and clay fractions were dewatered using a continuous flow CF 35M Microseparator. Samples from each size fraction were analyzed on the Coulter Counter to evaluate particle size distribution.

The size separation was performed only once for each sediment; however, where sufficient quantities of material were available, replicate samples of each operational size fraction were taken for chemical and size distribution analysis. Wet solids were placed in amber glass jars with Teflon-lined lids for chemical and physical analysis. No preservatives were added. Samples were maintained at 4°C.

RESULTS

Physical Characterization. Physical properties of the three sediments and results of the x-ray diffraction analysis are summarized in Chapter 5, Table 5-1. A short synopsis is provided here. All three sediments are classified as sandy silt (ML). Calumet is the coarsest sediment, with a comparatively low organic fraction, and a trace of gravel. New Bedford contains the highest proportion of organic materials, followed by New York. New York is the finest sediment with the highest proportion of clay. Smectite and mixed layer clays were present in all three sediments. Cation exchange capacity was comparable for the three sediments.

Chemical Characterization. Results of the chemical characterization of the bulk sediments and pore water are also summarized in Chapter 5, Table 5-2. Sediment and pore water PCB concentrations reported represent there are the mean of two replicates, with the exception of

TOC, DOC and O&G in the pore water which were not replicated due to limited pore water volume. Data in Table 5-2 is raw data.

Mass Balance. Recovery of all solids for gravimetric mass balance was not feasible due to processing losses and slurry volumes generated in the cyclone separation. The relative distribution of sediment mass to each size and density fraction was estimated based on measured properties of the bulk sediment and the resulting fractions. The procedure was described in Chapter 5, Equations 5-1 through 5-10. Mass of sediment reporting to each fraction is illustrated in Figure 5-1.

Distribution of Sorptive Phases. The distribution of OG, soot and OC in the study sediments is summarized in Chapter 5 and illustrated in Figures 5-2 through 5-4. The mass of organic carbon was much larger than either OG or soot (ranging from 1.4 to 82 times as much) in all fractions for all sediments except the organic fraction of Calumet. Here, the mass of soot was found to be approximately 14 times greater than OC. The relative distribution of the phases between the size and density fractions was distinctly different for each sediment, as can be seen by examining Figures 5-2 through 5-4.

PCB DISTRIBUTION

Calumet. Mean PCB concentration was approximately an order of magnitude higher in the organic fraction (4.3 percent of the sediment mass) than in the mineral fraction (Figure 6-1). In the size fractions, mean PCB concentration in the clay (16.7 percent of the sediment mass) was approximately two times the concentrations in the sand (44.2 percent of the sediment mass), and three times concentrations in the silt (39.1 percent of the sediment mass). This was true on an individual congener basis as well, with concentration in the clay ranging from approximately 1.5 to 9 times the concentrations in the silt and sand fractions (Table 6-1).

On a mass basis, mean PCB mass was highest in the mineral fraction, which comprises 95.7 percent of the sediment mass (Figure 6-1). On an individual basis, PCB mass was also highest in the mineral fraction, except for PCB 54 (30.6 percent) and PCB 206 (49.7 percent). In the size fractions, mean PCB mass was approximately equal in the sand and clay fractions. On an individual basis, highest PCB mass was found in the sand for 28 PCBs and in the clay for the remaining 10 PCBs. PCB mass in silt was about 70-80 percent of the mass in sand and clay fractions individually. Mean PCB mass in clay was 95 percent of mass in sand (Table 6-1).

New Bedford. Mean PCB concentration in the organic fraction (13.3 percent of the sediment mass) was approximately two times the concentration in the mineral fraction (Figure 6-2). Concentrations between the density fractions differed by as much as an order of magnitude for some congeners, but were always higher in the organic fraction (Table 6-2). In the size fractions, mean PCB concentration in the clay (22.9 percent of the sediment mass) was approximately two times the mean concentration in the sand (35.1 percent of the sediment mass) and approximately 4 times higher than the mean concentration in the silt (42.1 percent of the sediment mass).

On a mass basis, 76.9 percent of the PCBs were in the mineral fraction, which comprises 86.7 percent of the sediment mass (Figure 6-2). This distribution was also relatively consistent for individual congeners in the density fractions. In the size fractions, mean PCB mass was approximately equal in the sand and clay fractions (37.4 percent and 41.2 percent of total PCB mass respectively). Mean PCB mass in the silt was 21.4 percent, and ranged from 14.9 to 29.9 percent for the individual congeners. On an individual congener basis, highest PCB mass was found consistently in the sand for 15 congeners and in the clay for the remaining 30 congeners (Table 6-2).

New York. Mean PCB concentration in the organic fraction (10.8 percent of the sediment mass) was approximately two times the concentration in the mineral fraction (Figure 6-3). Concentrations of individual congeners were as much as an order of magnitude higher in the organic fraction than the mineral fraction, except for PCBs 8, 18, 49 and 52, which were higher in the mineral fraction. Mean PCB concentrations in sand (23.3 percent of sediment mass) were slightly higher than in the clay (54.6 percent of sediment mass) and approximately two times the concentration in the silt (22.1 percent of sediment mass). Concentration of individual congeners in sand ranged from 0.1 to 9 times that of clay concentrations, and 0.8 to 7 times that of silt concentrations. Concentration of PCBs 7, 8, 18, 28, 44, 49, and 52 were highest in the clay (Table 6-3). Composite PCB concentration for the size fractions (Figure 6-3) does not fall within the same range as the composite concentration for the density fractions. This is attributed to greater sample variability for this sediment, and the influence of one outlier in the density fraction data.

On a mass basis, 67.8 percent of the PCBs were in the mineral fraction, which comprises 89.2% of the sediment mass (Figure 6-3). Mass distribution of individual congeners in the mineral fraction varied widely from 0 to effectively 100 percent. Mass of PCBs 189 and 206 were slightly higher in the organic fraction. PCB 208 was found only in the organic fraction. In the size fractions, mass distribution of individual congeners varied widely, ranging from 18 to 91.6 percent in the clay, 5 to 71.1 percent in the sand, and 3.3 to 20.2 percent in the silt (Table 6-3).

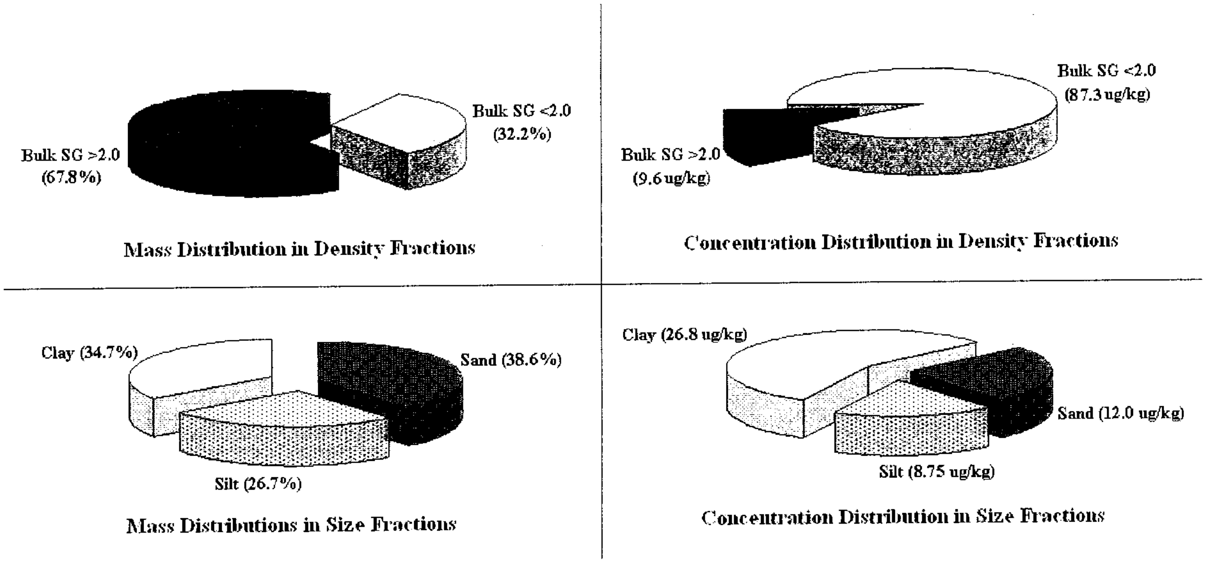


FIGURE 6-1. Calumet mean PCB mass and concentration distribution.

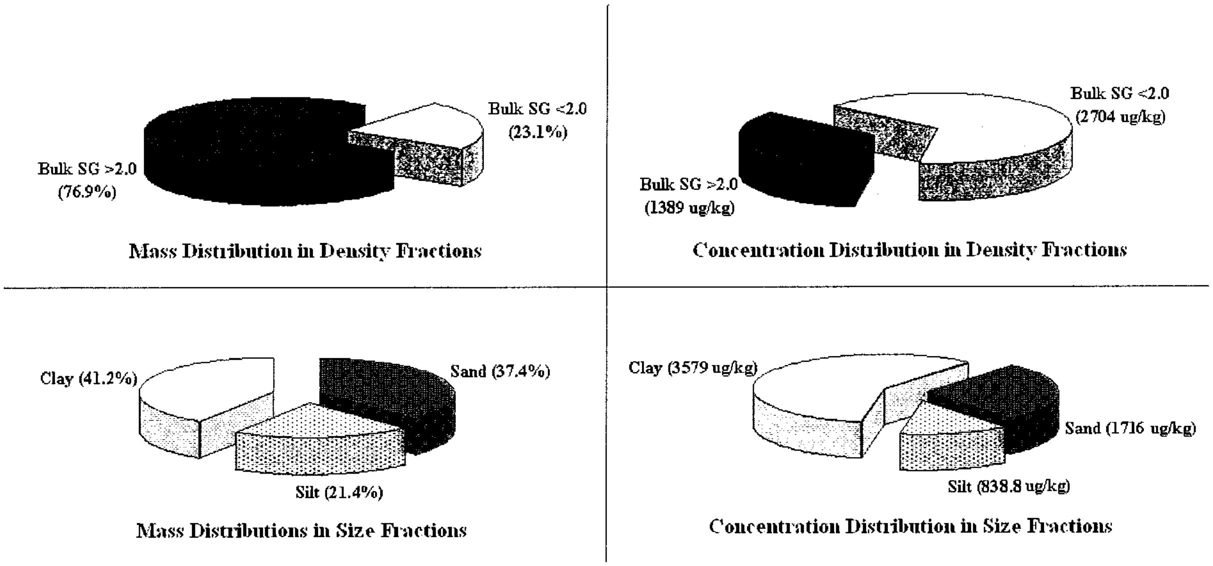


FIGURE 6-2. New Bedford mean PCB mass and concentration distribution.

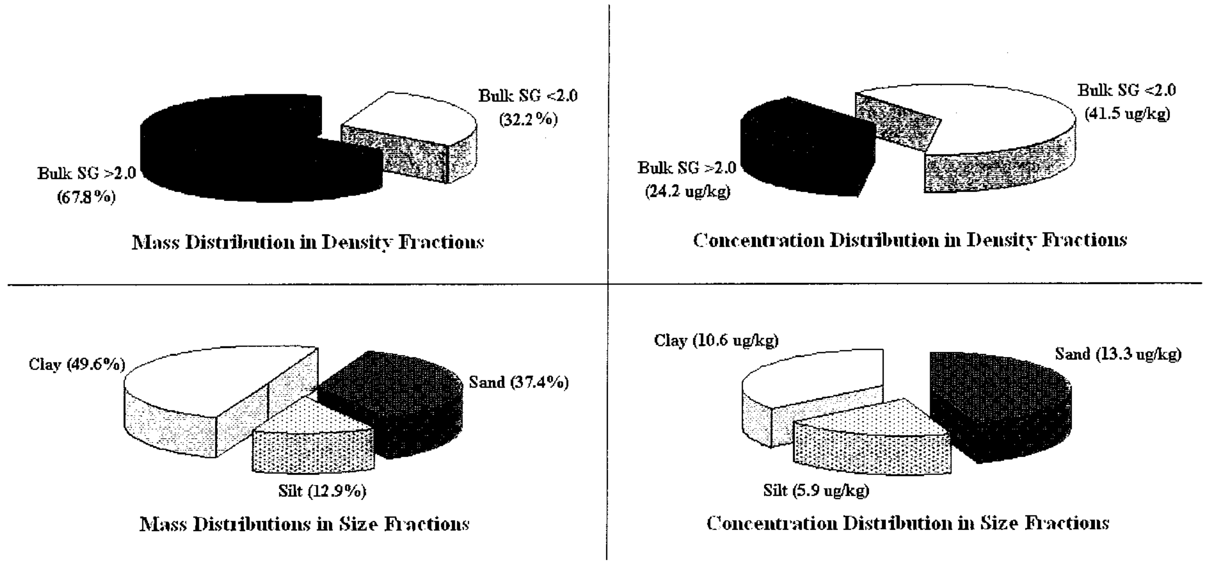


FIGURE 6-3. New York mean PCB mass and concentration distribution in fractions.

TABLE 6-1. Calumet Mean PCB Mass and Concentration in Size and Density Fractions

							Density Fractions						Size Fractions														
	Units		Bulk				Bulk SG<2			Bulk SG>2			Sand					Silt					Clay				
	Mass	Conc	Mass	Concentration			Mass			Mass			Mass		Concentration			Mass		Concentration			Mass		Concentration		
				Conc	SD	COV	Mass	%	Conc[b]	Mass	%	Conc[b]	Mass	%	Conc	SD	COV	Mass	%	Conc	SD	COV	Mass	%	Conc	SD	COV
Sediment Mass[a]	kg		0.667				0.039	4.30		0.866	95.7		0.350	44.2				0.309	39.1				0.132	16.7			
PCB101	µg	µg/kg	40.6	60.8	0.04	0.001	9.83	34.3	252	18.8	65.7	21.7	8.56	35.0	24.5	7.00	0.29	6.57	26.9	21.3	3.46	0.163	9.33	38.1	70.7	16.5	0.233
PCB114	µg	µg/kg		<5.15					<10.6	1.46	81.9	1.69	0.51	39.9	1.47	0.29	0.20	0.36	28.0	1.17	0.15	0.131	0.41	32.1	3.13	0.31	0.098
PCB118	µg	µg/kg	30.7	46.0	1.27	0.028	6.71	30.7	172	15.2	69.3	17.5	6.20	35.1	17.7	5.63	0.32	5.36	30.3	17.3	1.70	0.098	6.12	34.6	46.4	1.75	0.038
PCB128	µg	µg/kg	6.00	9.00	0.40	0.045	1.21	34.7	31.1	2.28	65.3	2.63	1.02	33.7	2.90	0.44	0.15	0.89	29.4	2.87	0.25	0.088	1.11	36.8	8.40	0.44	0.052
PCB136	µg	µg/kg	3.64	5.45	3.21	0.589			<10.6	3.57	94.5	4.12	0.98	34.4	2.80	1.65	0.59	0.61	21.4	1.97	0.45	0.229	1.26	44.2	9.53	3.27	0.343
PCB137	µg	µg/kg					0.53	32.0	13.7	1.13	68.0	1.31	0.44	35.4	1.25	0.28	0.22	0.36	29.5	1.18	0.02	0.015	0.43	35.1	3.28	0.16	0.048
PCB138	µg	µg/kg	26.8	40.2	0.07	0.002	5.62	31.4	144	12.3	68.6	14.2	4.69	33.4	13.4	2.69	0.20	4.13	29.5	13.4	1.21	0.090	5.20	37.1	39.4	1.65	0.042
PCB141	µg	µg/kg	5.85	8.78	1.01	0.115	1.03	25.5	26.4	3.01	74.5	3.47	1.09	38.9	3.10	1.31	0.42	0.76	27.3	2.47	0.06	0.023	0.94	33.8	7.13	0.38	0.053
PCB151	µg	µg/kg	6.88	10.3	2.52	0.245	1.66	35.9	42.6	2.96	64.1	3.42	1.39	40.0	3.97	0.90	0.23	0.99	28.5	3.20	0.35	0.108	1.09	31.5	8.27	0.57	0.069
PCB156	µg	µg/kg		<5.15	0.09	0.021			<10.6	1.03	73.7	1.19	0.68	39.5	1.93	0.92	0.48	0.50	29.4	1.63	0.12	0.071	0.53	31.1	4.03	0.15	0.038
PCB170	µg	µg/kg		<5.15			0.94	39.2	24.2	1.46	60.8	1.69	0.75	35.3	2.13	0.32	0.15	0.59	27.8	1.90	0.36	0.190	0.78	36.9	5.90	0.72	0.122
PCB 18	µg	µg/kg	57.8	86.6	4.24	0.049	10.0	26.8	257	27.4	73.2	31.6	17.7	44.6	50.6	24.7	0.49	9.35	23.6	30.3	3.89	0.129	12.6	31.8	95.4	24.7	0.259
PCB180	µg	µg/kg	5.21	7.81	0.73	0.093	1.46	38.2	37.4	2.36	61.8	2.73	1.67	43.2	4.77	1.42	0.30	1.01	26.1	3.27	0.49	0.151	1.18	30.7	8.97	0.32	0.036
PCB183	µg	µg/kg		<5.15	0.25	0.130	0.50	41.0	12.8	0.72	59.0	0.83	0.41	37.1	1.17	0.31	0.26	0.29	26.2	0.93	0.06	0.062	0.40	36.7	3.07	0.21	0.068
PCB189	µg	µg/kg		<5.15					<10.6			<0.46			<0.47					<0.45					<0.69		
PCB194	µg	µg/kg		<5.15	0.11	0.063	0.31	29.4	<10.6	0.74	70.6	0.86	0.40	41.7	1.13	0.25	0.22	0.28	29.2	0.90	0.10	0.111	0.28	29.1	2.10	0.20	0.095
PCB195	µg	µg/kg		<5.15					<10.6			<0.46			<0.47					<0.45			0.10	35.2	0.73	0.06	0.079
PCB196	µg	µg/kg		<5.15					<10.6						<0.47					<0.45			0.18	39.7	1.37	0.06	0.042
PCB199	µg	µg/kg		<5.15					<10.6			<0.46			<0.47					<0.45					<0.69		
PCB201	µg	µg/kg		<5.15			0.42	31.5	10.7	0.91	68.5	1.05	0.44	43.4	1.27	0.06	0.05	0.28	27.2	0.90	0.17	0.192	0.30	29.3	2.27	0.23	0.102
PCB203	µg	µg/kg		<5.15			0.47	32.0	12.1	1.00	68.0	1.16	0.26	41.1	0.73	0.15	0.21	0.16	26.4	0.53	0.15	0.286	0.20	32.4	1.53	0.49	0.322
PCB206	µg	µg/kg		<5.15					<10.6			<0.46	0.27	40.3	0.77	0.15	0.20	0.22	32.5	0.70	0.17	0.247	0.18	27.1	1.37	0.06	0.042
PCB208	µg	µg/kg		<5.15											<0.47					<0.45			0.10	33.1	0.75	0.07	0.094
PCB 28	µg	µg/kg	62.5	93.8	5.59	0.060	12.8	25.8	327	36.6	74.2	42.3	16.8	33.6	47.9	21.4	0.45	13.52	27.1	43.8	1.80	0.041	19.6	39.2	148.1	4.97	0.034

(continued)

TABLE 6-1. (Continued)

							Density Fractions						Size Fractions														
	Units		Bulk				Bulk SG<2			Bulk SG>2			Sand					Silt					Clay				
	Mass	Conc	Mass	Concentration			Mass			Mass			Mass		Concentration			Mass		Concentration			Mass		Concentration		
				Conc	SD	COV	Mass	%	Conc[b]	Mass	%	Conc[b]	Mass	%	Conc	SD	COV	Mass	%	Conc	SD	COV	Mass	%	Conc	SD	COV
PCB 40	µg	µg/kg	16.7	25.1	17.5	0.697	1.93	29.6	49.6	4.60	70.4	5.31	2.78	42.1	7.95	3.75	0.47	1.62	24.5	5.25	0.21	0.040	2.21	33.4	16.8	1.63	0.097
PCB 44	µg	µg/kg	45.3	67.9	13.15	0.194	8.46	30.9	217	19.0	69.1	21.9	13.0	45.4	37.1	24.3	0.66	6.29	22.0	20.4	2.05	0.101	9.33	32.6	70.7	14.1	0.199
PCB 49	µg	µg/kg	38.2	57.2	2.76	0.048	7.41	29.0	190	18.1	71.0	20.9	10.3	43.7	29.6	16.2	0.55	6.07	25.6	19.7	1.63	0.083	7.27	30.7	55.1	5.59	0.101
PCB 52	µg	µg/kg	56.9	85.2	2.69	0.032	11.7	30.5	301	26.8	69.5	30.9	16.7	44.4	47.8	32.1	0.67	8.50	22.5	27.5	0.71	0.026	12.5	33.1	94.5	27.5	0.291
PCB 54	µg	µg/kg		<5.15					<10.6			<0.46	0.20	41.1	0.57	b	b	0.06		<0.45	b	b	0.22	46.2	1.70	b	b
PCB 66	µg	µg/kg	13.8	20.7	2.47	0.120	7.80	31.7	200	16.8	68.3	19.4	12.8	50.4	36.6	b	b	5.56	21.9	18.0	b	b	7.02	27.7	53.2	b	b
PCB 7	µg	µg/kg		<5.15					<10.6			<0.46	0.40	42.2	1.13	0.72	0.64	0.32	34.0	1.03	0.72	0.700	0.22	23.9	1.70	0.66	0.386
PCB 70	µg	µg/kg	50.3	75.5	6.08	0.081	10.1	31.7	259	21.7	68.3	25.1	14.4	43.3	41.1	26.3	0.64	8.16	24.6	26.4	3.11	0.118	10.7	32.2	81.0	14.5	0.179
PCB 8	µg	µg/kg	22.8	34.2	2.40	0.070	4.56	20.2	117	18.0	79.8	20.8	7.98	37.2	22.8	3.04	0.13	6.73	31.4	21.8	1.79	0.082	6.73	31.4	51.0	2.31	0.045
PCB 82	µg	µg/kg	18.3	27.4	3.54	0.129	3.68	38.8	94.4	5.81	61.2	6.71	1.57	37.9	4.49	3.01	0.67	1.17	28.3	3.80	0.85	0.224	1.40	33.8	10.6	1.40	0.132
PCB 86	µg	µg/kg	4.79	7.19	1.48	0.206	3.26	27.8	83.6	8.47	72.2	9.78	3.45	36.0	9.87	4.11	0.42	2.75	28.6	8.90	0.92	0.103	3.40	35.4	25.7	2.36	0.092
PCB 87	µg	µg/kg	16.4	24.7	0.21	0.009	4.95	34.8	127	9.27	65.2	10.7	3.86	33.3	11.0	2.84	0.26	3.43	29.6	11.1	1.47	0.133	4.30	37.1	32.6	1.93	0.059
PCB 97	µg	µg/kg	4.79	7.19	1.48	0.206	3.26	27.8	83.6	8.47	72.2	9.78	3.45	36.0	9.87	4.11	0.42	2.75	28.6	8.90	0.92	0.103	3.40	35.4	25.7	2.36	0.092
		Mean	25.4	38.1			Mean	31.6	123	Mean	70.0	11.5	Mean	39.3	13.9			Mean	27.4	10.4			Mean	34.0	28.4		
		Max	62.5	93.8			Max	41.0	327	Max	94.5	42.3	Max	50.4	50.6			Max	34.0	43.8			Max	46.2	148.1		
		Min	3.64	5.45			Min	20.2	10.7	Min	59.0	0.83	Min	33.3	0.57			Min	21.4	0.53			Min	23.9	0.73		
		SD	20.1	30.1			SD	4.73	102	SD	7.02	11.4	SD	4.29	16.4			SD	3.07	11.3			SD	4.46	35.9		

[a] Dry fraction mass, assuming a starting mass of 1 kg wet bulk sediment. Difference in dry sediment mass for sum of density fractions, sum of size fractions and bulk sediment are due to differences in moisture content assumed in smoothed mass balance.

[b] Unreplicated values

TABLE 6-2. New Bedford Mean PCB Mass and Concentration in Size and Density Fractions

							Density Fractions						Size Fractions														
	Units		Bulk				Bulk SG<2			Bulk SG>2			Sand					Silt					Clay				
	Mass	Conc	Mass	Concentration			Mass			Mass			Mass		Concentration			Mass		Concentration			Mass		Concentration		
				Conc	SD	COV	Mass	%	Conc^b	Mass	%	Conc^b	Mass	%	Conc	SD	COV	Mass	%	Conc	SD	COV	Mass	%	Conc	SD	COV
Sediment Mass	kg		0.395				0.120	13.3		0.780	86.7		0.135	35.1				0.162	42.1				0.088	22.9			
PCB1	μg	μg/kg		<8.70			15.24	22.9	127	51.3	77.1	65.8	11.0	40.2	81.5	3.61	0.044	4.06	14.9	25.05	1.20	0.048	12.3	44.9	139.5	27.8	0.199
PCB101	μg	μg/kg	3420	8647.5	541	0.063	956	25.7	7970	2770	74.3	3550	773	36.2	5730	83.2	0.015	419	19.6	2590	152	0.059	944	44.2	10700	1020	0.095
PCB103	μg	μg/kg	121	306.0	84.9	0.277	28.08	30.6	234	63.6	69.4	81.5	22.3	34.9	165	9.05	0.055	12.3	19.3	75.9	5.23	0.069	29.2	45.8	332	44.0	0.133
PCB114	μg	μg/kg	42.5	107.5	7.78	0.072	14.88	22.7	124	50.6	77.3	64.9	12.4	35.9	92.1	3.68	0.040	7.2	20.9	44.7	3.04	0.068	15.0	43.2	170	28.3	0.166
PCB118	μg	μg/kg	2550	6447.0	460	0.071	628	22.7	5230	2140	77.3	2740	713	37.1	5280	9.05	0.002	402	20.9	2480	110	0.044	808	42.0	9180	985	0.107
PCB126	μg	μg/kg	13.8	35.0	2.05	0.059	4.34	28.5	36.2	10.9	71.5	14.0	6.8	42.9	50.0	1.41	0.028	4.0	25.4	24.7	1.84	0.074	4.99	31.7	56.7	9.33	0.165
PCB128	μg	μg/kg	115	291.0	14.1	0.049	40.4	21.6	337	147	78.4	188	36.5	35.0	271	8.13	0.030	22.5	21.5	139	9.40	0.068	45.3	43.4	514	88.7	0.172
PCB136	μg	μg/kg	365	923.5	51.6	0.056	128	23.4	1070	420	76.6	538	103	35.6	759	24.0	0.032	52.7	18.3	326	22.3	0.068	132	46.0	1500	144	0.095
PCB137	μg	μg/kg	72.1	182.5	13.4	0.074	21.96	21.5	183	80.3	78.5	103	21.9	41.3	163	6.36	0.039	12.3	23.2	76.1	3.75	0.049	18.8	35.5	214	39.6	0.185
PCB138	μg	μg/kg	913	2310.0	141	0.061	290	22.2	2413	1010	77.8	1300	323	38.0	2390	60.3	0.025	177	20.8	1090	73.3	0.067	351	41.2	3980	408	0.102
PCB141	μg	μg/kg	141	356.0	25.5	0.072	28.8	22.0	240	102	78.0	131	31.8	38.7	236	7.42	0.031	18.0	21.8	111	7.99	0.072	32.5	39.5	369	14.7	0.040
PCB151	μg	μg/kg	374	947.0	163	0.172	99.2	22.4	827	343	77.6	440	104	37.6	768	32.3	0.042	53.4	19.4	330	21.8	0.066	119	43.0	1350	140	0.104
PCB156	μg	μg/kg	120	304.5	65.8	0.216	36.8	22.6	307	126	77.4	162	35.6	35.5	264	13.1	0.050	23.0	23.0	142	6.22	0.044	41.7	41.6	474	69.9	0.147
PCB167	μg	μg/kg	112	282.5	20.5	0.073	31.4	22.7	262	107	77.3	137	32.6	39.9	242	13.2	0.054	17.5	21.4	108	6.58	0.061	31.6	38.6	359	59.3	0.165
PCB170	μg	μg/kg	120	304.5	37.5	0.123	33.0	22.3	275	115	77.7	147	38.0	37.7	282	17.2	0.061	22.0	21.8	136	9.69	0.071	40.8	40.5	464	61.6	0.133
PCB18	μg	μg/kg	6190	15662.2	923	0.059	1690	22.5	14100	5840	77.5	7490	929	32.5	6880	524	0.076	508	17.8	3140	187	0.060	1420	49.7	16100	1430	0.089
PCB180	μg	μg/kg	201	507.5	24.7	0.049	55.3	22.4	461	191	77.6	245	70.0	42.5	519	14.8	0.028	38.1	23.1	235	14.6	0.062	56.5	34.3	642	111	0.173
PCB183	μg	μg/kg	63.6	161.0	5.66	0.035	22.7	22.5	189	78.0	77.5	100	22.3	38.4	166	8.77	0.053	12.5	21.5	77.2	4.38	0.057	23.3	40.1	265	42.8	0.161
PCB185	μg	μg/kg	13.8	35.0	2.83	0.081	4.37	20.1	36.4	17.4	79.9	22.3	5.4	39.7	39.9	0.28	0.007	2.90	21.4	17.9	0.71	0.040	5.29	39.0	60.1	11.0	0.184
PCB189	μg	μg/kg	11.2	28.4	1.27	0.045	1.57	16.9	13.1	7.72	83.1	9.90	2.80	36.9	20.8	0.35	0.017	1.94	25.6	12.0	0.71	0.059	2.85	37.5	32.4	7.07	0.218
PCB191	μg	μg/kg	9.5	24.1	2.05	0.085	1.06	24.4	8.80	3.28	75.6	4.20	2.30	40.3	17.0	0.42	0.025	1.70	29.9	10.5	2.97	0.283	1.69	29.8	19.3	4.74	0.246
PCB194	μg	μg/kg	30.2	76.5	2.83	0.037	9.14	39.3	76.2	14.1	60.7	18.1	11.4	42.3	84.6	6.08	0.072	6.2	23.2	38.6	3.18	0.083	9.3	34.5	106	18.5	0.175
PCB195	μg	μg/kg	12.6	32.0	2.33	0.073	3.54	21.8	29.5	12.7	78.2	16.3	6.5	39.4	48.4	3.25	0.067	3.75	22.6	23.2	1.77	0.076	6.28	37.9	71.4	14.8	0.207
PCB196	μg	μg/kg	14.4	36.4	2.83	0.078	3.82	21.9	31.8	13.6	78.1	17.4	6.1	40.1	44.9	2.83	0.063	3.20	21.2	19.8	1.34	0.068	5.87	38.8	66.7	20.3	0.304
PCB199	μg	μg/kg	7.5	19.0	1.70	0.089	2.12	19.8	17.7	8.58	80.2	11.0	2.61	38.5	19.4	0.78	0.040	1.36	20.1	8.40	0.28	0.034	2.81	41.4	31.9	3.96	0.124

(continued)

TABLE 6-2. (Continued)

							Density Fractions						Size Fractions														
	Units		Bulk				Bulk SG<2			Bulk SG>2			Sand					Silt					Clay				
	Mass	Conc	Mass	Concentration			Mass			Mass			Mass		Concentration			Mass		Concentration			Mass		Concentration		
				Conc	SD	COV	Mass	%	Conc[b]	Mass	%	Conc[b]	Mass	%	Conc	SD	COV	Mass	%	Conc	SD	COV	Mass	%	Conc	SD	COV
PCB201	μg	μg/kg	26.4	66.8	3.54	0.053	6.53	21.0	54.4	24.5	79.0	31.4	9.9	39.5	73.0	4.67	0.064	5.7	22.8	35.2	2.05	0.058	9.4	37.6	107	16.3	0.153
PCB202	μg	μg/kg	8.0	20.3	1.27	0.063	3.06	20.4	25.5	11.9	79.6	15.3	3.26	38.1	24.2	5.16	0.214	1.73	20.2	10.7	0.14	0.013	3.57	41.7	40.6	11.1	0.274
PCB203	μg	μg/kg	16.1	40.9	1.77	0.043	5.77	22.4	48.1	20.0	77.6	25.7	10.6	44.1	78.2	5.02	0.064	5.7	23.6	34.9	2.26	0.065	7.7	32.2	87.7	18.5	0.211
PCB206	μg	μg/kg	17.2	43.5	5.44	0.125	4.15	23.0	34.6	13.9	77.0	17.8	7.2	44.2	53.7	5.44	0.101	4.03	24.6	24.9	0.92	0.037	5.12	31.2	58.2	10.3	0.176
PCB207	μg	μg/kg	3.89	9.85	2.05	0.208	0.73	14.8	6.10	4.21	85.2	5.40	1.33	38.1	9.85	2.19	0.223	0.93	26.7	5.75	0.07	0.012	1.23	35.3	14.0	3.11	0.222
PCB208	μg	μg/kg	7.4	18.85	1.63	0.086	1.19	22.7	9.90	4.06	77.3	5.20	3.35	45.9	24.9	1.91	0.077	1.71	23.4	10.6	0.64	0.060	2.24	30.7	25.5	8.77	0.344
PCB28	μg	μg/kg	8430	21400	1060	0.050	2120	22.0	17700	7510	78.0	9630	1450	30.7	10800	933.7	0.087	1000	21.2	6190	338.7	0.055	2270	48.1	25800	512.6	0.020
PCB40	μg	μg/kg	319	808	50.9	0.063	104	22.8	869	353	77.2	452	78.3	32.9	580	11.7	0.020	46.4	19.5	287	11.5	0.040	113	47.6	1290	121.9	0.095
PCB44	μg	μg/kg	2990	7570	467	0.062	896	25.7	7470	2590	74.3	3320	593	33.2	4390	131.1	0.030	332	18.6	2050	115.5	0.056	859	48.2	9760	905.5	0.093
PCB49	μg	μg/kg	7350	18600	1700	0.091	2120	22.5	17700	7320	77.5	9390	1250	33.1	9230	680.5	0.074	756	20.1	4670	418.9	0.090	1760	46.8	20000	19.0	0.001
PCB52	μg	μg/kg	7590	19200	1110	0.058	2080	22.2	17300	7260	77.8	9310	1240	33.8	9150	689.4	0.075	698	19.1	4310	244.7	0.057	1720	47.1	19600	9.76	0.000
PCB66	μg	μg/kg	1020	2590	179	0.069	572	23.7	4770	1840	76.3	2360	512	35.3	3800	148.5	0.039	312	21.5	1930	77.8	0.040	627	43.2	7130	70.7	0.010
PCB7	μg	μg/kg		<8.70			27.7	27.0	231	75.0	73.0	96.2	25.9	34.8	192	9.26	0.048	14.3	19.2	88.2	5.37	0.061	34.3	46.0	389	57.6	0.148
PCB70	μg	μg/kg	1720	4350	306	0.070	484	22.5	4030	1670	77.5	2140	438	34.7	3250	81.6	0.025	262	20.7	1620	94.5	0.058	565	44.7	6410	614.1	0.096
PCB8	μg	μg/kg	3580	9070	547	0.060	1020	26.0	8490	2900	74.0	3720	605	32.5	4480	194.7	0.043	351	18.9	2170	86.6	0.040	903	48.6	10300	896.3	0.087
PCB82	μg	μg/kg	77.6	197	12.0	0.061	24.5	25.1	204	73.2	74.9	93.9	17.5	32.4	130	6.51	0.050	11.1	20.5	68.3	2.55	0.037	25.4	47.1	289	63.0	0.218
PCB86	μg	μg/kg					295	22.3	2460	1030	77.7	1320	274	35.7	2030	42.4	0.021	149	19.5	922	59.4	0.064	344	44.8	3910	367.7	0.094
PCB87	μg	μg/kg	232	588	32.5	0.055	60.1	21.9	501	215	78.1	275	70.1	34.5	519	4.6	0.009	44.3	21.8	273	33.9	0.124	88.8	43.7	1010	108.4	0.107
PCB97	μg	μg/kg	361	913	41.0	0.045	295	22.3	2460	1030	77.7	1320	285	35.7	2110	47.6	0.023	155	19.5	958	63.3	0.066	357	44.8	4060	388.7	0.096
		Mean	1190	3010			Mean	23.1	2700	Mean	76.9	1390	Mean	37.4	1720			Mean	21.4	839			Mean	41.2	3580		
		Max	8430	21400			Max	39.3	17700	Max	85.2	9630	Max	45.9	10800			Max	29.9	6190			Max	49.7	25800		
		Min	3.89	9.85			Min	14.8	6.10	Min	60.7	4.20	Min	30.7	9.85			Min	14.9	5.75			Min	29.8	14.0		
		SD	2280	5780			SD	3.6	5020	SD	3.6	2640	SD	3.6	2830			SD	2.6	1440			SD	5.4	6280		

[a] Dry fraction mass, assuming a starting mass of 1 kg wet bulk sediment. Difference in dry sediment mass for sum of density fractions, sum of size fractions and bulk sediment are due to differences in moisture content assumed in smoothed mass balance.

[b] Unreplicated values

TABLE 6-3. New York Mean PCB Mass and Concentration in Size and Density Fractions

							Density Fractions						Size Fractions														
	Units		Bulk				Bulk SG<2			Bulk SG>2			Sand					Silt					Clay				
	Mass	Conc	Mass	Concentration			Mass			Mass			Mass		Concentration			Mass		Concentration			Mass		Concentration		
				Conc	SD	COV	Mass	%	Conc[b]	Mass	%	Conc[b]	Mass	%	Conc	SD	COV	Mass	%	Conc	SD	COV	Mass	%	Conc	SD	COV
Sediment Mass	kg		0.367				0.027	10.8		0.223	89.2		0.117	23.3				0.111	22.1				0.274	54.6			
PCB101	µg	µg/kg	13.0	35.4	3.75	0.106	2.9	20.2	107	11.4	79.8	51.2	3.4	29.8	28.8	5.94	0.206	1.58	14.0	14.2	0.57	0.040	6.34	56.2	23.2	2.76	0.119
PCB118	µg	µg/kg	11.9	32.6	2.33	0.072	2.2	19.7	80.6	8.9	80.3	39.7	3.00	26.9	25.6	2.83	0.110	1.80	16.1	16.2	0.42	0.026	6.34	57.0	23.2	0.64	0.027
PCB128	µg	µg/kg		<4.6			0.6	35.9	22.7	1.09	64.1	4.90	0.45	29.6	3.85	0.07	0.018	0.22	14.6	2.00	0.00	0.000	0.85	55.8	3.10	0.28	0.091
PCB138	µg	µg/kg	10.4	28.3	0.92	0.033	2.8	31.3	103	6.10	68.7	27.4	2.66	30.2	22.7	0.28	0.012	1.43	16.2	12.9	0.07	0.006	4.70	53.5	17.2	0.92	0.054
PCB141	µg	µg/kg	2.1	5.86	0.30	0.052	0.61	37.9	22.7	1.00	62.1	4.50	0.81	33.5	6.90	0.28	0.041	0.37	15.2	3.30	0.85	0.257	1.23	51.2	4.50	0.14	0.031
PCB151	µg	µg/kg	3.4	9.24	1.64	0.178	0.8	29.2	29.7	1.94	70.8	8.70	0.89	32.1	7.60	1.27	0.167	0.40	14.4	3.60	0.00	0.000	1.48	53.4	5.40	0.57	0.105
PCB156	µg	µg/kg		<4.6			0.3	30.5	10.5	0.65	69.5	2.90	0.30	28.3	2.60	0.42	0.163	0.18	17.0	1.65	0.07	0.043	0.59	54.7	2.15	0.07	0.033
PCB167	µg	µg/kg		<4.6			0.2	29.2	8.50	0.56	70.8	2.50	0.13	27.2	1.15	0.35	0.307	0.10	20.2	0.90	0.28	0.314	0.26	52.6	0.95	0.21	0.223
PCB170	µg	µg/kg	2.3	6.38	0.10	0.016	0.5	33.0	20.3	1.12	67.0	5.00	0.77	29.6	6.60	1.84	0.279	0.41	15.7	3.70	0.14	0.038	1.42	54.6	5.20	0.14	0.027
PCB18	µg	µg/kg	12.9	35.0	3.25	0.093	1.5	7.8	54.2	17.3	92.2	77.7	1.81	18.7	15.5	0.57	0.036	1.06	10.9	9.55	0.21	0.022	6.81	70.3	24.9	0.64	0.026
PCB180	µg	µg/kg	5.1	14.0	0.35	0.025	1.7	41.6	61.2	2.32	58.4	10.4	2.48	43.8	21.2	13.72	0.647	0.81	14.3	7.30	0.57	0.077	2.37	41.9	8.65	0.21	0.025
PCB183	µg	µg/kg		<4.6			0.44	33.6	16.3	0.87	66.4	3.90	0.63	39.8	5.40	3.11	0.576	0.23	14.4	2.05	0.07	0.034	0.73	45.8	2.65	0.21	0.080
PCB185	µg	µg/kg		<4.6			0.15	30.7	5.50	0.33	69.3	1.50	0.33	39.8	2.80	1.56	0.556	0.14	16.9	1.25	0.21	0.170	0.36	43.3	1.30	0.14	0.109
PCB189	µg	µg/kg		<4.6			0.16	53.9	5.80			<0.66	0.15	39.7	1.25	0.49	0.396			<0.48					<0.80		
PCB194	µg	µg/kg		<4.6			0.47	46.9	17.5	0.54	53.1	2.40	1.39	63.1	11.9	12.0	1.008	0.25	11.4	2.25	0.21	0.094	0.56	25.6	2.05	0.21	0.103
PCB195	µg	µg/kg		<4.6			0.13	35.0	4.90	0.25	65.0	1.10	0.35	46.7	2.95	2.62	0.887	0.11	14.3	0.95	0.07	0.074	0.29	39.0	1.05	0.07	0.067
PCB196	µg	µg/kg		<4.6			0.28	48.7	10.2	0.29	51.3	1.30	0.95	61.6	8.10	6.65	0.821	0.17	10.8	1.50	0.14	0.094	0.42	27.6	1.55	0.21	0.137
PCB199	µg	µg/kg		<4.6			0.09	51.4	3.50			<0.66	0.29	55.1	2.45	2.33	0.952	0.06	10.7	0.50	0.14	0.283			<0.80		
PCB201	µg	µg/kg	1.7	4.64	0.72	0.155	0.68	47.8	25.0	0.74	52.2	3.30	1.94	64.8	16.6	15.6	0.944	0.28	9.5	2.55	0.21	0.083	0.77	25.7	2.80	0.28	0.101
PCB202	µg	µg/kg		<4.6			0.17	46.3	6.40	0.20	53.7	0.90	0.38	56.2	3.25	2.62	0.805	0.08	11.5	0.70	0.14	0.202	0.22	32.4	0.80	0.00	0.000
PCB203	µg	µg/kg		<4.6			0.42	38.3	15.4	0.67	61.7	3.00	1.56	65.4	13.3	11.9	0.893	0.22	9.3	2.00	0.28	0.141	0.60	25.3	2.20	0.14	0.064
PCB206	µg	µg/kg		<4.6			0.65	52.8	24.0	0.58	47.2	2.60	1.60	67.6	13.7	12.8	0.938	0.21	8.7	1.85	0.07	0.038	0.56	23.8	2.05	0.07	0.034
PCB207	µg	µg/kg		<4.6			0.09	37.0	3.40	0.16	63.0	0.70	0.22	71.1	1.85	1.63	0.879			<0.48					<0.80		
PCB208	µg	µg/kg		<4.6			0.44	100.0	16.2	0.00	0.0		0.73	59.0	6.20	4.24	0.684	0.16	13.1	1.45	0.21	0.146	0.34	27.9	1.25	0.21	0.170

(continued)

TABLE 6-3. (Continued)

							Density Fractions						Size Fractions														
	Units		Bulk				Bulk SG<2			Bulk SG>2			Sand					Silt					Clay				
	Mass	Conc	Mass	Concentration			Mass			Mass			Mass		Concentration			Mass		Concentration			Mass		Concentration		
				Conc	SD	COV	Mass	%	Conc[b]	Mass	%	Conc[b]	Mass	%	Conc	SD	COV	Mass	%	Conc	SD	COV	Mass	%	Conc	SD	COV
PCB28	µg	µg/kg	20.0	54.5	3.54	0.065	3.7	11.5	136	28.3	88.5	127	3.01	17.2	25.7	2.40	0.094	2.30	13.2	20.8	1.20	0.058	12.2	69.6	44.4	1.77	0.040
PCB40	µg	µg/kg	4.7	12.8	0.07	0.006	0.5	22.0	19.1	1.83	78.0	8.20	0.75	32.1	6.40	0.85	0.133	0.26	10.9	2.30	0.14	0.061	1.33	57.0	4.85	0.21	0.044
PCB44	µg	µg/kg	13.3	36.3	1.34	0.037	2.1	18.1	77.7	9.5	81.9	42.6	2.59	25.6	22.1	0.14	0.006	1.19	11.8	10.8	0.78	0.072	6.30	62.5	23.0	0.99	0.043
PCB49	µg	µg/kg	16.7	45.5	8.77	0.193	2.0	7.9	75.6	23.6	92.1	106	2.23	19.8	19.1	1.06	0.056	1.55	13.8	14.0	0.71	0.051	7.47	66.4	27.3	0.64	0.023
PCB52	µg	µg/kg	24.3	66.1	3.54	0.053			<0.84	24.8	100	111	3.12	22.9	26.7	0.92	0.034	1.71	12.6	15.5	0.35	0.023	8.77	64.5	32.0	1.56	0.049
PCB66	µg	µg/kg	13.3	36.4	4.17	0.115	6.7	29.1	249	16.3	70.9	73.3	10.2	37.2	87.4	19.23	0.220	2.81	10.2	25.4	0.35	0.014	14.4	52.5	52.7	0.64	0.012
PCB7	µg	µg/kg					0.04	15.8	1.40	0.20	84.2	0.90			<0.68					<0.48					<0.80		
PCB70	µg	µg/kg	16.1	43.9	3.39	0.077	3.3	28.2	124	8.5	71.8	38.3	3.18	29.5	27.2	0.64	0.023	1.38	12.9	12.5	1.34	0.108	6.19	57.6	22.6	4.10	0.181
PCB8	µg	µg/kg	6.1	16.6	1.20	0.073	0.7	8.2	25.2	7.6	91.8	34.0	0.46	9.2	3.95	1.20	0.304	0.53	10.6	4.80	0.00	0.000	4.06	80.3	14.8	0.99	0.067
PCB82	µg	µg/kg	4.3	11.7	0.42	0.036	0.64	39.6	23.8	0.98	60.4	4.40	0.74	33.0	6.30	0.85	0.135	0.37	16.7	3.35	0.49	0.148	1.12	50.3	4.10	0.71	0.172
PCB86	µg	µg/kg					1.2	19.5	43.7	4.9	80.5	21.8	1.23	27.8	10.6	0.35	0.034	0.61	13.7	5.49	0.05	0.009	2.59	58.4	9.46	0.69	0.073
PCB97	µg	µg/kg		<4.6			1.2	19.5	43.7	4.9	80.5	21.8	1.25	27.9	10.7	0.35	0.033	0.62	13.8	5.55	0.07	0.013	2.60	58.3	9.50	0.71	0.074
		Mean	10.1	27.5			Mean	33.1	42.7	Mean	71.1	25.6	Mean	38.3	13.7			Mean	13.3	6.40			Mean	49.8	11.9		
		Max	24.3	66.1			Max	100	249	Max	100	127	Max	71.1	87.4			Max	20.2	25.4			Max	80.3	52.7		
		Min	1.70	4.64			Min	7.80	1.40	Min	7.80	0.70	Min	9.2	1.15			Min	8.70	0.50			Min	23.8	0.80		
		SD	6.70	18.2			SD	17.5	51.3	SD	17.5	35.4	SD	16.4	15.5			SD	2.63	6.53			SD	14.8	13.5		

[a] Dry fraction mass, assuming a starting mass of 1 kg wet bulk sediment. Difference in dry sediment mass for sum of density fractions, sum of size fractions and bulk sediment are due to differences in moisture content assumed in smoothed mass balance.

[b] Unreplicated values

DISCUSSION

Clay appears to play a larger role in PCBs sorption than for PAHs. Mean mass PCBs reporting to the mineral fraction was higher than mass percent of PAHs, for all three sediments. Further, contaminant concentrations were two to four times higher in the clay fraction of New Bedford, than in either the silt or sand fractions, and two to three times higher in the clay fraction for Calumet. Distribution was slightly different with New York, where highest contaminant concentration was in the sand, but only slightly higher than in the clay fraction. The relative influence of organic and clay materials is difficult to determine without statistical analysis. However, comparison of the organic and mineral fraction concentrations for the New Bedford sediment suggests that clay minerals are at least partly responsible for the high PCBs concentrations observed in the clay fraction for this sediment. Contaminant concentrations in the organic fraction were approximately twice that of the mineral fraction in New Bedford, while contaminant concentrations in the clay fraction were over four times that in the silt, suggesting organics may not fully explain the high concentrations seen in the clay fraction. There were also some PCBs present at higher concentrations in the mineral fraction than in the organic fraction, suggesting an association with either hard carbon or clay mineral phases, rather than natural organic material of low density. The observed distribution seems most consistent with sorption to the external surfaces of the clay, for the following reasons: Molecular volume of PCBs ranges from approximately 177 to 323 Å^3 (Mackay, Shiu and Ma 1992). The larger PCBs are too big to be accommodated in the clay mineral silicate pores (10-20 Å) or soot pores (<4-10 Å) (Cornelissen et al 2004). Moreover, while both may play a role, surface sorption to soot is unlikely to be as important as surface sorption to clay, given their respective surface areas. Specific surface area of soot was estimated to range from 58 m^2/g (Lastoskie and Gubbins 2000 as cited in Cornelissen et al. 2004) to 100 m^2/g (Gustafsson and Gschwend 1997). Internal surface area of vermiculite, for example, was estimated to range from 570-700 m^2/g (Hwang and Cutright 2004). Large PCBs may sorb primarily to the outer surface of clays through interaction between the dipole moment of the PCBs and the clay surface charge. Smaller PCBs could exchange in the clay interlayers as well.

High concentrations of contaminants in the sand fraction are thought to be due to either a coarse (non-black carbon) organic phase, hard carbon phase, or an oil and grease phase. Correlations between PCBs, OG, soot and OC will be further explored using statistical techniques in Chapter 7.

Some general relationships can be derived based on the results of the fractionation study which are of utility in assessing feasibility of contaminant reduction by size or density separation. Final contaminant concentration resulting from removal of a selected size or density fraction can be expressed as:

$$C_F = C_I * \left(\frac{1 - f_i}{1 - f_{sed}} \right) \tag{6-1}$$

where

f_i = fraction contaminant mass in size or density fraction removed
f_{sed} = fraction of sediment mass comprised by size or density fraction removed
C_I = contaminant concentration in bulk sediment, µg/kg

C_F = contaminant concentration in treated sediment, µg/kg

The percent reduction (R) in contaminant concentration is given by

$$R = \left(1 - \left(\frac{1 - f_i}{1 - f_{sed}}\right) * 100\right) \qquad (6\text{-}2)$$

A summary of the contaminant reduction resulting from removal of operationally defined clay and organic fractions for the three sediments studied is given in Table 6-4. Negative values indicate that higher concentrations would be expected in the treated sediment than in the untreated sediment. If the proportionality in Equation 6-1 is greater than 1, higher concentrations will result in the residuals. For Calumet, there were no instances where higher concentrations were predicted in the treated sediment. Highest mean reduction of PCBs resulted from removal of the organic fraction, but removal of the clay fraction would result in nearly comparable contaminant reduction. For New Bedford, removal of the clay resulted in positive contaminant reduction for all PCBs, as did removal of the organic fraction. Mean contaminant reduction in New Bedford was higher with removal of the clay fraction, however. For New York, removal of the clay fraction resulted in negative reduction for 20 of 36 PCBs. Removal of the organic fraction resulted in negative reduction for four PCBs, but a positive mean reduction overall.

TABLE 6-4. Percent reduction in PCB concentration (R) with removal of selected operationally defined fractions

	Clay Fraction Removed			Organic Fraction Removed		
Sediment	**Min**[a]	**Max**[a]	**Mean**[b]	**Min**[a]	**Max**[a]	**Mean**[b]
Calumet	8.6	57.2	21.6	1.3	68.0	29.2
New Bedford	9	34.8	23.8	1.7	30	11.3
New York	-80.6	81.6	-10.9	-12.1	100	24.0

[a] Minimum or maximum percent removal for an individual compound
[b] Mean percent removal for all PCBs

SUMMARY AND CONCLUSIONS

Both clay and organic fractions appear to be important to PCB sorption for these sediments to varying degrees. Higher contaminant reduction appears to be achievable with removal of the operationally defined clay fraction for PCBs than was reported for PAHs in Chapter 5. Conversely, PCBs reduction with removal of the organic fraction, while still appreciable for two sediments, was lower for PCBs than for PAHs for all three sediments.

PCBs present at higher concentrations in the mineral fraction than in the organic fraction suggest an association with higher density hard carbon phases or clay mineral phases, rather than natural organic material of low density. Such materials may be difficult to separate from similar size mineral particles using physical separation, as density differences may not be sufficient for the process to discriminate. Certainly, particulate associated contaminants cannot be separated from clean sediment using a screening method alone where particle sizes are similar. Separation processes such as a hydrocyclone or upflow column are typically needed to capitalize on density differences as well. Correlation of contaminant concentrations to sorptive phases is therefore potentially very important to designing a successful treatment train. Fractionation studies provide a good foundation for this, but may need to be augmented with more rigorous statistical analysis in order to evaluate a particular contaminant distribution trend and obtain phase specific contaminant concentrations.

REFERENCES

Brannon, J. M., Davis, W. M., McFarland, V. A., and Hayes, C. (1998). "Organic matter quality and partitioning of PCB," *Bull. Environ. Contam. Toxicol.,* 61: 333-338.

Cornelissen, G., Elmquist, M., Groth, I. and Gustafsson, O. (2004a). "Effect of sorbate planarity on environmental black carbon sorption," *Environ. Sci. Technol.,* 38: 3574-3580.

EPA 1999. "Physical Separation (Soil Washing) for Volume Reduction of Contaminated Soils and Sediments – Processes and Equipment", USEPA-905-R-99-006, Great Lakes National Program Office, Chicago, IL.

Girvin, D. C., and Scott, A. J. (1997). "Polychlorinated biphenyl sorption by soils: Measurement of soil-water partition coefficients at equilibrium," *Chemosphere*, 34:9, 2007-2025.

Gustafsson, O., Haghseta, F., Chan, C., MacFarlane, J., and Gschwend, P. (1997). "Quantification of the dilute sedimentary soot phase: Implications for PAH speciation and bioavailability," *Environ. Sci. Technol.,* 31(1): 203-209.

Gustafsson, Ő. and Gschwend, P. M. (1997). "Soot as a strong partition medium for polycyclic aromatic hydrocarbons in aquatic systems", *Molecular Markers in Environmental Geochemistry*, American Chemical Society Symposium Series 671; Eganhouse, R.P., Ed.; American Chemical Society; Washington, DC. pp 365-381.

Hansen, B. G., Paya-Perez, A. B., Rahman, M. and Larsen, B. R. (1999). "QSARs for K_{ow} and K_{oc} of PCB congeners: A critical examination of data, assumptions and statistical approaches," *Chemosphere*, 39(13): 2201-2228.

Hutzinger, O. H., Safe, S., and Zitko, V. (1983). *The Chemistry of the PCBs.* R. E. Krieger Publishing Company, Melbourne, FL.

Hwang, S. and Cutright, T. J. (2004). "Evidence of underestimation in PAH sorption/desorption due to system nonequilibrium and interaction with soil constituents," *Jour. Envir. Sci. and Health, Part A-Toxic/Haz. Subs. Environ. Eng.*, A39(5): 1147-1162.

Hwang, B-G., Jun, D-S., Lee, Y-D., and Lung,W-S.. (1998). "Importance of DOC in sediments for contaminant transport modeling," *Wat. Sci. Tech.*, 38(11): 193-199.

Karickhoff, S.W. (1984). "Organic pollutant sorption in aquatic systems," *J. Hydraulic Eng.*, 10:6, 708-735.

Latoskie, C. M., Gubbins, K. E. (2000). *Stud. Surf. Sci. Catal.*, 128, 41.

Mackay, D., Shiu, W-Y., and Ma, K-C. (1992). *Illustrated Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals, Volume II – Polynuclear Aromatic Hydrocarbons, Polychlorinated Dioxins, and Dibenzofurans.* Lewis Publishers, Boca Raton, FL.

Olin-Estes, T. J., and Palermo, M. R. (2001) "Recovery of dredged material for beneficial use: the future role of physical separation processes," *Journal of Hazardous Materials*, 85(2001): 39-51

Olin, T. J., Bailey, S. E., Mann, M. A., Lutes, C. C., Seward, C. A., and Singer, C. F. (1999). "Physical separation (soil washing) equipment for volume reduction of contaminated soils and sediments," EPA-905-R-99-006, Assessment and Remediation of Contaminated Sediments Program, Great Lakes National Program Office, Chicago, IL.

EEDP-02-22
August 1997

Environmental Effects of Dredging Technical Notes

Organic Matter Quality and Partitioning of Polychlorinated Biphenyls

Purpose

This technical note reports the initial results of laboratory testing conducted to examine the partitioning of polychlorinated biphenyls (PCBs) to organic carbon of differing degrees of aromaticity.

Background

Over the past 10 years, the U.S. Environmental Protection Agency (EPA) has pursued development of single-chemical sediment quality criteria (SQC). Equilibrium partitioning of neutral organic chemicals between the organic carbon fraction of bedded sediments and the interstitial water of the sediments provides the theoretical basis for the most popular approach to development of SQC. The solution phase of the chemical in equilibrium with the sediment is considered to represent the bioavailable fraction and to enable the conversion of existing water quality criteria (WQC) into SQC or sediment quality standards.

In this approach, sediment total organic carbon (TOC) is considered to be the primary sediment phase accounting for sorption of neutral organic chemicals, and concentrations of these chemicals are therefore normalized to the TOC fraction. A chemical-unique partition coefficient (K_{OC}), applied to the TOC-normalized chemical concentration, is used to estimate the solution-phase concentration for calculation of the bioavailable fraction, which is then compared with WQC. Criteria documents for the pesticides endrin and dieldrin, and for several polynuclear aromatic hydrocarbons, have been released by the EPA for public review and may soon be promulgated.

The promulgation of SQCs with the intent that they be used as standards will result in confounding of effects-based testing procedures as they are now practiced in dredged sediment regulation under the Ocean Dumping Act and

US Army Engineer Waterways Experiment Station
3909 Halls Ferry Road, Vicksburg, MS 39180-6199

the Clean Water Act (Wright, Engler, and Miller 1992; Wright and Wilson 1995). Under such circumstances, it is imperative that the accuracy of the SQC estimations and the degree of uncertainty surrounding them be clearly understood.

The Corps of Engineers is presently investigating the link between contaminant levels in sediment and sediment geochemistry, as well as the utility of equilibrium partitioning approaches for predicting toxicity. In the equilibrium partitioning approach, toxicity is assumed to be related to pore water concentrations of contaminants.

The study reported in this technical note compared measured values of K_{OC} for organic matter isolated from sediment with determinations of the degree of aromaticity in sediment organic carbon.

Additional Information

For additional information contact one of the authors, Dr. James M. Brannon, (601) 634-3725, Dr. William M. Davis, (601) 634-3786, Dr. Victor A. McFarland, (601) 634-3721, and Ms. Charolett Hayes, (601) 634-3428, or the manager of the Environmental Effects of Dredging Programs, Dr. Robert M. Engler, (601) 634-3624.

Introduction

Concentrations of truly dissolved organic contaminants in sediment pore water are regarded as the contaminant fraction available for organism uptake (Landrum and others 1985; Kukkonen, McCarthy, and Oikari 1990). The nature of sediment organic carbon can potentially affect partitioning of nonpolar organic contaminants. Evidence suggests that K_{OC} values increase as the aromaticity of sediment organic matter increases (Garbarini and Lion 1986; Chiou and others 1987; Gauthier, Seitz, and Grant 1987; Grathwohl 1990; Murphy, Zachara, and Smith 1990; Zhou, Rowland, and Mantoura 1995). However, Davis (1993) observed a nonlinear relationship between K_{DOC} (partition coefficient normalized to colloidal plus dissolved organic carbon, DOC) and the fraction of aromatic carbon for humic acids extracted from Florida soils and waters.

Kile and others (1995) reported that the K_{OC} values for carbon tetrachloride and 1,2-dichlorobenzene were relatively invariant for both bed sediments and soils, with the values of bed sediments averaging about twice those of soils. However, Kile and others (1995) also reported much higher values of K_{OC} for sediments impacted by anthropogenic contamination than for pristine sediments. Dredged sediments, by virtue of their location, are almost always subject to anthropogenic inputs.

The K_{OC} values for a particular compound have been reported to vary widely between sediments (Schrap and Opperhuizen 1989; Brannon and others 1993, 1995a). Similar wide variations in K_{DOC} for sediment pore waters from different sediments have been observed (Chin and Gschwend 1992; Brannon and others 1995b). These results imply that partitioning of nonpolar organic contaminants to sediments is much more complex than assumed in the SQC model.

If organic matter quality differs between sediments and the differences affect partitioning, then many of the assumptions used in modeling interactions between nonpolar organic contaminants in sediment and pore waters in aquatic systems are invalid. This study was conducted to examine the changes in aromaticity of organic carbon in sediments and the effects of organic matter aromaticity on partitioning of PCBs.

Materials and Methods

Humic acids were isolated from sediments used in the study of McFarland and others (1996) or planned for later use by the methods of Davis (1993). Isolation procedures included extraction with sodium hydroxide, precipitation, and cleanup of the humic acids. Isolated humic acids were prepared for Fourier Transform Infrared (FTIR) analysis by dissolving the isolated humic substances (approximately 10 mg/ml) into a solution containing a fixed amount of potassium thiocyanate (KSCN) (1.97 mg/ml) at pH 4.0 in distilled deionized water. The KSCN served as an internal standard to normalize the adsorption in the 1,600 to 1,650 cm^{-1} region, where adsorption results mainly from the aromatic carbon content of the humic substances investigated. The internal standard facilitates quantitative comparison of peak intensities between different humic sources. This allows FTIR spectra of humic substances to be used for semiquantitative comparisons of different humic sources.

Where sufficient humic material remained after determination of relative aromatic peak heights (FP-0.331, BL-0.963, NY-0.055, and NY-1.28), the humic acid was dissolved in water and partitioning of PCBs was determined. A commercially available Aldrich humic acid, as well as three humic acids (Orange Heights soil, Orange Heights DOC, and Pine Mountain) isolated in the same manner by Davis (1993), was also tested.

Aliquots from each dissolved humic acid were spiked with ^{14}C-labeled PCB 52 at three concentrations (0.01, 0.007, and 0.004 mg/L) in each of three replicates. Total ^{14}C-labeled PCB 52 in solution was determined by liquid scintillation-counting 1 ml of the original solution. The remainder was then centrifuged for 1 hr at 7,400 × g. A 2-ml aliquot of the centrifugate was then passed through a C-18 Sep-Pak, and a 1-ml aliquot of the eluant was counted to determine the concentration of PCB 52 bound to DOC (Landrum and others 1984). Truly dissolved PCB 52 was determined as the difference between the total counts in the original solution and the counts following passage through the C-18 Sep-Pak. Truly dissolved PCB 52 is that not associated with dissolved or colloidal humic acid.

The DOC content of the humic acids in distilled water was determined using an Astro Total Organic Carbon Analyzer model 2100. The DOC was used to calculate the K_{DOC}.

Results and Discussion

The internal standard normalized FTIR peak heights of the humic substances investigated indicated that there are significant differences in the aromatic character of the materials (Table 1). The relative peak height for the Aldrich humic acid was similar to the value (1.03) determined by Davis (1993). Of the materials isolated and characterized in this study, FP-0.331 had the highest peak height ratio for humic substance aromatic carbon functional groups. The relative aromatic peak heights of the humics isolated by Davis (1993) ranged from 0.39 to 0.95, compared with the range of 2.21 to 5.76 for the humics isolated from sediments. The materials isolated in this study showed higher relative content of aromatic carbon than either the Aldrich humic acid or the humics isolated and characterized by Davis (1993).

Table 1. Peak Height Ratios for Humic Substance Aromatic Carbon (1,600 cm^{-1}) Functional Groups

Humic Acid Source	Sediment TOC, percent	Peak Height Ratio (1,600 cm^{-1})
Aldrich humic acid	NA[1]	0.90
Orange Heights DOC	NA	0.57[2]
Orange Heights soil	NA	0.60[2]
Pine Mountain	NA	0.39[2]
FP-0.331	0.331	5.76
NY-0.055	0.055	3.23
BL-0.963	0.963	2.70
NY-1.28	1.280	2.21

Note: Peak heights are normalized to the response of the internal standard (KSCN) at 2,050 cm^{-1} and are in units of milligrams KSCN/milligram humic C.

[1] Not available.

[2] Data from Davis (1993).

The largest differences were between the materials from soils and river water isolated by Davis (1993) and the sediment humics isolated in this study. This suggests that sediments may be more aromatic in character than humics isolated from soils and water. This may be the reason that Kile and others (1995) found that sediments have K_{OC} values for nonpolar organic contaminants twice those of soils.

McFarland and others (1996) concluded that bioavailability of PCB 52 was highly variable and not linear with sediment organic carbon content at low TOC levels. One reason for these findings may have been the differences in relative aromatic peak height of the humic acids isolated from the sediments. The total organic carbon content of the sediments was not related to the relative degree of aromaticity of these sediments. For example, NY-0.055 (containing 0.055 percent TOC) showed a higher peak height ratio for humic substance aromatic carbon functional groups than did BL-0.963 and NY-1.28. Both these sediments contained higher levels of TOC, but were lower in peak height ratios for humic substance aromatic carbon (Table 1). These results suggest that the aromatic character of TOC may explain many of the contradictions noted in investigations of sediments involving partitioning of nonpolar organic contaminants to sediment organic matter.

Partitioning, or distribution of a hydrophobic organic compound between dissolved organic carbon and water at equilibrium, is mathematically described as follows:

$$K_{DOC} = C_{DOC}/C_W$$

where

K_{DOC} = distribution coefficient, L/kg

C_{DOC} = concentration of contaminant sorbed to the dissolved organic carbon, mg/kg

C_W = truly dissolved aqueous phase PCB 52 concentration, mg/L

Values of K_{DOC} were computed by regression of sorbed (normalized to DOC concentrations) versus truly dissolved PCB. Slopes, standard error of the slope, y-intercepts, and regression coefficients (r^2) are also presented in Table 2. Error in estimates of the slopes averaged 33 percent for all humic acid solutions. Error included differences between replicates and experimental procedure. Regression coefficients ranged from 0.44 to 0.90.

Table 2. Coefficients for Regression (n = 9) of Truly Dissolved and Bound PCBs in DOC

Humic Acid Source	Slope	Standard Error of Slope	Intercept	r^2
Aldrich humic acid	5,604	2,537	4.82	0.49
Orange Heights DOC	6,194	918	-5.4	0.90
Orange Heights soil	5,682	1,642	-0.12	0.66
Pine Mountain	50,934	19,020	68.34	0.51
FP-0.331	80,305	52,664	137	0.44
NY-0.055	73,426	10,471	-74.3	0.88
BL-0.963	22,600	5,410	31.8	0.85
NY-1.28	19,982	6,800	3.07	0.63

K_{DOC} values for PCB 52 varied from 5,604 to 80,305 L/kg. PCB 52 partitioning to materials isolated and characterized by Davis (1993) was generally lower than partitioning to humic material isolated from sediment, with the exception of the Pine Mountain material. However, Davis (1993) observed that the Pine Mountain material behaved in an anomalous manner during partitioning studies. Comparison of the K_{DOC} values measured during this study with projected values derived from the data of Davis (1993), who related K_{DOC} to log solubility for a series of PCBs other than PCB 52, showed good agreement except for the Pine Mountain humic material. The Pine Mountain projected value of log K_{DOC} was much lower (3.2) than the measured value in this study (4.71). Therefore, because of the anomalous behavior previously reported for the Pine Mountain material (Davis 1993) and the divergence in partitioning behavior of this material from that projected by the results of Davis (1993), K_{DOC} values for Pine Mountain material measured in this study were not used.

Estimated values of K_{DOC} were computed by substituting K_{OW} or log K_{OW} (octanol/water partition coefficient) for PCB 52 into the equation $K_{OC} = 0.411 K_{OW}$ (Karickhoff 1981) or $\log_{10} K_{OC} = 0.00028 + 0.983 \log_{10} K_{OW}$ (DiToro and others 1991), respectively. The value of log $K_{OW} = 5.84$ for PCB 52 was obtained from Hawker and Connell (1988). The measured values of K_{DOC} were consistently lower than the estimated K_{DOC} value (5.74), calculated using the method of DiToro and others (1991). The method of Karickhoff (1981) also somewhat overestimated measured values of K_{DOC} (5.45).

Measured values of K_{DOC} in humic materials extracted from soils, water, and sediment were not constant and were consistently lower than the value estimated by the method of DiToro and others (1991) or Karickhoff (1981). However, a strong linear relationship ($r^2 = 0.85$) existed between measured log K_{DOC} values of PCB 52 and the FTIR peak height ratios for humic substance aromatic carbon functional groups (Figure 1). These results demonstrate that the quality of organic carbon strongly affected K_{DOC} values of PCB 52. This relationship indicates that differences between measured K_{DOC} values can be caused by variations in the composition of natural organic matter, specifically variations in the aromaticity of TOC, as postulated by others (Gauthier, Seitz, and Grant 1987; Grathwohl 1990; Davis 1993).

Results indicate that the relative degree of aromaticity in sediments is not constant and differs markedly from that measured in humic acids isolated from soils and river waters. Equilibrium partitioning models that are used to predict concentrations of nonpolar organic contaminants in sediment pore water and which assume that all organic carbon is equal in sorptive capacity are making an erroneous assumption.

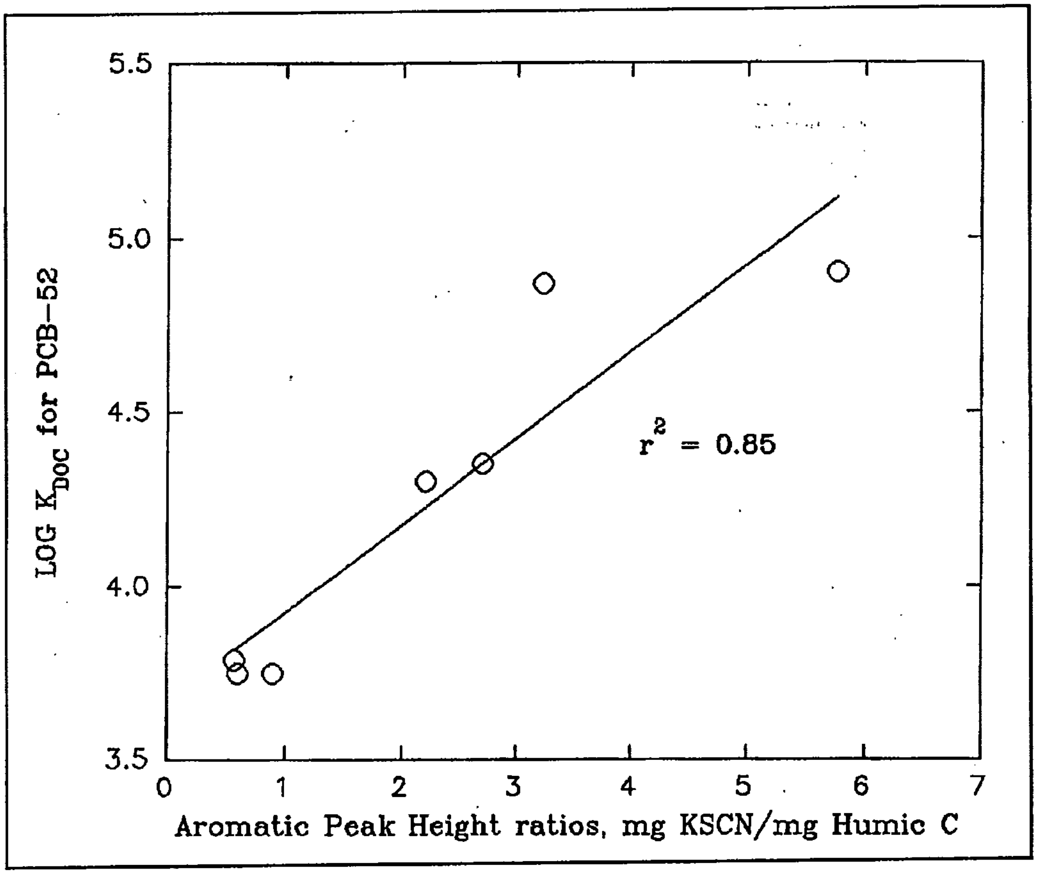


Figure 1. Plot of log K_{DOC} for PCB-52 versus aromatic peak height ratios for extracted humic materials

References

Brannon, J. M., Price, C. B., Reilly, F. J., Jr., Pennington, J. C., and McFarland, V. A. (1993). "Effects of sediment organic carbon on distribution of radiolabeled fluoranthene and PCBs among sediment interstitial water and biota," *Bulletin of Environmental Contamination and Toxicology* 51, 873-89.

Brannon, J. M., Pennington, J. C., Davis, W. M., and Hayes, C. (1995a). "Fluoranthene K_{DOC} in sediment pore waters," *Chemosphere* 30, 419-28.

Brannon, J. M., Pennington, J. C., McFarland, V. A., and Hayes, C. (1995b). "The effects of sediment contact time on K_{OC} of nonpolar organic contaminants," *Chemosphere* 31, 3465-73.

Chin, Y., and Gschwend, P. M. (1992). "Partitioning of polycyclic aromatic hydrocarbons to marine porewater organic colloids," *Environmental Science and Technology* 26, 1621-26.

Chiou, C. T., Kile, D. E., Brinton, T. I., and Malcolm, R. L. (1987). "A comparison of water solubility enhancements of organic solutes by aquatic humic materials and commercial humic acids," *Environmental Science and Technology* 21:1231-34.

Davis, W. M. (1993). "Influence of humic substance structure and composition on interactions with hydrophobic organic compounds," PhD diss., University of Florida, Gainesville.

DiToro, D. M., Zarba, C. S., Hansen, D. J., Berry, W. J., Swartz, R. C., Cowan, C. E., Pavlou, S. P., Allen, H. E., Thomas, N. A., and Paquin, P. R. (1991). "Technical basis for establishing sediment quality criteria for nonionic organic chemicals using equilibrium partitioning," *Environmental Toxicology and Chemistry* 10:1541-83.

Garbarini, D. R., and Lion, L. W. (1986). "Influence of the nature of soil organics on the sorption of toluene and trichloroethylene," *Environmental Science and Technology* 20, 1263-69.

Gauthier, T. D., Seitz, W. R., and Grant, C. L. (1987). "Effects of structural and compositional variations of dissolved humic materials on pyrene K_{OC} values," *Environmental Science and Technology* 21:243-48.

Grathwohl, P. (1990). "Influence of organic matter from soils and sediments from various origins on the sorption of some chlorinated aliphatic hydrocarbons: Implications on K_{OC} correlations," *Environmental Science and Technology* 24:1687-93.

Hawker, D. W., and Connell, D. W. (1988). "Octanol-water partition coefficients of polychlorinated biphenyl congeners," *Environmental Science and Technology* 22:382-87.

Karickhoff, S. W. (1981). "Semi-empirical estimation of sorption of hydrophobic pollutants on natural sediments and soils," *Chemosphere* 10:833-46.

Kile, D. M., Chiou, C. T., Zhou, H., Li, H., and Xu, O. (1995). "Partition of nonpolar organic pollutants from water to soil and sediment organic matters," *Environmental Science and Technology* 29, 1401-6.

Kukkonen, J., McCarthy, J. F., and Oikari, A. (1990). "Effects of XAD-8 fractions of dissolved organic carbon on the sorption and bioavailability of organic micropollutants," *Archives of Environmental Contamination and Toxicology* 19:551-57.

Landrum, P. F., Nihart, S. R., Eadie, B. J., and Gardner, W. S. (1984). "Reverse phase separation method for determining pollutant binding to Aldrich humic acid and dissolved organic carbon of natural waters," *Environmental Science and Technology* 18:187-92.

Landrum, P. F., Reinhold, M. D., Nihart, S. R., and Eadie, B. J. (1985). "Predicting the bioavailability of organic xenobiotics to *Pontoporeia hoyi* in the presence of humic and fulvic materials and natural dissolved organic matter," *Environmental Toxicology and Chemistry* 4:459-67.

McFarland, V. A., Honeycutt, M. E., Feldhaus, J., Ace, L. N., Weiss, C. A., Brannon, J. M., Clarke, J. U., McCant, D., and Jones, J. (1996). "Lower limits of organic carbon normalization: Results of fish/sediment/water equilibrium partitioning studies," *Environmental Effects of Dredging Technical Notes* EEDP-01-38, U.S. Army Engineer Waterways Experiment Station, Vicksburg, MS.

Murphy, E. M., Zachara, J. M., and Smith, S. S. (1990). "Influence of mineral-bound humic substances on the sorption of hydrophobic organic compounds," *Environmental Science and Technology* 24, 1507-16.

Schrap, S. M., and Opperhuizen, A. (1989). "Quantifying the sorption of organic chemicals on sediments," *Chemosphere* 18, 1883-93.

Wright, T. D., and Wilson, J. W. (1995). "Contaminant evaluation of dredged material," *Proceedings of the Western Dredging Association 16th technical conference*. R. E. Randall, ed., Center for Dredging Studies, Texas A&M University, College Station, TX, 125-32.

Wright, T. D., Engler, R. M., and Miller, J. A. (1992). "Effects-based testing and sediment quality criteria for dredged material," *Water quality standards in the 21st century; Proceedings of the 3rd national conference*, EPA 823-92-009. Office of Science and Technology, U.S. Environmental Protection Agency, Washington, DC, 207-18.

Zhou, J. L., Rowland, S., and Mantoura, R. F. C. (1995). "Partition of synthetic pyrethroid insecticides between dissolved and particulate phases," *Water Research* 29, 1023-31.

INTERNET DOCUMENT INFORMATION FORM

A . Report Title: ORGANIC MATTER QUALITY AND PARTITIONING OF POLYCHLORINATED BIPHENYLS

B. DATE Report Downloaded From the Internet: 08/15/00

C. Report's Point of Contact: (Name, Organization, Address, Office Symbol, & Ph #):

US Army Engineer Waterways Experiment Station
Environmental Laboratory
PO Box 631
Vicksburg, Mississippi 39181-0631

D. Currently Applicable Classification Level: Unclassified

E. Distribution Statement A: Approved for Public Release

F. The foregoing information was compiled and provided by:
DTIC-OCA, Initials: __LF__ **Preparation Date 08/21/00**

The foregoing information should exactly correspond to the Title, Report Number, and the Date on the accompanying report document. If there are mismatches, or other questions, contact the above OCA Representative for resolution.

Factors Affecting Sorption of Organic Compounds in Natural Sorbent/Water Systems and Sorption Coefficients for Selected Pollutants. A Review

Alessandro Delle Site[a)]
ENEA, Environmental Department, AMB-TEIN, Via Anguillarese 301, 00060 Rome, Italy

(Received 11 August 1999; revised manuscript received 25 October 2000)

Factors affecting sorption of organic pollutants by natural sorbents (soils, sediments, clays, humic materials, and dissolved organic matters) and sorption coefficients for selected pollutants are reviewed on the basis of the literature results and interpretations; with 681 references examined. The most significant aspects of the sorption process are discussed: sorption isotherms and sorption kinetics; effects of sorbent physico-chemical characteristics (pH, cation exchange capacity, ionic strength, surface area, etc.); effect of the temperature; sorption of volatile compounds; effect of the presence of a cosolvent; association with dissolved organic matter; effect of the sorbent concentration; "hysteresis" or nonsingularity in the sorption–desorption process, and its implications in the transport of these contaminants through soil columns. The experimental and prediction methods adopted for the determination and estimation of the sorption coefficients are also described. Literature sorption coefficients for selected hydrophobic, polar, and ionizable compounds are collected. The compounds taken into consideration belong to the following classes: monoaromatic hydrocarbons, polycyclic aromatic hydrocarbons, chlorinated alkyl and aryl compounds, phenol and chlorinated phenols, polychlorobiphenyls, dioxins, and pesticides. The respective sorption coefficients ($\log K_d$) and organic carbon-referenced sorption coefficients ($\log K_{oc}$) are tabulated together with the most relevant characteristics of the respective sorbent, the measurement temperature, and the experimental methods. The $\log K_{oc}$ values are averaged and compared with other experimental and estimated literature data. Differences of sorption coefficients on soils and sediments and effect of pH on sorption coefficients for ionizable compounds are evidentiated. *© 2001 American Institute of Physics.*

Key words: halogenated alkyl hydrocarbons; halogenated benzenes; chlorinated biphenyls; chlorinated dioxins; chlorinated phenols; critical review; monoaromatic hydrocarbons; pesticides; polyaromatic hydrocarbons; sorption coefficients.

Contents

[a)] Electronic mail: montc@casaccia.enea.it

0047-2689/2001/30(1)/187/253/$35.00

List of Tables

List of Figures

1. Introduction

Accurate procedures for estimating the behavior and fate of chemical pollutants in the environment have been developed in the last tens of years. The interest is justified by the awareness that chemical substances may constitute serious risks for the health of man and other living organisms. This is the reason why organizations like the Environmental Protection Agency and the U.S. Department of Agriculture require, for the registration of new chemicals, information on their environmental behavior and have published relevant test guidelines as those for pesticides.[1–3]

The prediction of transport, distribution, accumulation, and fate of a chemical is possible with the use of environmental models,[4–6] as those based on the concept of fugacity proposed by Mackay.[7–9] They require a number of equilibrium parameters characteristic of the chemical of interest, which are essentially water solubility, vapor pressure, Henry's law constant, octanol/water partition coefficient, adsorption coefficient and bioconcentration factor. Rate of transformation (chemical, biochemical and photochemical) should also be taken into consideration.[10] Such parameters can be obtained with a series of experimental methods or can be estimated using prediction methods.[11] Their values for a large number of organic pollutants have been collected and are available in the literature.[12–17]

The persistence of organic pollutants in topsoil,[18,19] their migration to groundwater,[20–22] and the evaluation of the degree of contamination expected in a groundwater system after an accidental spill or as consequence of the presence of a waste disposal site,[23–25] are problems of particular environmental concern which require the knowledge of the sorption characteristics of the pollutants to be investigated as well as the knowledge of the type of soil and of its characteristics.[26–28] Sorption also affects volatility of organic pollutants,[29–34] their bioavailability and bioactivity,[35,36] phytotoxicity,[37–44] and chemical or microbial transformations.[33,45–48]

In an aquatic system, the residence time of a pollutant and its distribution between water, sediments, and biota depends on its capacity to bound to suspended particles[49] and accumulate in sediments. Thus, the affinity of hydrophobic organic compounds for biotic and abiotic phases is an important determinant of both the rate of a lake's detoxification and its response time to changing loadings.[50] Pesticide–sediment–water interactions occurring within a watershed and the associated aquatic system have been reviewed.[51]

The sorption of an organic chemical on a natural solid is a very complicated process,[52,53] which involves many sorbent properties, besides the physico-chemical properties of the chemical itself. These properties are especially the relative amount of the mineral and organic material in soil/sediment and their respective composition with associated physical characteristics.[28] Also, different regions of a soil or sediment matrix may contain different types, amounts, and distributions of surfaces and of soil organic material, even at the particle scale.[54]

In this paper many studies regarding the distribution of organic chemicals between natural sorbent and water have been reviewed with the aim of examining the various physico-chemical aspects of the sorption process. The values of sorption coefficients available from the literature for several significant organic pollutants have also been collected together with the most relevant experimental conditions used for their measurement. An analysis of these data has been carried out to get information on their variability and accuracy. Differences between sorption on soils and sorption on sediments have also been examined as well as the effect of pH in sorption of ionizable compounds. A comparison of the data obtained by prediction methods with average experimental data collected in this work allowed to evaluate the reliability of those methods.

2. Sorption Isotherms and Sorption Coefficients

The sorption of a chemical on a solid from a water solution may be seen as the result of a reversible reaction (sorption–desorption) which reaches a final equilibrium condition between the concentration of the chemical in the two phases.

Often terms like ''sorptive,'' ''sorbate,'' and ''sorbent'' are used to refer, in the order, to the free solute in solution, solute which undergo sorption by solid material (soil, sediment, etc.), and the sorbing phase. The interaction solid–solute may be generally termed ''sorption,'' while the terms ''adsorption'' and ''absorption'' can be differentiated by the degree to which the sorbate molecule interacts with and is free to migrate between the sorbent phase.[28] Chiou[55] suggested the term ''partition'' for the distribution of a chemical between the organic fraction of the sorbent and the water phase, while ''adsorption'' for the interaction of the chemical with the sorbent mineral fraction. However, often the sorption process is indicated in the literature with various terms like ''sorption,'' ''adsorption,'' or ''partition'' without taking into account the mechanism involved, and the same happens with the sorption coefficient, which is indicated also as ''adsorption coefficient,'' ''partition coefficient,'' or ''distribution coefficient.''

To have reliable and reproducible data, sorption tests require an initial accurate preparation of the soil/sediment sample including sieving, homogenization and sterilization procedure; the latter is used to avoid microbial degradation of the chemical under investigation during the experiment.[56–58] The sorption capacity of a given sorbent may depend on a series of properties, which are grain-size distribution, specific surface area, cation exchange capacity, pH, organic matter or organic carbon content, and mineral constituents. These properties may affect sorption more or less depending on chemical characteristics of the sorbate. Methods of measurement of soil/sediment properties are reported in a series of publications of the American Society of Agronomy and American Soil Science Society.[59–61] The JRC Ispra of the European Commission[62,63] published in 1994 the results of the EURO-SOIL project for the identification, collection, preparation, and characterization of five regionally representative soils as reference soils for chemical testing in the European Union (EU), according to the respective OECD test guidelines[56] and Annex V of the EU-Directive 79/831/EEC.[64] Ball *et al.*[65] reported a detailed study for the characterization of a sandy aquifer material at the grain scale. The study included particle density, porosity, pore size distribution, specific surface area, and organic carbon content.

Specific surface area (SA) is measured by gas adsorption on dry sorbent; the low temperature nitrogen adsorption method (BET method)[66] gives only external surface area because nitrogen does not penetrate pores less than 5 Å in diameter. Krypton[67] and carbon dioxide,[68] on the contrary, are able to penetrate pores less than 5 Å in diameter, but are not able to measure interlayer surfaces of soils and clays. Finally, ethylene glycol monoethyl ether (EGME method) has the capacity to measure both external and interlayer surfaces of soils and clays.[69,70] Other methods, based on methylene blue[71] and water vapor[72,73] adsorption, have been adopted.

Organic carbon (OC) content can be obtained with different methods. The wet procedures are based on dichromate (Walkley–Black method)[74,75] or persulfate[76] oxidation of the sorbent organic matter (OM), while the dry combustion methods use high temperature to oxidize OM to carbon dioxide.[74,77] The OC content can be converted to OM content using the factor 1.724 for mineral soils[74,78] and 1.862 for peats.[78]

The sorption process is generally studied by plotting the equilibrium concentration of a compound in the sorbent as a function of its equilibrium concentration in gas phase or in solution at a given temperature. Sorption isotherms are often nonlinear. A classification of isotherms has been reported[79–81] and each isotherm has been interpreted by a specific model. However, some of them, such as the Langmuir,[82] BET,[66] and Gibbs[83,84] models often fail to describe sorption data in water phase adequately[81] and only Freundlich[85] and linear models seem to better fit the sorption data. However, all the models approach linear model at low sorbate concentration. Figure 1 shows some of these isotherms of interest in sorption of organic compounds in water solution by natural sorbents. In particular, BET isotherm will be met in sorption of organic compounds in vapor phase (Sec. 4.3).

O'Connor and Connolly[86] reported the basis of calculation of the Langmuir isotherm, originally derived for describing sorption of gases by solids, but adopted also for some cases of sorption of a chemical by natural solids from an aqueous solution.

A sorbing system has a sorption capacity, q_c, defined as the ratio of the mass of sorbate to the unit mass of sorbent. The total sorption capacity is therefore $q_c m$, in which m equals the mass of the sorbent. The rate of sorption is assumed to be proportional to the dissolved concentration of the chemical C and to the difference between the total capacity, $q_c m$, and the amount sorbed, $q\ m$, where q is the actual concentration of the sorbate in the solid phase. Thus the kinetic equation may be written

$$\mathrm{d}C/\mathrm{d}t = -k_1 m\ \ C(qc - q) + k_2 q\ \ m, \tag{1}$$

where k_1 and k_2 are the rate constants for the sorption and desorption, respectively.

At equilibrium, Eq. (1) reduces to the Langmuir isotherm

$$q = q_c C\, b/(1 + b\, C), \tag{2}$$

in which

$$b = k_1/k_2.$$

In the Langmuir model the mass of solute sorbed per unit mass of sorbent, q, increases linearly by increasing the solute concentration C at low surface coverages, approaching to an asymptotic value q_c when adsorption sites approach saturation. Three important assumptions made in deriving Eq. (2) are:[87] (i) the energy of sorption is the same for all sites and is independent of degree of surface coverage, (ii) sorption occurs only on localized "sites," with no interaction between adjoining sorbed molecules, and (iii) the sorption maximum (q_c) represents a monolayer coverage. Given these restrictive assumptions, it is not surprising that the Langmuir isotherms are observed only in a few cases[88–94] for the sorption of organic compounds in such a complex and heterogeneous media as soils. They are the most useful to represent the adsorption of polycyclic aromatic hydrocarbons (PAH) from water onto activated carbon.[95]

In natural systems, q_c is invariably an order of magnitude greater than q, and, in many cases, many orders of magnitude greater. Under this condition, Eq. (2) reduces to the linear equation

$$b\, q_c = K_d = q/C, \tag{3}$$

where K_d is the partition coefficient equal to the ratio of the solute (sorbate) concentration in the solid phase at equilibrium, q (indicated also as x/m, where x is the amount of compound sorbed on the mass m of sorbent), to the solute concentration in the aqueous phase at equilibrium C. By convention, concentration units are chosen with the volume unit in solution equivalent in mass to the mass unit for soil/sediment; typical units for K_d are $\mathrm{dm^3\,kg^{-1}}$ or $\mathrm{cm^3\,g^{-1}}$.[52]

Mackay[8] described the environmental behavior of a chemical on a thermodynamic basis using the fugacity approach. Fugacity (f) can be regarded as the "escaping tendency" of a chemical substance from a phase. It has units of pressure and can be related to concentration. Karickhoff[52,96] reported the thermodynamic treatment of the sorption process for dilute systems (linear isotherms) based on these concepts. Sorption equilibrium can be defined as the state at which the pollutant fugacities in the sorbed and solution phases are equal; thus

$$f^s = f^w,$$

where the superscripts s and w refer to the sorbed and solution phases, respectively. In composite systems, as soil and sediments, the fugacity within each sorptive compartment must be equal at equilibrium

$$f_i^s = f^w,$$

which is valid for all sorptive compartments (i). The fugacity can be related to pollutant concentration in each phase. For example, for the aqueous phase,

$$f^w = \phi^w C,$$

where ϕ^w is the fugacity coefficient (ϕ^w, ϕ^s, ϕ_i^s, for water, total sorbent, and single fraction of sorbent, respectively) commonly expressed as the product of an activity coefficient (γ) and the corresponding reference state fugacity (f_0). This fugacity coefficient is the reciprocal of the fugacity capacity used by Mackay.[8] For example

$$\phi^w = \gamma^w f_0^w.$$

The numerical evaluation of any given fugacity coefficient (ϕ) requires the specification of the standard or reference state and its associated fugacity. Concentrations must be in mole fraction units but, for low concentrations, more conventional units can be used; unit conversion factors are incorporated into the fugacity coefficient, but are only required for numerical evaluation of the individual coefficients. The sorbed and solution pollutant concentrations are related by

$$q = C\phi^w/\phi^s.$$

In general, fugacity coefficients are dependent upon pollutant concentration and, therefore, the corresponding sorption isotherms are nonlinear. In "sufficiently" dilute systems, however, these coefficients approach limiting values and the isotherms approach linearity. In simplistic terms, this is the limit in which solute–solute interactions can be ignored in each phase; the molecular environment of the pollutant within each phase remains relatively constant with changes in solute concentration. It is this "low loading" limit that should be quite typical of most environmental situations for which Eq. (3) is valid, where $K_d = \phi^w/\phi^s$ or $K_d = \phi^w \Sigma_i Y_i/\phi_i^s$, for composite sorbent.

Often the experimental data do not follow Eq. (3) but may be fitted by the empirical Freundlich isotherm[85]

$$q = K_f C^{1/n}, \tag{4}$$

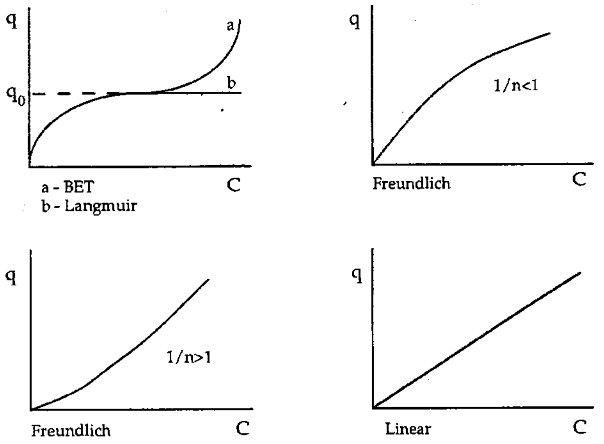


FIG. 1. Typical isotherms describing sorption of organic compounds in water and vapor phase (BET) by natural sorbents.

where K_f and $1/n$ are constants, and q and C have the same meaning as in Eq. (3). Equation (4) can be given in the linearized logarithmic form

$$\log q = \log K_f + 1/n \log C. \qquad (5)$$

The plot of $\log q$ as a function of $\log C$ has a slope equal to $1/n$ and an intercept equal to $\log K_f$. $\mathrm{Log}\, K_f$ equals $\log q$ when C equals unity. When $1/n \neq 1$, the value of K_f depends on the units with which q and C are expressed. In most papers q is given in μg/g of sorbent and C in $\mu\mathrm{g\,cm}^{-3}$ of solution; thus, $K_f(\mu\mathrm{g}^{1-1/n}\,\mathrm{cm}^{3/n}\,\mathrm{g}^{-1})$ is equal to q when $C = 1\ \mu\mathrm{g\,cm}^{-3}$. Hassett *et al.*[97] observed that K_d may be expressed on a mass basis or a molar basis, while K_f should be expressed on a molar basis (typically, q in $\mu\mathrm{mol\,g}^{-1}$ and C in $\mu\mathrm{mol\,cm}^{-3}$).

The value of $1/n$ represents a joint measure of both the relative magnitude and diversity of energies associated with a particular sorption process.[54,98] A $1/n = 1$ indicates linear adsorption and, therefore, equal adsorption energies for all sites. Linear adsorption generally occurs at very low solute concentrations and low loading of the sorbent. A value of $1/n > 1$ represents a concave, curved upward, S-type (Solvent affinity-type)[78,79] isotherm, where the marginal sorption energy increases with increasing surface concentration.[98] It can be interpreted also with strong adsorption of the solvent, strong intermolecular attraction within the adsorbent layers, penetration of the solute in the adsorbent, and monofunctional nature of the adsorbate.[99] S-type isotherms, characteristic of cooperative sorption, are more common for the soil fine fractions, which have a higher total amount of associated organic matter, than for the coarse fractions.[100,101] A value of $1/n < 1$ represents a convex, curved downward, L-type (Langmuir-type)[78,79] isotherm, where the marginal sorption energy decreases with increasing surface concentration.[98] It may arise where the competition of solvent for sites is minimum or the absorbate is a planar molecule.[99] When $1/n$ values are lower than 1 the mobility of a compound in soil columns can be significantly greater for the higher concentrations.[102] Thus, serious errors may be introduced by assuming a linear sorption isotherm.

The Freundlich-type isotherms can result from the overlapping patterns of several Langmuir-type sorption phenomena occurring at different sites on complex sorbent and showing different interaction energies.[54] Although previous attempts to interpret the Freundlich equation theoretically have had only limited success, a meaningful thermodynamic interpretation of this equation has been developed[103] using a fugacity approach with a proposed standard state for sorbed herbicide, which assumes that soil organic matter forms a solid solution with the herbicide.

It has been pointed out[87] that the error factor introduced by assuming the Freundlich isotherm to be linear can be represented as the ratio of Eq. (4) on Eq. (3) and is equal to $C^{(1/n)-1}$. This error factor has been evaluated by plotting $C^{(1/n)-1}$ versus C in the range of $0.1-10\ \mu\mathrm{g\,cm}^{-3}$ and for $1/n$ values ranging from 0.5 to 1.0 (Fig. 2). In this way, it is shown that an error factor of 1.0 represents perfect agreement between linear and nonlinear isotherms, while for $C < 1.0$ the amount sorbed is underpredicted, and for $C > 1.0$ the amount sorbed is overpredicted by assuming linearity. The maximum deviation for $0.1 < C < 10.0\ \mu\mathrm{g\,cm}^{-3}$ and $0.5 < 1/n < 1.0$ will be by a factor of 3 if linear isotherm is assumed. Such error factors may be tolerable for many practical applications as in nonpoint source models, but for large solution concentrations, such as those encountered under waste disposal sites, the amount sorbed could easily be overestimated by an order of magnitude or more.[102,104] Lyman[105] tabulated the values of deviation from linearity for the Freundlich adsorption isotherm as a function of equilibrium concentration in $\mu\mathrm{g\,cm}^{-3}$ and the value of $1/n$.

All the three empirical models (Freundlich, linear, linear with nonzero intercept) and the theoretically based Langmuir sorption model, were able to describe the observed results of batch experiments, carried out with pentachlorophenol (PCP)–soil systems ($r^2 > 0.92$).[106] The conclusion was that, if the measured $1/n$ value in Freundlich equation is in the range of 0.75 and 0.95, a linear isotherm can be used in lieu of the Freundlich isotherm without incurring unacceptable error. However, it was found[107] that sorption coefficients of hydrophobic chemicals with aquifer materials derived from column experiments were consistent with the batch-derived Freundlich isotherms, thus demonstrating the importance of isotherm type on breakthrough curves and solute transport in ground water.

How dilute the system must be to show linear isotherm varies from system to system depending upon the nature of the solute and type of sorption interaction. Sorption isotherms for hydrophobic chemicals were linear when the equilibrium water concentration was kept below 10^{-5} M or below one half of the solute water solubility.[52,108,109] Chiou *et al.*[55] found no isotherm curvature at equilibrium concentrations extending to 60%–90% of saturation with benzene and its two Cl derivatives on soil.

Ball and Roberts[88] reported that nonlinear isotherms

(Langmuir and Freundlich) of tetrachloroethene (PCE) and 1,2,4,5-tetrachlorobenzene (TeCBz) on sandy aquifer solids fit the entire range of data much better than does the simple linear relationship, although selection between the two nonlinear isotherm types is difficult. At the low concentrations ($<50\ \mu g\,dm^{-3}$) relevant to the rate studies[110,111] and field experiment[24,112] the isotherm data appear more linear. Isotherm nonlinearity of PCE and TeCBz observed at higher solute concentrations suggests that physical adsorption may be important in sorbent having a low content of organic matter (0.021%).[88] Young and Ball[113] observed that although PCE sorption on aquifer material follows isotherm nonlinearity, a linear approximation of sorption capacity might be adequate for modeling purposes.

Due to the heterogeneous composition of natural sorbents, sorption may be expressed by composite linear isotherms.[52,114,115] The relative equation may be of the type

$$q=\sum_{i=1}^{m} x_i q_i \left(\sum_{i=1}^{m} x_i K_{di} \right) C = K_d C,$$

where q is the total solute mass sorbed per unit mass of bulk solid at equilibrium, x_i is the mass fraction of the soil comprising reaction region or component i, q_i is the sorbed phase concentration at equilibrium expressed per unit mass of that region or component, K_{di} is the partition coefficient for reaction i expressed on a per mass of component i basis, and K_d is the mass-averaged partition coefficient.

If one or more of the component elements of sorption is governed by a nonlinear relationship between the solution and sorbed phases expressed by Freundlich isotherms, then the composite isotherm will deviate from linearity. Weber *et al.*[54] proposed the "distributed reactivity model" which takes the form

$$q=x_1 K_d C+\sum_{i=1}^{m} (x_{nl})_i K_{fi} C^{ni},$$

where x_1 is the summed mass fraction of solid phase exhibiting linear sorption, K_d is the mass-averaged sorption coefficient for the summed linear components, $(x_{nl})_i$ is the mass fraction of the ith nonlinear sorbing component, and K_{fi} is the Freundlich sorption coefficient for reaction i expressed on a per mass of component i basis. The model has been applied to soil having components with different organic matter content.

Another way to express nonlinear isotherms has been suggested by Lambert[116] who proposed an equation of the type

$$x/m=\alpha C+\beta C^2+\gamma C^3+\cdots, \tag{6}$$

where α, β, γ are the adjustable coefficients used to fit the data, x is the quantity of chemical sorbed, and m the mass of sorbing medium and C is the concentration of solute in solution at equilibrium. For most practical purposes, when C becomes very small and β and γ are small numbers the series converge without the second and third terms and α may be taken as a measure of K_d. Equation (6) accounted for the curvature observed in the adsorption isotherm of metribuzin better than the Freundlich equation[117] and has been proved valid for the first desorption equilibration of fluometuron from soils.[118]

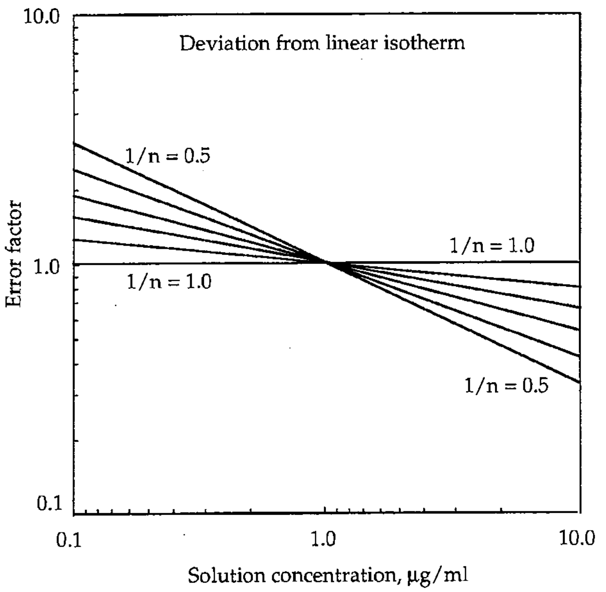


FIG. 2. Plot of the error factor as the ratio between Freundlich and linear isotherms as a function of solution concentration (after Rao and Davidson[87]).

Isotherm models describing equilibrium distribution of a solute between a solid phase and an aqueous phase are depicted in Fig. 1. The different shape of the isotherms depend on the sorption mechanism involved and the associated sorption energy. In particular, linear model is characterized by uniformly distributed sorption energy with increasing concentration. At low solute concentration all models reduce to linear. Therefore, linear model can be applied to cases of environmental contamination where concentration is low, so producing a simplification of the mathematical treatment of environmental models. However, when sorption isotherm cannot be considered linear, the appropriate isotherm model must be used. Finally, sorption coefficients have to be measured at equilibrium; therefore, a previous kinetic study is necessary to know the time required to reach equilibrium.

3. Sorption Kinetics

Sorption measurements must be carried out when equilibrium has been reached. It has been reported that times of 1 h or few hours[119–129] to 1 day are often sufficient to reach equilibrium, but sometimes are necessary some days[130–133] or several days, months, or years.[110,113,134–136]

Many examples exist of rapid equilibration time. The adsorption kinetics for bromacil and napropamide on air-dried clay soil with high OC content (7.3%–9.1%) indicated that bromacil attains equilibrium almost instantaneously.[137] Napropamide, however, does not reach equilibrium for 2–3 h. When napropamide was added to a prewet soil, the system was still not at equilibrium after 48 h.

No significant increase in adsorption of aldrin by soils and clays was observed between 5 min and 5 days of contact time.[138] Also with parathion equilibrium is quickly reached within 1 min.[139] The rapid equilibration (2 h) of organophosphorous and carbamate insecticides with soils has been interpreted as due to a physical type adsorption mechanism.[122]

A study of cyanazine adsorption on peat saturated with cations showed that equilibrium is reached within 1 h.[140] The thermodynamic parameters seem to point to an adsorption mechanism by hydrogen bonds.[141]

The rate of binding of diquat and paraquat on humic acid was rapid;[142] equilibrium was reached within 3 h. The sorption data suggested that the interaction between the herbicides and humic acid was mainly electrostatic in nature.

The adsorption of several insecticides and herbicides of different nature on inorganic sorbents (kaolinite, sand) was very fast (minutes), while the adsorption on substrates containing organic matter increased with time; equilibrium was not reached in 10^4 min, but extrapolation suggested it could be reached before 10^5 min, indicating that sorption is a multistage process.[114] Kookana *et al.*,[143] in a study of simazine and linuron adsorption by soils, reported that a well structured soil with high OM content showed slower rate of sorption compared with a dispersed soil with low OM content. Moreover, a comparison of sorption data obtained by a batch technique and a flow technique revealed that sorption occurs at a much faster rate under batch conditions, presumably because of shaking and high solution to soil ratio. Under batch conditions, the instantaneous component of sorption was very high (up to 90% of 24 h sorption value).

Hance[144] studied the sorption of four herbicides on six different sorbents. Equilibration time ranged from 1 to 24 h. Nylon and silica gel, which do not possess a crumb structure, came to equilibrium with linuron very quickly. The slow adsorption by some sorbents may depend on: the slow solvent action of the aqueous solution which causes the unmasking of some adsorbing sites; the slow chemical fixation processes which may operate in some instance; swelling of the sorbent after long exposure to water and, in some cases, the slow diffusion of the solute into the sorbent.

Hamaker and Thompson[123] postulated that the sorption kinetics depends on the sorption process and on the transport of the compound to the sorption sites which consists of transport to the outer sorption sites (macrotransport) and diffusion into micropores and capillaries. Talbert and Fletchall[145] suggested that the small increases in sorption of triazines by soils may be due to: delay in the wetting of small interior capillaries; slow diffusion of the solute into these interior surfaces; slow irreversible fixation reaction due to chemical forces; mechanical breakage of solid particles; formation of complexes.

A detailed study of 2,4-D adsorption kinetics on clay minerals indicated that the rate-limiting step in adsorption was diffusion to the reactive sites within the clay matrix and not the kinetics of reaction at the site.[146] The adsorption of 2,4-D and picloram on humic acid revealed an initial rapid rate followed by slower rates at longer times.[125] The amount of pesticide adsorbed was plotted as a function of the square root of time. In each instance the linearity in the plots was usually attained after about 1 or 1.5 h. Thus it appears that, at longer times, intraparticle diffusion of the compounds into the interior of the humic acid particles was the dominant rate-limiting process. The rate-limiting step for sorption of parathion on soil organic matter was the diffusion of the insecticide molecules to the surface of the adsorbent for the first 10 min of adsorption.[147] At longer times, intraparticle diffusion of the adsorbate into the interior of the adsorbent particles was rate limiting.

Thus, the sorption kinetics of organic pollutants on natural sorbents shows often a rapid initial uptake followed by a slow approach to equilibrium.[148–155] Karickhoff and Morris[156] described sorption dynamics of hydrophobic chemicals on sediments by a two compartment model that distinguish rapid or "labile" exchange (requiring at most a few hours to achieve) from highly retarded or "nonlabile" sorption requiring days or weeks to occur. They collected kinetic and sorption data for hydrophobic compounds with several sediments obtained in two studies.[151,156] When these data were combined, an equation relating the characteristic time ($1/k_2$) for nonlabile sorption to K_d ($\mathrm{cm^3\,g^{-1}}$) was found that seemed to hold over a range of characteristic times in excess of 3 orders of magnitude (hours to months):

$$1/k_2(\mathrm{h}) \approx 0.03 K_\mathrm{d} \quad r=0.87. \tag{7}$$

The authors observed that individual data deviate from Eq. (7) by as much as a factor of 3, but the relationship clearly defines the appropriate time frame for nonlabile sorptive events. In conclusion, times to reach equilibrium can be on the order of 0.1 K_d (h). For chemical/sediment systems with $K_\mathrm{d} > 10^5$, equilibration times in excess of 1 year would be expected. The fraction of the total sorption that was labile was typically 0.25–0.60, but decreased to 0.1 or less for highly sorbed chemicals at high solid concentrations.

A mathematical approximation of such a two-step sorption reaction for batch experiments can be simplified[152] to

$$x/c = K_\mathrm{d}(1 - e^{-k_2 t}), \tag{8}$$

where the time constant k_2 for accessing compartment 2 can be estimated by an iterative least-squares approximation based on a Taylor progression of k_2. Equation (8) has been proved valid for polychlorobiphenyl (PCB) congeners.[153] The results demonstrated that with strongly adsorbing PCB congeners equilibrium cannot be obtained even after 7 days.

Wu and Gschwend,[155] in order to develop an accurate description of hydrophobic compound transport, proposed a model of sorption kinetics ("radial diffusion" model) based on known physical and chemical processes, molecular diffusion, and phase partitioning. The effects of sorbate hydrophobicity, sorbent particle size, and system temperature on solid–solution exchange were examined. The results demonstrated that the bigger aggregates have lower uptake rates, that compounds with higher values of octanol/water partition coefficient (K_ow) show slower sorption, as already found by Karickhoff[151] with PAHs, and that desorption rates are consistent with a reversible diffusive exchange mechanism. Model simulation analysis indicate that a single effective diffusivity parameter, which is predictable from compound solution diffusivity, octanol–water partition coefficient, and sorbent organic content, density, and porosity, can be used to quantify the sorption kinetics.

Thus, diffusion limitations seem the most likely explanation for the long time often necessary to attain equilibrium in sorption process. However, Ball and Roberts[157] observed that accurate *a priori* estimation of sorption rates does not appear to be feasible.

Sorption of PCE and 1,2,4,5-TeCBz by sandy aquifer solids required contacting times on the order of tens to hundreds of days to reach equilibrium. However, equilibrium was approached much faster when pulverized material was used.[88] For a given solute, the distribution coefficients differed by a factor of 30 among the various size fractions, being greatest for the largest grains. The results have been interpreted[110] with an "intraparticle diffusion" model and diffusive rate constants were determined for different size fractions of the sorbent as well as with pulverized material. Based on measured particle size and independent estimates of porosity and internal retardation, effective pore diffusion coefficients were estimated to be roughly 2–3 orders of magnitude lower than bulk aqueous diffusivities.

Alachlor retention follows Freundlich isotherm;[158–160] it seems to react at different rates with different sites on sorbent, suggesting that a multireaction kinetic approach may be considered to describe alachlor retention kinetics in soils.[159] On this basis, Xue and Selim[161] presented a "multireaction kinetic" model to determine both the kinetics of alachlor retention and the nonreversibility of the adsorption–desorption in soils. The model also was capable of predicting alachlor desorption kinetics based solely on parameters obtained from adsorption experiments.

Some effects of the complexity of the sorption kinetics are:

(a) Sorption may not be reversible showing the existence of "hysteresis" in the sorption–desorption process[162] (Sec. 9). Sometimes, part of the sorbed compound may be strongly retained; covalent binding with soil surface may be one reason for the formation of nonextractable residues.[163] Quantitative recovery of paraquat from a field soil required chemical "dissolution" of the sorbent matrix to achieve chemical release.[89]

(b) Experimental sorption measurements may require long times and, therefore, special attention is necessary, due to the possibility of continuing losses of chemical from the system, chemical or biological transformations, and possible artifacts in experimental sorption and desorption work.[157,164] In addition, soil properties may change after many treatments.[165]

(c) Due to rate-limited sorption, models which assume equilibrium between dissolved and sorbed species, may result in significant error in prediction of fate, especially when the sorptive exchange "reactions" or mass transfer are slow with respect to advective flow of the pore fluid.[155] A nonequilibrium model can successfully simulate transport in aquifer materials performed at a faster velocity ($\sim 1\ \mathrm{cm\,h^{-1}}$), whereas the equilibrium model was adequate for the slower-velocity ($\sim 0.2\ \mathrm{cm\,h^{-1}}$) experiments[166] (Secs. 9 and 10).

4. Factors Affecting Sorption of Organic Compounds

The distribution of an organic solute between sorbent and solvent phases results from its relative affinity for each phase, which in turn relates to the nature of forces which exist between molecules of the solute and those of the solvent and sorbent phases. The type of interaction depends on the nature of the sorbent as well as the physico-chemical features of the sorbate (hydrophobic or polar at various degrees).[123]

Weber *et al.*[28] summarized the possible interactions between solute and sorbent included into three loosely defined categories of sorption: physical, chemical, and electrostatic. The physical sorption processes involve interactions between dipole (permanent or induced) moments of sorbate and sorbent molecules. The relatively weak bonding forces associated with physical sorption are often amplified in the case of hydrophobic molecules by substantial thermodynamic gradients for repulsion from the solution in which they are dissolved. Chemical interactions involve covalent bond and hydrogen bond. Finally, electrostatic interactions involve ion–ion and ion–dipole forces. In a more detailed way, the type of interactions and the approximate values of energy associated are:[163] van der Waals interactions (4–8 $\mathrm{kJ\,mol^{-1}}$), hydrophobic bonding (4 $\mathrm{kJ\,mol^{-1}}$), hydrogen bonding (2–40 $\mathrm{kJ\,mol^{-1}}$), charge transfer, ligand-exchange and ion bonding (40 $\mathrm{kJ\,mol^{-1}}$), direct and induced ion–dipole and dipole–dipole interactions (2–29 $\mathrm{kJ\,mol^{-1}}$), and chemisorption (covalent bond) (60–80 $\mathrm{kJ\,mol^{-1}}$).

Sorption of organic pollutants sometimes can be explained with the simultaneous contribution of two of more of these mechanisms, especially when the nonpolar or polar character of the compounds is not well defined.

4.1. Nonpolar Compounds

Clay minerals can be considered good sorbents for nonionic compounds. It is hypothesized[167,168] that the methylene groups of the aliphatic chain may form a kind of hydrogen bonding with the clay mineral (Ca-montmorillonite) of the type C–H$\cdots$O–Si. The degree of adsorption depends on the activity of the methylene groups and on chain length.[168]

Sorption of acetoaceticethylester and β,β-oxydipropionitrile on clay minerals (gibbsite, kaolinite, Ca- and Na-montmorillonite) was studied by Brindley *et al.*[169] The order of decreasing sorption per unit of surface was gibbsite>kaolinite>montmorillonite. It was suggested that the hydroxyl surfaces, which comprise the basal area of gibbsite and half the basal area of kaolinite, sorb more effectively than the oxygen surfaces which occur in montmorillonite and comprise half the basal area of kaolinite. Sorption may occur through hydrogen bonding from the hydroxyl surfaces toward oxygen atoms in the organic molecules. It may be that oxygen surfaces of montmorillonite are less effective in sorbing organic molecules by hydrogen bonding, due to the competition of water molecules. Moreover, the exchangeable cations of montmorillonite, Ca and Na, readily form hydration complexes which may screen an appreciable portion of the available surface. Kaolinite is thought to have relatively few exchangeable cations in the extended basal surfaces, and gibbsite probably has none. Therefore, it appears reasonable from this point of view that these minerals should exhibit higher surface sorption than does montmorillonite. However, benzene sorption on Al-saturated montmorillonite clay was seven times greater than for soils and three times greater than for Ca-saturated clay.[170] The reason of this behavior has not been explained.

SA may be an important factor in sorption of aromatic hydrocarbons by clay materials. Hydrogen bonding with the oxygen of the clay surface may occur. The K_f values for benzene, toluene, and xylenes were lower in kaolinite than in montmorillonite or illite.[171] This result, already reported by Bailey and White,[172] may be explained on the basis of the following considerations: montmorillonite is a 2:1 expandable lattice clay with a large SA ($8\times10^6\,\mathrm{m}^2\,\mathrm{kg}^{-1}$); illite is nonexpandable 2:1 clay with SA of $10^5\,\mathrm{m}^2\,\mathrm{kg}^{-1}$; kaolinite is a nonexpandable 1:1 clay with a SA of $3\times10^4\,\mathrm{m}^2\,\mathrm{kg}^{-1}$. Another significant result was that the amount of toluene adsorbed from a hydrocarbon mixture was smaller than the amount of toluene adsorbed from a single hydrocarbon solution, showing thereby a competitive adsorption in a mixture of hydrocarbons. Pierce *et al.*[173] found that montmorillonite adsorbed four times as much DDT as did kaolinite. Adsorption on clay was inversely proportional to temperature, which is indicative of physical adsorption. This was substantiated by the similarity of the adsorption and desorption isotherms.

The type of solvent may affect sorption of nonpolar compounds. Sorption of lindane on several sorbents from various solutions increased in the order ethanol$<$benzene$<$hexane $\leqslant$water.[174] The sorption differences were assumed due in part to the differing solubilities of lindane in the different solvents, and in part to the structure and affinity of the solvent molecule for the particular sorbent. It appears that lindane competes for sorption sites most effectively with water and least effectively with ethanol. This was attributed to the importance of dipole–dipole interactions in the lindane sorption. Griffin and Chou[175] investigated the adsorption of PCBs in hexane and ethanol solutions on soils. The results showed virtually no adsorption, indicating that potential migration of PCBs and other similar compounds could occur in a landfill if these compounds were dissolved in organic solvents.

The contribution of the OM of soils or sediments to the sorption of nonpolar compounds was found much more relevant than the contribution of other components.[26,116,176] The K_d values of a chemical with different sorbents were found directly proportional to the OM (or OC) content. The strong tendency of humic acid extracted from soils to retain hydrophobic organic compounds (HOC) was investigated by Khan and Schnitzer.[177] They found that 100 g of humic acid can firmly retain up to 2 g, and possibly more, of hydrophobic organic compounds by a mechanism that most likely involves sorption on external surfaces and in internal voids of a molecular sieve-type structural arrangement. The order of increasing adsorption rates for PCB congeners has been found to be: Del Monte sand, illite clay, Woodburn soil, and humic acid.[178] The vapor loss of Aroclor 1254 is significant from the sand but negligible from the soil.[30]

A good correlation between sorption of HOCs and OC content of the soil and sediment was found by Hassett *et al.*[179] with dibenzothiophene on 14 soils and sediments ($r^2=0.904$). The other factors tested [e.g., total clay, clay mineralogy, cation exchange capacity (CE), SA, pH], were nonsignificant. Similar results were obtained by Means *et al.*[180] investigating the sorption of four PAHs on 14 EPA soils. Also the variability in lindane sorption on soils was almost entirely due to OC.[119]

The sorption behavior of naphthalene, 2,4-D, p-chloroaniline, hexachlorobenzene (HCBz), and lindane on several organic and inorganic materials and natural soils have shown that the organic constituents of the soils were mainly responsible for their sorption properties.[181] Cellulose appeared to be a well-suited model sorbent for simulating the relative sorption behavior of the chemicals.

Sorption of PCBs on three marine sediments increased with the hydrophobicity of the PCBs and with the OC content of the sediments.[182] However, the removal of OM resulted in a decrease of the sorption coefficients, more marked for those congeners with a relative lower degree of chlorination.[183] Sorption of PCBs on the mineral particles whose OM has been removed becomes increasingly significant as the hydrophobicity of the PCBs and the percentage of silt–clay fraction of the sediments increase.

The role of OM has been also demonstrated by removing the soil OM using a series of extractants (ether, ethanol, hot water, 2% HCl)[185] or by oxidation with hydrogen peroxide.[138,184,185] These procedures reduced the amount of sorbed HOCs. However, other soil properties, besides OM, appeared responsible for adsorption,[185] but their role could be masked by that of the OM, as reported for parathion.[129] At low OM content, clay content and free iron oxide seemed implicated in lindane sorption on soils.[185] The decreased sorption of lindane by anaerobic soils low in OM content is attributed to the decrease in inorganic surface area caused by the reduction of ferric to ferrous ion and the high state of hydration attained by ferric oxides upon flooding.[186] On the basis of the relevant importance of the OM in controlling adsorption of organic nonpolar compounds of limited water solubility ($<10^{-3}$ M),[52] the following constants have been defined:

$$K_{\mathrm{om}}=K_{\mathrm{d}}/f_{\mathrm{om}} \quad \text{or} \quad K_{\mathrm{oc}}=K_{\mathrm{d}}/f_{\mathrm{oc}}, \tag{9}$$

where f_{om} and f_{oc} are the fractions of OM or OC in the solid sorbent respectively. K_{om} and K_{oc} are expressed in $\mathrm{cm}^3\,\mathrm{g}^{-1}$ or $\mathrm{dm}^3\,\mathrm{kg}^{-1}$ of OM or OC, respectively. In Eq. (9) the OC content in soil is assumed constant and K_{oc} is expected to have an equal value, within the experimental errors, for a chemical in sorption with different soils.

Wershaw *et al.*[187] reported that the adsorption of DDT to humic acid was not affected by the addition of sodium chloride, indicating that the association was not due to coulombic attraction. Khan and Schnitzer[177] suggested that hydrophobic molecules could be trapped by internal voids formed through hydrogen bonding between humic polymers. The high adsorbing capacity of humic acid was due to hydrophobic bonding in humic acid–DDT interaction, because of the presence of nonpolar portions of the humic acid polymer and lipoidal molecules trapped within the polymer, or to trapping of DDT molecules within voids in the polymer.[173] Thus, the association of nonpolar organic compounds to soil OM is attributable to ''hydrophobic bonding.''[123] This type of bonding is due to the combination of van der Waals forces and a ''thermodynamic gradient'' driving nonpolar organics of low solubility out of solution, because the interactions of these compounds with natural OM are energetically preferred to interactions compound/water or compound/compound.[28,188]

In comparing several sorbents, the PCB concentration factors were found to be inversely related to their average particle size and linearly related to their SA.[189] The concentrations of chlorinated hydrocarbons from Los Angeles Arbor are closely related to the OC content and to particles of 8 μm or less in size.[190] Retention of DDT, endosulfan and methoxichlor was studied with two soils.[191] A portion of each soil was treated with hydrogen peroxide to study the effect of OM on pesticide retention. In the untreated soils the greatest retention of the three insecticides was on the colloidal (< 0.08 μm) and 0.08–0.5 μm fractions. Removing the OM from both soils reduced the retention on these fractions.

Karickhoff *et al.*[108] also have identified, in addition to the primary effect of OC, sediment particle size as a secondary factor in the sorption of hydrophobic chemicals on natural sediments. The K_{oc} for the whole sediment approximates that of the fines fraction, which contains the majority of the organic carbon. The K_d for a series of PAHs was determined and correlated to the fraction of OC of sediments.[96] Correlation coefficients (r) exceeded 0.90 in all cases. Moreover, the zero intercept in the plot K_d–f_{oc} showed clearly that an inorganic sorption contribution was contraindicated. Nkedi-Kizza *et al.*[192] also found that OC content in soil increases exponentially with decreasing particle size; the K_d values for diuròn and 2, 4, 5 T increase accordingly.

Sorption of toluene by two samples of soil (0.23% and 0.41% OC, respectively) and by commercial humic acid and the same humic acid coated Al_2O_3 was investigated.[193] K_{oc} values varied by a factor of 2.5, with the sorbents of highest and lowest OC content (humic acid and a soil). Moreover, the K_{oc} values for trichloroethene (TCE) and toluene onto humic acid were more than 2.5 times greater than those determined for the same humic acids when coated onto Al_2O_3. The same authors[194] carried out sorption experiments with TCE and toluene on soil and on humin fraction extracted from the same soil. The results indicated that the humin fraction shows an increased sorption capacity over the whole soil, thus suggesting the possibility that the intimate association of soil OM with the soil inorganic matrix strongly modifies the particle surfaces and/or the nature and properties of soil OM, thus influencing its binding capacity.

Chiou *et al.*,[55] on the basis of their own results,[195–198] observed that sorption of nonionic organic compounds from water on soil consists primarily of partition into the soil organic phase; adsorption by the soil mineral fraction is relatively unimportant in wet soils presumably because of the strong dipole interaction between soil minerals and water, which excludes neutral organic solutes from this portion of the soil. The linear isotherms obtained with single and binary compound indicated no competition in the sorption process of the two compounds. Therefore, partitioning of organic solutes between the soil organic phase and water may be treated in a manner similar to that between an organic solvent phase and water. Also the adsorption of naphthalene and fluorene in a mixture with other PAHs was linear and was suppressed slightly compared to measurements when only one compound was in solution.[199] Partitioning of organic solutes between soil and water was analyzed[195,196] by using the conventional solution concept for solutes in water and the Flory–Huggins[200,201] treatment for solutes in the polymeric humic phase. Sorption determined for 12 aromatic and chlorinated compounds on soil shows that the extent of solute insolubility in water is the primary factor affecting the soil OM–water partition coefficient (K_{om}) and that the effect of solute incompatibility with soil OM is significant but secondary. This explains the commonly observed correlations of $\log K_{om}$ vs $\log K_{ow}$ (octanol–water partition coefficient) and of $\log K_{om}$ vs $\log S$ (water solubility) (Secs. 12.1 and 12.2).

However, Spurlock and Biggar[202] pointed out that isotherm linearity is not a prerequisite for partitioning, because: (i) nonlinear uptake (dissolution) of organic vapors and gases in polymers is often observed, (ii) a number of studies on nonionic organic compound–humic acid sorption have reported nonlinear isotherms, and (iii) solvent–polymer interactions sometimes vary with concentration.[203] On the basis of the chemically heterogeneous macromolecular nature of humic substances, a more general view of partitioning has been taken into consideration;[202,204,205] organic carbon-based sorption is viewed as a solute distribution between a three-dimensional macromolecular humic phase and the bulk solution phase and the solute–sorbent interactions are not necessarily restricted to nonspecific London interactions. A general thermodynamic partition model for organic carbon-based linear and nonlinear sorption from solution was formulated in order to characterize sorbate partial molar free energies.

Chin and Weber[206] applied the modified Flory–Huggins model in conjunction with solute aqueous activity coefficient data to estimate the association of organic contaminants to humic and other organic polymers in the aqueous phase. The correlation between $\log(K_{oc})_{obsd}$ and $\log(K_{oc})_{pred}$ for 14 aromatic and chlorinated hydrocarbons showed good agreement (Sec. 12.7.).

For sorbents with OC content greater than 0.1%,[207] a highly significant correlation was found between the K_ds of some halogenated alkenes and benzenes and the OC contents of a series of sediment samples. These findings indicate a very similar lipophilicity of the organic materials present in these natural sorbents. Small K_d values have been found for ''organic poor'' sorbents ($OC<0.1\%$), even for those with a high SA. Therefore, the compounds investigated are quite mobile in such media. The limit of about 0.1% OC has been indicated also by other authors,[208,209] although others[88] found that the K_d values of PCE and 1,2,4,5 TeCBz on different size fractions of an aquifer material low in OC content (0.021%) correlate linearly with the f_{oc} values of the single fractions; however, this occurs at low sorbate concentrations while physical adsorption to heterogeneous sites may be present at higher concentrations where nonlinear relationship is observed. Khan *et al.*[210] studied the adsorption of acetophenone on 14 sediment and soil samples of different composition. The linear partition coefficient was correlated significantly with percent OC. The amount of clay appeared to be important in some cases, where OC was too low and did not mask the effect of the clay minerals.

The adsorption on mineral surface (clay) dominates organic matter partitioning at high clay to OM ratio.[52,54,98] Karickhoff[52] collected the data regarding the role of mineral in pollutant sorption[38,129,185,211,212] and defined a threshold for onset of mineral contribution, given by the ratio cm/oc $=30$, where cm and oc are the fractional masses of swelling clay minerals and organic carbon in the whole sediment. That is, for $cm/oc<30$ mineral contributions are masked, regardless of the mineral content. However, this ratio depends on hydrophobicity of the sorbate. For a compound having a value of $\log K_{ow}=2.14$, the critical clay to OM ratio is 15:1, which corresponds to $cm/oc=30$. Mc Carty *et al.*[115] suggested that the critical $f_{oc}(f_{oc}^*)$ below which mineral adsorption dominates over OM partitioning can be calculated by the equation

$$f_{oc}^*=\mathrm{SA}/[200(K_{ow})^{0.84}],$$

where SA is the mineral-specific surface area.

Sorption isotherms for naphthalene, 1-methylnaphthalene, and o-dichlorobenzene (DCBz) were measured on seven subsurface aquifer materials having OC content ranging from 0.0096 to 0.156%.[213] Multivariate statistic was used to investigate possible relationships between sorption coefficients and OC content and other sorbent properties (percentage sand, percentage silt, percentage clay, CE, SA, etc.). The sorption coefficient, for aquifer materials containing less than 0.10% OC, does not correlate with any of the properties of the sorbent, including the OC content. No single surface appears to control sorption on the aquifer material and, therefore, it is recommended that sorption coefficients be determined experimentally on each different sorbent of this type. Humic acid-modified silica shows similarities with these aquifer materials and has been proposed as a simplified model to examine organic solute transport processes in ground water.[107]

Lara and Ernst[182] reported that K_{oc} values for PCB congeners with three different sediment samples, having OC contents of 0.50%, 1.47%, and 2.33%, respectively, depart considerably from constancy with the degree of chlorination, increasing with decreasing f_{oc}. This is probably a result of the assumption that OM is the sole sorbent, whereas significant sorption of highly hydrophobic congeners is also taking place on exposed mineral surfaces of the sediments.

The contribution of the mineral fraction to the sorption of nonionic compounds may be computed by plotting K_d versus f_{oc} for the adsorption of a compound on a series of sorbents. A more general formulation of Eq. (9) can be[153,214,215]

$$K_d=K'_{oc}f_{oc}+K^0,$$

where the intercept K^0 expresses a fraction of adsorption by soil constituents other than OC. This fraction may be significant especially in soils with a low OC content and can be subtracted to the K_d values of all soils to get amended K_{oc} values.[153]

Although all this evidence that K_{oc} or K_{om} is constant for each chemical when $f_{oc}>0.001$, it has been found that the K_{om} values for a single compound may show differences ranging from a factor of 3 to over an order of magnitude from soil to soil.[123,163,216,217]

A study of partitioning of two PCBs and fluoranthene between sediments and interstitial water demonstrated a marked dependence of K_{oc} on the source of organic carbon and a two to 17-fold deviation of measured K_{oc} values from those predicted by $\log K_{oc}-\log K_{ow}$ empirical relationships (Sec. 12.1).[218]

The diversity in composition and structure of the organic matter can give a variation in the sorptivity of organic compounds, due to the presence of different fractions such as humic and fulvic acids, lipids, and humins.[188,194,219,220] Garbarini and Lion[194] investigated the sorption behavior of TCE and toluene on two humic acid samples extracted from soils, tannic acid, lignin, corn protein zein, cellulose, and Aldrich humic acid. The K_d values for the two compounds on these sorbents do not converge to a similar K_{oc} value, when normalized by the fraction of OC, indicating that components of OM found in soils may have affinities for nonionic organic compounds which cannot simply be explained by their OC content. The results are consistent with the observation[221] that an organic material's ability to sorb organic pesticides was related to its relative hydrophilic/hydrophobic balance as indicated, in part, by its number of oxygen-containing functional groups. Lignin, as compared to humic and fulvic acids, has a notable lack of carboxylic groups, making it less hydrophilic and possibly accounting for its higher K_ds and K_{oc}s. Thus, a decrease greater than an order of magnitude in sorption can be found using humin, humic acid, or fulvic acid in the order.

However, sorption of naphthalene on EPA-6 sediment modified by sorption of poly (N, N-dimethylaminoethyl methacrylate) (PDAM) showed an unexpected behavior.[132] PDAM has a high carbon-to-oxygen ratio of 4-to-1. Preadsorption of PDAM increased K_d values of naphthalene from 3.35 to 56 mL/g, an increase of about a factor of 17, but K_{oc} values were 940 for the modified sediment and 465 for the unmodified sediment.

Soils exchanged with organic cations of the form $[(CH_3)_3NR]^+$, where R is a C9–C16 hydrocarbon, have significantly higher OM contents and display high sorptive uptake of common groundwater contaminants (benzene, toluene, chlorobenzenes, and alogenated alkanes).[222] The isotherms were linear. The organic phase derived from exchanged hexadecyltrimethylammonium (HDTMA) was at least ten times more effective than natural OM for removing these compounds from water. This simple soil modification might be used to improve the retardation capabilities of low OM soils and aquifer materials, and to enhance the containment capabilities of clay landfill liners and bentonite slurry walls.[223]

Other studies regarding the sorption of tetrachloromethane (TeCM) on clay modified by replacing inorganic ions by different quaternary ammonium compounds have been reported.[92,93,224] Decyltrimethyldiammonium (DTMDA) cations, in particular, have both ends attached to the silica surface of the clay mineral.[92] TeCM sorption to DTMDA–clay is characterized by nonlinear isotherms, competitive sorption, strong solute uptake, and relatively high, exothermic heat of sorption. An adsorption-dominated process instead of a partition-dominated process is suggested.

HDTMA is adsorbed on different clay minerals up to the CE.[225] X-ray diffraction analysis of the HDTMA clays revealed basal spacings higher for vermiculite and decreasing in the order for high-charge, intermediate-charge, and low-charge smectites. In general, both the greater HDTMA content and the larger basal spacings of high-charge HDTMA clays increased the partition of benzene, alkylbenzenes, naphthalene, and biphenyl. Alkylbenzenes showed greater sorption than the other compounds by high-charge HDTMA clays. This was attributed to the capability of the large basal spacings to accommodate larger solute molecules.

Grathwohl[226] studied sorption of trichloromethane (TCM), 1,1,1-trichloroethane (TCA), TCE, and PCE on 39 soil and sediment samples from different geological formations and areas. The results indicate a decrease in sorption with increasing proportions of oxygen-containing functional groups in sorbent OM of the most recent soils. A first approximation to estimate sorption coefficients for various OM compositions is provided by an empirical correlation between the hydrogen/oxygen (H/O) atomic ratio as an index of the oxidation of the OM and the K_{oc} values for TCE

$$\log K_{oc} = 1.52 \log([H]/[O]) + 1.54 \quad r^2 = 0.95.$$

Therefore, many of the experimental and estimated K_{oc} values reported in the literature for nonionic compounds fail to account for variations in the composition of natural OM and are therefore likely to be misleading when used to predict sorption coefficients such as K_d. Moreover, differences between OC content obtained using both high- and low-temperature methods are found with respect to the sorption capacity.[54]

The composition of the OM shows a decrease of the polar groups also by increasing the depth of a soil horizon. Since the concentration of OM in soils is typically decreasing with the depth, a nonlinear correlation between K_d and f_{oc} is expected[227]

$$K_d = K_{oc} f_{oc}^n,$$

where n is less than unity. This behavior has been demonstrated with atrazine sorption on 24 soil profiles, comprising 109 soil horizons. In a logarithmic correlation between K_d and f_{oc} the nonlinearity constant proved statistically significant from unity

$$\log K_d = 1.81 + 0.75 \log f_{oc},$$

which indicates that not only the concentration, but also the composition of the OM play important roles in soil sorption of atrazine. Moreover a multiple linear regression analysis between K_d and the various OM fractions revealed that humic acid explained 71% of the variance compared to 26% for humin plus free organic matter and 3% for manganese oxide.

Sorption of carbazole, dibenzothiophene, and anthracene was investigated on hematite and kaolinite that had been coated with natural humic substances over a mass percent carbon range of 0.01%–0.5%.[228] Humic acids were invariably more strongly adsorbed than fulvic acids on mineral surfaces and increasing quantities of sorbed humic substances greatly enhanced HOC sorption, with anthracene, the most hydrophobic compound, showing the greatest sorption enhancement. The type of humic coating influenced the amount of HOC adsorbed, and the most aromatic substance, peat humic acid, was the strongest sorbent. The mineral surface also influenced the amount of HOC adsorbed on the organic coating, with hematite giving the greater adsorption due to the distribution of surface hydroxyl sites, which represents points of attachment for carboxyl groups on the humic substance.

Sorption of benzene and TeCM from water on three high-organic-content soils (muck, peat, and peat extracted with NaOH) and on cellolose was determined in order to evaluate the effect of sorbent polarity on the solute partition coefficient.[229] The isotherms are highly linear for both solutes on all the OM samples, which is consistent with a partition model. The K_{om} values increase by decreasing the polar-nonpolar group ratio $[(O+N)/C]$ of the sorbent samples from cellulose to extracted peat. The relative increase is similar for both solutes and the limiting sorption capacity (LSC, Q_{om}^0) on a given OM sample is comparable between the solutes. LSC is defined by the following expression

$$Q_{om}^0 = K_{om} S,$$

where S is the water solubility of the solute. This observation suggests that one can estimate the polarity effect of a soil OM on the value of K_{om} for various nonpolar solutes by determining the partition coefficient of single nonpolar solute when compositional analysis of the OM is not available. The observed dependence of K_{om} on sample polarity is used to account for the variation of K_{om} values of individual compounds on different soils that results from change in the polar group content of OM. On the assumpion that the carbon content of OM in "ordinary soils" is 53%–63%, the calculated variation of K_{om} is a factor of ~3.[123,217] This value is in agreement with the limit of variation of most K_{om} data with soils of relatively high OM content. Karickhoff *et al.*[108] reported an average K_{oc} of 83 for benzene with the coarse silt fractions of two sediment samples, which is far greater than the values obtained with muck and peat (7.67 and 12.5, respectively). Following the above discussion, the authors[229] concluded that sediment OM should have extremely low polar group content, with the partition efficiency approaching that of a good organic solvent.

Thus, K_{oc} values depend on the nature of the sorbent, which influences the amount of compound sorbed on it. However, for all nonpolar compounds, which have comparable sorption mechanisms, this influence will be the same. Schrap and Opperhuizen,[209] selecting the sorption coefficients of nine nonpolar organic compounds from the literature, demonstrated that the ratio of the K_d values for two compounds, independent of the sediment, is constant. When this ratio is known, it is possible, by the knowledge of K_d for a reference compound, to obtain K_d for a second compound without knowing the f_{oc} value of the sorbent. This result is valid for chemicals which are not sensitive to the third phase ($K_{ow}<5$) (Sec. 10), which have aqueous solubilities in the μg/dm^3 range and which have relatively high sorption coefficients. Although the simplicity of the procedure and the restricted number of compounds to which it is devoted, this method would require more proofs that the influence of the nature of the sorbent is the same for all nonpolar compounds.

Kile *et al.*[230] determined the partition coefficients (K_{oc}) of TeCM and 1,2 DCBz for a large set of soils, bed sediments, and suspended solids from the United States and the People's Republic of China. The values for both solutes are quite invariant either for the soils or for the bed sediments; the values on bed sediments are about twice those on soils. The similarity of K_{oc} values between normal soils and between normal bed sediments suggests that natural organic matters in soils (or sediments) of different geographic origins exhibit comparable polarities and possibly comparable compositions. The results also suggest that the process that converts eroded soils into bed sediments brings about a change in the organic matter property. The difference between soil and sediment K_{oc} values provides a basis for identifying the source of suspended solids in river waters. The very high K_{oc} values observed for some special soils and sediments are diagnostic of severe anthropogenic contamination.

In conclusion, both clay minerals and soils or sediments can sorb nonpolar compounds. Different types of bonds are involved in sorption of organic chemicals by clay, while, in the case of sorption of these compounds by soils or sediments, hydrophobic interactions are prevailing and K_d values depend linearly on the OC content in sorbent. Thus, sorption may be assimilated to a partitioning of the solute between an organic phase and an aqueous phase. Relationships between sorption coefficients ($\log K_{oc}$) by soils or sediments and partitioning into n-octanol ($\log K_{ow}$) were derived on this basis (Sec. 12.1). Therefore, if the organic phase is the same for a series of sorbents, K_{oc} is expected to be the same; however, often this is not the case, and K_{oc} decreases by increasing the polar character of the organic matter. This is the reason why K_{oc}s for nonpolar compounds on sediments are normally higher than those on soils.

4.2. Polar and Ionizable Compounds

Sorption of polar and ionizable compounds depends at various degrees on moisture content in sorbing system, the presence of exchangeable cations,[221] electrolyte concentration and pH.[231] Water solubility may also affect sorption. Bailey and White[35] published a review on adsorption and desorption of these compounds by soil colloids as a function several factors as colloid type, physicochemical nature of the pesticide, soil moisture content, and others, with implications concerning pesticide bioactivity.

Hance[221] demonstrated a significant competition for sorption sites between diuron and water. The mineral fraction of an oxidized soil adsorbed considerably more diuron from petroleum spirit solution than from aqueous solution. The organic matter from a peat soil, on the other hand, showed greater sorption from aqueous than from petroleum solution. So, presumably, in the first case water competed more efficiently with diuron for mineral fraction than does petroleum spirit, while in the second petroleum competes more efficiently with diuron for organic matter than does water. These results suggest that under field conditions, when excess water is not always present, the soil mineral fraction may play a more important part in adsorption than is indicated by the slurry type sorption experiments.

Sorption of atraton and monuron by soil did not change significantly by reducing water content until the level approached that needed to produce a monolayer on the soil surfaces, when it increased sharply.[232]

The strong competition of water molecules in adsorption of 52 aniline, acetalinide, and carbamate pesticide analogs[233] and of hexazinone[234] on cellulose from aqueous solutions was evidentiated. In the absence of water, hexazinone was adsorbed from hexane solution, thus suggesting that it can be adsorbed to cellulose in the absence of competing water molecules through hydrogen bond formation between the carbonyl groups of hexazinone and the hydroxyl groups of cellulose.

Adsorption of parathion by attapulgite clay was studied in both organic and aqueous media.[235] In hexane solution the presence of hygroscopic moisture resulted in competition between parathion and water so that an increase in the clay's moisture content reduced parathion adsorption.

The same effect was detected for adsorption of parathion[139] and parathion and lindane[198] on soils. In a dry soil–hexane–parathion system the slightly polar parathion molecules efficiently compete with the apolar hexane molecules for adsorption sites.[139] Generally as the soil water content increases, parathion adsorption decreases because of the decreasing contribution of the soil mineral fraction. When soils are fully hydrated, adsorption of the organic solutes by soil minerals becomes relatively insignificant compared to the uptake by partitioning into soil organic matter, presumably because water is preferentially adsorbed by minerals.[198] Lindane shows an uptake on dry soil which is lower than that of parathion and a reduced amount adsorbed at 2.5% water in soil. These differences are consistent with the low polarity of lindane relative to parathion, making lindane a less potent adsorbate, and thus a weak competitor against water, for adsorption on mineral surfaces.

It was suggested[236] that the sorption of parathion on dry soils occurs by cation–dipole interaction, which is much stronger than the hydrogen bonding interaction in wet soils.

Bowman *et al.*[237] studied the adsorptive behavior of malathion on Na-, Ca-, Cu-, Fe-, and Al-montmorillonite by IR spectroscopy and x-ray diffraction. At RH exceeding 40%, malathion penetrated the interlayer region of the clay and was adsorbed as a double layer, giving an expansion of 5.6 –6.5 Å. The mechanism of adsorption was through a H-bonding interaction between the carbonyl O atoms and the hydration shell of the saturating cation. In dehydrated systems, a direct ion–dipole interaction occurred between the carbonyl O atoms and the saturating cations. The magnitude of both interactions increased with cationic valence.

Spencer *et al.*[238,239] found that the vapor density of lindane and dieldrin was high when more than a monomolecular layer of water was present in soil and decreased markedly by decreasing the soil water content.

Diffusion coefficients of disulfoton and dimethoate in a silt loam soil varied little with concentration of both compounds, but increased rapidly for dimethoate with increasing moisture content from 10% to 41%.[240] In contrast, for disulfoton, which is more volatile, less soluble, and more strongly sorbed than dimethoate, diffusion coefficients were smaller but did not change much as the soil became drier.

Dao and Lavy[241] reported that a decrease in water:soil ratio and in soil moisture content led to an increased adsorption of atrazine. At water to soil ratio equal to 0.4:1, adsorption of atrazine increased by increasing the $CaCl_2$ concentration.

The pH values of the clay systems did not appear to affect adsorption of slightly polar linuron and malathion.[242]

Hance[212] studied the effect of pH and exchangeable cation on the adsorption of two substituted urea and five triazines by a montmorillonite. The adsorption of the ureas was virtually independent of pH and exchangeable cation, whereas the adsorption of the triazines was influenced by both factors. It was postulated that the less polar ureas are adsorbed by physical forces and possibly the formation of coordination complexes with exchangeable cations, while the basic triazines are adsorbed by a combination of these two mechanisms plus protonation and consequent ion exchange reactions, the relative importance of each process being determined by pH, exchangeable cation and the characteristics of the sorbate molecule. Infrared studies[243] suggested that adsorption of diuron among other phenyl ureas on montmorillonite may be attributed to an interaction of the carbonyl of the herbicide with exchangeable cations on external surfaces and with edge aluminum groups.

In general, the adsorption of substituted ureas on clays increased with the polarizing power of the exchangeable cation, indicating that electrostructured water molecules play an important role in the adsorption process.[244] The effect of salt concentration was almost negligible up to 1.0 N; above that range the adsorption increased and became very dependent on the ionic strength. The salting-out effect was due to a decrease in solubility of the nonelectrolyte in water upon the addition of a salt.[244,245]

The K–clay systems showed a greater adsorption capacity for linuron and malathion than Ca-, Mg-, and H/Al–clay systems, due to the greater dispersing effect of K ion.[242] The reduced adsorption of the pesticides by Mg and Ca homoionic clays, particularly with linuron, was ascribed to the formation of polyplatelets.

Bowman and Sans[246] investigated the influence of the saturating cation on the adsorption of organo-phosphoric pesticides, parathion, methyl parathion, fenitrothion, aminoparathion, and paraoxon by montmorillonite suspensions. In all cases the saturating cation distinctly influenced the Freundlich-type adsorption, with adsorption decreasing in the following sequence: Fe_{-}^{3+}, Ca_{-}^{2+}, Na_{-}^{+} montmorillonite. Adsorption of these compounds at low concentrations varied inversely with their water solubilities in Na^{+}- and Ca^{2+}–montmorillonite suspensions. Only paraoxon adsorption was slightly greater than the compound with the next lower solubility, aminoparathion. Aminoparathion was more than 99.9% adsorbed from solution by Fe^{3+}–montmorillonite, suggesting the possibility of protonation of the $-NH_2$ group by the acidic clay surfaces.

The effect of pH on the adsorption of basic s-triazines by montmorillonite clay was very similar for all compounds.[247] The amount of each compound adsorbed increased as the pH of the solution was lowered, until an adsorption maximum was reached. Lowering the pH still further resulted in releasing a portion of each of the compounds into solution. The maximum adsorption of each compound by the montmorillonite clay occurs in the vicinity of the pK_a value.[248,249] At pH values higher than pK_a the compound is present primarily in the molecular form and is adsorbed by H bonding or through polar adsorption forces. A decrease of pH results in increasing the protonation; the adsorption of the resulting monovalent cation occurs by displacing a Na^{+} ion from the clay surface. At pH values lower than the pK_a the increased concentration of H^{+} ions may compete with the cation for sites on the clay. The presence of other ions like Na^{+} or Ba^{++} has the effect of decreasing the amount of protonated compound adsorbed because of some competition effect at the sorption sites (e.g., carboxyl groups) of the organic colloids.

Several mechanisms can be postulated for adsorption of organic compounds (basic or acidic) by clay alumino-silicates:[250] physical adsorption, hydrogen bonding, coordination complexes, association or bridging complexes and chemical adsorption. Some of them may occur simultaneously, depending on the nature of the functional groups of the molecules, the type of clay mineral, and the acidity of the system. The authors studied the adsorption of members of herbicide families as s-triazines, substituted ureas, phenylcarbamates, aniline, anilides, phenylalkanoic acids, benzoic acids, and picolinic acids on 1–0.2 μm montmorillonite clay adjusted to two pH values: 3.35 and 6.80. Regardless of chemical character, adsorption occurred to the greatest extent on the highly acid H–montmorillonite compared to the near neutral Na–montmorillonite. The magnitude of adsorption of organic compounds with widely different chemical character is governed by the degree of water solubility, the dissociation constant of the adsorbate, and the pH of the clay system. A basic compound can be considered 100% associated or completely dissociated when the pH is approximately 2 units below or above the pK_a, respectively. For atrazine, pK_a is 1.68. If the pH of the clay surface is equal to the pH of the suspension (3.35), then it would be expected that $<10\%$ of the compound would be adsorbed. However, experimentally it was found that the material was completely adsorbed. This would indicate that the surface acidity would be approximately 3 units lower than the suspension pH. If the surface pH is greater than the pK_a by a magnitude of 1.5–2 pH units, then adsorption will be principally due to van der Waals' forces. For acidic compounds, on the contrary, adsorption is principally dependent upon the pH of the bulk solution; positive adsorption will commence when the pH of the bulk solution is approximately 1–1.5 pH units above the pK_a. Adsorption increases by decreasing the pH. It seems that the primary mechanism of acid adsorption is due to proton association and adsorption occurring by van der Waals' type adsorption, that is, the compound is adsorbed in the molecular form. Hydrogen bonding between the carbonyl group of the acidic compound and the surface also may occur.

Thermodynamic parameters for adsorption of cyanazine by peat and montmorillonite saturated with several cations ($H^+, K^+, Mg^{2+}, Ca^{2+}, Co^{2+}, Cu^{2+}$) seem to indicate that adsorption occurs with a mechanism involving hydrogen bonds.[140] However, for peat in the acidic (pH 6) and Cu^{2+} samples, a protonation process and adsorption of the protonated species is also likely. For montmorillonite–cation systems the thermodynamic parameters seem to point to the following mechanisms: for montmorillonite–Cu^{2+} samples a direct coordination cyanazine–Cu^{2+}; for montmorillonite–Co^{2+} samples physical bonding; for montmorillonite–H^+ samples physical adsorption plus ionic adsorption.

The chemical characteristics of the sorbate strongly affects the sorption behavior. Harris and Warren[251] studied the adsorption of herbicides, diquat, 4,6-dinitro-o-sec-butylphenol (DNBP), atrazine, isopropyl N-(3-chlorophenyl)carbamate (CIPC), and monuron, from aqueous solution by muck (organic soil), bentonite, an anion exchanger, and a cation exchanger. Lowering of the pH resulted in increased adsorption by bentonite of all of the herbicides, except the organic cation, diquat, which was completely adsorbed at both a high and a low pH. The influence of pH was greatest for DNBP and atrazine. The DNBP was adsorbed by an anion exchanger, but not by a cation exchanger, while CIPC, monuron, and atrazine were adsorbed by both. Diquat was completely adsorbed by the cation exchanger and only slightly by an anion exchanger. All were adsorbed by muck but to varying extents. Diquat and paraquat, both organic cations, were adsorbed by montmorillonite and kaolinite at pH 6 up to to the cation-exchange capacity.[249]

Dioctahedral montmorillonite exhibited a high affinity for paraquat, since when less than 50 me/100 g were adsorbed, no paraquat was detected in the solution, irrespective of the saturating cation.[252] Interlamellar adsorption of paraquat was detected. Weber and Weed[253] investigated the adsorption of diquat, paraquat, and prometone by montmorillonite and kaolinite clays and their desorption using several extracting solutions. The two compounds were adsorbed by the clay minerals to approximately the cation exchange capacity of the clays. Approximately 80% of each of herbicides was replaced from kaolinite clay with Ba^{2+} ions, while a total of 5% of each of the compounds was removed from montmorillonite using 1 M $BaCl_2$ solution. Paraquat was preferentially adsorbed over diquat by both clays in competitive ion studies. Prometone adsorbed on clays was more readily desorbed with de-ionized water than with $BaCl_2$.

Hayes *et al.*[254] reviewed the interaction between clay minerals and bipyridylium herbicides.

Sorption of low polarity pesticides, like monuron and diuron, by soils depends only little by soil pH and the presence of soluble anions and cations.[255] OM (or OC) content in soils was found to be of primary importance. High correlations between sorption on soils and sediments and OM content were observed for diuron,[245,256,257] fluometuron,[258] alkyl-, chloro-, and chlorophenoxy-urea,[259] phenyl-urea herbicides,[260] fensulfothion and its sulfide and sulfone derivatives,[261] disulfoton,[262] and organochloride pesticides.[263] Sorption of linuron and malathion by humic acid was higher than that in clay systems.[242] Sorption of a series of insecticides, representative of the organochlorine, organophosphorus, and carbamate groups, was studied using three soils and a stream sediment and was found inversely correlated with solubility in water[264] and significantly correlated with the OC content in soils and sediment. Similar results were found with carbofuran[265,266] and dieldrin.[265] Positive correlation was also found between K_d and CE, because OM is known to contribute from 25% to 90% of the total exchange capacity of many soils.[265]

Organophosphorous and carbamate insecticides were adsorbed to greater extents as the OM content of the soil increased.[122] Destruction of OM by oxidation with H_2O_2 markedly reduced adsorption. Similar results were already found with parathion adsorption by soils.[129,267,268] It was suggested that, in OM rich soils ($>2\%$), the contribution of other factors affecting parathion sorption may be masked, because the inorganic adsorption surface is covered up by OM.[129] When the OM was destroyed by oxidation, the sorption decreased considerably. However, with two soils sorption remained very high, in spite of the considerable decrease of the OM to less than 0.1%. It was hypothesized that the inorganic soil constituents are very important in parathion sorption in soils with very low OM. Biggar *et al.*[269] observed that parathion has highly polar $P^{\delta+}-O^{\delta-}$ and P=S bonds, as well as a conjugated ring and a polar $-NO_2$ group and is strongly adsorbed on the clay surface as well as on the OM.

Soil OM content was the most important factor influencing the sorption of phenylurea herbicides by soils.[72] Hance[259] studied the adsorption of urea and a number of its derivatives by different soils. Increasing chain length in the alkyl substituents and choro- and chlorophenoxy substitution in the aryl substituent increased adsorption. There was no relationship between sorption and water solubility; OM content was the only soil property that could be related to sorptive capacity. Then, model adsorbents were prepared by treating cellulose phosphate powder with a series of alkyltrimethylammonium compounds in which the size of the alkyl group was varied from C8 to C18. The adsorption of linuron, atrazine and EPTC by these materials increased logarithmically with increasing chain length and was large compared with the adsorption of these herbicides by a humic acid and by peat organic matter. Since soil organic matter is thought to contain alkyl groups, it was concluded that the possible influence of such groups should be considered in discussing the mechanisms involved in the adsorption of organic molecules by soil.[270]

Sorption of diuron was studied with a series of several arid-zone soil samples having different composition, pH values ranging from 6.5 to 9.3, and low OM percentage ranging from 0.1 to 1.7.[271] Statistical analysis rendered r^2 values for diuron adsorbed in relation to CE, SA, and OC equal to 0.785, 0.754, and 0.476, respectively. It was concluded that CE or SA can account for the variability of diuron adsorption in these soils. Several mechanisms were postulated for the sorption of diuron by soils.[243,250,272] Mainly these include physical adsorption by van der Waals forces and H bonding that could occur via both the carbonyl oxygen and the amino hydrogen. Electrophoretic studies[272] showed that substituted urea molecules become positively charged upon dissociation in water. Thus, sorption on soils could be explained as an ion-exchange process. Sorption of monuron is highly correlated with soil OM content, while the correlation with pH, percent silt, and percent clay is not significant.[273] However, Savage[274] did not detect any significant linear correlation between the Freundlich constant values of chlorbromuron and soil texture, OM content, pH, or water-holding capacity.

OM arising from cane leaf burning in topsoil have been found factors of considerable importance in sorption of PCP, linuron, diuron, simazine, monuron, and atrazine, in the order, on sugar cane soils.[275]

No correlations were found between K_d values measured for napropamide on 36 samples of a soil and soil OC fraction measurements.[276] The distribution of K_{oc} values was more variable than the original K_ds. However, Gerstl and Yaron[277] found that adsorption of napropamide and bromacil was only slightly correlated with the soil clay content but was highly correlated with soil OM content. The mobility of napropamide in soil columns was reduced with an increase in clay and OM content.[278]

Kozak *et al.*[279] studied the adsorption of prometryn and metolachlor by different fractions of soil OM, including humic substances (humic and fulvic acids), humin, and nonoxidable soil organic matter. At pH 6 most of the prometryn in solution is in the molecular form, while metolachlor, which is a nonionic compound, is totally in this form. Humic substances showed high affinity for both herbicides. Humin fractions adsorbed significant amounts of prometryn, but not metolachlor. These differences were interpreted on the basis of different sorption mechanisms due to the different structure of the two molecules.

Alachlor and metolachlor adsorption on soils was found positively correlated with soil OM content, clay content, and SA(EGME) and inversely correlated with herbicidal activity.[280] Other authors[281] found that OM content was the predominant adsorbent for metolachlor in soils. Application of carbon-rich wastes to sandy soil increases sorption of alachlor and may be useful for reducing pesticide leaching to groundwater.[282]

In a recent review paper, Senesi[283] discussed the nature of the binding forces involved and the types of mechanisms operating, often simultaneously, in the adsorption processes of several pesticides onto soil humic substances, humic acids, and fulvic acids. These include ionic, hydrogen and covalent bonding, charge transfer or electron donor–acceptor mechanisms, van der Waals forces, ligand exchange, and hydrophobic bonding or partitioning. Experimental evidence obtained and interpretation provided for the various adsorption processes proposed were presented and commented. Senesi *et al.*[160] showed that multifunctional hydrogen bonds and charge-transfer bonds were preferentially involved in the adsorption of alachlor at low concentrations, especially onto well humified, highly aromatic soil humic acids rich in O-containing groups. Hydrophobic bonding appeared to predominate at higher alachlor concentration, especially onto low-humified, highly aliphatic sludge humic acids. Senesi and Testini[141] studied the adsorption of two s-triazines and two substituted urea herbicides by three different humic acids (HA) using elementary analysis and infrared spectroscopy. Adsorption involved ionic bonds for s-triazines and hydrogen-bonding, van der Waals forces, and possibly charge transfer in both s-triazines- and substituted urea-HA complexes.

Weber *et al.*[284] studied the adsorption of seven s-triazines by organic soil colloids at pH levels from 1.0 to 5.2. Maximum adsorption occurred at pH levels in the vicinity of the pK_a values of the respective compounds. It was concluded that the adsorption of s-triazines was due to complexing of the triazine molecules with functional groups on the organic colloids and/or adsorption of s-triazine cations by ion exchange forces. These mechanisms, based on protonation of such weakly basic compounds, may be less important with metribuzin, which is a weaker base than the s-triazine herbicides.[285] The K_d value for atrazine on soil at pH 3.9 was more than twice that at pH 8.[286] It was observed that for atrazine it is unlikely that ionic forces are appreciable until the pH nears the pK_a value (1.68 at 22 °C). Therefore, this increased sorption can be attributed to van der Waals forces and adsorption via SiOH groups. Adsorption of four herbicides having basic properties (buthidazole, $pK_a=0.6$; VEL 3510; $pK_a=0.9$; tebuthiuron, $pK_a=1.2$; fluridone, $pK_a=1.7$) by H-organic matter, Ca-organic matter, Ca-montmorillonite, and Cape Fear sandy loam soil, increased with decreasing pH, suggesting that the adsorption mechanism was molecular under neutral pH conditions and ionic under acidic conditions.[287]

Sorption of metribuzin, an asymmetrical triazine herbicide, was measured in surface and subsurface soils.[288] The results showed that clay was the single best predictor. The combination of two variables most related to sorption was clay and pH ($r^2=0.860$), while organic matter was not one of the primary variables related to sorption. Savage[117] found that metribuzin sorption and mobility were significantly associated with clay content, OM, and water content. This compound has a $pK_a=0.99$.[289] As atrazine, the adsorption of metribuzin increased gradually and its mobility decreased as the soil pH decreased toward the pK_a value. However, metribuzin had greater mobility than atrazine because of differences in water solubility and basicity. Degradation of metribuzin by soil microrganisms decreased as the soil pH decreased. This compound is more phytotoxic in high pH soils than at lower pH levels.[290] Soil OM, clay content and SA (EGME) were correlated with metribuzin adsorption in soils and activity.[291]

The K_d values of atrazine were strongly and significantly correlated to the OC content of sandy soils ($r^2=0.84$).[292] Also, clay contents in the lower subsoil horizons were significantly correlated to the K_d ($r^2=0.51$). The K_{oc} values varied considerably among soils and within soils with depth, and this was attributed to differences in the ability of OM to adsorb atrazine and in contributions from clay minerals in the lower subsoil horizons.

Binding of atrazine with fulvic acid (FA)[293] and HA[294] extracted from Laurentian soil, and with the whole soil[94] did not follow the phase distribution model (partition) often discussed for hydrophobic organic compounds. Binding isotherms were clearly of the Langmuir type with a definite stoichiometric complexing capacity limit, which was found at low solution atrazine concentration. The concentration at which bound atrazine reached a saturation limit became smaller as pH increased. The difference in behavior between the atrazine–soil and the atrazine–FA and atrazine–HA has been interpreted as due to the simultaneous adsorption on organic fractions and on clay mineral fraction of the soil, with the clay term being less pH dependent.

The complexing of atrazine by fulvic acid was studied at 25 °C and over the pH range of 1.3–6.0 with and without addition of 0.1 M KCl or Cu(II).[295] The results indicated that atrazine is hydrogen bonded in a labile equilibrium to an identifiable set of protonated carboxyl groups, which act as Brönsted acid catalyst for hydrolysis.

In general, the order of increasing sorption by 25 soils for five triazines was propazine, atrazine, simazine, prometone, and prometryne.[145] Correlation coefficients between the properties of the soils and K_d values of these triazines have shown that sorption was most closely related to OM content, clay content, CE and exchangeable magnesium and hydrogen. However, the sorption of prometone and prometryne was less closely associated with percent OM than the chlorotriazines. There was a tendency for pH to be negatively correlated with K_d values. For atrazine, sorption studies[296] indicate that, besides OM, the noncrystalline to poorly crystalline Al and Fe components and other inorganic constituents present in a series of particle size fractions of the soils, especially <20 μm fractions, provide adsorption sites.

It has been demonstrated that the sorption ability for atrazine and trifluralin was decreased considerably when the soil with high OM content was treated with sodium hypochlorite.[297] However, the K_{oc} values for atrazine sorption by oxidized soil were three times greater than those for untreated soil, indicating that the soil mineral components might have affected sorption of this herbicide.[298]

Sorption isotherms of dipropetryn and prometryn were determined using six adsorbent materials possessing a wide range in CE, percent OM, clay levels, and pH values between 7.3 and 5.3.[299] They showed increasing sorption with increasing clay content, CE, and OM levels, and decreasing pH values. Prometryne sorption was increased and mobility was decreased by increasing the $CaCl_2$ concentration from 0.01 to 0.5 N, the pH value remaining constant.[300] This effect of increasing sorption by increasing salt concentration appeared to be due to an increase of the activity coefficient of the herbicide in solution without significantly affecting that near the clay surface. On the contrary, fluometuron sorption decreases by increasing salt concentration. If ion exchange is assumed to be the primary mechanism of fluometuron sorption in an acid environment (pH 5.9–6.4), the reduction in sorption with an increase in salt concentration could result from an increase in the ratio of Ca^{++} to fluometuron ions present in the double layer.

Hexazinone is the most water-soluble triazine herbicide and acts like a very weak base ($pK_a \sim 1$) by accepting a proton at low pH.[234] Sorption of hexazinone correlates to soil OC.[234,301]

Sorption of benzidine, which also may form cations by protonation of the amino groups, by "whole" soils and sediments was controlled primarily by the concentration of the ionized species and was highly correlated with pH, since pH controls the ratio of neutral to ionized benzidine in the aqueous phase.[302] When the isotherms were corrected for sorption of the neutral species, sorption of the ionized benzidine was highly correlated with surface area and negatively correlated with OC content. The OM appeared to coat and hence mask ionized benzidine sorption sites. On the contrary, the sorption of three nitrogen–heterocyclic compounds (acridine, biquinoline, and dibenzocarbazole) on 14 soils and sediments was significantly correlated only with the percentage of OC in the soils or sediments.[303]

Sorption of prometryn, sencor, fluometuron and 2,4-D on 48 soils[304] was found highly correlated with OM content. Also CE was significantly correlated with sorption of the first three compounds. Correlation between clay content and sorption was statistically significant only for fluometuron and sencor. The effect of pH on the sorption of ametryne by soil was significantly greater than that of diuron.[256] K_d values for ametryne decrease from about 28 to about 3 when pH increases from 4 to 8. In the same range of pH, K_d values for diuron range between about 8 and 13. Both compounds were positively correlated with soil OM content. For ametryne, a multiple regression analysis including OM, silt content, and pH of the soil gave a good explanation for adsorption. For diuron, a correlation was found between adsorption and OM content, and CE.

Organic cations show a different behavior. Diquat and paraquat sorption–desorption behavior was studied by Tucker *et al.*[305] Each compound was adsorbed on loam, muck, sand, and silt loam soils, which were then washed with water and ammonium chloride solution in sequence. The soil was then treated with 18 N sulfuric acid by refluxing for 5 h. The analysis of these solutions allowed to establish the amount of "unbound," "loosely bound," and "tightly bound" compound, respectively. At high levels of compound in soils, some of the paraquat or diquat is unbound and can be leached with water. The ratio of loosely to tightly bound compound adsorption capacities varies greatly among soil types, being approximately 4, 27, and 107 for loam, sand, and muck, respectively. While the loosely bound fraction was the result of an ion exchange process, the tightly bound compound became trapped in the lattice structure of the soil particles. In particular, for muck soil, the high total cation exchange capacity parallels its high loosely bound compound capacity.

Paraquat sorption on a series of sorbents[306] decreases in the following order: Fuller's earth (Ca–montmorillonite) >humic acids>peat soils>lignin>sandy loam soil >cellulose. Fuller's earth adsorbed paraquat almost up to the CE. Adsorption on peat is low in the presence of high level of calcium. The results indicated that paraquat sorbed on weak sorption sites of organic matter can be inactivated, after incorporation into the soil, by transfer to the strong adsorption sites of clays. The adsorption of paraquat by a range of soils follows the Langmuir isotherm. Up to a limiting value, defined as the strong adsorption capacity (SAC), the solution concentration of paraquat is reduced below the level of chemical detection by suspended soil: this strongly adsorbed paraquat is preferentially held against 0.1–0.2 N solutions of ammonium ion. Removal of soil OM by treatment with hydrogen peroxide usually does not greatly change the SAC. Thus, strong adsorption of paraquat is primarily a property of clay minerals, and the presence of expanding lattice minerals is of particular importance. Taken with the difficulty of displacement, this indicates that the adsorption of paraquat is strongly influenced by factors other than simple electrostatic interaction. Another study[45] indicated that paraquat adsorption by the soil organic fraction is faster than that by the clay. Possibly surface adsorption is instantaneous while penetration into the crystal lattice of the clay is relatively slow. Ultimately of course, as demonstrated in the dialysis experiments, all the paraquat ends up in the clay lattice. Paraquat adsorbed into the interstices of the clay particle is completely unavailable to microbial attack[45] and almost de-activated herbicidally,[306] while the paraquat reversibly adsorbed on the surface of the organic colloid particles during the early transfer stages can be degraded.

Best *et al.*[307] demonstrated competitive adsorption of paraquat, diquat, and Ca on various adsorbents. A Histosol and its humic and humin fractions showed preference in order: paraquat⩾diquat>Ca when adsorption occurred on strong acid sites and Ca>paraquat⩾diquat when adsorption occurred with weaker acid groups.

Sorption of diquat and paraquat on soils conformed quite well with the linear form of the Langmuir isotherm.[308] Sorption maxima obtained for eight soils ranged from 17 to 47 me/100 g. The cation exchange capacity of a soil was found to be the determining factor of adsorption for the two compounds. Paraquat sorbs on sediments by ion exchange following Langmuir isotherms, and sorption coefficients show a definite correlation with the cation exchange capacity of individual size fractions.[89,309] However, exchange sites in different fractions differed in their effectiveness in sorbing paraquat, with the fine silt and clay exchange sites being more effective than those of the larger separates. The adsorption mechanisms of paraquat by soil organic colloids largely depend on the Donnan properties of the adsorbent. The primary adsorption mechanism appears to involve ion-exchange processes where the adsorbents have well-defined cation-exchange capacities.[309] However, secondary specific interactions are possible when Donnan potentials in adsorbents are low (e.g., hydrogen bonding, van der Waals forces, charge tranfer processes, etc.). Such interactions determine the high affinity of paraquat for humic substances.

Khan[310] studied the binding or complexing of diquat and paraquat by humic acid and fulvic acid. Paraquat was complexed by humic compounds in greater amounts than was diquat, but the amounts of the two herbicides complexed by humic acid were higher than those complexed by fulvic acid. Evidence is presented for the formation of charge-transfer complexes between the two herbicides and humic compounds. Binding of diquat and paraquat to humic acid was mainly electrostatic in nature.[142] Two binding sites are involved. Variation in pH suggested that hydrogen ions competed strongly with the herbicides for the binding sites. The acidic functional groups on humic acid (carboxylic and phenolic) are characterized by an average pK_a value of 5.0; therefore at pH values lower than 5.0 an extensive protonation is expected. This is reflected in the large reduction in binding of both paraquat and diquat at low pHs.

Sorption of an organic cation, dodecylpyridinium, on clay, aquifer materials, and soil strongly depends upon the nature and concentration of the inorganic cations in solution, but virtually independent of solution pH.[311] Two types of sorption reactions were found to be significant: exchange of pyridinium with an alkaly–metal cation, and sorption of pyridinium with chloride counterion. The sorption behavior of acidic compounds, when undissociated, resembles that of hydrophobic compounds; on the other hand, much lower sorption coefficients are expected for dissociated compounds due to their high water solubility and possibly the repulsion by the surface negative charge of the OM.[195]

The importance of OC content on sorption of α-naphthol ($pK_a=9.34$) by soils and sediments was evidentiated by Hassett *et al.*[97] However, when the ratio %OC/% clay is below 0.1, clay surfaces are more accessible, and sorption of this compound is apparently controlled by the clay fraction and the K_{oc} values do not converge. Also bromacil behaves like a weak acid ($pK_a=9.3$). At pH values lower than 9.3 the major fraction of bromacil is present as neutral molecules. Therefore, at these pH values it is adsorbed in this form and correlates with OC content.[312] However, as the pH approaches 9.3, the portion of bromacil present as anionic form increases, and thus adsorption is retarded.

Picloram is an herbicide of acidic character ($pK_a=3.4$). Its sorption by soils and hydrated metal oxides increases by decreasing the pH.[313,314] OM is responsible for sorption by soils, but, when OM content is lower than 0.3%, metal oxides are the main sorbing agents.[314] Biggar *et al.*[269] estimated the relative quantities of picloram adsorbed by the clay (0.14%), OM (93.79%) and free iron oxide (6.07%) fractions of the Palouse soil (3% OM, pH 5.9). The low total adsorption in general and, on clay in particular, may be attributed to the fact that most of picloram is in its anionic form and, therefore, interactions with the negatively charged clay surface is highly unfavorable. Sorption on iron oxide can be explained considering that anionic picloram is capable of chelating with metal ions with its pyridinium nitrogen and the carboxyl group forming a five-membered ring. Other authors[313] reported that K_f values for picloram in soils were correlated with extractable Al and clay content. Picloram molecule may undergo protonation of the carbonyl group or annular nitrogen from water associated with adsorbed Al^{3+}.

The effect of pH on sorption of picloram by soils has been studied by other authors,[315–317] who demonstrated that this compound is sorbed on soil OM especially in the molecular form, while in the ionized form is not readily sorbed. The addition of salt to the aqueous solution produces an increase of adsorption.[316] Also the pH-dependent adsorption of picloram by humic acids and humin is largely due to the uncharged molecules.[318] However it has been demonstrated[315] that on a sandy loam soil with pH 7.2 and on a silty loam soil with pH 5.9 the percentage of sorption was 1.9%–3.6%, and 26%–33%, respectively, where the range was depending on the concentration of the solution. These results for so high pH values indicate a significant adsorption of picloram in the anionic form.

Picloram sorption was determined on an Aiken silt loam, on three cation exchange resins and on a single anion exchange resin.[319] The study was extended to the same soil saturated with some cations ($Fe^{3+}, Al^{3+}, Cu^{2+}, Zn^{2+}, Ca^{2+}$), which showed increased picloram adsorption compared to the native soil. This result was explained on the basis of decreases in the equilibrium solution pH, except for Fe, Zn, and especially the Cu treatment, which could not be explained readily by pH changes. The possibility of complexing of the polyvalent cation with soil organic colloids and picloram was suggested.

Sorption of picloram was observed at pH values between 6.0 and 7.8, while dicamba was not adsorbed.[320,321] Dicamba is a benzoic acid herbicide with $pK_a=1.9$. Low sorption of dicamba was detected on a soil at pH 6.1, but no sorption on other soils at higher pH values.[322] However, dicamba may be adsorbed strongly by soils dominated by variable charge (''pH dependent'') clays which can have large anion exchange capacities due to a net positive charge.[323] Alkylammonium–clay complexes are effective sorbents for dicamba.[324] Solution pH significantly affected the sorption of dicamba by organo-clays, with the isotherm inflection point near the pK_a value. Nearly twice as much dicamba could be sorbed in the molecular form as compared to its anionic, deprotonated form. Sorption and desorption of basic, acidic, and nonionic pesticides were studied with OM prepared from a peaty muck soil and with Ca–montmorillonite.[121] Asulam ($pK_a=4.82$), like dicamba, is an organic acid; dicamba was not adsorbed by OM, whereas asulam was adsorbed slightly. Although the pH of the water suspension was 5.5, the pH at the colloid surface was probably much lower due to hydrogen saturation. At the lower pH, a majority of asulam molecules in solution would be in their molecular form, while a majority of dicamba molecules would be in anionic form. Since OM has a net negative charge, dicamba anions would be repelled by the OM and asulam molecules would be adsorbed by weak physical forces or through hydrogen bonding. Dicamba was adsorbed by Ca–montmorillonite, while asulam was not. Both herbicides are 100% ionized at the pH of the clay suspension. One possible explanation of this difference is that the negatively charged dicamba ion complexes with the Ca ion on the clay surface, while asulam ion cannot form complexes due to some type of steric interference.

Bentazon is a herbicide of acidic character due to the possible ionization of the N–H group ($pK_a=3.2$).[325] The herbicide was not adsorbed by any of twelve selected soils or by cation exchange resin, but was almost completely adsorbed by charcoal and by an anion exchanger. Bentazon is very mobile in soils due to its high water solubility and strong anionic characteristics which result in a lack of attraction to the predominately negatively charged soil colloids. Tillage practices affect sorption of bentazon and its degradation.[46] Under no-tillage, accumulation of plant residue leads to increased soil organic matter near the soil surface, which tends to enhance sorption of nonpolar or moderately polar organics and affects degradation processes.

Chlorsulfuron is a sulfonylurea herbicide of acidic character ($pK_a=3.58$)[326] owing to the acidic sulfonamide group. Its adsorption is positively correlated with soil organic matter and negatively correlated with pH, while no or negligible adsorption occurs to clay silicates.[326–328] Also, chlorsulfuron phytotoxicity increased with increasing soil pH and reached a maximum at pH 6.9.[329] Chlorimuron, belonging to the same class, has a $pK_a=4.2$ and behaves in the same way.[330,331] Its adsorption was higher in no-tilled soils, due to enhanced plant residue accumulation, than in tilled soils. Its adsorption in soil decreased with increased soil pH.

2,4-D is a weak acid with a pK_a of 2.73[332] or 2.99.[181] In the soil slurries the pH of the solutions is normally near neutral or slightly alkaline, so that very little of the 2,4-D is in the molecular form. Thus, a reduced sorption is expected, considering that the buffering capacity of the soils should be sufficient to prevent a measurable shift in the pH value as a result of the addition of the compound in the experiments. However, in some cases it was observed that the pH value at the surface of the soil can be significantly reduced, with a certain amount of compound being adsorbed. Another possible explanation of anomalous partition coefficients may be the biotic decomposition of 2,4-D in the soil.

In general, soil OM ($r=0.83$), exchangeable aluminum ($r=0.82$), and low soil pH ($r=-0.79$) promote 2,4-D adsorption.[333] By considering only the surface horizons, the correlation of adsorption with soil organic matter was 0.77, but improved markedly with soil pH ($r=-0.92$). For subsoil horizons the exchangeable aluminum becomes the most significant soil parameter ($r=0.93$), whereas the correlation with soil OM was 0.83. Sorption data were obtained at an ionic strength $\mu=0.075\,(CaCl_2)$. By increasing μ in solution, adsorption is enhanced: this result is probably due to a corresponding decrease of the pH value of the suspension due to replacing of acidic hydronium and aluminum ions by $CaCl_2$. This mechanism may promote the molecular 2,4-D sorption to the colloid surfaces through hydrogen bonding. The results of a ring test[124] indicated that the influence of pH, which is important for atrazine, dominates the sorption behavior of 2,4-D in soils. Clay content and OM content are only of limited importance.

Montmorillonite (M) and vermiculite (V) were modified by treatment with decyammonium (D) chloride to obtain the respective organo–clay sample.[334] Langmuir and Freundich sorption parameters indicated an increase of sorption capacity for 2,4-D of clays after decyammonium exchange. The sorption at different pHs showed that molecular forms were preferentially adsorbed on D–M, whereas anionic forms were adsorbed on D–V. The D–V sample showed much higher and stronger sorption capacity than D–M, due to the different arrangement of D cations in the interlayer of both minerals, as a consequence of their different layer charge.

Boyd[335] studied sorption of undissociated phenol and its derivatives on a soil sample at pH 5.7 to evaluate the effect of the presence of other functional groups in the phenol molecule. Introduction of $-CH_3$, $-OCH_3$, $-NO_2$, or –Cl groups resulted in increased sorption due to decreased water solubility. Moreover, sorption of substituted phenols, with the exception of o-nitrophenol, was generally greater than predicted for hydrophobic sorption ($\log K_{oc}-\log S$) (Sec. 12.2), probably due to H-bond formation. In particular, for meta- and para-substituted phenols a positive relationship was observed between substituent electron-donating ability and sorption. These phenols apparently formed H bonds with sites on soil surfaces by acting as a proton acceptor. Ortho-substitution of $-CH_3$, $-OCH_3$, and –Cl resulted in less sorption than para-substitution, suggesting steric hindrance by the ortho substituents of H-bond formation.

Sorption and desorption of phenol, 2-chlorophenol (2-MCP), and 2,4-dichlorophenol (2,4-DCP) by a fine and coarse sediment fraction were measured in a continuous flow stirred cell.[100] The pHs of uninteracted sediment suspensions were in the range 6.21–6.35. The extensive sorption, the shape of the isotherms (S-type), and the very high K_{oc} values with respect to those predicted on the basis of the solubility and the octanol/water partition coefficient (Secs. 12.1 and 12.2), indicate a substantial contribution to sorption by more specific sorbate–sorbent interaction than by general hydrophobic forces. The mechanism of sorption is likely, therefore, to involve extensive hydrogen-bond formation between the sorbate phenolic hydroxyl groups and the hydrogen-bonding sites on the sediment organic matter. The sorption of these phenolic compounds was also greater than that found by Boyd[335] with soil samples. This result should be interpreted on the basis of the complex relationship between the behavior of soils and sediments. Sorption of some phenols on soils has been found dependent on the percentage iron oxides and solution pH.[336]

Laboratory experiments have been conducted to study the sorption of nine chlorinated phenols (from di- to penta-) by sediments and aquifer materials in the pH range between 6.5 and 8.5.[337] It was shown that sorption not only of the non-dissociated phenols but also of their conjugate bases (phenolates) can occur. However, the marked increase of the overall distribution coefficients with decreasing pH suggests that, under the conditions used, the contribution of the sorption of the deprotonated species is generally small except for those cases where the difference between pH and pK_a is large. This happens with 2,3,4,6-tetrachlorophenol (2,3,4,6-TeCP) and PCP. Thus, as a first approximation, the experimental data were analyzed by using a simple partitioning model neglecting phenolate sorption as well as a possible dissociation of the phenol in the organic phase. The sorption of these compounds can be examined by the following equations:

$$\text{sorption:}\quad K_d=[AH]_s/[AH]_w,$$

$$\text{dissociation:}\quad K_a=[A^-]_w[H^+]_w/[AH]_w,$$

$$A_t=[A^-]_w+[AH]_w+(M_s/V_w)[AH]_s,$$

$$A_w^*=[A^-]_w+[AH]_w,$$

where the subscripts w and s refer to water and sorbent phases, respectively, A_t is the total initial concentration of the phenol in the aqueous phase (before sorbent is added), A_w^* is the total equilibrium concentration in the aqueous phase (after equilibration with sorbent), V_w is the volume of the aqueous phase, and M_s is the mass of the sorbent phase. Combination of the previous equations yields the relation

$$D = K_d Q, \tag{10}$$

where D is the experimentally determined overall distribution ratio

$$D = [(A_t - A_w^*)/A_w^*](V_w/M_s)$$

and Q is the degree of protonation

$$Q = 1/(1 + K_a/[\mathrm{H}^+]_w). \tag{11}$$

Thus, sorption coefficient K_d for nonionized phenol can be obtained from the linear regression of D vs Q [Eq. (10)]. A good fit was obtained for all compounds except 2,3,4,6-TeCP and PCP, which are almost fully deprotonated in the pH range of the experiments. For these two compounds K_d values of protonated species were derived from the linear relationship between $\log K_d$ of the remaining phenols and the logarithms of their corresponding relative retention in reversed-phase liquid chromatography, using methanol/water, 1/1 v/v at an apparent pH~2. In natural waters of low ionic strength (i.e., $\mu \leq \sim 10^{-3}$ M) and of pH not exceeding the pK_a of the compound by more than one log unit (i.e., pH$-$p$K_a \leq 1$), the contribution of phenolate sorption may be neglected and the overall distribution coefficient may be expressed by Eq. (10). However, the results of the experiments conducted with these systems indicate that, in certain cases, the sorption of the phenolate species must be taken into consideration. This indication derives from the significantly positive intercepts found when the experimental data are analyzed with a linear regression according to Eq. (10). Similarly to the nonionized species, the degree of phenolate sorption is strongly dependent on the OC content of the sorbent. It depends also on the ionic strength in the aqueous phase.

Lagas[111] conducted a series of sorption experiments with five chlorophenols and natural and synthetic soils having different composition and pHs ranging from 3.4 and 7.5. The K_d values were obtained for 3-MCP, 3,4-DCP, 2,4,5-trichlorophenol (TCP), 2,3,4,6-TeCP, and PCP. The K_{oc} values for the undissociated species were obtained with the relation

$$K_{oc} = K_d / f_{oc} f_{nd},$$

where f_{nd} is the fraction of undissociated species calculated as in Eq. (11). The calculation has been conducted only when pH(soil)<pK_a+1. The $\log K_{oc}$ values for the five compounds were then correlated with $\log K_{ow}$. The standard error of fit was $s = 0.19$. The K_d values corresponding to TeCP and PCP on loamy soils (pH>pK_a+1) allowed to calculate K_{oc}s for the dissociated species of these two compounds (280 and 500, respectively). These values resulted in about 15–30 times lower than those of the undissociated species, calculated with the correlation $\log K_{oc} - \log K_{ow}$ (8000 and 25 000, respectively). Bellin *et al.*[338] adopted the same procedure to calculate K_{oc} for undissociated species of PCP from the K_f values, using the relation $\log K_{oc}(\text{und.}) = \log(K_{foc}/Q)$.

Lee *et al.*[339] derived an equation which allows us to discriminate sorption of dissociated and undissociated species to obtain the total K_d value.

The fraction of neutral phenol in aqueous solution, Q, can be expressed also in terms of pH ($-\log[\mathrm{H}^+]$) and pK_a ($-\log K_a$)

$$Q = [A\mathrm{H}]/([A\mathrm{H}] + [A^-]) = (1 + 10^{\mathrm{pH} - \mathrm{p}K_a})^{-1}$$

PCP (pK_a~5) is essentially 100% neutral at pH<3 and is completely ionized at pH>7.

For sorption by soils, the distribution of the molecular form of phenol and phenolate between the sorbed and solution phases may be defined as

$$K_d = ([A\mathrm{H}]_s + [A^-]_s)/([A\mathrm{H}]_w + [A^-]_w),$$

where the subscripts s and w refer to sorbed and solution phases, respectively.

The predicted K_d for the neutral (n) and ionized (i) form of a weak organic acid can be expressed as

$$K_{dn} = [A\mathrm{H}]_s/[A\mathrm{H}]_w$$

and

$$K_{di} = [A^-]_s/[A^-]_w,$$

respectively.

Assuming that only the neutral form is sorbed and that the OC content of the sorbent predominantly determines the extent of sorption, then

$$K_{oc,p} = K_{oc,n} Q, \tag{12}$$

where $K_{oc,n} = K_{dn}/f_{oc}$, and the subscript p refers to the predicted value. If there is a transfer of the ionized species to the organic phase, the predicted sorption would be underestimated by Eq. (12).

Assuming that also the ionized forms can be sorbed to a hydrophobic surface (by formation of neutral ion pair or by sorption of the hydrophobic part of the organic anion), then

$$K_{oc,p} = K_{oc,n} Q + K_{oc,i}(1 - Q), \tag{13}$$

where $K_{oc,i} = K_{di}/f_{oc}$. The sorption predicted for a weak organic acid in its ionized form would be less than that for the neutral form because of the difference in their hydrophobicities. Equation (13) may better describe sorption of a weak organic acid than Eq. (12), because sorption of both the neutral and the ionized forms are accounted for, while allowing the magnitude of the individual sorption coefficients $K_{oc,n}$ and $K_{oc,i}$ to be different. If the anionic species does not contribute significantly to the overall sorption process (i.e., if $K_{oc,n} \gg K_{oc,i}$), Eq. (13) reduces to Eq. (12). The authors[339] reported several PCP sorption data, some of which collected from the literature, and plotted $\log K_{oc}$ values as a function of pH. The model given by Eq. (13), where the sorption of the ionized species is also considered, describes better than Eq. (12) the data over the entire pH range. $\log K_{oc}$ shows a constant value of about 4.3 between pH 0 and pH 3.5 (sorption of neutral species), then a gradual decrease until pH 7, and finally a constant value of about 2.6 until pH 14 (sorption of ionized species). In this study an increased sorption of PCP^- with increasing ionic strength for batch experiments conducted in aqueous $CaCl_2$ solutions was observed. The K_d values for PCP by Eustis soil in the pH<3 increased by a factor of 1.3 over the μ range of 0.0015–1.5. A value of 1.5 was predicted by Karickhoff.[52] For the pH>7 region sorption by the same soil was studied from aqueous solutions with $\mu=0.01-1.4$. PCP sorption increased by a factor of ~6 over this μ range. Moreover, the data by the same authors[339] and those by Westall *et al.*[340] on the distribution of PCP in octanol–water systems and by Schellenberg *et al.*[337] on the retention of chlorophenols on a C-18 column, supported the conclusion that for pH>7 the formation of neutral metal–phenolate ion pair must be involved in these processes. The ionic strength of most environmental settings does not exceed 10^{-3} M; thus, ionic strength effects can usually be neglected.

A recent study[106] regarding the effect of dissolved organic matter (DOM) on sorption of PCP by soil confirmed the results obtained in previous investigations. The K_f, K_d, and K_{oc} values were generally lower at pH 6.1 than at pH 5.4. The Q values were 0.183 and 0.043 at pH 5.4 and 6.1, respectively. In the DOM-poor fraction, the K_{oc} for nonionized and that for ionized PCP were found to be 27800 and 305, respectively, at the ionic strength of 0.02. These results agree quite well with the predicted or measured values obtained from solutions of $\mu=0.015$.[339] The contribution of neutral ion pair in the sorption of PCP^- is possible but needs to be evaluated.

The average K_{oc} values for 2,4,6-TCP with two soils at pH 6,7, and 7.7 were 2.200, 620, and 170, respectively.[341] Sorption isotherms followed Freundlich equation with $1/n=0.76$. Sorption of the phenolate anion was considered negligible. The $K_{oc,n}$ value for the undissociated form was calculated as follows:

$$
\begin{aligned}
[AH]_{oc} &= K_{oc,n}[AH]_w^{1/n} \\
&= K_{oc,n}\{([AH]_w+[A^-]_w)Q\}^{1/n} \\
&= K_{oc}([AH]_w+[A^-]_w)^{1/n}.
\end{aligned}
$$

Therefore, $K_{oc,n}$ is given by

$$K_{oc,n}=K_{oc}/Q^{1/n},$$

which is Eq. (10) applied to a nonlinear isotherm. The calculated value of $K_{oc,n}$ was 3590.

Jafvert[342] examined the sorption to sediments and saturated soils of selected organic acid compounds, 4-(2,4-dichlorophenoxy)butiric acid and silvex. By varying intrinsic compound properties (pK_a and hydrophobic character) and sediment properties (ionic strength and composition, organic carbon content and aqueous pH) sorption of both the neutral and anionic forms of these compounds was shown to occur.

Stapleton *et al.*[343] observed that the pH range of surface and groundwater is approximately from 4 to 9. Therefore, ionizable organic compounds with a pK_a in the same range are of special interest because both the protonated and deprotonated species may be found in the aqueous phase. They investigated the sorption of PCP to a surfactant-modified clay (hexadecyltrimethylammonium-montmorillonite) and the solubility of PCP as a function of pH and ionic strength and developed a model that described the sorption across the experimental pH range (4–8.5). The model represented the sorption of the deprotonated species by a Langmuir-type isotherm and the sorption of the protonated species by a linear isotherm. It was suggested a partitioning mechanism between the hydrophobic section of the modified clay and water for the undissociated species, and sorption to the two-dimensional lipophilic surface with a counterion in the double layer for the phenolate species. Between pH 4 and pH 8.5, the sorption decreased by three times and the solubility increased by 3 orders of magnitude as the dominant aqueous species changed from the protonated to the deprotonated form. Sorption of the phenolate species increased with ionic strength when pH was >8.

Seip *et al.*[344] found that at pH 7.4, TCPs, TeCPs, PCP, and tetrachloroguaiacol, which are almost completely dissociated, move fairly easily through the soil.

In conclusion, OM may have a great importance in sorption of polar organic compounds.[39,262,275,345] However, the spread in K_{oc} values is generally greater than that found for hydrophobic compounds. A comparison of the literature K_{oc} values showed a variance of a factor of 40.[163] For the most polar and ionizable compounds, like amines, amides or carboxilic acids on soils, the variation in K_{oc} values was up to 2 orders of magnitude.

Stevenson[48] reported the literature results indicating the major role played by the OM in sorption of herbicides in soils. The conclusion of his analysis was that divalent cations (diquat and paraquat) would be expected to be the most strongly bound due to their large affinities for soil organic colloids, followed by the weakly basic s-triazines capable of being protonated under moderately acidic conditions. For the s-triazines, differences in sorption can be accounted for by variations in pK_a, with the more basic compounds (high pK_a) being the strongest sorbed. Herbicides included in the next order of sorption are those having very low pK_a values but which contain one or more polar groups suitable for H bonding (phenylcarbamates, substituted ureas). Finally anionic pesticides (alkanoic acids) may or may not be sorbed, depending upon the soil reaction.

The K_{oc} values for α-naphthol decreased from ~436 to ~3 $cm^3\ g^{-1}$ with increasing polarity index [(O+N)/C] and decreasing aromaticity of organic sorbents, lignin (organosolv), lignin (alkali), collagen, chitin, cellulose, and collagen–tannic acid mixture).[346] It was concluded that the quality of organic sorbents significantly influences partitioning of hydrophobic organic chemicals in aqueous systems. Atrazine and terbuthylazine have greater K_{oc} values with a loamy clay soil showing the highest degree of humified organic matter (85.9%) compared to a calcareous clay soil (73.1%) and a high clay soil (68.3%).[347]

Nonionic surfactants are often added to post-emergence herbicide sprays. They affect herbicide–plant interactions by increasing the area of contact between herbicide and plant, and by assisting in plant uptake of the herbicide. The effect of three nonionic surfactant on 2,4-D adsorption and degradation in soil was investigated.[348] Adsorption of 2,4-D was significantly decreased by the least water-soluble surfactant and degradation was also significantly delayed. Several cationic surfactants increase the adsorption of diuron onto soil, while the nonionic surfactants did not affect this adsorption.[349] It is suggested that, due to the cationic nature of the surfactant, it is chemically adsorbed by ionic attraction onto soil particles which are negative, thus leaving the alkyl chains to form lipophilic layers on these particles. Diuron, which shows affinity for lipophilic materials, is thus adsorbed into these layers by physical van der Waals forces.

In an attempt to find a way to reduce the soil contamination by pesticides, the effect of the presence of a cationic, anionic or nonionic surfactant on sorption of diazinon, acephate, atrazine, and ethofumesate by a sandy loam soil was investigated.[350] Although the increase in the apparent water solubility, this effect is extremely complex, because it depends on the degree of hydrophobicity of the pesticide and the type of surfactant, as well as on the concentration of surfactant in the system. For instance, picloram adsorption from aqueous solutions and from nonionic and anionic surfactant solutions was greater on soils at pH 5 than at pH 7.[313] The anionic surfactant competed with picloram for adsorption sites on the soils at pH 5. Picloram adsorption from solutions containing 0.1% and 1% cationic surfactant was greater than that from aqueous and anionic and nonionic surfactant solutions.

Several important results regarding sorption of polar and ionizable compounds have been obtained: (i) water competes with chemicals for sorption sites; sorption increases by decreasing water content. Such an effect, already mentioned for nonpolar compounds, will be evidentiated much better in sorption of volatile compounds (Sec. 4.3); (ii) also for polar compounds organic matter is involved in sorption, but K_{oc} values show variations larger than those found for nonpolar compounds; (iii) K_{oc} values for ionizable compounds, basic or acidic, which can exist as dissociated or neutral forms, depend on pH and on pK_a of the compound. A different value of K_{oc} is found for the two forms, due to different sorption mechanisms, with the undissociated form behaving like a nonpolar compound.

4.3. Volatile Compounds

Ehlers *et al.*[352] developed equations to describe the combined vapor and "nonvapor" phase diffusion of lindane in soils. The quantity of diffused lindane appears to increase linearly with increased lindane concentration in air-dried Gila silt-loam soil up to about 20 ppm, when lindane will reach maximal vapor density. Then, vapor diffusion approaches zero and all the diffusion is in the "nonvapor" phase. At a 10% soil water content, 50% of lindane diffuses in the Gila silt loam in the vapor phase, and 50% in the "nonvapor" phase. At near saturation, total diffusion is in the "nonvapor" phase. In a second paper the authors[353] gave further information on how lindane diffusion is influenced by soil water content, bulk density, and temperature. The diffusion coefficient is nearly zero in soil of 1% water content. With an increase to 3% water content, which is equivalent to two layers of water between the montmorillonite clay plates, water is able to displace the lindane from the adsorbing surface so that the diffusion coefficient becomes maximal. A small additional increase in water content reduces the diffusion coefficient to about one-half of the maximal value, which remains constant up to saturation. Decreasing bulk density or increasing temperature raises the diffusion coefficient.

Harvey[351] studied the adsorption of seven dinitroaniline herbicides to a silt loam soil in relation to their respective phytotoxicity. The results indicated that absorption of vapors of these herbicides by plants may be more important than absorption of them from soil solution.

The movement of organic vapors in the gaseous headspace of unsaturated aquifers may be a significant aspect of volatile organic compounds (VOCs) transport. It has been demonstrated that dry soils and clays have sizeable adsorption capacities for VOCs, but the presence of water may strongly reduce these adsorption capacities.[35,354,355] Therefore, the water content in soil plays a very important role in volatilization of organic compounds. The vapor density of dieldrin,[239] lindane[238] and trifluralin[356] decreases by decreasing the water content in soils and it is reduced to minimum values in the presence of dry soils. For example, at 19% soil water content, the trifluralin vapor density, or potential volatility, was 3000–5000 times greater than when the soil was air dry. As the soil water content was reduced, trifluralin vapor density began to decrease. Vapor densities of dieldrin[239] at 100 $\mu g\ g^{-1}$ or lindane[238] at 10 $\mu g\ g^{-1}$ in Gila silt loam did not decrease until the soil water content was reduced below approximately one molecular layer or water equivalent to approximately 2.7% water in Gila silt loam.

Wade[357] studied sorption on soils of ethylene dibromide (ED) in the vapor phase as a function of moisture content, starting from soil samples dried in a current of air at 32 °C. The results were calculated as the number of mg of fumigant sorbed per 100 g of dry soil from a constant concentration in air of 10 mg dm^{-3}. The curves, amount adsorbed-moisture content, were at first linear, and represented a sharp drop in the amount of fumigant sorbed for an initial small increase in moisture content. The rate of fall became less step as the moisture content continued to increase, passed through a minimum, and then became linear again, the amount sorbed rising slightly with increasing moisture content. This last linear part of the curve ranged roughly from 40% to 70% moisture content with the Black Fen soil and could be taken to correspond with the field range of moisture content. The small increase of amount sorbed was attributed to the solution of the fumigant in the increasing amount of soil water. Comparison of ED sorption on three soils, over the field range of moisture content, demonstrated that the factor governing the amount of fumigant sorbed by a soil is its OC content.

The sorption isotherms of ED on dry soils[354] appeared to be of BET type II (BET-BDDT classification).[358] The isotherms for the 5% and 10% relative humidity (RH) were similar but showed progressively lower sorption. Above 20% RH, the isotherms passed over into type III, the knee of the curve having disappeared. The isotherms for 30%–50% RH were mostly linear. The great influence of small percentages of water at lower humidities seems to indicate that water is competing more successfully for the soil surface than does ED. Experimental results indicated that water alone formed a monolayer at about 10% RH. At this value of water content sorption of ED is approximately halved with respect to that on dry soil and at humidities greater than 10%–20% the mechanism of sorption appears no longer predominantly competitive. The competitive nature of sorption at low humidities was further demonstrated showing that ED sorbed on dry soil can be displaced by water vapor. Finally, it has been shown that, when the water content in soil is that corresponding to field capacity, solution of ED in soil water can account for a fraction of the material sorbed, while the additional ED is sorbing on the water interfaces. The isotherms for ED sorption on Ca-montmorillonite at 5%, 10%, and 20% RH lie above that for the dry clay, indicating an expansion of the crystal lattice which allows entry to ED molecules. Jurinak and Volman[359] studied the thermodynamics of ED vapor adsorption by Ca–montmorillonite and Ca–kaolinite.

Sorption of ED in the vapor phase was studied in the presence of air on 20 different soils at moisture contents corresponding to field capacity.[360] All isotherms were linear and the sorption coefficient (slope of the isotherm) could be correlated with SA, OM content, moisture content and less closely with clay content. In a study of the diffusion of ED vapor through soil, the importance of blocked pores and the dynamic equilibrium existing between vapor and sorbed phases has been evidentiated.[361]

Chiou *et al.*[362] determined vapor sorption isotherms on oven-dried (140 °C) Woodburn soil at 20–30 °C for benzene, chlorobenzene (MCBz), m- and p-DCBz, 1,2,4-trichlorobenzene (TCBz), and water as single vapors and as functions of RH. Isotherms were plotted as milligrams taken up per gram of whole soil versus the relative vapor concentration of the compound (P/P^0), where P is the equilibrium partial pressure and P^0 the saturation vapor pressure at the system temperature. The use of P/P^0 in the isotherm normalizes the activity (or chemical potential) of each compound with respect to its own pure state. The isotherms for all compounds on dry soil samples are distinctively nonlinear (BET type-II isotherms), with water showing the greatest capacity. The coincidence of two isotherms for m-DCBz and 1,2,4-TCBz on dry soil at 20 and 30 °C at $P/P^0>0.05$ is evidence that the enthalpies of (mineral) adsorption are essentially the same as the enthalpies of vapor condensation. This is the basic assumption in the BET adsorption theory with adsorbates approaching and exceeding the monolayer capacity. The BET equation is

$$(P/P^0)/[Q(1-P/P^0)]=[(C-1)P/P^0]/CQ_m+1/CQ_m, \tag{14}$$

where Q_m is the monolayer adsorption capacity (mg g^{-1} of soil) and C is related to the net molar enthalpy (ΔH_m, kJ mol^{-1}) of adsorption at $Q \leqslant Q_m$

$$-\ln C \sim (\Delta H_m+\Delta H_v)/RT,$$

where ΔH_v is the enthalpy of vaporization of the compound, R is the gas constant, and T is the system temperature. A plot of $(P/P^0)/[Q(1-P/P^0)$ vs P/P^0 should yield a straight line, with a slope of $(C-1)/(CQ_m)$ and an intercept of $1/(CQ_m)$, from which Q_m and C can be determined. The isotherms are very well described by Eq. (14) over the range $P/P^0=0.05$–0.30. The BET monolayer adsorption capacities for all compounds with dry soil were established at relatively low P/P^0 ($\leqslant 0.18$), except for benzene which occurred at $P/P^0 \sim 0.23$. Q_m values ranged between 5.54 and 9.53 mg g^{-1} for alkylbenzenes and that for water was equal to 11.7 mg g^{-1}. The ΔH_m values at $Q \leqslant Q_m$ were noticeably more exothermic than respective $-\Delta H_v$ values by about 6.3–10.5 kJ mol^{-1}; these enthalpy effects are consistent with the dominance of mineral adsorption with dry Woodburn soil. Sorption on dry soil increases by increasing the polarity of the sorbate; thus it increases by increasing the chlorine number in the benzene ring. Water vapor sharply reduced the sorption capacities of organic compounds with the dry soil; on water-saturated soil, the reduction was about 2 orders of magnitude and the isotherms become linear. The markedly higher sorption of organic vapors at subsaturation humidities is attributed to adsorption on the mineral matter, which predominates over the simultaneous uptake by partition into the organic matter. At about 90% RH, the sorption capacities of organic compounds become comparable to those in aqueous systems, because of the effect of displacement by water of organics adsorbed on the mineral matter. However, the amont of these compounds sorbed from vapor phase at 90% RH was still more than that sorbed in water phase, with benzene showing the higher deviation by more than a factor of 5.

Vapor sorption of water, ethanol, benzene, hexane, TeCM, 1,1,1-TCA, TCE, PCE, and ED on soil humic acid has been determined.[363] The uptake (mg g^{-1}) of these compounds is highly linear over a wide range of relative pressure (P/P^0), characteristic of the partitioning (dissolution) of the organic compounds in soil humic acid. Isotherms approaching $P/P^0=1$ show a general steep rise due to an induced vapor condensation onto the exterior surface of the humic sample. The overall vapor sorption is essentially reversible. Extrapolating the linear portion of the vapor phase isotherms at $P/P^0=1$ the "limiting sorption (partition) capacity" (LSC) is obtained (Q^0_{ha}). The values of LCSs are used to predict the K_{om}s for nonpolar organic compounds following the procedure described in Sec. 12.6.

Rhue *et al.*[366] studied the vapor-phase sorption of toluene, p-xylene (p-X), and ethylbenzene (EBz) on bentonite, kaolin, two soil samples, an aquifer material, and a silica gel ovendied at 140 °C prior to use. Sorption (mg g^{-1}) was reported as a function of P/P^0; the isotherms conformed to the BET type-II isotherms. Differences in the amounts of the three alkylbenzenes adsorbed on a given adsorbent were generally quite small. With the exception of bentonite, the isotherms for water adsorption were also BET type-II isotherms. Q_m and C [Eq. (14)] were estimated; the values of C are indicative of the low interaction energies associated with physical adsorption process. Surface areas calculated from BET monolayer capacities indicated that the surface available for alkylbenzene adsorption was essentially that measured by N_2 adsorption except for silica gel. Plots of the relative adsorption (Q/Q_m) vs P/P^0 for water and p-X were similar for several of the adsorbents used. Overlapping isotherms were also reported for p-X and TCE adsorption on oven-dry soils and clays.[367] This suggests that sorbent surface area has a predominant effect on VOC adsorption on anhydrous sorbents. In another paper[368] the competitive adsorption of EBz and water on bentonite and of p-X and water on kaolin and silica gel was reported. EBz adsorption on bentonite was not affected by water at RH near 0.23, but was reduced significantly at RHs near 0.50. p-X adsorption on kaolin and silica gel decreased with increasing RH, especially above a RH of about 0.2. Increasing RH not only decreased the amount of alkylbenzene adsorption but also resulted in a change from type-II isotherms to ones that were essentially linear. Linear isotherms could not be attributed to organic matter, since the clays and oxide used had very low to trace amounts of OC. Based on solubility considerations alone, partitioning of EBz and p-X into adsorbed water films was not considered to be an important adsorption mechanism in this study. p-X and TCE adsorption on air-dry soils and clays (water contents 25–40 mg g^{-1}) was about 1000-fold less than that on oven-dry sorbents, indicating that water effectively competes with VOCs for the sorbent surface.[367] Isotherms of p-X adsorption on air dry sorbents (water content: 30 mg g^{-1} for Webster soil, 25 mg g^{-1} for Lula aquifer, 25 mg g^{-1} for kaolin, corresponding to values in equilibrium at RH>50%) were linear. The temperature dependence of adsorption coefficients K_d was used to calculate the enthalpy of adsorption for several VOCs. These values ranged from -30 to -40 kJ mol^{-1}, and were more similar to enthalpies of vaporization than to enthalpies of solution.

Sorption of TCE and benzene on a desert soil has been investigated at two different temperatures and various moisture content, using a gas-chromatographic method.[369] Sorption of these two VOCs to the unmodified soil was compared to sorption onto the same soil that was alternately treated with hydrogen peroxide (to remove organic carbon) or with humic acid (to add organic carbon) in order to examine the role of soil organic matter in vapor phase sorption. Results from this study indicate that organic carbon plays only a minor role in sorption at low moisture content.

Also Smith *et al.*[370] agreed with this result. Using vadose zone soil, at 0% RH, soil uptake of TCE appears to be caused mainly by adsorption onto mineral surfaces (BET type-II isotherms). At higher relative humidity the competition of water reduces TCE adsorption by the minerals and isotherms become more linear. At 100% RH, TCE uptake by soils is in all likelihood predominated by partition into the soil organic matter. The moisture content of soil samples collected from the vadose zone was found to be greater than the saturation soil-moisture content, suggesting that adsorption of TCE by the mineral fraction of the vadose zone soil should be minimal relative to the partition uptake by soil organic matter. Analysis of TCE in soil and gas samples collected from the field indicated that the ratio of the concentration of TCE on the vadose-zone soil to its concentration in the soil gas was 1–3 orders of magnitude greater than the ratio predicted by using an assumpion of equilibrium conditions. This apparent disequilibrium presumably results from the slow desorption of TCE from the organic matter of the vadose-zone soil relative to the dissipation of TCE vapor from the soil gas.

When sorption takes place from the vapor phase, a vapor sorption analog to K_d can be derived.[98] The linear sorbed/vapor distribution parameter K_{sg} can be defined similarly to K_d as

$$q = K_{sg} C_g, \tag{15}$$

where q is the concentration of solute in sorbent (μg kg^{-1}), C_g is the equilibrium concentration of solute in vapor phase (μg dm^{-3}).

Vapor phase sorption of TCE by a porous aluminum oxide surface coated with humic acid (to simulate an aquifer material) was observed to be highly dependent on moisture content.[364] The authors used an experimental headspace procedure to measure linear solid-vapor sorption coefficient (K_{sg}) of TCE onto the oven-dried simulated soil, which was 11 870 cm^3 g^{-1}. This value was over 10^5 times greater than the aqueous-phase linear sorption coefficient. The soil region overlying the water table could conceivably contain moisture from a few percent to near saturation. A typical field moisture content for the intermediate zone of a partially saturated soil layer is approximately 10%. The authors[364] found that the TCE sorption coefficient (K_{sg}) for the synthetic soil at 8.2% water content was 207 cm^3 g^{-1}, and at 11.6% the value decreased to 53.9 cm^3 g^{-1}. Both of these values are still 2 or more orders of magnitude greater than that determined for the saturated synthetic soil ($K_d = 0.29\,cm^3\,g^{-1}$). Obviously the magnitude of TCE vapor sorption coefficients and their dependence on moisture content will be different on different sorbents. However, these results indicate that the assumption that vapor sorption coefficients may be equated with saturated sorption coefficients can lead to large errors in modelling TCE transport through unsaturated zone, unless experimental data are available, demonstrating that this assumpion is reasonable for the soil of interest.

Alumina coated with humic acid was used to evaluate the sorption of mixtures of organic vapors (chorinated and nonchlorinated hydrocarbons) under partially saturated conditions.[365] Vapor interactions resulted in both enhanced and suppressed sorption relative to the uptake of single vapors. These interactions may result from interaction between adjacent molecules at the surface, solvophobic effects, or nonlinear sorption isotherms.

Ong and Lion[371] observed that the validity of application of the Henry's law constant in vadose zone transport models for organic chemicals required specific investigations due to the poor information available in the literature.[238,362] The Henry's law constant is a measure of the equilibrium distribution of a pollutant between the aqueous and vapor phases, and is coupled with the sorption distribution coefficient of the same pollutant dissolved in water phase (soil/water equilibrium) to describe uptake of organic vapors in that zone. The authors carried out a detailed study on TCE vapor ($P/P^0 < 2\%$) sorption on several minerals (alumina, alumina coated with humic acid, iron oxide, kaolinite, and montmorillonite) over a wide range of moisture contents. For oven-dry minerals, surface area was found to be a good indicator of the sorptive capacity of the solid phase. As moisture content was increased, the partition coefficients of TCE vapor decreased by several orders of magnitude, attained a minimum, and then gradually increased. Mechanisms of TCE vapor sorption were proposed corresponding to three regions of sorbent moisture content. In region 1, from oven-dried conditions to one monolayer coverage of water on the solid surface, direct solid–vapor sorption was evident with strong competition between water and TCE for adsorption sites of the sorbents. Enthalpy of sorption for all oven-dried solids were between -40 and -80 kJ mol^{-1}, with the humic-coated alumina having the highest value of the five solids at -69 kJ mol^{-1}. Values of this magnitude indicate that sorption of TCE on oven-dried solids was a physical sorption process. In region 2, between a monolayer coverage to approximately five layers of water molecules, likely interactions between TCE vapor and water include sorption of TCE onto surface-bound water and limited TCE dissolution into sorbed water with some "salting out" effects caused by water structure. In region 3, extending from a minimum of approximately five layers of water molecules to the water retention capacity of the soil, TCE dissolution into condensed water-dominated vapor uptake along with sorption at the water solid interface. Enthalpy of sorption in this region increases to the same magnitude as the enthalpy of dissolution (-39 kJ mol^{-1}). Application of Henry's law and aqueous phase partitioning coefficients to model TCE vapor interaction with water condensed on the solid surface is possible only after ≈ 5 layers of water molecules have formed. This assumption may not be valid for soils in arid or semiarid regions or for the top surface soil layer in temperate regions on a seasonal basis. The implications of these results are that, for low moisture content soils, volatilization loss of organic vapors to the atmosphere will be more highly retarded than when they are at their water retention capacity.

Petersen *et al.*[372] measured the K_{sg}s of TCE using four oven-dry soils. They ranged between 61 and 3400 cm^3 g^{-1}. In the dry range, adsorption was dominated by soils with higher specific areas (i.e., high clay content), while soils with higher organic carbon content manifested higher adsorption amounts in the wet moisture range. The adsorption behavior from dry to wet conditions was similar to that reported by Ong and Lion.[371] The point at which measured K_{sg} falls on the line where Henry's law can be applied seems to be located at approximately four molecular layers of water.

Goss[373] studied the sorption of 17 volatile and semivolatile organic compounds on quartz sand at different relative humidities and temperatures. The enthalpy of sorption was determined for each substance and compared with the corresponding enthalpy of condensation. At relative humidities generally present in the environment, quartz was covered by at least a monolayer of water. In this case adsorption of organic compounds took place on the liquid-gas interface of an adsorbed water film. The results suggest higher binding forces for polar than for nonpolar compounds, probably due to hydrogen bonds. Above the water monolayer coverage, sorption occurred on the adsorbed water film and showed an exponential decrease with increasing relative humidity.

The adsorption of organic vapors on polar surfaces (quartz sand, Ca–kaolinite) depends primarily on two environmental parameters: ambient temperature and relative humidity. Goss[374] presented an empirical model to predict sorption on these sorbents when they are covered by at least 1 monolayer of water (RH above 30%). It has been shown that the model is still valid at 100% RH and that this interesting special case corresponds to the adsorption on a bulk water surface. At RHs above 100% RH condensation of water occurs, leading to an unlimited increase of water film. In this case, adsorption on the water film is equivalent to that on a bulk water surface.

Pennell *et al.*[375] studied the adsorption of p-X vapors on oven-dried silica gel, kaolinite, and Webster soil. The results demonstrated that dissolution of p-X into adsorbed water films was insignificant at 67 and 90% RH. In contrast, the adsorption of p-X at the gas-liquid interface, predicted by the Gibbs equation, contributed significantly to p-X sorption in the presence of water vapor. All these results indicate that a multimechanistic approach should be used to describe sorption of nonpolar organic vapors by hydrated soil materials. It incorporates adsorption on mineral surfaces, adsorption at the gas-liquid interface, dissolution into adsorbed water, and partitioning into soil organic matter.

The vapor phase sorption of several VOCs by a calcareous soil has been measured using inverse gas chromatography.[376] For dry soil, sorption isotherms are apparently nonlinear, and finite desorption kinetics contribute to the chromatographic peak shapes. Even a small addition of water (1.5%–15% RHs) drastically decreased the sorption of nonhydrogen-bonding VOCs by the soil, chromatographic peaks became symmetrical and the sorption isotherms became linear. The results seem to indicate that the effect of additional water is to simply reduce the available surface area of the soil by filling some of the soil pores. Because water can substantially reduce the surface activities of inorganic surfaces by occupying the high-energy sorption sites, it is possible that at high humidity only organic carbon would be responsible for vapor-phase sorption. Hydrogen-bonding compounds (diethylether, acetone, acetonitrile), on the contrary, still exhibited nonlinear sorption isotherms and finite sorption and desorption kinetics in the presence of water. The values of enthalpy of sorption obtained at 52% RH (1.65% w/w) for silt and clay fractions ranged between −37.6 and −64.8 kJ mol^{-1} for six nonpolar VOCs, while enthalpy of condensation of the neat compounds ranged between −30.8 and −38.7 kJ mol^{-1}.

The sorption isotherms of MCBz and toluene on a standard EPA soil at different relative humidities were measured using a dynamic technique based on frontal analysis chromatography.[377] A mechanistic approach to evaluate the contribution of the possible sorption mechanisms to the total sorption indicated that adsorption at the gas-liquid interface was important, while dissolution in liquid water and partitioning into organic matter from the adsorbed water phase were negligible. However, these three mechanisms could not account for the total sorption which suggests that the VOC may be competing with water for available sites on the surface at high VOC partial pressure.

Farrell and Reinhard[98] measured the sorption–desorption isotherms spanning 4–5 orders of magnitude in vapor concentration for TCM, TCE, and PCE under unsaturated conditions at 100% RH. The mechanisms affecting isotherm shape were investigated using model solids, aquifer materials, and soil spanning a range in physical properties. Isotherms in log–log scale for the total uptake of all three sorbates coincided on the montmorillonite, Norwood, and Livermore soils. On all but the Norwood soil, where the organic matter (1.4% OC) was likely responsible for most of the uptake, mineral adsorption was the dominant sorption mechanism. Linear isotherms were observed on the nonporous solid (montmorillonite) and on the solids with the highest external surface area (Livermore clay and silt) absent of microporosity. The adsorption was nonlinear on microporous solids, like silica gels, glass beads, and soil sand, which show structural heterogeneity in the form of micropores. Moreover, for organic species adsorbed in a lipophilic environment created by their own adsorption in a micropore, desorption is not expected to follow the same path as adsorption and hysteresis between adsorption and desorption may result due to cooperative adsorption on micropores. This is the case of the Santa Clara aquifer solids (0.15% OC). Finally, the adsorption isotherm of a soil with $f_{oc}=1.4\%$ is more linear than those regarding soils with $f_{oc}\sim 0.1\%$; this greater linearity may indicate that organic matter partitioning dominate sorbate uptake. The contribution of mineral uptake in soils is greater when the organic matter content is lower.

Batterman *et al.*[378] described models and measurements of diffusion, dispersion, and retardation parameters developed for several hydrocarbon vapors in unsaturated soils using laboratory column systems. The experiments clearly demonstrated the role of humidity in absorption and transport of vapors in soils. Soil gas humidities below 30% resulted in considerable retardation of hydrocarbon vapors in all media. Retardation factors ranged up to 80 for toluene and to 46 for trichloroethylene. Retardation coefficients decrease but remain large with increasing humidity in organic rich soils. No significant retardation is seen for methane. Based on soil–water isotherms, these results suggest competitive sorption between hydrocarbon and water vapors on soil surfaces, especially the mineral fraction.

Sorption of benzene, toluene, and EBz in vapor phase at infinite dilution on soils was studied by inverse gas chromatography in the Henry's law region.[379] The results indicated that the adsorption processes was exothermic and depended mainly on the chemical nature, pore size distribution and pore shape, and especially on the microporous structures of the soils. Intraparticle mass transfer might play a significant role in the adsorption of VOCs on soils.

It has been demonstrated that various VOCs may be firmly bound to natural sorbents with sufficient exposure time, because they are entrapped in soil micropores so that they are difficult to extract.[380–382] Incubation of soil samples with volatile organic solvents (benzene, toluene, EBz and 1,1,1-TCA) at part-per-thousand concentrations leads to the formation of a residual firmly bound fraction that resists evaporation and may persist in the soil for long periods of time.[383] The concentration of this fraction increases with temperature and solvent concentration. Its formation is not greatly affected by the water concentration in the soil.

In conclusion, dry soils and clays show sizable sorption capacities for volatile organic compounds. Water competes with them for sorption sites; therefore the presence of water may strongly reduce the sorption capacities. Sorption isotherms, which are of the BET type II, change to linear when relative humidity is in the range 30%–50%. Due to this behavior, sorption of volatile compounds may be important in their transport through soil columns, especially in the unsaturated zone of soils and aquifers. Shoemaker *et al.*[384] proposed analytical models to describe subsurface transport of volatile chemicals.

5. Temperature Effect

Sorption of a chemical on a solid sorbent occurs when the free energy of the sorptive exchange is negative[163,385,386]

$$\Delta G=\Delta H-T\Delta S, \tag{16}$$

where ΔG is the change of the Gibbs free energy (kJ mol^{-1}); ΔH is the change in enthalpy (kJ mol^{-1}), and ΔS is the change in entropy (kJ mol^{-1} K^{-1}). ΔH represents the difference in binding energies between the sorbent and the sorbate (solute) and between the solvent and the solute.

Thus, sorption may occur as the result of two types of forces: enthalpy-related and entropy-related forces.[123] Hydrophobic bonding is an example of an entropy-driven process; it is due to a combination of London dispersion forces (instantaneous dipole-induced dipole) associated with large entropy changes resulting from the removal of the sorbate from the solution. For polar chemicals, the enthalpy-related forces are greater, due to the additional contribution of electrostatic interactions.

Generally sorption coefficients decrease with increasing temperature. However, some examples of increasing equilibrium sorption with increasing temperature and of no effect of temperature on sorption equilibrium were also found.[386] Chiou *et al.*[195] observed that an inverse relationship exists for organic compounds between sorption coefficients and solubilities. Lower K_d values are found at higher temperatures for most organic compounds for which solubility increases with temperature, while increased sorption at higher temperatures can be expected for compounds for which solubility decreases with temperature. Therefore, due to the dependence of both sorption coefficients and solubility on temperature, the measured effect of temperature on sorption isotherms is the result of combined sorption and solubility contributions.[387]

Podoll *et al.*[132] reported that adsorption of naphthalene (K_d) on soil decreases with increasing temperature from 15 to 50 °C and isosteric enthalpy of adsorption is exothermic. The heat evolved during adsorption (between −8.8 and −12 kJ mol^{-1}) is probably dominated by the heat of dilution of liquid naphthalene in water, evaluable to about 7.5 kJ mol^{-1} between 5 and 30 °C. Assuming this value constant in the range of 15–50 °C, the corresponding enthalpy of solution in the sorbent phase would be between −1.3 and −4.6 kJ mol^{-1}. These data indicate that the enthalpy of solution in the sorbent phase is smaller and of opposite sign to the enthalpy of solution in bulk water. Therefore, the displacement of water by naphthalene at the soil surface is slightly favored energetically.

He *et al.*[388] studied the sorption of fluoranthene on soils and lava. The sorption coefficients of fluoranthene were found to decrease with temperature between 5 and 25 °C. The measured decreasing extent of sorption corresponds to that evaluated introducing ΔH_s (26.1 kJ mol^{-1}), the enthalpic contribution to excess free energy of the solution calculated from the relation between aqueous solubility of fluoranthene and the corresponding temperature, in the equation reported by Schwarzenbach *et al.*[389]

The temperature effect on Freundlich adsorption isotherms of β and γ isomers of hexachlorocyclohexane was studied in the temperature range of 10–40 °C.[390] Sorbents were: a high organic soil with mixed mineral fraction, a clay soil high in montmorillonite containing a little organic matter, a montmorillonite clay (Ca–bentonite), and a crystalline silica. Plots of x/m against C for the two isomers show that an increase in temperature lowers sorption uniformly for each system. Proportionally, the decrease is least with silica gel and greatest with Ca–bentonite. Contributing to this net effect of isotherm displacement downward with temperature are not only the energy contributions in the sorption reaction itself, but also the change in solubility of the solute as a result of the temperature change. This change is closely related to the change in the reduced concentration, C/C_0, with temperature, where C, the solute concentration, may be considered constant, and C_0 is the solubility of the solute in the solvent at a specified temperature. In addition to the Freundlich constant K_f, another constant, K_f', is obtained when $\log(x/m)$ is plotted against $\log(C/C_0)$. The K_f' values can be considered as the hypothetical amount sorbed from solutions having a nearly constant equilibrium solute fugacity. While the K_f values decrease with temperature, the solubility corrected intercept values, K_f', increase in each case as temperature increases. Thus it appears that the sorption process, which is indicated to be exothermic by the normal isotherms, is at least partially so because of the solubility–temperature interaction. The $1/n$ constants of the Freundlich equation increased with temperature according to the theory of dilute solutions.

On the basis of these considerations, Yaron and Saltzman[139] reported the amount of solute adsorbed as a function of its reduced concentration in water. They found that the reduced adsorption isotherms for parathion with three soils at temperatures of 10, 30, and 50 °C overlap, showing that parathion is adsorbed by soils without any appreciable thermic effect.

Sorption of fenuron and monuron on montmorillonite and bentonite was studied as a function of exchangeable alkali or earth–alkali cation, temperature, and ionic strength.[244] Normal adsorption isotherms were exothermic but, when the temperature effect on solubility was accounted for, the adsorption reaction changed to endothermic and tended to be more and more temperature independent as electronegativity of the exchangeable cation increased. It was postulated that substituted urea is associated with the metal ions through a bridging effect of coordinated water.

However, the use of reduced concentration concept, as well as the terms organophilic and hydrophilic applied to the adsorption of organic molecules, appears not universally justified because it lacks theoretical and experimental support.[391] The concept of reduced concentration can be used for those systems where it has been proven to apply.

Anyway, the temperature effect on sorption isotherms is normally low for both hydrophobic and polar organic compounds.

A negative enthalpy of sorption (−14.6 kJ mol^{-1}) has been derived from the Gibbs–Helmholtz equation for the partition coefficients of 1,2,3,4-TeCBz in water/sediments systems at temperatures ranging from 24 to 55 °C, indicating an exothermic binding reaction.[155]

Wauchope *et al.*[392] studied the sorption of naphthalene by a loam soil with 1% organic matter content. Because the solubility and vapor pressure of naphthalene were precisely known over the range of temperature taken into consideration (6.5–37 °C), a complete thermodynamic description of the differences between standard vapor, crystal, solution, and soil-adsorbed states was possible. The results indicate that enthalpies and entropies of the solution and surface standard states are quite similar resulting in a near-zero standard enthalpy difference and a small standard entropy increase for adsorption from solution. The results emphasize the importance of the unique structured nature of water acting as a solvent, and the competition of water for adsorption sites.

An increase of ΔH from −10.9 to −8.4 kJ mol^{-1} was observed when the sorbed concentration varied from 0.01 to 0.07 mmol g^{-1} in TeCM/DTMDA–clay system.[92]

Sorption of p,p′-DDT to marine sediment, montmorillonite clay and humic acid was studied in the temperature range between 5 and 25 °C.[173] The respective isosteric enthalpies were found to be 12, 16, and -8 kJ mol^{-1}.

Binding of 2,2′,5,5′-tetrachlorobiphenyl (TeCB) by dissolved humic acid was not significantly correlated with temperature.[393] This indicates a low enthalpy of interaction of this compound with humic acid and implies that the binding is primarily entropy driven.

Also sorption of PAHs to dissolved organic carbon from a lake decreased with increasing temperature over a temperature range between 16 and 45 °C.[394] $\Delta H°$ values ranged from -18.3 kJ mol^{-1} for fluoranthene to -40.6 kJ mol^{-1} for benzo(ghi)perylene. A temperature decrease of 10 °C leads to an average increase of K_{doc} with 60%.

A study was carried out with alachlor adsorption on montmorillonite saturated with several cations (Al^{3+}, Cu^{2+}, Ca^{2+}, Mg^{2+}, NH_4^+, Na^+, Li^+, Rb^+, and Cs^+,) at 5 and 22 °C.[395] A decrease in temperature from 22 to 5 °C resulted in an increase in adsorption except for Al-, Rb-, and Cs–montmorillonite, for which the adsorption process was endothermic. The isosteric changes of enthalpy were in the range between -1.97 and 11.2 kJ mol^{-1} for all systems and indicated that the interaction energy of homoionic montmorillonite was weak and consistent with physical bonding (hydrogen bond or van der Waals forces). A correlation between adsorption (Freundlich isotherms) and the polarizing power of the exchangeable cation was observed. The interaction of alachlor with homoionic montmorillonites was also studied by Fourier transform infrared spectroscopy in an organic solvent. The results indicated that the molecule is adsorbed on monoionic montmorillonite by a coordination bond, through a water bridge, between C═O groups and the exchangeable cation of the clay. Further, the coordination strength is directly correlated with the polarizing power of the cation. X-ray diffraction analyses showed that the herbicide was able to penetrate the interlayer space of montmorillonite saturated with polyvalent cations.

Measurements of K_f values for diuron on three sediments at 5, 25, and 40 °C showed that sorption was inversely related to temperature; ΔH values of -9.6 kJ mol^{-1} for two sediments and -12.6 kJ mol^{-1} for the third were considered characteristic of weak sorption forces of the van der Waals type.[257] Temperature appeared to have a greater effect on the sorption of diuron than on the sorption of ametryne.[256] K_d values of diuron with a clay soil (3.2% OM) decrease from about 9 to about 7 cm^3 g^{-1} by increasing temperature from 5 to 45 °C. Those of ametryne remain practically constant ($K_d \sim 2$) at the same conditions. The same effect of temperature on diuron was found by other authors.[245]

The isosteric enthalpy of adsorption of linuron on humic acid saturated with several cations was calculated from the adsorption data at 5 and 25 °C[396] and ranged from about -0.71 to -3.1 kJ mol^{-1}. These values are relatively small and are of the order which is consistent with a physical type of adsorption.

A thermodynamic study was carried out by Spurlock[397] on substituted phenylureas–soil interactions for understanding various aspects of sorption phenomena, including isotherm nonlinearity. The results suggest that specific interactions between the phenylureas and soil organic matter moieties are dominant at low sorbed phase concentrations, but become less important relative to nonspecific London–van der Waals forces as sorbed phase concentration increases. The urea isotherms are therefore nonlinear, with nonlinearity fundamentally related to the nature of substituted phenylurea-sorbed phase interactions.

The adsorption of monuron, atrazine, simazine, CIPC and DNBP by bentonite was greater at 0 °C than at 50 °C.[251] Adsorption by muck was similar at the two temperatures for all compounds. Comparisons between the muck soil and bentonite results should be valid since both received identical treatment, and temperature effects on solute–solvent interactions would be expected to be the same. Adsorption by bentonite exhibited a greater temperature dependence than adsorption by muck. This result suggests a higher bonding energy on bentonite than on muck.

The K_d values for simazine and atrazine sorbed by a silty–clay–loam soil (OM=4.2%) decreased of about 60% and 45%, respectively, with increasing temperature from 0 to 50 °C.[145] A small temperature effect was detected with adsorption of atrazine[286] by soil; the average K_d value (in the range of pH 3.9–8) at 30 and 40 °C was 7.2 cm^3 g^{-1} while at 0.5 °C was 9.6 cm^3 g^{-1}. Sorptive processes are exothermic; therefore, an increase in temperature should reduce sorption, especially if sorption forces are weak. Ionic sorption, however, tends to be less temperature dependent than physical sorption. If ionic forces are involved in sorption of atrazine over the soil pH range studied, then the temperature effect should be less at the lower pH values. This was not true for atrazine–soil system where there was a greater temperature effect at a low than at a high pH. Sorption of atrazine on acid humic acid (pH 2.5) was ten times greater ($K_d = 627$ cm^3 g^{-1}) than on neutral humic acid (pH=7.0) ($K_d = 62.2$ cm^3 g^{-1}). This pH effect was attributed to increased ionic bonding caused by protonation of the amino groups on the atrazine molecule at low pH. The effect of temperature on the sorption of atrazine on humic acid was quite marked; sorption was nearly twice as great at 40 °C as at 0.5 °C. This is opposite of what usually occurs with mineral systems.

Dao and Lavy[241] reported that greater amounts of atrazine were adsorbed at 30 °C than at 5 °C on four soils at 0.1 bar moisture content. This indicated an endothermic reaction which was observed both before and after correction for differential atrazine solubility due to temperature. The standard free energy change $\Delta G°$ of the adsorption reaction was negative in all four soils indicating the spontaneity of the process. The standard enthalpy change $\Delta H°$ was positive, ranging from 0.016 to 2.78 kJ mol^{-1} and indicating the endothermic nature of the reaction. There was an increase in the entropy of the system as shown by the positive values of $\Delta S°$(0.010–0.017 kJ K^{-1} mol^{-1}).

The effect of equilibration temperature (5 and 28 °C) on sorption of metribuzin and metolachlor by Alaskan subartic soils was investigated.[398] For surface soil, metribuzin showed increased sorption at lower temperature, whereas metolachlor had greater sorption at 28 °C. However, for both herbicides equilibration temperature did not affect K_f values from the lower soil depth. Furthermore, of the total variation of K_f values within the surface soil, temperature accounted for less than 10%, while soil type accounted for greater than 80% for both herbicides.

Sorption of isocil and bromacil on silica, clays and humic acid is exothermic.[99] The sorption enthalpies calculated as a function of chemical sorbed become more positive with increasing surface coverage. The behavior of humic acid surface is quite different as far as the magnitude and change of ΔH is concerned. The ΔH value is small and also its change with surface coverage is insignificant. For most of the surfaces the probable mechanism of the adsorption is a physical or van der Waals-type adsorption as indicated by the magnitude of ΔH. Some hydrogen bonding is also probable at very low surface coverage.

Temperature was shown to exert a small influence on the binding of diquat and paraquat to humic acid.[142] On bentonite diquat was completely adsorbed at 0 and 50 °C.[251]

A slight effect of temperature on adsorption has also been found with picloram[315,316] and this behavior has been interpreted as due to physical adsorption. Also, the negative values of $\Delta G°$ and $\Delta S°$ for the same systems evidentiated adsorption-type processes and stable adsorption complexes, respectively. Biggar *et al.*[269] studied the sorption kinetics of picloram on Palouse silt (pH 5.9) and of parathion on Panoche clay (pH 7.5) and Palouse silt. From the temperature dependence of the relative sorption constant, they obtained the activation energies associated with the sorption kinetics of the three systems equal to 11.3, 5.4, and 18 kJ mol^{-1}. Such energy levels are comparable to van der Waals bonding (2–8 kJ mol^{-1}) and hydrogen bonding (17–21 kJ mol^{-1}) that occur on clay surfaces and with such groups as the carboxyl, hydroxyl, and amino groups of the organic fraction. Mechanisms of interaction based on experimental results and thermodynamic considerations emphasize the importance of organic matter for picloram sorption and both clay and organic matter in sorption of parathion.

Temperature had little effect on the amount of 2,4-D sorbed on clay materials.[146] Activation energies for the sorption process laid between 12.5 and 21 kJ mol^{-1}, with clays of larger surface area giving higher activation energies. These values are characteristic of diffusion controlled processes.

In conclusion, sorption processes are generally exothermic; therefore sorption coefficients decrease with increasing temperature. However, this effect is inversely related to water solubility which, on the contrary, increases with temperature for most organic compounds. Therefore, the measured variation of sorption coefficients with temperature is the result of both the contribution of sorption effect and solubility effect.

A review on the effect of temperature on sorption equilibrium and sorption kinetics of organic micropollutants has been recently published.[386] The conclusions of this study are in summary: (a) the transfer of hydrophobic organic compounds from solution to sediment generally involves slightly negative enthalpy changes (on the average −0.25 kJ mol^{-1}); (b) when favorable electrostatic interactions (e.g., H bonding) are possible, equilibrium sorption enthalpies were found to be more exothermic (on the average −8 kJ mol^{-1}); (c) the activation energies for fast adsorption and desorption were found to be between 0 and 50 kJ mol^{-1} (on the average 18 kJ mol^{-1}), while the activation energy for slow desorption was found to be of 66 kJ mol^{-1}, similar to the activation energies for diffusion in polymers, which averaged 60 kJ mol^{-1}. This was interpreted as an indication that diffusion causes nonequilibrium sorption effects.

6. Binding to Dissolved Organic Matter

Natural waters contain various concentrations of high-molecular-weight organic substances (humic and fulvic acid, humine) indicated as dissolved organic matter (DOM) or as dissolved organic carbon (DOC), which may bind organic chemicals.

The association constant DOM- or DOC-organic chemical can be defined as

$$K_{\mathrm{dom}} \text{ or } K_{\mathrm{doc}} = (\mu\text{g compound bound/g or kg DOM or DOC})/(\mu\text{g compound freely dissolved/cm}^3 \text{ or dm}^3 \text{ solution}) \quad (17)$$

K_{dom} and K_{doc} (cm^3 g^{-1} or dm^3 kg^{-1}) of Eq. (17) are similar to K_{om} and K_{oc} are measures of the binding affinity of DOM or DOC for the organic chemical. The possible interactions chemical–DOM may be hydrogen bonding, van der Waals forces or hydrophobic association.[399] For neutral PAH molecules it is believed that binding is dominated by van der Waals type interactions.[188] The binding of benzo(a)pyrene (BaP) to dissolved humic material (DHM) is completely reversible and the extent of reversibility is unrelated to the sorption time.[400] The rate of binding of BaP to DHM, measured by the quenching of BaP fluorescence, is very rapid and the equilibrium is reached within 5–10 min. The authors found a relationship between the hydrophobicity of BaP (K_{ow}) and the bonding affinity.

Johnsen[401] studied the interactions between PAHs and natural aquatic humic substances (NHS) as a function of contact time. Eight PAH compounds were sorbed on NHS and recovered by cyclohexane extraction after storage times ranging from 4 to 70 d. In general, the recoveries decreased with increasing storage time. The results suggested that strong bonds were formed between PAH and NHS. In the early part of the experiment (4 and 7 d) the recoveries of the different PAHs decreased with increasing K_{ow} or decreasing water solubility of the compounds.

Carter and Suffet[402] observed that a significant fraction of the dissolved DDT found in natural waters may be bound to DHM and that the extent of binding depends on the source of the humic material, the pH, the calcium concentration, the ionic strength, and the concentration of humic materials. The increase of the hydrogen and metal ion concentration change the structure of the humic polymer, which becomes less hydrophilic as its charge is neutralized. It seems reasonable that the less hydrophilic form of the polymer would bind hydrophobic compounds more effectively.

Sorption of anthracene on estuarine colloids significantly decreased when the experimental pH of 8.01 was increased to 9.0 or decreased to 5.0.[399] The decrease in K_{oc} values was attributed to changes occurring within the polymeric structure of the colloids.

The addition of ammonia to soil produces an increase of both the soil pH and the concentration of DOC in the soil solution.[403] These ammonia-induced changes appeared to decrease atrazine sorption and to increase atrazine desorption, thus increasing atrazine movement through soil.

The binding of benzene, naphthalene, and anthracene with estuarine colloids has been found at least an order of magnitude higher than those reported for corresponding soil/sediment systems.[399] A possible explanation of this behavior is that soil/sediment OM may often be occluded by the inorganic components, thus making fewer sites available for hydrophobic association. The amount of diuron, bromacil, and chlorotoluron complexed by water soluble soil organic material was about 70 times the amount sorbed by the soil from which the organic material was extracted.[404]

Natural estuarine colloids bind atrazine and hold the resulting aggregate of molecules in stable colloidal suspension.[405] The high K_{doc} values of atrazine and linuron for colloidal matter suggest that the two compounds are strongly bound.[406] On an OC basis, the colloidal material is on the order of 10–35 times better as a sorptive substrate for the herbicides than sediment or soil OM. However, the relative strengths of sorption of the two compounds on colloidal matter as reflected in the ratio of the K_{doc} value of atrazine to linuron appear to be the same as the ratio of the K_{oc} values on soil–sediment (170 vs 670 for soil as opposed to 1850 vs 6750 for colloids). Two hypotheses that may explain the difference between the values observed on soil–sediment and on colloidal matter are suggested. First, although K_{oc} values are reported on the basis of total OC for a soil or sediment, all the OC is not available as a sorptive surface. Alternatively, the surface acidity of sediment or soil clay particles may have the effect of decreasing the sorptive capacity of the OM.

However, it has been observed[407] that, when the nature of the DOM released from the soil/sediment bulk organic matter is similar to that of the soil/sediment bulk organic matter, the ratios of K_{doc}/K_{oc} of solutes will be close to 1. If the DOM is more hydrophilic than the soil/sediment bulk organic matter, the ratios of K_{doc}/K_{oc} of these solutes will be less than 1. The K_{doc}s to nonsettling colloids were 0.5–1 times the K_{oc}s to sediments of the Lake Superior for PCB congeners.[50,408] When the sources and nature of the DOM and soil/sediment OM are different, the ratios K_{doc}/K_{oc} of solutes will have a broad range.

A recent study[394] on the sorption of PAHs to particulate and dissolved organic carbon from Lake Ketelmeer, the Netherlands, has shown a linear relationship between $\log K_{oc}$ and $\log K_{doc}$ with a slope of nearly one.

Great Lakes waters freshly collected were inoculated with radiolabelled hydrophobic organic compounds and, after equilibration, separated into particle bound, DOM bound, and freely dissolved phases.[409] The mass distribution measurements among the three phases have shown that in all cases (73 water samples) most of the compound was in the freely dissolved phase, with only a small fraction (rarely >5%) associated with the DOC. About 40% of the least water soluble compounds, BaP and 2,2′,4,4′,5,5′-hexachlorobiphenyl (HCB), were particle associated. The results demonstrated that DOC could be different from particle organic matter and that the associations of the compounds with the two phases were unrelated. As a matter of fact there was no correlation between $\log K_{doc}$ and $\log K_{oc}$. Similar results were obtained with the same compounds in Green Bay waters,[410] except for the binding to DOC that was approximately 2–3 times the average for open Great Lakes waters.

Brannon *et al.*[411] examined the K_{doc} values of fluoranthene in pore water from 11 sediments. Concentrations of truly dissolved organic contaminants in pore waters are commonly estimated[412] by assuming constant partitioning between pore water (truly dissolved) and organic carbon in pore water. Measured values of K_{doc} for fluoranthene were not constant over the 11 sediments, and were over or underestimated by assuming that $K_{doc}=K_{oc}$. Therefore, current models[96,412] used to predict the fate of hydrophobic organic compounds may require modifications to account for the observed difference between K_{doc} and K_{oc}.

The DOM concentration may affect the value of the association constant. A decrease of the association constant of DDT by increasing the humic acid concentration has been observed.[402] The same effect has been detected in measuring the association constants for 26 PCB congeners with marine humic substances (HS).[413] A possible reason for this observation could be that an increase in HS concentration may increase humic–humic interaction, thus reducing the number of available sites for humic-hydrophobe association.

Also the binding affinity for BaP, benzanthracene, and anthracene to DHM decreases slightly as the concentration of DHM increases.[400] Landrum *et al.*[414] found that K_{doc} of some PAHs and PCBs does not depend on pollutant concentration but is inversely proportional to the concentration of DOC in solution. However, the trend toward decreased partition coefficients with increased HA concentration is relatively slight; it may be due to conformational differences of the HAs altering the pollutant binding and/or competition of the humics for binding sites on other humics.

However, Gauthier *et al.*,[415] using the fluorescence quenching method, did not detect any variation in the association constants of PAHs with the DOM concentration. The authors believed that this effect may be an artifact of the reverse phase method.[414]

Also Hassett and Milicic[416] in their study of

2,2′,5,5′-TeCB binding by Aldrich HA by gas purge technique found that K_{doc} is apparently independent of DOC concentration. On the contrary, Yin and Hassett[417] reported that, with increased HA concentration, the fraction of bound mirex increased, but K_{doc} showed a declining trend. This result was obtained using the same technique and indicated that binding may involve more complicated mechanisms than simple phase partitioning.

The magnitude of the binding interaction of DOM with 2,2′,5,5′-TeCB is affected by several parameters:[393] (i) K_{doc} decreases by increasing the pH of the medium, probably due to increased ionization of HA with increased pH; (ii) increasing ionic strength K_{doc} increases as a result of salting-out; (iii) K_{doc} decreases with decreasing molecular weight of Aldrich HA; (iv) HA extracted from soil and water samples has lower binding capabilities than Aldrich HA, but higher binding capabilities than fulvic acid (FA). Moreover, the K_{doc} increases with the degree of chlorination of the PCBs and decreases in general by increasing the number of the ortho-chlorines within groups of isomers; this latter result may be attributed to the fact that o-substitution increases the solubility of PCB isomers.[413]

An effect of the organic pollutant/DOM association is a general enhancement of the apparent water solubility of the pollutant.[187]

The solubility enhancement can be expressed[219,220] as

$$S_{\mathrm{w}}^{*}=S_{\mathrm{w}}(1+XK_{\mathrm{dom}}), \tag{18}$$

or

$$S_{\mathrm{w}}^{*}=S_{\mathrm{w}}(1+XK_{\mathrm{doc}}), \tag{19}$$

where S_{w}^{*} and S_{w} are the apparent water solubility in DOM or DOC solution and solubility in distilled water, respectively, X is the concentration of DOM or DOC. The apparent solute solubilities increase linearly with DOM concentration and show no competitive effect between solutes.

Webster *et al.*[418] measured by the generator column procedure the solubility of three dioxins in pure water and in water containing known amounts of HA. Three HAs were used, one isolated from soil, a second from water (peat bog), and a third commercial (Aldrich). The solubility of dioxin compounds increases in the presence of HA and also by increasing the temperature in the absence and in the presence of HA. The enhanced solubility in the presence of HA was employed to calculate the association constants of the dioxin compounds. The association constants decrease with the temperature. However, the data do not allow calculation of the exact value for ΔH of association, which is expected to be very low ($\leqslant$40 kJ mol^{-1}).

The aqueous solubilities of 1,2,3-TCBz, pentachlorobenzene (PCBz), and hexachlorobenzene (HCBz) in an aqueous phase isolated from a sediment–water suspension are significantly higher than those measured in distilled water. This effect has been attributed to the presence of a ''third phase'' material originating from the sediment,[133] which produces also a reduction of the experimental adsorption coefficient (K_{d}).

The effect of enhancing solubility is more pronounced with hydrophobic organic compounds exhibiting extremely low water solubilities, and high values of K_{ow} (p,p′-DDT, PCBs, etc.), while no noticeable water solubility enhancement is found for compounds like lindane and 1,2,3-TCBz.[220] The K_{dom} values of solutes with soil-derived HA are approximately four times greater than with soil FA and 5–7 times greater than with aquatic HA and FA. The effectiveness of DOM in enhancing solute solubility appears to be largely controlled by the DOM molecular size and polarity; less polar DOM forms stronger associations with organic chemicals and produces higher solubility effects. The K_{doc} values for pyrene with six marine HAs, five soil HAs, three soil FAs and Aldrich HA varied by as much as a factor of 10 depending upon the degree of aromaticity in the humic material.[188] An increase in aromaticity of the dissolved humic material may serve to increase the polarizability of the polymer and increase the strength of PAH binding. Thus, different sources of dissolved humic material in natural waters can have different affinities for binding organic contaminants.[400]

Chin and Gschwend[419] used fluorescence quenching to measure the binding of pyrene and phenanthrene to marine interstitial water organic colloids from two sites. Both compounds were sorbed by porewater colloids. Sediments and porewater colloids from a contaminated nearshore site were particularly effective sorbents for these compounds. It was observed that the high sorption coefficients may be due to the high lipid content of these sediments and colloids. Alternatively, they may be due to a very substantial nonpolar character of the natural organic matter there.

Fluorescence enhancement of pyrene in the presence of different HAs showed significant variations, leading to the conclusion that large soil HAs are more effective in isolating small molecules than smaller aquatic or structurally rigid HAs.[420]

Caron *et al.*[421] reported that the addition of HA extracted from sediments to the aqueous phase reduced the sorption of DDT to sediments, but had no effect on the sorption of lindane. In the absence of added DOC, the sediment–water sorption coefficient (K_{d},cm^3 g^{-1}) for DDT was 20 650, while in the presence of 6.95 mg dm^{-3} of DOC it was 5170. Using the free DDT concentration rather than the total aqueous phase DDT concentration, the value of K_{d} (19 776) was indistinguishable from the value obtained in the absence of added DOC (20,650). For lindane at the same conditions, the values of K_{d} were 84 and 90 in the absence and in the presence of added DOC, respectively. This result is consistent with the observation that the compound does not associate with humic material to any great extent.[220] Also sodium humate can solubilize DDT, whereas HA strongly adsorbs 2,4,5-T from solution.[187]

No enhanced solubility effects, due to the presence of DOM up to 100 ppm organic carbon, has been found for simazine, which shows a relatively high water solubility at 20 °C (3.5 ng/ml).[422] Adsorption experiments on sandy loam soil also demonstrated no statistically significant effect for simazine concentrations between 30 and 1900 mg ml^{-1} in the presence of 45 ppm soluble OC. Other authors[404,405] previously demonstrated a substantial effect of DOM on s-triazine adsorption. These contrasting results suggest the possibility that the interaction between DOM and nonionic organic compounds may be a function of the source from which the DOM is obtained.

Napropamide, which is more water soluble and therefore considered less hydrophobic than lindane and prometryn, had a greater extent of association with peat-dissolved humic acid (DHA), suggesting that hydrophobicity of nonionic pesticides is not the only factor governing their interaction with DOM.[423] When comparing DOM from several sources, DHA had a higher affinity than dissolved fulvic acid (DFA) for napropamide, DDT, and lindane. Association of napropamide with peat-DHA increased with increasing pH above pH 6.4, decreasing ionic strength, and decreasing charge on cations added to the system. In addition, DHA and DFA released from two soils showed a different affinity for napropamide compared to bulk soil organic matter. The relative efficiency of OM fractions taken from two soils in associating with napropamide is DHA>bulk OM>DFA. Dissociation studies showed that the interaction between napropamide and peat-DHA was not fully reversible.

Thus, the interaction PAH–DOM, measured on the basis of increased solubility, is dependent upon the "quality" of naturally occurring DOM.[424] An investigation carried out with a series of PAH indicated that these compounds do not undergo significant interaction with oceanic DOM at natural concentrations, while significant interactions are observed when terrestrial DOM is employed at naturally occurring concentrations. This difference seems due to the higher molecular weight of the terrestrial DOM. Also terrestrial humic substances are believed to originate from lignin whereas marine humics are believed to be primarily derived from marine plancton. These different origins result in marine humic substances having less aromatic and more aliphatic character, along with more protein and carbohydrate components.

The K_{doc} values of BaP and PCP with HAs and FAs extracted from river sediments and sea sediments or isolated from river water and sea water have been measured at pH values of 5.0, 6.5, and 8.0.[425] The results showed that HAs have a greater affinity for binding hydrophobic compounds than FAs and that K_{doc} values decreased as the polarity of the sorbent, measured by the ratio [(O+N)/C], increased. The binding of PCP with HAs strongly decreased with increasing pH, suggesting that only unionized form can interact with the humic material. Change in pH only weakly affects K_{doc} values for BaP.

Hassett and Anderson[426] found that DOM derived from natural water and sewage reduces the sorption of hydrophobic organic compounds by river- and sewage-borne particulate matter. They suggest that this observation is due to the formation of soluble complexes between the DOM and the compounds. DOM in water solution reduces also the amount of a nonpolar compound bound to soil or sediment. Therefore, the presence of DOM in natural systems can significantly affect the mobility of organic pollutants by increasing their transfer to groundwaters.[427]

Experiments[428] were carried out to evaluate the effectiveness of a solution of HA to enhance the removal of six aromatic hydrocarbons (benzene, toluene, p-xylene, ethyltoluene, sec-butylbenzene, and tetramethylbenzene) from a sandy material. None of the compounds were completely removed from the material. Nonetheless, the compounds with the highest water solubility, benzene and toluene, were removed effectively (up to 99%) with the use of either the HA solution or water. For the less soluble compounds, removal was more difficult and was enhanced by the HA solution compared to water.

Pierce *et al.*[173] reported that humic particles associated with chlorinated hydrocarbons may contribute to the transport of these pollutants from the water column to the sediment.

The effect of natural DOM on K_{d} values of PCP with soil was negligible at pH 5.2–6.1 and low concentration of PCP (<0.4 nmol cm^{3}).[106] At these conditions DOM showed no significant effect on PCP transport in a soil column. However, the PCP adsorption isotherms obtained from a higher concentration range of PCP (<3 nmol cm^{3}) showed that DOM may increase the adsorption of PCP on soil at pH 5.4 and 6.1. It appears that natural DOM may play an increasingly important role in the adsorption of PCP as the number of free "sites" decreases with higher PCP concentration. However the mechanism responsible for such a possible effect remains unclear and needs to be investigated.

Thus, if colloids are stabilizing hydrophobic organic contaminants in porewaters, then the transport of organic pollutants from sediments to overlying waters could be enhanced through a combination of bioirrigation and colloid sorption effecs.[419] They may also alter the transport of contaminants in the subsurface environment.[21] Column experiments demonstrated that the effect of the presence of macromolecules on the mobility of HCBz through soil was in the order: groundwater DOC>humic acid>dextran at respective concentrations of 50, 50, and 500 mg dm^{-3}.[429] Also the retardation factor of phenanthrene in a sand column was reduced by an average factor of 1.8 in the presence of DOM derived from soil, suggesting that a phenanthrene-DOM "complex" enhanced the transport of phenanthrene.[430] The same effect of enhanced mobility in the presence of DOC was evidentiated studying 2,2′,4,4′,5,5′-HCB transport through columns containing aquifer material.[431] Contaminant mobility was found to increase as solution DOC concentrations were incrementally changed from 0 to 20.4 mg dm^{-3}. Thus, the fate and transport of contaminants in groundwaters can be studied on the basis of three-phase distribution (immobile solid phase, mobile solution phase, and mobile colloidal phase or DOC).

The one-dimensional transport of a single solute in porous media, assuming constant fluid flow in a homogeneous matrix, can be described by a convection–dispersion equation

$$(\rho/\theta)\partial q/\partial t+\partial C/\partial t=D\partial^2 C/\partial X^2-V\partial C/\partial X, \quad (20)$$

where ρ is the porous medium bulk density, θ is the volumetric water content, q is the total adsorbed solute per unit mass of solid, t is time, C is the resident concentration of solute in the mobile phase, D is the dispersion coefficient reflecting the combined effects of diffusion and hydrodynamic dispersion on transport, X is the distance, and V is the mean pore water velocity. Contaminant distributions in field samples are usually characterized by total solution and solid phase measurements; thus, C can contain solutes in the truly dissolved form and/or solutes in a colloidal or colloid-associated phase. It has been shown[432] that for solutions containing DOC, the "three-phase" distribution relationships, represented by Eqs. (21)–(23), can be incorporated into Eq. (20) using Eq. (25) to account for the presence of two mobile solute phases in porous media

$$K_d = q/C_{aq}, \tag{21}$$

$$K_{app} = q/(C_{aq} + C_{doc}[\mathrm{DOC}]), \tag{22}$$

$$K_{app} = K_d/(1 + K_{doc}[\mathrm{DOC}]), \tag{23}$$

$$R_t = 1 + (\rho K_{app}/\theta), \tag{24}$$

$$R_t = 1 + (\rho/\theta)[K_d/(1 + K_{doc}[\mathrm{DOC}])]. \tag{25}$$

In Eqs. (21)–(25), K_d is the equilibrium distribution of the contaminant in the absence of mobile DOC, K_{app} (apparent K_d) is the equilibrium distribution of the contaminant in the presence of mobile DOC, q is the solid-phase contaminant concentration, C_{aq} is the aqueous phase contaminant concentration, C_{doc} is the colloidal-associated contaminant in the mobile phase, R_t is the net retardation factor, [DOC] is the concentration of dissolved organic carbon in the mobile phase, and $K_{doc} = C_{doc}/C_{aq}$ is the distribution coefficient of the contaminant between DOC and water.

The general form of the transport equation can be obtained combining Eqs. (20) and (24)

$$R_t \partial C/\partial t = D\partial^2 C/\partial X^2 - V\partial C/\partial X. \tag{26}$$

Selection of Eq. (21) or Eq. (23) for use with Eq. (26) will depend on the presence or absence of mobile DOC. The authors[431] then introduced the two-sites transport model[433] (Sec. 10), which assumes instantaneous adsorption on type-1 sites and first-order kinetic controlled adsorption on type-2 sites to account of possible nonequilibrium for contaminant interactions with the solid phase (Sec. 9). The adsorption rate for type-2 sites is described by

$$\partial q_2/\partial t = \alpha[(1-F)K_{app}C - q_2],$$

where q_2 is the concentration of adsorbed solute on type-2 sites, F is the fraction of type-1 sites, and α is the first order rate coefficient. For a two-site adsorption process, Eq. (26) now takes the form of

$$\beta R_t \partial C/\partial t + \rho/\theta\, \partial q_2/\partial t = D\, \partial^2 C/\partial X^2 - V\, \partial C/\partial X,$$

where $\beta = (\theta + F\rho K_{app})/(\theta + \rho K_{app})$ is a dimensionless variable related to the fraction of type-1 sites.

Equation (23) was used to obtain K_d and K_{doc} values for anthracene, HCBz, and pyrene from batch and column experiments with soil and aqueous solutions containing dextran, humic acid, and groundwater DOC.[429]

Binding of BaP to DOM and to particles was measured for each sorbent and in a mixed system containing both dissolved and particulate sorbents.[434] DOM competed with particles for binding of the dissolved contaminant and reduced the amount bound to particles. Binding was independent and noninteractive. Significant errors in estimating the environmental partitioning and bioavailability of very hydrophobic compounds can result if the role of DOM as a competitive sorbent is ignored. The influence of DOM is greatest when suspended particle concentrations are low, such as in lakes and streams, or when DOM levels are high, such as in swamps and bogs. In most cases, only the very hydrophobic contaminants ($K_{ow} > 10^5$) will be significantly affected by binding to DOM, but these compounds constitute the greatest concerns in terms of human health and environmental persistence.

Thus, association of organic contaminants with dissolved humic substances reduce their bioavailability and toxicity.[435–438] The bioconcentration of dehydroabietic acid and BaP into Daphnia magna is significantly lower in the presence of such substances when compared with a standardized soft freshwater.[439] Moreover, an increase in humus concentration decreases the bioavailability of BaP in a logarithmic manner.[440] However, this effect is not observed with PCP, because at the pH of the experiment (6.6) it is in ionic form and does not associate with humic materials.[439] Association constants of hydrophobic chemicals with three fractions (hydrophobic-acid, hydrophobic-neutral, and hydrophilic subcomponents) of DOC from a stream water were measured.[441] The total water and the different DOC fractions reduced the uptake and accumulation of benzo(a) pyrene and 2,2′,5,5′-HCB by Daphnia magna in proportion to the capacity of the DOC for binding the contaminants.[442] Besides the quantity the qualitative differences in the nature of organic material from different sources also have a large effect on its affinity for binding lipophilic organic xenobiotics.[443] The aromaticity and the portion of hydrophobic acids in DOM can play an important role.

7. Cosolvent Effect

Sorption coefficients for HOC are generally measured in aqueous systems and, therefore, may not be always applicable to the prediction of groundwater contamination due to the presence of waste disposal or treatment sites. In these situations often pollutants are in solution of water and various water-miscible organic solvents. It is therefore necessary to develop a more general approach for describing sorption of HOC on soils from aqueous and mixed solvent systems.[444] Rao *et al.*[445] applied the "solvophobic theory" for predicting sorption of HOC by soils from both water and aqueous–organic solvent mixtures. This approach was already adopted by Amidon *et al.*[446] and Yalkowsky *et al.*[447] for predicting the solubility of nonpolar and polar solutes in polar solvent mixtures.

Yalkowsky *et al.*[448] have shown that the solubility of a hydrophobic organic compound in a binary mixed solvent (water and water-miscible organic solvent) can be related to the aqueous solubility through the equation

$$\log X^{\mathrm{m}} = \log X^{\mathrm{w}} + \sigma^{\mathrm{c}} f^{\mathrm{c}}, \tag{27}$$

where X is the solubility in mole fraction with superscripts m and w indicating "mixed solvent" and "water;" f^{c} is the volume fraction of cosolvent. The parameter σ^{c} is a function of the solvent surface tension and of the solute hydrophobic characteristics. Yalkowsky *et al.*[447] suggested for the value of σ^{c} the following expression:

$$\sigma^{\mathrm{c}} = (\Delta\gamma^{\mathrm{c}}\mathrm{HSA}/kT) + (\Delta\varepsilon^{\mathrm{c}}\mathrm{PSA}/kT), \tag{28}$$

where HSA and PSA are the hydrocarbonaceous and polar surface areas of the solute molecule (nm^2), respectively; $\Delta\gamma^{\mathrm{c}}$ and $\Delta\varepsilon^{\mathrm{c}}$ are the interfacial free energies ($\mathrm{J\ nm^{-2}}$) of the solvent at the hydrocarbonaceous and polar surface areas at contact with the solute, respectively; k is the Boltzman constant ($\mathrm{J\ K^{-1}}$); and T is the absolute temperature (K). Equation (28) for many HOC can be approximated to[448]

$$\sigma^{\mathrm{c}} = (\Delta\gamma^{\mathrm{c}}\mathrm{HSA}/kT),$$

σ^{c} may be determined by the logarithm of the ratio of the hydrophobic compound solubilities in pure cosolvent (X^{c}) and in pure water (X^{w})[449,450]

$$\sigma^{\mathrm{c}} = \log(X^{\mathrm{c}}/X^{\mathrm{w}}).$$

Morris *et al.*[451] have demonstrated that σ^{c} can be correlated to K_{ow}

$$\sigma^{\mathrm{c}} = a \log K_{\mathrm{ow}} + b,$$

where a and b are empirical constants unique for a given cosolvent.

For multiple cosolvent systems, Eq. (27) becomes

$$\log X^{\mathrm{m}} = \log X^{\mathrm{w}} + \Sigma \sigma_{\mathrm{i}} f_{\mathrm{i}},$$

where f_{i} is the volume fraction of cosolvent i and σ_{i} corresponds to the logarithm of the ratio of the solubilities of the chemical in the pure solvent i and in water.

This approach was then adopted[445] to explain the decrease of the sorption coefficients and, consequently, the enhanced mobility of the organic chemicals through porous media due to the presence of a cosolvent in the aqueous solution.

Karickhoff[52,96] derived the following equation, relating K_{oc} to water solubility and including a "crystal energy" term (Sec. 12.2) for solutes which are solid at ambient temperature

$$\log K_{\mathrm{oc}}^{\mathrm{w}} = -\alpha \log X^{\mathrm{w}} - [\Delta S_{\mathrm{f}}(T_{\mathrm{m}} - T)]/(2.303RT) + \beta, \tag{29}$$

in which α and β are regression-fitted parameters. Equation (29) has been extended for binary solvent mixture[444]

$$\log K_{\mathrm{oc}}^{\mathrm{m}} = -\alpha \log X^{\mathrm{m}} - [\Delta S_{\mathrm{f}}(T_{\mathrm{m}} - T)]/(2.303RT) + \beta. \tag{30}$$

Replacing $\log X^{\mathrm{m}}$ by Eq. (27) and rearranging terms

$$\log K_{\mathrm{oc}}^{\mathrm{m}} = \log K_{\mathrm{oc}}^{\mathrm{w}} - \alpha\sigma^{\mathrm{c}} f^{\mathrm{c}}.$$

Taking into consideration that $K_{\mathrm{d}} = K_{\mathrm{oc}} f_{\mathrm{oc}}$, we obtain

$$\log K_{\mathrm{oc}}^{\mathrm{m}}/K_{\mathrm{oc}}^{\mathrm{w}} = \log K_{\mathrm{d}}^{\mathrm{m}}/K_{\mathrm{d}}^{\mathrm{w}} = -\alpha\sigma^{\mathrm{c}} f^{\mathrm{c}}. \tag{31}$$

In these equations, K_{d} is the sorption coefficient and the superscripts m and w refer to mixed solvent and water, respectively. The parameter σ^{c} explicitly accounts for sorbate–solvent interactions and is assumed to be independent of the sorbent.[445] α is an empirical constant which accounts for solute–sorbent or cosolvent–sorbent interactions. It should approach unity if the fugacity coefficient for solute in soil/sediment organic carbon is relatively independent of solute,[52] and if the soil organic carbon properties are independent of change in solution phase composition. Equation (31) shows that the relative sorption coefficient ($K_{\mathrm{d}}^{\mathrm{m}}/K_{\mathrm{d}}^{\mathrm{w}}$) decreases exponentially as the fraction of organic cosolvent (f^{c}) increases.[340,452–454]

For a mixture of water and multiple cosolvents Eq. (31) becomes[446]

$$\log K_{\mathrm{d}}^{\mathrm{m}} = \log K_{\mathrm{d}}^{\mathrm{w}} - \alpha \Sigma \sigma^{\mathrm{c}} f^{\mathrm{c}},$$

where f^{c} and σ^{c} refer to each solvent in the mixture. Therefore, $(f^{\mathrm{w}} + \Sigma f^{\mathrm{c}}) = 1$.

It is important to recognize[454] that in Eqs. (29)–(31) the units of K_{oc} must be consistent with the expression of solubility in terms of mole fraction. This is not strictly necessary when Eq. (29) is used to compare different values of $\log K_{\mathrm{oc}}^{\mathrm{w}}$ (Sec. 12.2). In this case the partition coefficient may be employed with customary units of $\mathrm{dm^3\ kg^{-1}}$; the number of moles per liter is constant for dilute aqueous systems, i.e., 55.34 $\mathrm{mol\ dm^{-3}}$, and this value becomes incorporated in the regression constant β. However, for the case of solvent/water mixtures, the total number of moles per liter is not constant and the partition coefficient must be expressed in units of $\mathrm{mol\ kg^{-1}}$. Thus, Eq. (31) becomes

$$\log\{[K_{\mathrm{d}}(V^{\mathrm{w}}/q^{\mathrm{w}} + V^{\mathrm{s}}/q^{\mathrm{s}})]/[(K_{\mathrm{d}}^{\mathrm{w}}(55.34)]\} = -\alpha\sigma^{\mathrm{c}} f^{\mathrm{c}},$$

where V refers to the solute-free volume of water or solvent in the mixtures, and q represents the molar volume of water or solvent.

The solvophobic theory was tested by Nkedi-Kizza *et al.*[455] measuring the sorption of anthracene and two herbicides (diuron and atrazine) by five soils from aqueous solutions and binary solvent mixtures consisting of methanol–water and acetone–water. Using the batch equilibration method, the Freundlich constants were obtained for a given sorbate–soil combination and for each solvent mixture. For each sorbate, the $\log K_{\mathrm{d}}^{\mathrm{m}}$ ($\mathrm{dm^3\ kg^{-1}}$) value decreased log linearly as the fraction organic cosolvent (f^{c}) increased. The slope of $\log K_{\mathrm{d}}^{\mathrm{m}}$ vs f^{c} plots, designed as σ^{c}, was unique to each sorbate–solvent combination and was independent of the soil (sorbent). Thus, the organic cosolvent effects on sorption could be specified by a single parameter (σ^c), which combines the coefficients characterizing solvent and the sorbate properties. The solvophobic model does not explicitly account for the possible effects of the solvent on the sorbent. Deviations from log-linear relation between K_d^m and f^c for sorption from acetone–water mixtures were attributed to this effect. The sorption coefficients of low solubility compounds (anthracene) from aqueous solutions (K_d^w) are difficult to measure. However their value can be derived by extrapolating the values obtained from mixed solvents to $f^c = 0$. The same authors[452] verified this theory also by measuring the sorption and leaching of diuron and atrazine in soil columns eluted with aqueous solutions and binary solvent mixtures of methanol and water. The retardation factor (R^m) for both herbicides decreased drastically as the volumetric fraction of organic cosolvent (f^c) was increased in the binary solvent mixture. The log-linear decrease in ($R^m - 1$) observed with increasing f^c was well predicted by the solvophobic theory. All breakthrough curves (BTCs) were asymmetrical in shape, but the extent of asymmetry decreased with increasing f^c for $0 \leq f^c \leq 0.5$. At $f^c = 0.5$, the BTCs for both diuron and atrazine were similar in shape (symmetrical and sigmoidal) and location ($R^m = 1$) to that of tritiated water, a nonadsorbed tracer.

In a further study[444] the application of a solvophobic approach for predicting the sorption of HOC was evaluated with data collected using synthetic sorbents and soils. The experimental data consisted of batch equilibrium sorption coefficients, as well as soil-thin layer chromatography (TLC) and reversed-phase liquid chromatographic (RPLC) retention factors. All data were collected using aqueous solutions and binary or ternary solvent mixtures of water, methanol, acetone, and acetonitrile. As predicted by the theory, the chromatographic retention factors and sorption coefficients for HOC decreased log-linearly with increasing fraction of organic cosolvent in binary solvents. Reasonable agreement was found between model parameters reported in the literature and those estimated using the data from batch sorption, soil-TLC and RPLC studies.

Fu and Luthy[454] measured sorption of naphthalene, naphthol, quinoline, 3,5-dichloroaniline onto three different soils from methanol-water and acetone-water mixtures. It was observed that the sorption partition coefficients, expressed in units of mol kg^{-1}, decreased semilogarithmically with increase in volume fraction of solvent in the aqueous phase. The decrease of the sorption partition coefficients were expressed in terms of the parameter σ and the value $\alpha\sigma$, which is the logarithmic term with which sorbent sorption coefficient decreases with volume fraction solvent in water. It was concluded from this evaluation that the parameter α was typically in the range of 0.44–0.57 with an average value of 0.51. The magnitude of the α values show that the logarithmic decrease of sorption partition coefficient is about half of that which could be expected on the basis of the logarithmic increase in solute solubility in the solvent/water mixtures. This may be a result of the solvent/water mixture swelling the organic carbon associated with the soil, and thereby increasing solute accessibility to the organic matter. It was shown that the more hydrophobic the solute, the greater the effect of solvent in solvent/water mixtures on solute solubility enhancement, and hence the less the tendency to sorb onto soil. Thus the results of this investigation are particularly significant for those aromatic solutes exhibiting lowest aqueous phase solubility. The authors recalculated the sorption coefficients (dm^3 kg^{-1}) reported by Nkedi-Kizza *et al.*[455] for anthracene in terms of mol kg^{-1}. Then, to compute the α value for anthracene sorption onto soil, they regressed $\log K_d$ against volume fraction solvent and divided the regression coefficient by the appropriate value of σ. Values of $\alpha \approx 0.67$ for methanol/water system and $\alpha \approx 1.1$ for acetone/water system were found. These values, larger than those found by the authors[454] may signify that the solvent did not have as large an impact on improving the accessibility of the solute to the organic carbon.

Walters and Guiseppi-Elie[456] studied the sorption of 2,3,7,8-tetrachlorodibenzo-p-dioxin (TCDD) to soils from water methanol mixtures. Volume fraction methanol in the liquid phase (f^c) was varied between 0.25 and 1.0. Sorption isotherms were linear and, when sorption partition coefficients in cm^3 g^{-1} were converted to mol g^{-1}, their values were log-linearly related to f^c. The K_d^m values for two soils, when normalized on f_{oc}, gave values of K_{oc}^m that collapsed onto a single line having the equation determined by linear regression analysis

$$\log K_{oc}^m = -4.97 f^c + 5.30. \tag{32}$$

The intercept value of 5.30 in Eq. (32) is equal to the logarithm of the aqueous-phase partition coefficient for TCDD expressed in units of mol g^{-1}. This value can be converted to correspond to conventional dimensionless units by adding to it $\log V$ for water ($\log V = 1.26$). The value of $\log K_{oc}$ (cm^3 g^{-1}) for aqueous phase sorption of TCDD to soils determined in this way is 6.6±0.7. The slope of −4.97 corresponds to the term $-\alpha\sigma^c$ of Eq. (31). The value of σ^c for TCDD in water/methanol systems, which is estimated to be 6.2, corresponds to the slope of the log-linear relationship between mole fraction solubility and f^c. The apparent value of α was calculated by dividing $\alpha\sigma^c$ by σ^c. For water sorption of hydrophobic solutes, α is expected to range from 0.7 to 0.92. For sorption of TCDD from water/methanol mixtures, a value for α of 0.80 was observed. The authors reported for some compounds the α values which increase as $\log K_{ow}$ increases. The prewashing of the soils with methanol prior to use in sorption experiments apparently does not modify the sorptive behavior of TCDD.

The influence of an organic cosolvent (methanol) on the sorption and transport of three HOC, naphthalene, phenanthrene, and diuron in a sandy surface soil was investigated using both batch equilibration and column miscible displacement techniques.[457] The sorption constant values obtained from the two techniques were comparable and exhibited an inverse log-linear dependence on the volume fraction (f^c) of methanol in the mixed solvent. The slope of the plot was approximately equal to the logarithm of the ratio of the compound solubilities in neat cosolvent and water. Long-term exposure to methanol-water mixtures had little effect on sorption and transport properties of the soil, but column retardation factors were influenced by the short-term solvent exposure history prior to solute elution.

Equilibrium batch isotherms for neutral and ionized PCP with Weber soil were measured also in methanol-water systems at pH<3 where PCP is completely undissociated and at pH>9 where PCP is completely dissociated.[339] An inverse log-linear relationship, as described in Eq. (31), was observed between K_d and the volume fraction of methanol (f^c) for sorption of neutral and ionized PCP. The slope of the log-linear relationship ($\alpha\,\sigma^c$) for ionized PCP is smaller than that for neutral PCP. This reflects a change in the degree of hydrophobicity between the two species and also suggests the dominance of solute–solvent interactions with transfer of some type of neutral ion pair from solution.

The effect on the solubility of HOCs due to the presence of a partially miscible organic solvent (PMOS) in a completely miscible organic solvent (CMOS)/water system was examined.[458] It has been found that nonpolar PMOSs (e.g., toluene and TCE) did not appreciably increase HOC solubility, while polar PMOSs (e.g., o-cresol and nitrobenzene) did significantly enhance HOC solubility. Polar PMOSs have greater cosolvent effects because they are present in greater concentrations as a result of their higher aqueous solubilities. These changes in solubility of HOCs results in corresponding inverse variations of sorption coefficients on soil systems.[459] The presence of nonpolar PMOSs does not significantly influence HOC sorption by soils. In contrast, polar PMOSs have sufficiently high aqueous solubilities that significant decreases in HOC sorption can be measured.

The sorption data collected with mixed solvents can be extrapolated to provide reliable estimates of both equilibrium (solubility, K_d) and nonequilibrium parameters for sorption of organic chemicals from aqueous solutions.[460] The use of mixed solvents is advocated especially for the more hydrophobic compounds ($\log K_{ow}>4$), because it greatly facilitates batch and column experimentation and minimizes experimental artifacts. Methanol is recommended as the cosolvent of choice, because data from mixed-solvent systems best conform to the log-linear cosolvency model. Furthermore, this method of determination of K_d on sediments allows us to minimize the effects of the presence of colloids and DOC and the effect of the sediment concentration.[461]

8. Effect of Sorbent Concentration or "Solids Effect"

Sorption of a chemical on soil/sediment is generally treated as its distribution or partition between two homogeneous phases, which can be totally separated. Thus, the distribution coefficients should be independent on the concentration of sorbent.

However, the results of several laboratory studies[86] demonstrated an inverse relationship between partition coefficient and concentration of adsorbing solids. The "solids effect" is most pronounced for constituents characterized by large partitioning. For constituents that are represented by intermediate partitioning, the effect of the solid concentration is less pronounced, and the coefficient approaches a constant value for substances of low partitioning. This effect has been found with a variety of elements and organic compounds sorbed on various solids; the K_d values may decrease of some orders of magnitude when the range of solid concentration (10–10.000 mg dm^{-3}) covers values normally existing in natural water systems. It has been suggested a power-law dependence of the partition coefficient on the concentration of solids. This effect may have very serious consequences in assessing the fate of hydrophobic pollutants in natural water systems, because it means that the pollutant sorbed on suspended solids and accumulated in sediments can be released to the interstitial water.

The sorption of linuron and atrazine on Begbroke soil was studied as a function of the soil to water ratio.[462] A fivefold increase in the sorption of linuron was found under 1:10 than at 4:1 ratio. The sorption in a 1:1 soil:water mixture was intermediate. For atrazine the difference between slurry conditions and the 4:1 ratio was approximately threefold. Also lindane sorption was shown to be affected by sediment suspension concentration.[463] A 50-fold increase in the water-to-sediment ratio effects approximately a 1.5 times increase in adsorption at an equilibrium concentration of 1 ppm of lindane (K_f value).

Voice *et al.*[464] found that the linear regression of $\log K_d$ as a function of log (concentration) of three Lake Michigan sediments for MCBz, naphthalene, 2,5,2′-trichlorobiphenyl (TCB), and 2,4,5,2′,4′,5′-HCB had an average value of the slope of −0.47, indicating approximately an order of magnitude increase in partition coefficient for every 2 orders of magnitude decrease in solid concentration.

Weber *et al.*[465] found that the slope of the relationship varied from −0.16 to −0.92 with an average value of −0.40 with Aroclor 1254-river sediments or montmorillonite systems.

Di Toro *et al.*,[466] in order to quantify the effect of suspended solids in sediment interstitial water, determined the diffusion coefficient and the partition coefficient of 2,2′,4,4′,5,5′-HCB in a sediment by using a dual radio-tag experiment that extended over 2 yrs. They found that the partition coefficient is in close agreement with that predicted from hydrophobic sorption correlations based upon sediment organic carbon and K_{oc}. It also corresponds to the low particle concentration limit of the partition coefficients found when batch equilibrations of dilute suspensions of the same sediment were used. The conclusion is that, whatever the reason for this behavior is, it appears that the partition coefficient that applies to interstitial water-sediment sorption is the low particle concentration limit obtained in suspended sediment experiments. However, Horzempa and Di Toro[467] reported that, under approximately constant equilibrium concentration of the same HCB compound (~7 mg dm^{-3}), values of K_d for adsorbed HCB on Saginaw Bay sediment decreased by approximately a factor of 4, as sediment concentrations were increased from 10 to 1000 mg dm^{-3}.

Further evidence of the effect of suspended sediment concentration (SSC) on the K_d value was given by Servos and Muir[468] with their work regarding the sorption of 1,3,6,8-TCDD on lake sediments. The sediment to water partition coefficient was determined for suspended sediment concentrations ranging over 4 orders of magnitude. The truly dissolved (free) concentrations were estimated by four different methods: centrifugation at 6000 g for 15 min, centrifugation at 20 000 g for 30 min, reverse-phase C18 cartridges,[414] and dynamic headspace analysis.[417] The slope of the relationship between $\log K_d$ and log SSC resulted in being significantly less negative for the last two methods than for the first two. However, the four measurements did not completely eliminate the negative correlation. The data of the $\log K_d$s obtained as a function of log SSC were extrapolated at zero sediment concentration. Four values were obtained with the four methods; they ranged between 5.98 and 6.23 cm^3 g^{-1}.

Celorie *et al.*[469] demonstrated by batch sorption tests that, as the solid (kaolinite) concentration (SC) increased from 0.01 to 270 g dm^{-3}, the K_d for phenol decreased 4 orders of magnitude, demonstrating the solids effect. A regression of $\log K_d$ as a function of log SC gave a slope of -0.95. This value is consistent with similar data for heavy metal sorption to quartz and montmorillonite (-0.67, -0.91)[470] and for PCB sorption to lake sediments (-0.68).[471] It was observed[469] that the batch tests may be affected by the solids effect; therefore column studies may be conducted to estimate K_d values by modeling the generated breakthrough curves with a solute transport model. However, column studies conducted with fine grained soils require a long time to be completed. Thus a centrifugation procedure of the soil column was suggested to alleviate these disadvantages, by imposing a confining stress on the soil, and by producing a greater pore water velocity. K_d values obtained in the centrifuge experiments were compared with K_d values measured in batch equilibrium tests. Although the K_d values determined in the centrifuge were slightly lower than the values predicted by extrapolating the batch data, the results were consistent with the solids effect.

9. Desorption and Nonsingularity in Sorption–Desorption Process

A sorption process is sometimes reversible, however often a "hysteresis" effect is observed.

The lindane desorption from 32 soil samples, with the exception of a lacustrine soil, was complete and independent of all soil variables and the amount of lindane sorbed.[119]

Desorption of chlorinated benzenes from river sediments has the same time scale as the sorption process.[155] Both sorption and desorption processes were completed in about 2 d.

A variety of laboratory batch and column experiments have been conducted to elucidate the sorption behavior of halogenated alkenes and benzenes in a river water–groundwater infiltration system.[207] The results of this study indicated that, for concentrations typically encountered in natural waters, the sorption of these compounds by aquifer materials was reversible.

No significant differences were found by comparing constants of adsorption and desorption for halogenated aliphatic and aromatic compounds using several different soil materials.[472]

No hysteresis effects were observed in the desorption of pyrene and methoxychlor from sediment coarse silt fraction.[108]

Also the binding of BaP to dissolved humic material was completely reversible and the extent of reversibility was unrelated to the sorption time.[400]

Adsorption of napropamide and bromacil on soils[277] and adsorption of parathion on organic matter extracted from soil were all reversible.[147] Also metribuzin-soil systems showed little tendency for irreversible sorption.[288]

Desorption of PCE or 1,2-dibromo-3-chloropropane from aquifer sediment (0.19% OC) was monitored following sorption for 6 or 30 d.[473] The compounds were desorbed by a purge technique in which a third phase of Tenax polymeric adsorbent beads provided a sink for desorbed chemical, thereby simulating desorption to infinite dilution. More than 95% of the initial sorbed compound was desorbed within the first 4 d, but a persistent fraction (0.4%–1%) remained associated with the sediments for at least 35 d.

Rogers *et al.*[170] demonstrated with desorption experiments that 3% of the initial benzene remained sorbed to two soils, while 32% remained on the Al-saturated clays and 1% on the Ca-saturated clays. Also sorption-desorption of fluorene with aquifer materials showed hysteresis effect.[199]

Adsorption–desorption studies of DDT with clay minerals, marine sediment, and humic acid showed that adsorption on clays and sediment was almost reversible, while that on humic acid was not.[173] The very low apparent equilibrium shift observed for desorption from sediment probably was due to DDT desorption from the more abundant mineral fraction and to alteration of the humic acid polymer in the sediment, due to interaction with clay minerals.

Sorption of PAHs on sediments was achieved in few hours, but a drastic change in the ease of extraction with hexane of sorbed chemical was frequently observed with increased incubation time.[151]

Desorption of PCBs from Glendale soil was minimal, between 2% and 9.5% per cycle depending on the equilibrium solution concentration.[474] The addition of sewage sludge to the soil increased PCB adsorption, while desorption was minimal, although depended on the incubation time. These data suggest that the transport by soil water of PCBs associated with sewage sludge additions should be minimal.

Hance[144] reported that the desorption of four herbicides, monuron, linuron, atrazine, and chlorpropham, from two soils, a soil OM fraction and bentonite appeared to be somewhat slower than adsorption. A period of 24 h or less was taken for equilibria to be established in adsorption processes. However, in seven cases out of eighteen the desorption equilibrium had not been attained after 72 h. It appeared that, when the value of the Freundlich constant $1/n$ was 1 or nearly so, the desorption equilibrium was achieved in less than 24 h. The systems showing low values of $1/n$ were those involving the ureas and bentonite or soil, for which desorption is slower. This suggests the possibility that some mechanism involving penetration of the interlayers of expanding clay minerals may operate.

Urea herbicides were easily desorbed from a sandy loam soil (1.77% OM) and a heavy clay soil (4.15% OM), but not from a high organic loam soil (10.5% OM).[260] The same trend of decreasing desorption rate with increasing OM content in four soils was found for fensulfothion and its sulfide and sulfone derivatives.[261] Trifluralin and triallate were readily desorbed from montmorillonite by water, with minimal desorption for peat moss, cellulose triacetate, and wheat straw.[475]

The variability of diuron desorbed from arid-zone soils low in organic matter was basically due to diuron initially adsorbed.[271] As in adsorption, desorption could be predicted from SA or CE and not from OC content in soils. Other authors found that desorption of diuron from sediments was related to the amount of OM present.[257] As reflected in the difference between the sorption slope and the desorption slope, sediments low in organic matter readily desorbed diuron. As the organic matter increased, the differences between the slopes increased. The resistance to desorption, which can be considered a measure of the binding energy, of diuron and monuron sorbed on sugar cane soils has been found to be related to adsorptive capacity.[255] Thus, in highly adsorptive soils these herbicides are not active enough to be used.

Fluometuron sorbed on a loam soil showed hysteresis effect.[476] The same effect was found with fluometuron when a soil was subjected to seven consecutive desorption equilibrations.[118] It was suggested that the shift in the sorption equilibria with repeated equilibration was most likely due to a physical change in the sorptive character of the soil complex. This change may be associated with increased dispersion or weathering of the clay–organic matter microaggregates with repeated wetting and shaking, resulting in an increased number of sites available for sorption. This explanation was similar to that suggested by Grover and Hance[462] to explain the effect of soil/water ratio on sorption of linuron and atrazine.

Graham-Bryce[262] reported that adsorption of disulfoton by soil was fully reversible if desorption took place immediately after uptake when soils were still wet, but the release was modified when the soils were allowed to dry thoroughly between adsorption and desorption. However, with dried soils values of K_f were larger and values of $1/n$ smaller, indicating that drying made desorption more difficult. Moreover desorption became progressively more difficult as insecticide was removed.

Monuron, atrazine, and prometryne were reversibly adsorbed to montmorillonite even when the clay plus adsorbed herbicide was dried to a constant weight at 62% relative humidity.[477] With peat there was an indication that some monuron, linuron, atrazine, and prometryne became irreversibly sorbed after a period of time. Thus, irreversible sorption to the OM in soil may be a mechanism by which some herbicides become phytotoxically inactive in the field.

The sorption and desorption of atrazine and linuron with sediment/water (1:9) mixtures are initially very fast, approaching 75% of equilibrium values within 3–6 min.[478] Herbicide sorption on the sediments was completely reversible after 2 h of sorption time. Talbert and Fletchall[145] reported that s-triazines could be eluted gradually with water; however, the sorption reaction was not completely reversible as indicated by the small amounts of simazine (10%) and atrazine (19%) not released during the course of the experiment. Desorption of atrazine from geologic materials (0.09%–0.33% OC)[479] and soils (2.6% and 2.8% OC)[480] indicated hysteresis.

Soil samples containing residues of the herbicides atrazine and metolachlor were collected from fields 2–15 months after their application to assess the sorptive reversibility of these residues.[481] The results indicated that these contaminated samples can contain a fraction of labile compound ranging from 0.056 to 0.60 inversely related to the age of the residue.

Desorption of K_f values of atrazine from field aging residue increased slightly with aging.[482] Also Ma *et al.*[483] reported that desorption of atrazine from soil deviated significantly from adsorption data. The deviation was more pronounced as incubation time increased from 1 to 24 d.

Also atrazine adsorbed on two Ca^{2+}, Mg^{2+}, and Na^+ saturated soils shows hysteresis effects indicating that adsorption and desorption of this compound are irreversible reactions.[127] Desorption of atrazine from a clay loam soil is affected by temperature and pH.[286] The average recovery was 85% at 0.5 °C and 98% at 30 and 40 °C. An increase of temperature should increase desorption for two reasons: desorption is endothermic and solubility increases with the temperature. Desorption also increased as pH increased: the recovery was 89% from the soils at pH 3.9 and 4.7 while 98% was recovered from the soil at pH 8.0. Desorption of atrazine from humic acid was quite low. The average recovery was only 11% with humic acid at pH 2.5, while 69% was recovered when the pH was raised to 7.0. Desorption experiments were carried out in batch for the same time (2 h) as sorption experiments.

Clay and Koskinen[158] reported that nondesorbable alachlor (as determined after methanol extraction) generally increased on a Waukegan (W) silt loam and a Ves (V) clay loam during five 0.01 M $CaCl_2$ desorptions. Atrazine was totally extracted with methanol from W soil after one desorption with 0.01 M $CaCl_2$. However, after five desorptions with 0.01 M $CaCl_2$ an average of 5.5 and 15.5% of the total recovered atrazine from two atrazine application rates was methanol nondesorbable from the W and V soils, respectively.

Laboratory studies showed that more than 95% of applied permethrin was adsorbed on lake sediment with OM content of 43%, but less than 10% of the adsorbed insecticide was desorbed by four 10 mL water rinses.[126]

The desorption of dipropetryn and prometryn was investigated after a series of adsorption experiments using six adsorbent materials possessing a wide range of physicochemical characteristics (CE, clay content, OM content, pH).[299] Generally, less dipropetryn than prometryn was desorbed after any given extraction. The adsorbents showing the greatest amount of adsorption also showed the least amount of desorption. The clay and OM content in each soil appeared to significantly decrease the amount of herbicide desorbed from the soil matrix. The shape of the desorption isotherms also appeared to be influenced by the presence of the OM. With a sorbent of sand plus muck having an OM content of 2.1% and with a clay loam soil of 2.8% OM the isotherms were nearly flat ($1/n \sim 0.0$) at low herbicide concentrations. This suggests that the herbicide was firmly attached to the adsorbent and difficult to remove or irreversibly adsorbed.

The adsorption–desorption studies showed that the aqueous solution leached only a small quantity of the aldrin adsorbed by the soil.[138] The desorption rate from the soils was inversely proportional to their OM content. Also desorption of parathion from attapulgite modified with treatment with an organic cation (hexadecyltrimethylammonium) was lower than desorption from the unmodified clay.[235]

It has been demonstrated that parathion sorbed on OM extracted from soil is reversibly released,[147] while a hysteresis effect was found when parathion was sorbed on natural soils with high OM content.[267] The removal of the OM from the soils by hydrogen peroxide treatment followed by adsorption–desorption experiments, allowed us to evidentiate the differences in desorption between OM and mineral fraction. The results demonstrated that parathion–organic complexes are stronger than parathion–mineral ones. The hysteresis in the parathion adsorption–desorption process is especially due to the very small amounts of parathion released from the organic fraction, while the adsorption on the mineral fraction is easily and totally reversible. Similar results were reported by other authors with parathion,[129] organophosphorous and carbamate insecticides,[122] and hexachlorocyclohexane isomers.[185]

However, hysteresis effects were noted also in adsorption–desorption studies of parathion with clay suspensions.[246] These effects were greater in Fe^{3+}- than in Ca^{2+}–montmorillonite. The repeated desorption pathway was dependent only on the initial concentration. The volume of solution removed in each cycle did not alter the desorption pathway, but only the rate at which the desorption proceeded down the desorption isotherm.

Desorption of 12 insecticides, representative of organochlorine, organophosphorus, and carbamate groups, from three soils and a stream sediment was found proportional to their water solubility.[264] The compounds were desorbed in greatest amounts from the sand>sandy loam>sediment, but the order of desorption for the 12 chemicals remained the same.

Napropamide shows nonsingularity between adsorption and desorption in different soil–water systems.[278] Also the desorption data can be described by the Freundlich equation. As for the other reported systems, the value of K_f for desorption is not constant, but a function of the adsorbed concentration when desorption was initiated. The soils with high OM contents had a larger retention ability and the data suggest that some of the napropamide may be fixed or nonreversibly adsorbed.

Carringer *et al.*[121] compared the amounts of some pesticides of different nature desorbed from OM prepared from a peaty muck soil and from Ca–montmorillonite after three repeated desorption steps. Asulam, an acid herbicide, was weakly adsorbed by the OM. More asulam was desorbed by de-ionized water (84.4%) than by 1 N $CaCl_2$ (58.5%). This may have been due to a lower solubility of asulam in $CaCl_2$ than in water. Prometryn, a basic s-triazine herbicide, was adsorbed in great amount by the same OM. Desorption studies showed that much more prometryn was desorbed by 1 N $CaCl_2$ (69.4%) than by de-ionized water (5.89%). This verifies that the mechanism of adsorption was by cation exchange, since the excess Ca was very effective in displacing prometryn from the colloid surface. Prometryn, adsorbed in large amount also by clay mineral, was much more desorbed with 1 N $CaCl_2$ (100%) than with deionized water (37%), indicating that prometryn cations were probably being displaced by excess Ca ions. Desorption studies of dicamba, an acidic herbicide, adsorbed by clay minerals, have shown that little compound was desorbed by deionized water and 1 N $CaCl_2$ (32.8% and 41.6%, respectively). The desorbed amounts were collected almost totally in the first step. This suggests that part of dicamba was adsorbed very strongly.

A high hysteresis effect has been found in desorption of 2,4,5-T from a Glendale clay loam soil, having a pH of 7.9, and OC=0.47%.[484]

Desorption experiments were undertaken with 18 soils used in the adsorption studies to evaluate the stability of adsorption complexes between 2,4-D and colloid surfaces.[333] The effect of successive washings with solutions of 0.025 M $CaCl_2$ on desorption of 2,4-D was studied as a function of soil pH, soil OM, and exchangeable aluminum. The calculated r values were 0.81, −0.78, and −0.81, respectively.

Sorption and desorption of picloram with a loam soil having 1.7% OM content cannot be described by one equation and hence are not single valued.[485]

The sorption and desorption of phenol, 2-MCP, and 2,4-DCP by a fine and coarse sediment fraction were measured in a continuous flow stirred cell at pH values lower than the respective pK_as.[100] Desorption was slower than sorption, and in some cases up to 90% of the sorbate was irreversibly held. Peroxide treatment of the sediment decreased the amount of irreversible sorbate, but the partition coefficients referred to the residual organic matter increased. The increase in the percentage of reversible sorbate presumably is due in part to sorbate held at inorganic surface sites, and hence, these partition coefficients are overestimates.

The nonreversibility or nonsingularity of the sorption–desorption process may have serious consequences in studying the movement of organics in soil/sediment systems. Therefore, Rao and Davidson[87] evaluated the errors introduced by not accounting for this effect. For nonsingular isotherms, the Freundlich coefficients are different for sorption and desorption and the respective equations are

$$S_{\mathrm{a}}=K_{\mathrm{a}}C^{N_{\mathrm{a}}}, \tag{33}$$

$$S_{\mathrm{d}}=K_{\mathrm{d}}C^{N_{\mathrm{d}}}, \tag{34}$$

where the subscripts a and d denote, respectively, the sorption (adsorption) and desorption, S is the sorbed phase concentration [equal to q in Eq. (4)], C is the solution pesticide concentration at equilibrium, and N is equivalent to $1/n$ in Eq. (4). It has been demonstrated[485] that the degree of nonsingularity depends on the maximum amount sorbed (S_{m}) before initiation of desorption, to which corresponds the maximum concentration of the aqueous phase (C_{m})

$$K_{\mathrm{d}}=K_{\mathrm{a}}^{\beta}S_{\mathrm{m}}{}^{1-\beta}, \tag{35}$$

where $\beta=N_{\mathrm{d}}/N_{\mathrm{a}}$. Equation (35) can be expressed in terms of the maximum solution concentration (C_{m}) prior to desorption as follows:

$$K_{\mathrm{d}}=K_{\mathrm{a}}C_{\mathrm{m}}{}^{N_{\mathrm{a}}-N_{\mathrm{d}}}. \tag{36}$$

The ratio $S_{\mathrm{d}}/S_{\mathrm{a}}$ may be calculated introducing in Eq. (36) the respective Eqs. (33) and (34), thus obtaining

$$S_{\mathrm{d}}/S_{\mathrm{a}}=(C_{\mathrm{m}}{}^{N_{\mathrm{a}}-N_{\mathrm{d}}})(C^{N_{\mathrm{d}}-N_{\mathrm{a}}}). \tag{37}$$

Note that the ratio ($S_{\mathrm{d}}/S_{\mathrm{a}}$) in Eq. (37) is equal to 1.0 when $C=C_{\mathrm{m}}$, the point where desorption is initiated, or when $N_{\mathrm{a}}=N_{\mathrm{d}}$, i.e., when the isotherm are singular. It was shown[484] that the value of N_{d} was related to N_{a} and S_{m}; however an average value of $\beta=1/2.3$ was found satisfactory (i.e., $N_{\mathrm{a}}=2.3\ N_{\mathrm{d}}$). Introducing this relationship in Eq. (37)

$$S_{\mathrm{d}}/S_{\mathrm{a}}=(C_{\mathrm{m}}{}^{-0.565N_{\mathrm{a}}})(C^{-0.565N_{\mathrm{a}}})$$

and assuming $C_{\mathrm{m}}=10\ \mu\mathrm{g/mL}$ under normal agricultural field conditions, the authors have demonstrated graphically that the error ($S_{\mathrm{d}}/S_{\mathrm{a}}$) is greater at low solution concentrations and decreases with increasing nonlinearity ($N_{\mathrm{a}}<1$) of the sorption isotherm. The conclusion is that, if a factor of 2 or 3 is considered tolerable, then over a solution concentration range of 0.4–10 μg cm^{-3} the effects of nonsingularity may be ignored. Lyman[105] reported a table with the values of errors associated with assumption of reversible adsorption for $C=1.0$, 0.1, and 0.01 μg mL^{-1} and $C_{\mathrm{m}}=10\ \mu\mathrm{g\,cm}^{-3}$ and as a function of N_{a} between 0.5 and 1.1.

10. Interpretation of "Solids Effect" and Nonsingularity in Sorption–Desorption Process

These two apparent anomalies observed in the interaction of organic and inorganic sorbates with several sorbents are often discussed together, because a number of experimental results indicate that they may be due to the same cause.

A first interpretation of the solids effect and of the hysteresis effect is that they are due to artifacts connected to the experimental methods. Servos and Muir[468] suggested that the solids effect may be due to errors inherent in measuring free water concentrations, especially at high suspended sediment concentrations. Grover and Hance[462] evidentiated that the observed solids effect can be due to the dispersion of soil aggeregates in batch tests, which is greater at low particle concentration, thus resulting in greater adsorption.

Bowman and Sans[486] studied the sorbent concentration effect on sorption of some insecticides by soils and clays. They observed that: (a) for those compounds, such as dieldrin, exhibiting strong tendencies to adsorb to glassware, the conventional adsorption blank, used in batch-type sorption isotherm, is inadequate to properly compensate for glass adsorption. Since glass adsorption is quite irreversible in aqueous solution, they proposed a sequential blank/sample adsorption technique, whereby the stock solution was initially equilibrated in the glass bottle then a small aliquot was removed for analysis before adding the sorbent for its equilibration period; (b) to reduce the measurement error, it is preferable to adjust the sorbent concentration to a suitable value (Sec. 11.1.); (c) sorbent concentration does not appear to significantly affect the distribution coefficient of pesticides over a fairly wide range of values. Reported solids effects may be ascribed to incomplete phase separation or to accumulative relative errors in measuring concentrations; (d) the centrifugation process does not appear to change the distribution of pesticides between the sorbent and water phases. Thus, the same authors[487] proposed the use of a dilution method in batch equilibration (Sec. 11.1.), which allowed us to considerably reduce anomalous effects because it avoided physical separation of the two phases. The small amount of observed hysteresis in the dilution method may be ascribed to a combination of true hysteresis and/or small sorbate losses due to degradation, glass adsorption, and volatility, which occurred during equilibration period.

Rao and Davidson[87] identified three major causes for nonsingularity of the sorption–desorption processes: (i) artifacts due to the specific method, (ii) chemical and/or microbial transformations of the chemical during the experiment, and (iii) failure to establish complete equilibrium during sorption.

Artifacts (i) may be connected to the batch equilibrium method. It involves repeated centrifugation and resuspension of the soil followed by prolonged agitation, which may breakdown the soil particles, thus increasing the number of sorption sites during the desorption phase. A similar hypothesis was already suggested by other authors.[274] Modifications of the batch method have been identified to eliminate the centrifugation step:[488] (a) using a water immiscible organic solvent as a third phase to desorb the compound from the soil and aqueous phase, and (b) desorption by dilution of the soil–water-compound system (Sec. 11.1.). This second procedure was the same suggested by Bowman and Sans.[487]

The chemical and microbiological transformations of the compound (ii) may be sometimes important to explain nonsingularity in sorption–desorption isotherms, but cannot be a significant factor for the most persistent pesticides. It would be a good practice to sterilize or to add antibiotics to minimize the microbial activity in soils during the sorption experiments. Microbial decomposition is also responsible of the apparent increase of phenol adsorption by soils with the increase of the equilibration time.[489] When sterile soils are used, the K_f and $1/n$ values do not change with time.

Point (iii) will be discussed later.

Although artifacts may be important in some cases, the nonsingularity of sorption–desorption isotherms could be real and significant for certain compounds.[87] Di Toro and Horzempa[490] studied the desorption process using tritiated 2,4,5,2′,4′,5′-HCB and a series of lake sediment and clay mineral samples. They found that the K_d for desorption is significantly higher than that initially determined in the sorption experiment and that the results of consecutive desorption studies indicate a presence of a significant component of the adsorbed HCB extremely difficult to desorb. On this basis they have defined a "resistant" and a "reversible" fraction of it to build a model describing the desorption behavior. The resistant fraction does not desorb at all for the first few consecutive desorptions; its existence accounts for the observed hysteresis in the single desorption experiments. The authors have derived a computational method to allow prediction of the magnitude of the reversible and more strongly adsorbed HCB fractions, assuming linear the adsorption isotherm and the initial stages of the consecutive desorption isotherm. The kinetic data suggest that separate sites should be responsible for reversible and resistent binding of HCB. The results of a following study[491] suggest that nonsingular isotherm behavior cannot be attributable to microbiological, kinetic, or experimental effects. Moreover, while HCB sorption may ultimately be reversible, desorption coefficient values are substantially greater than those obtained for adsorption. Release from sediments by consecutive equilibrations appears to involve desorption along two distinct isotherms.

Sorption of lindane on chitin shows the same problems: sorbent concentration effect and nonsingularity of sorption–desorption.[492] The reversible and resistant components have been determined following the method by Di Toro and Horzempa.[490] The main results of this work were: (a) the reversible component sorption coefficient is fairly constant while the resistant component sorption coefficient is inversely related to the chitin concentration. When the chitin concentration is above 10 mg dm^{-3}, the sorption and desorption isotherms are almost the same; (b) at a fixed chitin concentration, the resistant component is inversely proportional to temperature and is directly related to the salinity. At high temperatures and low salinities, the process becomes reversible and the resistant component sorption coefficient becomes zero.

A second interpretation of the solids effect and the nonreversibility of the sorption process was that they are due to the presence of DOM released from the sorbents. The role of the DOM from natural water and sewage in reducing sorption of hydrophobic organic compounds by river- and sewage-borne particulate matter was suggested by Hassett and Anderson.[426]

Karickhoff and Brown[89] reported that UV spectra of paraquat in a hectorite suspension revealed the presence of more than 50% of this compound in the water phase sorbed on particulates not removed by centrifugation. They observed that, for highly sorbed compounds such as paraquat, conventional phase separation techniques for measuring sorption may not distinguish sorbed versus "free" compounds.

Significant interferences were apparent in the measurement of the water-phase concentrations of 2,3,7,8-TCDD for sorption experiments involving a high-f_{oc} soil.[109] They were attributed to the presence of nonseparable suspended particles. Prewashing this soil from one to five consecutive times with water appeared to reduce these interferences, as individual-point distribution ratios approached the K_{oc} value determined for the low-f_{oc} soil.

Gschwend and Wu[408] gave the same interpretation to both the nonreversible effect and the solids effect, which can be explained with the release of organic matter (natural microparticles or organic macromolecules) from the sorbent to water. It has been assumed that, if the phase separations in the sorption experiments are incomplete, noncentrifugable of nonfilterable microparticles or organic macromolecules (NSPs) released from the solids remain in the aqueous phase, sorbing some of the compound. Thus, these materials may cause the decline in partition coefficients with higher suspended solid loading, by increasing the amount of compound in "solution." This has been demonstrated by a series of experiments carried out with two lake and river sediments. After five washes of 12 000 mg dm^{-3} sediment (2.5% OC) the NSP content dropped by about an order of magnitude down to 100 mg dm^{-3}. It did not appear that washing significantly affected the sediment f_{oc} and, therefore, it may be reasonable to assign to NSPs a similar affinity for hydrophobic compounds as that exhibited by the larger mass of solids. On this basis the authors have proposed a model to predict the decline of K_d with the initial sediment concentration. This effect was strongest for the sediment with the greatest organic carbon content and for hydrophobic compounds with the strongest tendencies to sorb. The good fit of the model with the decreasing of the experimental K_d values by increasing the sediment concentration supported the hypothesis that the NSPs are the primary cause of this behavior. In desorption experiments, after the first sorptive batch equilibration, the aqueous layer is discarded and clean water is added to take its place for a new equilibration step. Thus, the NSPs in this inadvertently prewashed condition are reduced in quantity, and the resultant aqueous load contains proportionately less NPS-sorbed material. Hence the observed $K_{oc}^{desorption}$ is greater than the previous $K_{oc}^{sorption}$. Further successive desorption tests will continue to be effected by NSPs less and less. These results would lead to the erroneous conclusions that irreversible binding was occurring and that there was a hysteretic effect in the desorption process. Moreover the authors[408] have demonstrated that using prewashed sediments the results obtained by Di Toro and Horzempa[490] in desorption experiments could be reproduced and that, after repeated prewashes, the adsorption and the desorption isotherms were indistinguishable. The "three phase" model[408] was used to describe the sorption behavior of 1,2,3,4-TeCBz on three sediments at different sediment to water ratios.[493] On the same basis, another model was proposed by Voice and Weber.[464,494] The "solute complexation" model assumes that the liquid phase contains a certain amount of organic material (total organic carbon, TOC) which originates mainly from the solid phase but remains in solution following phase separation. The initial reaction that takes place in the system is an irreversible binding or complexation of solute molecules to TOC. As a result of this complexation phenomenon the solute can exist in two states within the liquid phase, "free" and "bound;" subsequent to the binding reaction, both free and bound solute can be sorbed by the organic fraction of the solid phase. The model predictions gave a good fit to experimental data regarding the sorption of some hydrophobic compounds on three Lake Michigan sediments. The authors concluded that the solute complexation model offers a plausible representation of the partitioning of hydrophobic organic compounds to sediments containing moderate levels of organic compounds.

The importance of colloidal-sized, nonsettling microparticles to the behavior of highly hydrophobic organic pollutants has been evidenced by measurements of the sediment–water partitioning of PCB congeners in Lake Superior.[50] The strong inverse variation of K_d with suspended solids (SS) concentration suggested the presence of this colloidal DOM. The authors, starting from the "three phase equilibrium" model by Gschwend and Wu,[408] introduced the inverse correlation between K_d and SS concentration observed in Lake Superior to show that colloids contributing to the "dissolved" concentration can explain PCB partitioning in natural waters. Their "three phase equilibrium speciation" model allow readily calculating the relative amounts of dissolved, colloid-associated, and particle-bound contaminant.

Eadie *et al.*[409] studied the distribution of hydrophobic chemicals in Great Lakes water and demonstrated the presence of these compounds as free, bound to particles, and bound to DOC. They noted a weak inverse relationship between the $\log K_d$ and ambient particle concentration.

Schrap *et al.*[495] attempted to quantify the "third phase" in the suspension water of sediments by turbidity, dry weight, and dissolved organic carbon measurements. Also, the apparent enhanced solubilities of HCBz and two PCBs were determined in the suspension water. Solubilities of these compounds were found to be considerably enhanced (up to about eight times). On the basis of these third-phase analyses, experimental sorption coefficients of HCBz were corrected for the third-phase influence. The sorption coefficients of less chlorinated benzenes did not decrease with increasing sediment/water ratios.

Di Toro *et al.*[470] examined the desorption reaction starting from some of the already reported results:

(a) the sorption reaction for heavy metals and organic compounds is not completely reversible;
(b) the sorption coefficient tends to decrease with increasing particle concentration;
(c) sorption data demonstrate that reversibility varies as a function of particle concentration.

They carried out resuspension and dilution experiments to demonstrate that explanations that rely on nonseparated particles and/or complexing ligands associated with the particles should be excluded. Then they hypothesized that the classically conceived sorption coefficient is indeed descriptive of reversible sorption at low particle concentrations and that, when the particle concentration increases above a certain concentration, which depends only on the type of chemical and of the sorbent, the reversible sorption coefficient starts to decrease. They presented a "particle interaction" model which assumes the existence of an additional desorption reaction that results from particle–particle interactions and is independent of ionic strength. This model[470,496] permits us to calculate K_d values consistent with the experimental data. Experimental results indicate that the particle concentration effect on reversible partitioning is not limited to just neutral organic chemicals and organic carbon containing particles, but is a ubiquitous feature of reversible component partitioning. However the authors admit that the model does not give indications on the mechanisms responsible for this desorption reaction which remain still uncertain.

Mackay and Powers[497] agreed with the principle that the particle concentration may be responsible for the desorption of hydrophobic organic chemicals from particulate organic matter. They assumed that the primary process is "loose sorption" in which an organic chemical reduces the total organic–water interfacial area, and hence free energy, by associating loosely with the natural organic surface, displacing the water from the surface and from part of the chemical. This process is easily reversible as a result of particle collisions, thus the apparent sorption partition coefficient decreases as the particle concentration and collision rate rise.

Lodge and Cook[498] applied the solid concentration effect to obtain the K_{oc} value for desorption of 2,3,7,8-TCDD from a contaminated lake sediment. To do this they modified the sorption equation introducing a factor for accounting of the fraction of compound associated with dissolved and suspended material. This fraction was assumed to depend in a linear way on solid concentration. The model used several experimental data of concentration of solute, sediment, suspended solid, dissolved organic carbon, as well as median size of the material and f_{oc}. The two K_{oc}values (7.59 and 7.25 $cm^3\,g^{-1}$) obtained using solids data or organic carbon data, respectively, were higher, as expected, than those reported in the literature without taking into account the solid concentration effect. Also, the authors observed that the contact period was likely too short for true desorption equilibrium to be reached. Therefore, the water concentrations were probably lower than at equilibrium, giving rise to a higher sorption coefficient.

Schrap and Opperhuizen[499] discussed the "third phase model," the "resistant component model" and the "particle interaction model.'' Their conclusion, based on the application of the three models to the experimental results, was that there was not any evidence to support the resistant component model or the particle interaction model, while the presence of a third phase could be demonstrated. However, more experimental data were needed to quantify the influence of the third phase on experimental sorption coefficients.

Another explanation of the sorption–desorption hysteresis and of the sorbent concentration effect is given by the ''implicit-adsorbate'' model.[500] The model is based on the competitive sorption between a sorbate under study, A, and an implicit sorbate, B, initially on the sorbent. During batch sorption–desorption experiments B desorbs and uncovers sites for binding A, increasing the apparent sorption coefficient. A similar interpretation was given by Hassett and Anderson,[426] who suggested the possibility that natural DOM can compete with organic compounds for the same sorption sites. This interpretation however implies that the sorption mechanism is not a simple partition like liquid–liquid partitioning, because this model predicts no role for competitive sorption.[195]

The point (iii) suggested by Rao and Davidson[87] as another explanation of the nonsingularity of the sorption–desorption process was the ''failure to establish complete equilibrium between the soil and the solute prior to initiation of desorption.''[156,501] Diffusion-controlled migration of the compound to sorption sites within the soil organic matter and/or clay matrix would result in a pseudoequilibrium.[144,502] Karickhoff[151] demonstrated that the approach to equilibrium, in both sorption and desorption, involves a fast and a much slower component. The slower process may be a diffusive transfer of the sorbate to sorption sites inaccessible to water. Karickhoff and Morris[156] studied the sorption–desorption kinetics of pyrene, pentachorobenzene (PCBz), and HCBz with sediment suspensions. The results demonstrated that part of the sorbing sites is readily accessible in minutes or hours, but part requires days or months for sorption or desorption. The reason for this behavior may be a slow diffusion within the organic matrix, which is a function of the square root of time. On the basis of these assumptions, a ''two-compartment'' first-order model was proposed as an approach to describe sorption dynamics. The model distinguished rapid or ''labile'' exchange from highly retarded or ''nonlabile'' sorption. In general, one-half or less of the total sorption is labile. For highly hydrophobic chemicals and high solid concentrations, the labile fraction decreases to 0.1 or less in some systems. The kinetic exchange constant for nonlabile sorption varies inversely with the sorption equilibrium constant. That is, the more highly sorbed chemicals sorbed more slowly. Similar results were obtained by Coates and Elzerman,[134] who conducted purge release experiments of chlorinated benzenes from sediments. However, plotting the increase of the nonextractable fraction for chlorophenols as a function of the square root of time and extrapolating to $t=0$, an intercept is evidentiated, which indicates that diffusion is not the only process for the formation of nonextractable residues.[111]

On the basis of the concept that sorption may occur both on ''labile'' soil surface sites and on ''restricted'' soil sites,[478] the early concept of ''hysteresis'' was revised. The adsorption/desorption kinetics and the reversibility of the sorption process of cyanazine and metribuzin in a suspension of soil was studied.[503] A mathematical model of pesticide sorption kinetics based on Freundlich isotherm was considered in attempts to describe measured adsorption kinetics. In this model, the sorption kinetics of two classes of site are considered. The sites of the first class equilibrate at a time scale of minutes, those of the second at a time scale of hours. Measured desorption kinetics and equilibria were found to be explained well, quantitatively, by the Freundlich model whose parameters were based on adsorption kinetics and equilibria. Thus, no hysteresis was found in the isotherms, and desorption kinetics was found to proceed as fast as adsorption kinetics.

It has been shown that various one- to three-carbon halogenated alkanes and alkenes form slowly reversible fractions in soils that comprise up to several percent of total sorbed chemical.[381] The slowly reversible fraction becomes greater in magnitude as the sorption period increases. The soil fumigant ED was found in agricultural topsoil up to 19 yr after its last known application.[380] This residual ED was highly resistent to both mobilization (desorption into air and water) and microbial degradation in contrast to freshly added ED. Pulverization promoted release, both to the aqueous and the gaseous phases. The results suggest that ED is entrapped in soil micropores and that release into bulk solution is diffusion controlled. Thus desorption is retarded by molecular diffusion of molecules from remote locations in the soil matrix.[382] It has been evidentiated that the residual is associated with organic matter and that this association is rate limiting. The mineral fraction, however, plays an important role by shielding some of the sorbate associated with the organic matter from equilibrium with bulk fluid. Hence, release of the residual is promoted by breakup of soil particles and by acidification of the soil suspension, which cause partial disaggregation of particles by dissolution of cementing agents (Fe and Al oxides) or hydrolysis of metal–humate linkages.

The ''intraparticle diffusion'' model was proposed to explain slow intraparticle mass transfer.[88,110,155,504] It assumes that diffusion occurs in water filled pores within homogeneous particles and that diffusion is retarded by equilibrium sorption within the pores. The breakthrough of TeCE through packed columns of Borden aquifer material was studied, and a transport model incorporating intraparticle diffusion was used to simulate the experimental results.[113] Model predictions showed excellent agreement with column breakthrough data, supporting the hypothesis of intraparticle pore diffusion as the causative mechanism of slow sorption in this material.

McCall and Agin[135] studied the desorption kinetics of picloram as a function of incubation time in seven soils incubated for up to 300 days in the presence of picloram. The amount of picloram readily released from the soil decreased significantly with incubation time. A two step sorption–

desorption mechanism was used to model the observed behavior that can be described in terms of external and internal sorption sites. Desorption from external sites is relatively fast, taking place in less than 5 h, whereas desorption from internal sites can take up to 300 h to reach equilibrium and is characterized by a first-order rate constant. The amount of picloram sorbed to internal sites increases with residence time in the soil.

Recently[505] the mechanisms controlling desorption rates of TCE from various sorbents under unsaturated conditions at 100% RH were investigated. The results indicated that desorption proceeds on two distinct time scales; at TCE concentrations near vapor saturation, the majority of TCE desorbs within 10 min while removal of the remaining fraction requires weeks or months. The kinetic and isotherm data implicate intragranular micropores of mineral solids as responsible for both isotherm nonlinearity and the slowly released fraction.

Pignatello[154] reviewed a number of studies regarding slow sorption or desorption kinetics of highly hydrophobic compounds as well as certain polar pesticides in soils. In some instances it has been demonstrated or predicted that weeks to years would be required to reach true equilibrium.

The nonsingularity of the sorption–desorption relation forced to revise the earlier modeling approach[155,207,506–508] to describe the movement of chemicals through porous media. Those models assumed instantaneous sorption and a linear and single-valued sorption–desorption relation (''one-site'' models), but showed considerable deviations from the experimental data especially at high flow velocities. Such deviations were due to the fact that those models predicted symmetrical breakthrough curves (BTC), while experimental results gave asymmetrical curves, as result of nonequilibrium sorption–desorption of chemicals in soils under steady-state flow conditions.

Thus, the two-stage approach to sorption equilibrium was taken into consideration in modeling pollutant transport through porous media. It was assumed a rapid initial rate of sorption or desorption, where roughly 30%–50% of the total sorption occurs within minutes to hours, followed by a much slower rate of sorption or desorption (days or months).[134–136,151,156]

The miscible displacement techniques were used to study the movement of picloram through soil.[485] The equilibrium sorption–desorption isotherms were not single-valued relations. Picloram mobility was reduced when the average pore-water velocity was decreased. Predictions were made with a simulation model using two kinetic rate equations and an equilibrium Freundlich equation. The two kinetic models and the equilibrium model gave satisfactory results only at low pore water velocities provided the nonsingle valued character of the sorption–desorption relation was included in the calculations, but were inadequate to predict the picloram movement at high pore water velocities.

In a following paper, the authors[148] proposed a new model for the movement of chemicals through a sorbing porous medium with lateral and intra-aggregates diffusion. The liquid phase in the porous medium was divided into mobile and immobile regions. Diffusional transfer between the two liquid regions was assumed to be proportional to the concentration difference between the mobile and immobile liquids. Sorption processes in both the dynamic and stagnant regions of the medium were assumed to be instantaneous and the sorption isotherm was assumed to be linear. The analytical model was able to describe the extensive tailing observed during flow through an unsaturated, aggregate sorbing medium and to explain the often observed early breakthrough of chemicals in the effluent. The model was then tested with 2,4,5-T.[509] On the same basis the ''two region'' model was developed by Coats and Smith.[510] Miller and Weber[91,511,512] proposed the ''dual resistance'' model which describes sorption as a series of mass transfer steps involving molecular diffusion through a boundary layer surrounding a soil particle followed by diffusion within the particle itself.

In another series of studies, instead of physical diffusion[148,510] or chemical nonequilibrium,[475,485] diffusion-controlled migration of pesticide to sorption sites within the soil organic matter and/or clay matrix was taken into consideration.[513] In these models sorption on one group of sites was assumed to be instantaneous, while the rate of sorption on the second group of sites followed nonlinear reversible kinetics (''bicontinuum'' or ''two-site'' models).[149,502,514]

Ma and Selim[515] presented a second-order model that was capable of describing both adsorption and desorption kinetics of atrazine in soils. The model assumed heterogeneity of adsorption sites and dominant nonequilibrium conditions. Also, Xue and Selim[161] studied the adsorption–desorption behavior of alachlor through a multireaction kinetic model, assuming that this compound reacts at different rates with different sites of a soil matrix. Adsorption and desorption isotherms showed extensive hysteretic behavior and were best described by a model version incorporating nonlinear equilibrium, a kinetic reversible mechanism, and a consecutive irreversible mechanism.

Examination of the literature data on nonequilibrium sorption of a broad spectrum of organic solutes by natural sorbents allowed to analyze values of equilibrium sorption coefficient (K_d) and sorption rate constant (k) with the linear free energy relationship approach.[516] An inverse linear relationship was found between $\log k$ and $\log K_d$. After examining the intercept value for hydrophobic organic chemicals and that for polar/ionizable organic chemicals, the experimental conditions under which the data were collected, and considering the nature of the sorbents and the sorbates, it was postulated that the following processes were responsible for the observed sorption nonequilibrium: intraorganic matter diffusion for hydrophobic chemicals; intraorganic matter diffusion and chemical nonequilibrium for polar/ionizable chemicals. A regression equation relating k and K_d may be used to estimate approximate values of the sorption rate constant for organic solutes. This provides a means to evaluate nonequilibrium potential and to attempt to predict nonequilibrium behavior.

Brannon *et al.*[218] measured the partitioning of BCB 52, PCB 151, and fluoranthene between sediments and interstitial water. The compounds were incubated and sampled periodically over a 6 month period. Interstitial water was analyzed for free compound and compound bound to dissolved organic matter. Results demonstrated that as time of contact increased, the value of K_{oc} increased, reflecting a decrease in the truly dissolved contaminant concentration in the interstitial water. Decreases in concentrations of free contaminant are consistent with movement of nonpolar organic contaminants into interparticle spaces of organic matter over time.

A long series of researches were carried out to successfully predict by the bicontinuum model the BTCs of organic chemicals and for investigating the transport of these solutes in soils and aquifers.[166,517–524] Experiments of elution of diuron, atrazine, and PAHs from soil columns[452,525] with aqueous solutions containing various fractions of methanol have demonstrated that the degree of BTC asymmetry (i.e., nonequilibrium sorption) decreases with increasing volume fraction (f_c) of cosolvent and that the nonequilibrium mechanism involves organic matter. Also the desorption rate constant (k_2) for the same compounds increases log-linearly with increasing volume fraction of organic cosolvent (f_c).[526] This relationship was expected, based on the existence of a log–log inverse relationship between k_2 and the equilibrium sorption constant (K_d), and a log-linear inverse relationship between K_d and f_c. It is suggested that decreased polarity of the mixed solvent, caused by the addition of a cosolvent, appears to influence the conformation of the polymeric organic matter and, hence, the rate of sorbate diffusion. Similar results were obtained with chlorophenols regardless of ionization status.[460]

A bicontinuum model was applied to describe experimentally determined breakthrough curves for atrazine, simazine, and cyanazine.[527] The model considers sorption in two domains and includes a description of first-order degradation.

In summary, two main anomalous effects have been detected in sorption and desorption processes: solids effect and nonsingularity in sorption–desorption. Some explanations were proposed for both effects. In particular, the solids effect may depend on: (i) dispersion of soil aggregates in batch tests which is greater at low particle concentration, so increasing the number of soil sites available for sorption; (ii) presence of DOM released by the sorbent, which increases with the concentration of the sorbent itself and associates with the compound in water; and (iii) particle interaction, which increases with the concentration of the sorbent inducing a partial release of the compound. However, at the moment, it does not seem that a single theory can explain all cases of solids effect. On the contrary, the nonsingularity in sorption–desorption found a satisfactory explanation when a two-step sorption process was evidentiated. A rapid sorption followed by a slower diffusion into the sorbent matrix were modeled to reproduce successfully the breakthrough curve of a sorbate in a sorbent matrix.

11. Experimental Methods for the Determination of Sorption Coefficients

11.1. Batch Equilibration (BE)

A known weight of sorbent (soil or sediment) is placed in a vial with a measured volume of solution containing a known concentration of the solute in water (distilled or containing known concentration of an electrolyte, NaCl, $CaCl_2$, etc., to simulate the ionic strength of soil solution and to improve phase separation). A minimum of headspace is left to avoid losses of solute in vapor phase. The vial is shaken for a time suitable to reach equilibrium, then is centrifuged and both phases are separated and analyzed to determine the concentration of the solute. The mass of sorbate per unit mass of sorbent may be obtained also by difference between the initial concentration of solute and the concentration after equilibrium has been reached. The first procedure seems more reliable because it takes into account the possibility of loss of solute by volatilization, degradation or by other processes causing disappearence or nonrecovery of the solute from the measurement system.[528] No differences were found between the two procedures with napropamide and lindane sorption by soil.[529] The K_d or K_f value are calculated using Eqs. (3) and (4). Often labeled (^{14}C or ^{3}H) compounds are used and their concentration is measured by liquid scintillation counting. However, much care is necessary in using radio-labeled compounds, especially when sorption coefficients are extremely high. Their purity should be checked accurately before use to avoid errors in measurement of the aqueous concentration after sorption. This can be termed the ''standard batch'' method.

Several sources of error may be introduced in determining sorption by this method:[530] losses of chemicals by volatilization and biological or chemical degradation; length of the experiment non sufficient to reach equilibrium; no complete separation between sorbent and water phase; water/sorbent ratio. To avoid bias in experiments requiring long contacting times, it is of paramount importance to avoid losses through volatilization or transformations.[88] Autoclaving has been found effective in inhibiting biotransformation, and employing fire-sealed glass ampules precluded volatilization losses. Boyd and King[531] recommended using anaerobic conditions during measurement of sorption coefficients of labile organic compounds to prohibit degradative losses. Autoclaving of soil was used to avoid the microbial degradation of phenol during the sorption experiments.[489,532] However, the use of autoclaved soil apparently resulted in a less accurate measurement of adsorption,[531] while the use of sodium azide treatment approximates sterilization without altering the soil physical and chemical properties.[58,113,289]

Bowman and Sans[486] observed that factors involved in selecting experimental adsorbent concentrations include: (i) relative partitioning of compound between sorbent and water phases, (ii) detection limits and working range of analytical methods, and (iii) concentrations at which the compound and adsorbent occur in natural aqueous environments. For maximum precision in adsorption experiments, it is preferable to adjust the adsorbent concentration so that the percent removed is in the 20%–80% range. Outside this range, relative measurement errors can become a dominant factor. Also Green and Yamane[533] reported that the precision expected in solute adsorption measurement (based on change of concentration in a solution equilibrated with an adsorbent) depends upon the magnitude of the solution concentration change. Improvements can sometimes be achieved by altering the soil:solution ratio to obtain larger concentration changes.

An accurate evaluation of the measurement error in the standard batch method has been reported.[534] The ratio mass sorbent/volume solution may vary in batch experiments, depending upon sorption coefficient of the chemical under study. By examining the literature reports[86,121,535] this ratio ranges between 10^{-4} and 1 g cm^{-3} with all the possible intermediate values between these two extremes. If sorption is derived from the difference in the concentration in liquid phase, the experimental error in the sorption coefficients becomes very large when this coefficient tends to zero. To minimize experimental errors, the solid/liquid ratio of the soil suspension should always be taken as large as possible (in practice 1 g cm^{-3}), unless this results in an equilibrium concentration that is too low to be measured accurately. If a solid/liquid ratio of about 0.2 g cm^{-3} is used, the error in the sorption coefficient will usually be unacceptable for sorption coefficients less than about 1 cm^3 g^{-1}. If the expected value of the sorption coefficient is below 0.3 cm^3 g^{-1}, it will usually be necessary to remove the liquid phase from the solid phase as far as possible and to extract the remaining mixture of solid and liquid phase in order to obtain an accurate sorption coefficient. However, in selecting the solid/liquid ratio it is necessary to take account of the possibility of a solids effect, especially when conditions already described (high ratio) (Sec. 8) are verified.

Ball and Roberts[88] measured by the batch technique the K_d values for TCE and 1,2,4,5-TeCBz sorption on sandy aquifer material. They developed an accurate data analysis technique to account for partitioning to sample headspace and glass surfaces of the ampules, monitored through the routine use of blank samples containing solute and water but no solids. Experimental errors were determined for all important batch measurements and these propagated through the calculations to provide estimates of error on reported apparent distribution coefficients. In their study, relative errors in the measurement of K_d^{app} were generally between 0.02 and 0.20 cm^3 g^{-1} and, for most cases, were sufficiently low as to be insignificant compared to sorption variability due to heterogeneity among samples.

With the standard batch method the upper limit of sorption data obtainable is dictated by affinity of the sorbent for the compound, compound water solubility, and sorbent/solution ratio. When the sorbent has a great affinity for the compound (>95% adsorption) it becomes difficult to generate an adsorption isotherm, since even the maximum solution concentration would be greatly depleted. Consequently, it would be impossible to obtain adsorption data at or near the solubility limit of the compound using this technique. Thus, Bowman[536] proposed another method which allows us to extend the isotherm to values of equilibrium aqueous concentrations closer to the water solubility of the compound under examination. For obtaining the sorption isotherm, after each equilibration and centrifugation a certain volume of supernatant is removed and substituted with an equal volume of preselected compound solution. The initial concentrations of the compound and the volume and concentrations of the solutions added in each step are selected to produce uniformly distributed data points. Usually, the compound concentration selected for the incremental additions is close to the solubility limit, but sometimes it can be established depending on the affinity of the compound for the sorbent. This can be termed the "repeated addition" method.

Ou *et al.*[537] proposed a continuous batch method which eliminated centrifugation with all the associated problems. The solid sorbent and the solution were stirred in a glass ampoule having a glass fiber filter on the bottom. At known time intervals the solution was circulated, using a syringe pump, through a closed system which allowed taking known aliquots of solution for analysis.

Desorption may be carried out by the following procedure:

(a) the sorbent is at first equilibrated with the aqueous solution;
(b) the compound-spiked sorbent is separated, resuspended in pure water, equilibrated under swirling; the phases are separated again for the analysis. This procedure is used to obtain one value of the desorption for each point of the sorption isotherm and allows to obtain a "single-point" desorption isotherm.
(c) the compound-spiked sorbent coming from (b) can be separated again and resuspended in pure water for a further determination of desorption. This procedure can be repeated many times to get a series of "consecutive" desorption steps.

However, method (c) is affected by two sources of error: (i) it is difficult to decant all the centrifuged supernatant solution without losing some sorbent, thereby affecting subsequent desorption steps; (ii) an indeterminate volume of solution is left behind, associated with the sorbent when the supernatant is decanted. This volume could be easily determined by weighing. However, Bowman[536] proposed another procedure to obtain the consecutive-desorption branch of the isotherm, similar to that used for the sorption isotherm (see above), by adding a water increment rather than another compound increment. When the sorption isotherm has been completed, the system is centrifuged, a volume of the supernatant is removed, and a volume of water is added; the system is equilibrated, centrifuged, and again a volume of supernatant is removed for a new addition of water. This procedure can be repeated many times, selecting volume increments to obtain successive desorption points suitably spaced. This procedure can be termed the "repeated dilution" method.

Finally, taking into consideration what has been exposed in this section and in Sec. 8, it can be evidentiated that two main problems may affect the BE procedure: the possibility of measurement error and solids effect. Consequently, the following suggestions may be given for a correct use of this procedure:

(i) To reduce experimental errors sorbent/solution ratio should be chosen so that the percent removed is in the 20%–80%[486] range or in the 15%–70%[563] range. However, this ratio depends on the value of K_d. When K_d(cm^3 g^{-1}) takes the values: 0.1; 1.0; 10; 100; 1000; 10,000; 100,000, the corresponding ranges of sorbent concentration (g/dm^3) have to be in the order: 2500–40 000; 250–4000; 25–400; 2.5–40; 0.25–4; 0.025–0.4; 0.0025–0.04, to stay in the range 20%–80% sorbate removed;

(ii) However, these ranges of sorbent concentration may give solids effect. Schrap *et al.*[495] found with PCBs and chlorobenzenes that, to minimize the solids effect due to the potential influence of nonsettling particles in BE, sediment concentrations should be $\leqslant 1$ g/dm^3. These values of concentration correspond to $K_d \geqslant 250$ cm^3 g^{-1} for 20% sorbate removed. For compounds having smaller K_ds, larger sorbent concentrations are necessary to remain into the range 20%–80% removed; therefore, a significant solids effect may be present. However, it has been specified that this effect is decreasing in intensity by decreasing sorption of the substance examined.[86]

Therefore, the two problems connected with this method: necessity to minimize both, experimental errors and solids effect due to the presence of nonsettling particles, could be approximately solved by selecting the sorbent concentration on the basis of the expected K_d as calculated above. However, when K_d is very low, the use of BE becomes problematic due to the very large concentrations of sorbent necessary to stay in the range; therefore, at these values of K_d, another method could be used (Secs. 11.2. and 11.4.).

Thus, taking into consideration these points, it can be worthwhile to list the main steps which are necessary to obtain a reliable value of K_d by BE:

(i) Define a rough value of K_d at ambient temperature for the compound under investigation, through the knowledge of K_d for the same compound or for similar compounds with other sorbing systems;

(ii) Carry out a kinetic investigation to establish the time necessary to reach equilibrium. To do this, select as said the sorbent concentration on the basis of the approximate value of K_d, and the aqueous concentration of the compound below its water solubility; shake the vial at time intervals, and measure the water concentration of the solute up to obtaining a constant value;

(iii) When these parameters, equilibration time, sorbent and solute concentration, and temperature are chosen, a batch experiment for the determination of K_d can be carried out following the procedure outlined at the beginning of this section;

(iv) In the absence of specific studies it would be better to control if there is any evidence of solids effect for the system under study. This can be made by repeating the K_d measurement at three or four concentrations of sorbent.

11.2. Equilibrium Head Space (HS)

This method,[364,371,372] was used for the determination of sorption coefficients [Eq. (15)] for vapors on oven-dry or moist sorbents in the absence of an aqueous phase. A system with known gas volume and mass of sorbent may be compared to a control, which contains no sorbent. The vials are sealed with Teflon-lined rubber disks and aluminum crimp caps. After equilibration at known temperature, a volume of the headspace vapor is withdrawn from the vials and analyzed. If the same mass of vapor is introduced into each system, the mass balance equation must be equal

$$C_{g1}V_{g1}=C_{g2}V_{g2}+X, \tag{38}$$

where C_{g1} is the vapor concentration for a control vial, C_{g2} is the vapor concentration at equilibrium for a sample vial, V_{g1} is the volume of the control vial, and V_{g2} is the available gas volume (total volume less than the volume occupied by solids and moisture) of a sample vial and X is the mass of vapor that is adsorbed. If linear sorption isotherm is assumed

$$X/M=K_{sg}C_{g2}, \tag{39}$$

where K_{sg} is the sorbent–vapor sorption coefficient and M is the mass of sorbent. Combining Eq. (38) and (39) results in

$$(C_{g1}C_{g2}/V_{g1}V_{g2})-1=K_{sg}(M/V_{g2}).$$

K_{sg} may be determined by calculating the slope of a plot of $[(C_{g1}C_{g2}/V_{g1}V_{g2})-1]$ vs M/V_{g2}.

Farrell and Reinhard[98] observed that K_{sg} for moist sorbent incorporates all sorption mechanisms, including partitioning into the surface-bound water and adsorption at the water/vapor interface—neither of which are incorporated by K_d. To compare adsorption from solution to partitioning from the vapor phase, K_{sg} can be converted into an equivalent K_d by subtracting the sorbate partitioned into the surface-bound water. If partitioning into the water layer obeys Henry's law and adsorption at the water/vapor interface is ignored, the relation between K_d and K_{sg} is

$$K_d=K_{sg}H-W,$$

where W is the water loading on the solid, i.e., the volume of water adsorbed per mass of dry solid.

Grathwohl[226] studied the sorption of TCM, 1,1,1-TCA, TCE, and PCE in gas phase on several natural sorbents at relative humidities (~98%) generally achieved at field conditions, when Henry's law is valid. He found that sorption isotherms follow the Freundlich equation

$$q = K'_{sg} C_g^{1/n},$$

$$\log q = 1/n \log C_g + \log K'_{sg},$$

where q is the sorbed concentration (μg kg^{-1}) and C_g is the vapor phase concentration (μg dm^{-3}), and K'_{sg} represents the Freundlich sorption coefficient K_f in the system soil–gas phase. The K_f values in aqueous systems ($K_f = q/C_w^{1/n}$) were obtained by using the Henry's law constant ($H = C_g/C_w$)

$$K_f = K'_{sg} H^{1/n}.$$

For experiments in sorbent-water systems, on top of a vial a free space is left in which a VOC is partitioned between water and vapor phase. Thus, two equilibria are established in the vial for the solute: sorbent–water and water–vapor phase. This second equilibrium follows the Henry's law.

A technique, named equilibrium partitioning in closed systems (EPICS)[193] was proposed for determining H of volatile organic compounds in water when the dimensionless H is less than 3. In a first step, the activity coefficient (γ) of the chemical is determined by comparing two identical bottles, containing the same compound mass and the same liquid and gas volumes, where the volatile solute in the first bottle behaves ideally (e.g., in distilled water) while the volatile solute in the second bottle behaves nonideally (e.g., in an electrolyte). From the equilibrium distribution of the compound in the gaseous and liquid phases of the two bottles and the value of the Henry's law constant, the activity coefficient of the chemical can be obtained using the relationship

$$H = C_g/\gamma C_l, \tag{40}$$

where C_l is the liquid concentration, C_g is the gaseous concentration, and γ is the aqueous activity coefficient correcting for nonideal behavior. When γ and H are known, the equilibrium gas concentration of a volatile chemical in a closed system serves as a direct measure of its liquid concentration and the EPICS method can logically be extended to the examination of sorption equilibria. Again, partitioning equilibria can be determined by comparing two similar systems containing the same liquid volume (V_l) and gas volume (V_g), but in this case one system would contain a sorbent, the other none. The final equation, obtained for equilibrium conditions and derived to calculate K_d is the following

$$(C_{g1}/C_{g2}) = (C_{l1}/C_{l2}) = K_d[M/(V_l + H\gamma V_g)] + 1, \tag{41}$$

where C_{g1} is the gas concentration of the chemical in equilibrium with C_{l1}, the concentration in the aqueous phase in the system without sorbent, and C_{g2} is the gas concentration in equilibrium with C_{l2}, the concentration in the aqueous phase in the system with sorbent, respectively; M is the mass of sorbent employed.

The authors[193] measured the H values at 25 °C for TCE (0.397) and for toluene (0.261). Both values are within the range in which the EPICS technique is considered reliable (i.e., $H < 3$). Activity coefficients were measured for both compounds in NaCl solutions of variable ionic strength. Both compounds showed behavior typical of neutral molecules, i.e., an increased salting out with increased ionic strengths

$$\log \gamma = k\mu,$$

where k is the "salting coefficient" and μ is the ionic strength of the solution (mol dm^{-3}). The salting coefficients (k) calculated for TCE and toluene in NaCl electrolyte were 0.194 and 0.208, respectively.

From Eq. (41), K_d values for VOC can be obtained by plotting the equilibrium ratio C_{l1}/C_{l2} as a function of $M/(V_l + V_g H\gamma)$. This should result in a straight line having 1 as the intercept.

This method has been used also by Peterson *et al.*[364] in their study on TCE vapor phase sorption by a porous aluminum oxide surface coated with humic acid. To evaluate the sorption process, a system with known liquid volume, gas volume, and mass of sorbent is compared to a control, which contains no sorbent, if the total mass of the volatile compound in each system is the same, then the mass balance equations for each system may be equated. If, in addition, a linear adsorption isotherm is used to describe the relationship between the sorbed and liquid concentrations, then

$$X/M = K_d C_l, \tag{42}$$

where X is the mass sorbed, M is the mass of solid sorbent, and K_d is the solid–liquid sorption coefficient (cm^3 g^{-1}). Thus, a combination of the mass balance equations for the control and the system containing sorbent, and substitution of Eqs. (40) and (42) can allow us to obtain a general form of Eq. (41)

$$\begin{aligned}(C_{g1}/C_{g2})[(V_{g1}H\gamma + V_{l1})/(V_{g2}H\gamma + V_{l2})] \\ = K_d[M/(V_{l2} + H\gamma V_{g2})] + 1,\end{aligned} \tag{43}$$

where V_{l1} and V_{g1} being the volume of liquid and gas in a standard control bottle without sorbent (mL), V_{l2} and V_{g2} being the liquid and gas volumes in bottles containing sorbent, C_{g1} being the headspace vapor concentration in the control, and C_{g2} being the vapor concentration in the bottle with sorbent. K_d can be determined by calculating the slope of a plot of the left-hand side of Eq. (43) versus $M/(V_{l2} + H\gamma V_{g2})$.

Since the gas phase is analyzed, the technique evades problems such as losses through volatilization, difficult extractions, the use of carrier solvents, and the incomplete solid separation (and therefore possible solid effects) which often burden other techniques.[193] Other advantages are that it does not require analysis of the aqueous phase, and that K_d is determined by a concentration ratio, thus, when the sorption is low, it is not necessary to determine the small amount sorbed by the difference between two large values, which may introduce large errors. This technique is most sensitive for solutes with low Henry's constants and sorbents with high sorption capacity (K_d). Sensitivity for measurement of compounds with low K_d values (approximately 0.5 cm^3 g^{-1} and less) may be increased by increasing the mass of sorbent employed in analyses. A major advantage of the EPICS technique is that knowledge of the total solute mass added to the system is not necessary for the determination of H, γ, and of K_d. However, H and γ must first be independently determined.

11.3. Leaching Equilibration (LE)

The solute dissolved in water is pumped at a given flow rate via the inlet port at the base of a column containing the sorbent.[132,428] The effluent samples are collected in vials and analyzed. When sorption equilibrium is reached (equal inlet and outlet concentrations) the inlet and outlet stopcocks are closed and the pump is shut off. The same column may be eventually used for desorption experiments. The K_d value is given by

$$K_d=[(m_i-m_0)/m_s]/C,$$

where m_i is the total mass (g) of the compound entering the column; m_0 is the total mass (g) of the compound leaving column; m_s is the mass (g) of sorbent in column; and C is the equilibrium breakthrough concentration of the compound (g cm^{-3}). The symmetry of the BTCs indicates uniform packing of the column and equilibrium of the sorption–desorption process.

For desorption experiments, the inlet solution is changed to either water or another water solution and pumped at a given flow rate through the column material. The effluent samples are collected as in sorption and analyzed.

Another way to use this technique is that[538] which involves equilibrating a known weight of soil (W, kg) in a weighable leaching tube with a solution of known concentration (C, μmoles dm^{-3}) until the effluent has attained the same concentration as the input solution. The volume of solution retained in the soil after equilibration (V, dm^3) is then determined gravimetrically; subsequently, the adsorbate remaining (adsorbed plus solution phase) is displaced with a suitable displacing solution or solvent (acetone for diuron, methanol for atrazine) into a known volume and measured quantitatively (D, μmoles). The quantity adsorbed (A, μmoles kg^{-1}) is calculated

$$A=(D-VC)/W.$$

With another procedure[268] a small volume of dilute ethanol solution containing the compound is added to the surface of the soil column. After the solution has entered into the surface of the soil, the column is slowly leached with water at the desired flow rate. The effluents are collected in fractions, which are analyzed. Distribution coefficients (K_d) can be calculated using the expression first described by Ketelle and Boyd[539]

$$K_d=[(V_p/V_v)-1]V_v/W,$$

where V_p is the volume of effluent to leach one-half of the solute through the column, V_v is the void volume in the column, and W is the weight of adsorbent in column. The results obtained with this method gave results comparable to those obtained by the standard batch equilibration procedure.[540]

11.4. Miscible Displacement (MD)

The experimental technique is similar to that of the leaching equilibration.[364,517,521,541] It consists of displacing, under saturated, steady water flow conditions, a solution containing the solute through a column packed with the soil. The influent solution is injected continuously until the concentration of the solute in the effluent (C) equals that in influent (C_0), i.e., $C/C_0=1$. The effluent may be collected with a fraction collector or connected to a flow-through detector. Tritiated water is employed as a nonsorbing tracer to characterize the hydrodynamic properties of the column.

The distribution coefficient (K_d) can be calculated with the following expression:[542]

$$R_t=1+(\rho/\theta)K_d, \tag{44}$$

where R_t is the retardation factor for water solutions, ρ is the bulk density (g cm^{-3}), and θ is the porosity or the volumetric soil–water content (cm^3 cm^{-3}).

R_t can be estimated[452] with a method which is based on the conservation of mass principle and involves computing the area above the breakthrough curve. It is given by

$$R_t=\int_0^{p_{\max}}(1-C^*)dp,$$

where C^* is C/C_0 and p is the dimensionless time in pore volume. The values of R_t determined in this manner are independent of the existence and degree of nonequilibrium, in contrast to the batch equilibration technique.[519]

Johnson and Farmer[529] reported that K_d values for napropamide and lindane estimated using the retardation factor from the column experiments were consistently larger than those determined by the batch equilibration method.

Seip *et al.*[344] determined the concentration profiles (breakthrough curves, C/C_0 as a function of pore volumes) of solutes after percolation through different soils. The relative retention with respect to tritiated water (R_f values) was calculated when a fairly stable concentration (C_s) level of compound is reached. The number of pore volumes necessary to reach $C_s/2$ is denoted R_x for compound X and R_w for tritiated water. R_f is equal to R_x/R_w and is used in Eq. (44) at the place of R_t.

Brousseau *et al.*[517] in comparing gas purge with miscible displacement technique, observed that the viability of MD is a function of the sorptivity of the solute/sorbent combination and of the texture/structure of the sorbent. This technique seems ideal for investigating the transport of solutes in soils and aquifer materials and, on the basis of some experimental results, it seems especially useful for low-sorptivity systems. Its efficacy, however, is greatly reduced for systems comprising highly sorptive chemicals or sorbents containing high levels of clay and/or OM. As the sorptivity of the solute increases, time constraints and other problems, such as sorption to the apparatus, become of increasing concern. These problems can be overcome with the use of a miscible organic cosolvent, which results in reduced values of K_d and increased value of k_2. Values of these constants in aqueous systems can be estimated successfully by extrapolation from column experiments performed with mixed-solvent systems.

11.5. Diffusion (DF)

This method[466] is based on the relationship, derived from the conventional reversible sorption theory, between the apparent diffusion coefficient of total chemical, $D_s^*(\mathrm{cm}^2\,\mathrm{day}^{-1})$ and the adsorption–desorption partition coefficient, $K_d(\mathrm{dm}^3\,\mathrm{kg}^{-1})$

$$D_s^* = D_s/(1+mK_d)/\phi,$$

where D_s is the aqueous diffusion coefficient ($\mathrm{cm}^2\,\mathrm{day}^{-1}$) in the interstitial water for nonadsorbing chemicals, m is the sorbent concentration $m=\rho_s(1-\phi)$, and ϕ is the porosity. For this equation to apply, adsorption and desorption are assumed to be described by a linear reversible isotherm. The value of D_s^* is related to the distance, l, from the initially contaminated sorbent layer and to the time, t, elapsed to reach this distance

$$\mathrm{l} \sim \sqrt{2D_s^* t}.$$

The experimental procedure is not without practical difficulties, because this process is very slow. Thus, it can be calculated that it would be necessary to measure changes of concentration in distances on the order of 0.1 mm and to wait for time periods on the order of 10^2 d. The detailed description of this procedure is available in the original paper.[466]

11.6. Gas Purge (GP)

This technique can provide equilibrium and kinetic information from the same experiment. Karickhoff[156] applied GP to study the sorption dynamics of hydrophobic organic compounds, which can be described by a two-compartment model. GP allowed us to obtain the kinetic constants for the short-term sorption and for the long-term desorptive release. The experimental apparatus was conceived to follow the desorption kinetics and consists of a purge cell, having a glass frit on the bottom, in which a sediment suspension containing the test chemical is placed. Desorption is induced by continuous stripping the chemical from the aqueous phase, using a purge gas (air) entering from the bottom of the cell. Head space is kept at a minimum. The sparged chemical is collected on a Tenax trap, which is changed and analyzed at sampling intervals chosen to provide the desired temporal resolution in the chemical release profile. Chemical concentration in the water phase is determined just prior to purge and the total chemical (sorbed plus solution phases) is determined at the termination of each experiment. Similar systems were used to study the desorption kinetics of naphthalene from soil[132] and of chlorinated hydrocarbons from freshwater sediments.[136] Nitrogen was used as purge gas. Oliver[136] used a purging apparatus in which a teflon-coated bar stirred the solution and a glass tubing entering from the top was used to introduce purging gas at a certain depth.

Hassett and Milicic[416] used GP for the determination of equilibrium and rate constants for binding of a PCB congener by dissolved humic substances. The binding of a hydrophobic compound at equilibrium can be described by a constant

$$K_d = C_b/C_{aq} = k_{21}/k_{12}, \tag{45}$$

where C_b is the concentration of bound compound in water, C_{aq} is the concentration of free compound, k_{21} and k_{12} are the first order rate constants for the reverse and direct sorption equilibrium reactions, respectively. In water containing no binding agent, the loss of compound from solution due to volatilization can be described as an irreversible first-order reaction with a rate constant equal to k_{23}. The value of k_{23} depends on temperature, gas flow rate, Henry's law constant, liquid volume, and, if the gas phase does not equilibrate with the liquid phase, the gas–water interfacial area and the overall liquid-phase mass-transfer coefficient.[543] In the study under examination[416] these parameters were held constant and the value of k_{23} was determined by experiment in pH-buffered distilled water. The total concentration of the test compound in solution (C_T) at any time is

$$C_T = C_b + C_{aq}. \tag{46}$$

The rate expressions for C_b, C_{aq}, C_T, and C_g are

$$\begin{aligned} dC_b/dt &= k_{21}C_{aq} - k_{12}C_b \\ dC_{aq}/dt &= k_{12}C_b - (k_{21}+k_{23})C_{aq} \\ dC_T/dt &= -k_{23}C_{aq} \\ dC_g/dt &= k_{23}C_{aq}. \end{aligned} \tag{47}$$

Implicit in this treatment are the following assumptions: (i) the binding reaction is a set of opposing first-order reactions; (ii) the bound test compound is not volatile; and (iii) dissolved organic matter does not affect the magnitude of k_{23}. This assumption is necessary only if the dissolved test compound does not equilibrate with the gas phase. Given these assumptions, the system can be solved for three special cases as well as the general case. Only the first two cases are reported here, because they refer especially to the determination of the sorption constants, while the last two provide values for the forward and reverse rate constants for the binding reaction.

1st case: "Equilibrium Binding" solution.

If the rate of gas purging is sufficiently slow so that equilibrium is mantained between C_b and C_{aq}, then Eq. (45) is applicable at any point in a purging experiment. Combining Eq. (45) with Eq. (46) and Eq. (47) yields an equation which in integrated form is

$$\ln C_T = -k_{23}t/(1+K_d) + \ln C_T^0,$$

where t is time and C_T^0 is the initial concentration of C_T. Since k_{23} can be determined by experiment using water without binding agent, K_d can be determined from the slope of a plot of $\ln C_T$ vs t. No rate information is provided by this approach. Note that a plot of $\ln C_T$ vs t should remain linear during the entire course of the experiment if the equilibrium binding solution is valid.

2nd case: "Initial Slope" solution.

If the initial rate of volatilization of the dissolved compound from solution is much greater than the rate of dissociation of the bound compound into true solution, then Eq. (40) can be written as

$$C_T = C_{aq} + C_b^0 \tag{48}$$

for a period of time after the start of the experiment. If the system is allowed to equilibrate before the start of an experiment, then the following initial $(t=0)$ conditions exist

$$C_T^0 = C_{aq}^0 + C_b^0, \tag{49}$$

$$K_b = C_b^0 / C_{aq}^0. \tag{50}$$

Solving Eq. (47) and Eqs. (48)–(50) simultaneously yields an expression which, upon integration, becomes

$$C_T = [C_T^0/(1+K_d)]e^{-k_{23}t} + [K_d C_T^0/(1+K_d)].$$

Thus, K_d can be obtained from the ratio of the intercept to the slope of a plot of C_T vs $e^{-k_{23}t}$. Again, no kinetic information is obtained. Note that in this case, a plot of C_T vs $e^{-k_{23}t}$ will be linear only during the initial phase of an experiment. As release of the bound compound becomes significant, the line will begin to curve.

Finally, it should be noted that K_d is a function of the concentration of the binding agent. If this concentration is expressed in terms of (DOC), then the usual partition coefficient is obtained

$$K_{doc} = C_{doc}/C_{aq} = K_d/(\mathrm{DOC}),$$

where C_{doc} is the amount of test compound bound per unit of DOC (e.g., g g^{-1} DOC) and (DOC) is the DOC concentration. If C_{doc}, C_{aq}, and (DOC) are expressed as weight fractions, then K_{doc} is unitless.

Jota and Hassett[393] used the previous equilibrium binding approach to obtain K_{doc} values for 2,2′,5,5′-TeCB binding with humic acids extracted from soil and Aldrich humic acid.

Yin and Hassett[417] determined the association constant of mirex with Aldrich humic acid by GP technique. The experimental apparatus was a 20 dm^3 glass carboy with a 13 cm (o.d.) metal screw cap, containing 19 dm^3 of water samples. The purging tubing was 3.3 mm o.d. stainless steel with six 0.7 mm holes at a depth of 28 cm. Nitrogen bubbling at this depth allowed sufficient time to approach equilibrium with the solute in the water phase. At this condition

$$C_g = HC_{aq}, \tag{51}$$

where C_g and C_{aq} have the same meaning as before and H is the nondimensional Henry's law constant. C_g can be related to the fugacity of the solute in the aqueous phase by the ideal gas law. During gas purging, the solution concentration will decline as described by

$$dC_{aq}/dt = -(F/V)C_g, \tag{52}$$

where F is the purge gas flow rate, and V is the water sample volume. Assuming that the gas and the aqueous phases equilibrate and that all solute in the aqueous phase is in true solution, C_g can be eliminated by combining Eqs. (51) and (52). Integration of the resulting equation yields

$$\ln C_{aq} = -(F/V)Ht + \ln C_{aq}^0, \tag{53}$$

where t is the duration of purging, and C_{aq}^0 is the initial concentration of the solute in water. Note that if an experiment is carried out with sufficiently small F or t or sufficiently large V, C_{aq} essentially equals C_{aq}^0. Under these conditions, determination of C_g will yield C_{aq}^0 from Eq. (51) if H is known and will yield fugacity even if H is not known. This approach is advantageous if particles or DOM are present in the sample since equilibria with these phases are not perturbed and, therefore, do not have to be considered. This approach is similar to static headspace methods in that the gas and water phases equilibrate, but it makes practical the use of large gas volumes. Therefore, this method was termed "dynamic headspace" technique. For operational purposes in this study, C_{aq} is considered essentially equal to C_{aq}^0 if $C_{aq}/C_{aq}^0 > 0.9$.

Preliminary experiments with mirex in distilled water solution allowed us to confirm reaching the equilibrium condition. After a purging time of 120 min at a flow rate of 0.56 dm^3 min^{-1}, the value of H was determined from C_g obtained by analysis of mirex on Tenax trap, and C_{aq} obtained by analysis of mirex in water phase. Substituting this value into Eq. (53) along with the flow rate, the sample volume (19 dm^3), and the purge time, yield $C_{aq}/C_{aq}^0 = 0.93$.

In Aldrich humic acid solution, the apparent Henry's law constant of mirex was significantly lower than that in distilled water, because one portion of mirex was bound to dissolved humic acid and, therefore, was not volatile. The association constant of mirex can be defined

$$K_{doc} = C_d/[C_{aq}(\mathrm{DOC})] \tag{54}$$

and the apparent Henry's law constant (H') in humic acid solution is

$$H' = C_g/(C_{aq} + C_b), \tag{55}$$

where symbols have been already defined and (DOC) is the dissolved organic carbon concentration expressed as a weight fraction. Equations (54) and (55) can be combined with Eq. (51) to give the expression

$$K_{doc} = [(H/H') - 1][1/(\mathrm{DOC})].$$

Since H, H' and (DOC) can all be measured, K_{doc} can be calculated.

Another system was used to study the sorption kinetics of chlorobenzenes to and from suspended sediment and soil particles.[155] It consists of a reaction vessel which is continuously stirred with a magnetic stirrer. Stripping air is pumped and recycled in a closed-loop all-glass system except that a small part of the flow is diverted through a parallel loop containing a photoionization detector (PID). The PID measures the chemical concentration in the gas phase, thereby reflecting the activity of the dissolved compound in the water phase through the Henry's law, and in the solid suspension. The sorption experiment is initiated by pouring the sorbent suspension into the reaction vessel containing a water solution of the compound. The activity of the compound in the solution is monitored continuously during the first hour and is measured intermittently afterwards. Typically, there is no measurable change in activity after 1–2 d. Desorption experiments are similar to sorption experiments except that contaminated sediments are poured into clean water in the reactor. K_d values for sorption or desorption can be calculated from the observed dissolved concentration at the end of the kinetic experiments.

Brusseau *et al.*[517] observed that a disadvantage of the Karickhoff[156] apparatus is that it can only be operated in the desorption mode. On the other hand disadvantages with the design used by Wu and Gschwend[155] are that: (i) desorption can only be studied by using the dilution approach, and (ii) the detection limit of the PID does not allow measurements with sparingly soluble solutes and for those with small Henry's constant values where small changes at minute concentration levels may not be discernable. The apparatus employed by the authors[517] was designed to combine the advantageous features of the two systems and to eliminate the associated disadvantages. It can operate in either closed or open modes using three-way valves placed in line, thus allowing, respectively, the performance of an adsorption experiment and then, with the same slurry, the performance of a desorption experiment. Moreover, a metering valve in-line controls the gas flux, thus enhancing the ability to optimize experimental conditions and an additional valve allows the use of trapping devices when concentrations were too small to be detected by PID. The equilibrium sorption constant K_d can be determined in the following way. Measured quantities of sorbent, water, and solute are placed in the reaction vessel, which is then sealed and shaken to allow the establishment of equilibrium. The vessel is attached to the GP apparatus and the system is operated in the closed mode to determine the equilibrium gas-phase concentration of the solute. With this value, K_d can be determined from the following data: gas volume, water volume, sorbent mass, solute mass, and Henry's constant.

The viability of the GP technique is a function of the Henry's constant of the chemical and the sorptivity of the solute/sorbent combination.[517] It appears ideal for investigating the sorption dynamic of organic contaminants in sediment/water systems. On the basis of some experimental results, it appears that the GP technique is viable for systems having K_d values ranging from over 10^5 to less than 1 dm^3/g and becomes unreliable for K_d values in the range of 0.1–1 dm^3/g.

11.7. Flow Equilibration (FE)

Sorption and desorption isotherms of phenol and chlorophenols have been obtained by using a thermostated continuous flow stirred cell apparatus.[100] This system consists of a suspension of sorbent contained by two hydrophilic membranes (one 0.45 μm and one 0.22 μm) in a glass cell (~100 cm^3) with entry and outlet ports. Eluent solutions are drawn through the cell from a reservoir containing a known concentration of sorptive (sorption) or containing distilled water (desorption) and then through the flow cell of a spectrophotometer by using a peristaltic pump at a known flow rate. Flow rates in the range of 0.03–1.00 $cm^3\ min^{-1}$ have been used to obtain mean residence times of 3000–100 min. The amount of sorptive sorbed at any given time in this system can be obtained through the mass balance around the cell, which can be calculated knowing the volume of reservoir solution input, and the concentration profile of the eluted solution. Sorptive concentration in the eluate is measured by continuous monitoring of absorbance at the wavelength characteristic for each compound in the spectrophotometer flow cell. Linear calibration curves of concentration versus absorbance are obtained for each sorptive, over the range of eluent concentrations used. The absorbance method is checked against quantitation by gas chromatography. Selected eluate fractions can be chromatographed to identify any degradation products formed during the course of interaction. All sorbent are preeluted with distilled water to remove material capable of passing through the end-of-cell membranes. Blank sorption and desorption experiments can be performed for each sorptive, in the absence of sorbent, to verify that there was no interaction with the flow system.

11.8. Field Measurement (FM)

Measurements of pollutant concentrations in samples collected in the field was used to investigate the influence of colloids on binding of PCBs by suspended sediments in an aquatic system.[50] Water samples were collected in bottles and the solute was isolated from the bulk water by passage through a precombusted XAD-2 resin in a glass column. Particles were isolated from bulk water samples with a glass fiber filter (0.6 μm pore size). Nonfilterable PCB concentrations (colloidal associated) were determined by difference. Filter and resin samples were extracted with 1/1 (v/v) hexane/acetone, and the resulting extracts were concentrated by solvent removal, fractionated on Florisil columns, concentrated, and analyzed by gas chromatography.

Sorption of PCBs and other chlorinated compounds by lake and river sediments was investigated.[49] Sediment samples were collected with traps, which consisted of plexiglass tubes fitted at the bottom with removable caps. The traps were suspended in holders on a cable and placed at a certain depth from the surface. The settling particulate samples were Soxhlet extracted with suitable solvent(s) and analyzed. Water samples were filtered and extracted with hexane.

This technique has been found satisfactory for compounds having $\log K_{ow} > 5.5$, but for compounds with lower partition coefficients the field values are considerably higher than the predicted values.[49] The lower the K_{ow}, the larger the observed deviation, up to 40 times for dichlorobenzenes. These results show the difficulties that can be encountered in applying laboratory predictions to field situations.

Adsorption of PAHs on river sediments[544] was determined by refluxing sediment or particulate samples with methanolic KOH, filtering, and extracting the filtrate with cyclohexane. Water filtrate samples were extracted with dichloromethane.

11.9. Batch Equilibration and Ultrafiltration (BU)

Batch equilibration was used also to measure sorption behavior of colloid materials.[399] Water samples are filtered through 0.45 μm filters to remove suspended particulates and then concentrated by ultrafiltration using a hollow fiber system having a nominal molecular weight cutoff of 5000. Sample volumes are thus reduced, resulting in an enriched colloidal fraction (ECF) and an ultrafiltrate. Solutions containing known amounts of the chemical are prepared in ultrafiltrate water, then sonicated, stirred in the dark at a given temperature for 24–36 h, and filtered through a 0.2 μm filter to remove any contaminant particle or crystals. The ECF fraction is divided in portions, and a given volume of ultrafiltrate containing a known amount of chemical is added to each. The spiked samples are equilibrated in a shaker and then recirculated through the hollow fiber system to separate the colloidal and ultrafiltrate fractions. The chemical in each fraction is concentrated and analyzed.

11.10. Fluorescence Quenching (FQ)

This method has been developed for determining equilibrium constants for the association of PAHs with dissolved humic and fulvic acids[188,415] and to follow the rate of association between PAHs and dissolved humic matter.[400] The measurement is based upon the observation that PAHs fluoresce in aqueous solution but not when associated with dissolved humic materials. If we assume that the fluorescence intensity is proportional to the concentration of free PAH in solution, then

$$F_0/F=[\mathrm{PAH_T}]/[\mathrm{PAH_D}]=1+K_d[\mathrm{Hu}], \qquad (56)$$

where F_0 and F are the fluorescence intensities in the absence and presence of humic material, respectively, $[\mathrm{PAH_T}]$ is the total initial concentration of PAH and $[\mathrm{PAH_D}]$ is the dissolved concentration of PAH in the presence of humic material. Since, at the concentrations used, a significant excess of humic acid is present, [Hu] can be taken as the amount of added humic acid without correction for the fraction of humic that is associated with PAH. K_d can be calculated from the slope of the plot of F_0/F as a function of the concentration of humic acid. A correction factor should be calculated to account of the apparent quenching due to an attenuation of the excitation beam and/or absorption of emitted radiation by an excess concentration of fluorophore or by the presence of an additional absorbing species in solution (''inner filter effect''). The maximum value of this factor for a 1×1×4 cm quartz fluorescence cuvette did not exceed 1.8, which was well within the recommended acceptable range.[415] In general, the binding of a PAH compound with dissolved organic carbon may be expressed as

$$F_0/F=1+K_{oc}[\mathrm{DOC}].$$

A very detailed study on the correct use of this method has been presented with modifications of Eq. (56), by taking into account the possibility of substantial wall losses from aqueous solutions and no full quenching of organic colloids-associated compound fluorescence.[545]

11.11. Equilibrium Dialysis (ED)

This method was used to measure the association constants of organic chemicals with DOM.[402,414]

A water sample with known characteristics (pH, ionic strength, etc.) is poured in a glass bottle and spiked with a solution of the compound under examination. A dialysis bag is filled with a solution of known concentration of humic material and transferred to the bottle. The bottle is shaken at a fixed temperature for a time necessary to reach equilibrium. At the end of this period aliquots are removed from both the dialysis bag and the solution outside the dialysis bag and analyzed for the compound. In a dialysis experiment it is assumed that the compound inside the dialysis bag consists of two fractions: one fraction is free, truly dissolved compound, while the other is bound to humic materials. Since the free compound can diffuse through the dialysis bag, the concentration of free compound will be the same both inside and outside the bag. The bound concentration can then be determined as the difference between the compound concentration inside and outside the dialysis bag. A dialysis experiment, therefore, measures the amount of bound compound as a function of the free compound concentration.

11.12. Reversed-Phase Separation (RS)

This method was also used to measure the association constants of organic chemicals with DOM.[414,546]

The [^{14}C] organic compound is added to humic acid solution and allowed to equilibrate at room temperature for at least 18 h. Aliquots of the test solution are taken and the total ^{14}C activity is measured by liquid scintillation counting. Separation of humic-bound compound from free compound can be made with a C-18 cartridge or C18 reverse-phase HPLC column. It is assumed that humic bound compounds would pass through the resin with the humic acid. Measurements of the organic matter as DOC before and after separation can confirm that humic acid quantitively pass through the cartridge. The partition coefficient can be calculated as the ratio of the g of pollutant per g of DOC (determined from the ^{14}C activity passing through the cartridge and measured DOC) divided by the g of pollutant per cm^3 trapped (freely dissolved). The amount trapped can be determined from the difference of the ^{14}C activity total per cm^3 minus the ^{14}C activity per cm^3 passing through the cartridge. Harkey *et al.*[547] used this procedure to measure the association constants for BaP, transchlordane, pyrene, and endrin in sediment porewater and elutriate. Before separation samples were filtered through two glass fiber filters or centrifugated to remove the particulate matter.

Great Lakes[409] and Green Bay[410] waters, freshly collected, were inoculated with radiolabeled hydrophobic compounds and, after batch equilibration, separated into particle-bound using glass fiber filter, DOC-bound using C-18 reverse phase Sep Pak, and freely dissolved phases, in order to determine the respective K_{oc} and K_{doc} values.

11.13. Solubility Enhancement (SE)

The K_{dom} values for chemicals on humic acids have been obtained by Chiou *et al.*[220] by measuring enhanced solubility due to the presence of various amounts of cosolutes and calculating the association constants by Eqs. (18) and (19). Solutions containing cosolutes were placed in centrifuge tubes with Teflon-line screw caps, and the test compound was subsequently added to each tube in amounts slightly more than required to saturate the solution. These samples were then equilibrated on a reciprocating shaker and centrifuged to separate the excess solute. Undissolved solute particles adhering to the meniscus were aspirated from the surface. Centrifugation and aspiration may be repeated to completely eliminate the excess solute. Subsequently, an aliquot of the supernatant was carefully withdrawn with a volumetric pipet and analyzed for determining solubility.

11.14. Adsorption on the Glass (AG)

This method has been used for the determination of the association constants of PCBs with humic material (HM).[413] It is based on the measurement of the fraction of compounds adsorbed on the glass walls of the flask containing a reference solution without HM and the measurement of the fractions of compounds adsorbed in the presence of known concentrations of HM. The PCBs adsorbed on the glass were determined by extraction with hexane and analysis of the hexane extracts. Equations derived to calculate sorption constants are available in the original paper.[413]

11.15. Humic Acid Titration (HT)

Carboxyl groups in humic acid are responsible both of the catalysis of atrazine hydrolysis to hydroxyatrazine and of the sorption of the two compounds by humic acid.[548] Titration of the carboxyl groups and separate measurements of the kinetics of atrazine hydrolysis allowed us to determine the equilibrium sorption constants for atrazine and hydroxyatrazine and the rate constant for atrazine conversion on the catalytic sites.

12. Prediction Methods for the Evaluation of Sorption Coefficients

The experimental methods for the determination of the environmental properties such as water solubility, bioconcentration factor, and soil sorption are expensive and time consuming and may be very inaccurate especially for compounds of low solubility. Therefore, some alternative methods were proposed for their prediction[120] based on the general Collander[549] equation

$$\log K_1 = a \log K_2 + b, \tag{57}$$

where K_1 and K_2 are organic solvent-water partition coefficients. The constants a and b can be calculated knowing only the water concentration in the two organic solvents. Equation (57) has been extended to the cited environmental properties, which all may be regarded as partition of a chemical between an organic phase and water.[120] The measurement or calculation of one property allows prediction of the other to within 1 order of magnitude.

Mc Gowan[550,551] proposed to calculate solubilities and partition coefficients for solutes not forming hydrogen bonds using correlations with the parachor; corrections were introduced to account for hydrogen-bonding interaction.[551] Other authors[116,552] applied these correlations to the prediction of K_{om} or K_{oc} for pesticides. K_{om} or K_{oc} values were also estimated using correlations with K_{ow}, solubility, specific surface area, indices of molecular structure, or capacity factors in reversed-phase high-pressure liquid chromatography. Some reviews are available on this matter.[105,553,554] Gawlik *et al.*[555] reviewed and classified more than 200 existing relationships for K_{oc} estimations.

12.1. Correlations with Octanol/Water Partition Coefficients

The role of organic matter of soils and sediments in controlling the sorption of hydrophobic compounds may be assumed to be similar of that of an organic phase in solvent extraction.[26,176] Octanol has been chosen to simulate natural organic phases and many authors have demonstrated that adsorption coefficients (K_{oc}) may be estimated from the octanol–water partition coefficients (K_{ow}) using suitable correlation equations.

The relative lipophilicity of organic phases may be determined by comparing the solubility of a hydrophobic compound in each of them. This may be accomplished by extrapolating the observed partitioning to the aqueous solubility limit (at saturation) (S_w), at which the sorbed concentration is designated as the "solubility" in OM (S_{om})[197]

$$S_{om} = K_{om} S_w .$$

Chiou[197] has reported that PCE solubilities (S_{om}) in soil OM and humic acid are 42 and 27 mg g^{-1}, respectively, and that the estimated solubility of PCE in octanol is 72 mg g^{-1}. A previous study[363] has shown that the soil humic acid is about half as effective as soil organic matter in sorption of relatively nonpolar organic compounds. Furthermore, both sorbents show a lower solubility power than octanol for PCE, thus demonstrating a lower lipophilicity. On the other hand, humic substances can absorb a larger amount of water than octanol, thus demonstrating a more polar character.[55] Therefore humic substances are less favorable partitioning phases than octanol for nonpolar chemicals. Accordingly, Chin and Weber[206] found that experimental binding constants of organic compounds with humic acid (K_{oc}) are consistently

0.2–1.5 log units lower than their respective K_{ow} and that these differences appear to increase with increasing hydrophobicity.

Karickhoff[96] derived the following equation relating K_{oc} to K_{ow} on the basis of the fugacity model[7]

$$K_{oc}=(\phi^0/\phi^{oc})K_{ow}, \qquad (58)$$

where the proportionality constant is the ratio of fugacity coefficients for the solute dissolved in octanol (saturated with water) (ϕ^0) on that bound to natural organic matter (ϕ^{oc}). For K_{oc} and K_{ow} to be linearly related, this ratio must be independent of solute. Karickhoff[96] found that sorption coefficients normalized to organic carbon, K_{oc}, for hydrophobic compounds were highly invariant over a set of sediments and soils and that their values for five compounds (benzene, naphthalene, phenanthrene, anthracene, and pyrene) were related to K_{ow} through a relationship of the type of Eq. (57)

$$\log K_{oc}=0.989 \log K_{ow}-0.364 \quad r^2=0.997.$$

The near-unity coefficient, a, for $\log K_{ow}$ substantiates the constancy of the ratio of fugacity coefficients in the organic phases for this series of compounds. Fitting the linear form, Eq. (58), gives

$$K_{oc}=0.411 K_{ow} \quad r^2=0.994.$$

This equation allowed us to estimate K_{oc} values for many compounds of a different chemical nature, which were compared with the experimental K_{oc}s. Compounds for which solute speciation could be expected (such as organic bases with $pK_a>3$) were excluded. The agreement between calculated and measured K_{oc} values was good, within a factor of 3 or 0.48 log units, comparable to typical deviations in K_{oc} reported for a given compound on widely differing sediments and soils.

A similar linear relationship ($a=1.00$ and $b=-0.21$; $r^2=1.00$) between K_{oc} and K_{ow} was derived in a study[108] concerning the sorption on sediments of 7 PAHs, benzene, and 2 chlorinated hydrocarbons (methoxychlor and 2,4,6,2′,4′,6′-HCB). The same relationship was used by Hassett *et al.*[179] to predict the K_{oc} value of dibenzothiophene, which was in good agreement with that obtained from the sorption experiments. An equation with constants very close to the previous ($a=1.029$ and $b=-0.18$) was found by Rao and Davidson[87] with several pesticides

Schwarzenbach and Westall[207] applied the linear free-energy relationships to partitioning of nonpolar solutes (6 alkylbenzenes and 7 chlorobenzenes) between water and soil organic matter. A highly significant linear correlation ($a=0.72$ and $b=0.49$) was found between the logarithms of the average K_{oc} values and the logarithms of the K_{ow} values for these compounds. The slope parameter is $a=0.72$, suggesting that the natural sorbents investigated in that study are less lipophilic than octanol and more similar to butanol.[556]

Dzombak and Luthy[553] observed that for hydrophobic compounds a series of parallel lines can be obtained when $\log K_{ow}$ is plotted against $\log K_d(K_f)$ for sorbents having single OC contents.

Vowles and Mantoura[128] determined by batch equilibration the K_d values for benzene and six alkylbenzenes and for naphthalene, four alkylnaphthalenes, phenanthrene and pyrene, using a surface estuarine sediment with an organic content of 4.02%. The correlation between $\log K_d$ values and the respective $\log K_{ow}$ values gives the equation with $a=1.15$ and $b=-2.53$ ($r^2=0.961$), which accommodating on organic carbon content of 4.0% gives the corresponding $\log K_{oc}-\log K_{ow}$ relationship in which b changes to 1.13. The authors demonstrated that the K_{oc} data are more sensibly correlated if the hydrocarbons are placed into homologous groups, like:

- benzene-naphthalene-phenenthrene-pyrene: $a=1.20$; $b=1.13$; $r^2=0.998$;
- alkylbenzenes: $a=0.904$; $b=-0.46$; $r^2=0.996$;
- alkylnaphthalenes: $a=0.774$; $b=0.37$; $r^2=0.992$.

The equation obtained for alkylbenzenes agrees very well with that found for benzene, chlorobenzenes and PCBs (12 compounds) sorbed on soils[55]

$$\log K_{om}=0.904 \log K_{ow}+0.779 \quad r^2=0.989. \qquad (59)$$

Lara and Ernst[182] found highly significant correlations between the experimental $\log K_{oc}$ values for several PCB congeners obtained with each of three sediments and the respective $\log K_{ow}$ values. However, if the K_{oc}s of the three sediments were pooled, lower correlations were obtained. The correlation became significantly higher if a multiple regression analysis were adopted, taking the pooled $\log K_d$ values of the same PCB congeners for the three sediments as dependent variable and $\log f_{oc}$ and $\log K_{ow}$ as independent variables.

Brown and Flagg[130] determined the K_{oc} values of nine chloro-s-triazine and dinitroaniline compounds with a coarse silt fraction of a pond sediment. These values, that were well correlated with the K_{ow} values, were compared with the work by Karickhoff *et al.*[108] The more polar character of the compounds under examination, however, reduced the precision of estimating sorption from octanol/water partition coefficients. A fit of the combined data sets for a total of 19 compounds of widely varied properties (5 orders of magnitude variation in solubility) yielded a relationship with $a=0.937$, $b=-0.006$, and $r^2=0.95$. Estimates of K_{oc} based on this empirical equation were within a factor of 2 or 3 of the measured values. The authors concluded that predictions of this quality would be adequate for many environmental modeling applications.

A significant relationship exists between K_{oc} and K_{ow}[97,180] for the sorption of 22 nonpolar compounds by various soils and sediments ($a=1.00$; $b=-0.317$; $r^2=0.980$), which is very similar to the Karickhoff[108] equation. However, when this equation is used to predict K_{oc} values for amino-substituted PAHs, the calculated values are significantly lower than the observed values.[557] These data suggest that, although the sorption of these aromatic amines is highly correlated with the OC content of the substrates, the strength of the sorption is greater than can be accounted for based on hydrophobic association of neutral aromatic nuclei to sediment OM, as was observed for neutral PAHs.

Some equations were derived for polar compounds sorbed on soils. They regard correlations $\log K_{oc}-\log K_{ow}$ for:

(i) 45 chemicals, mostly pesticides:[217] $a=0.544$; $b=1.377$; $r^2=0.74$;

(ii) 105 chemicals (anilines, anilides, nitrobenzenes, urea derivatives, carbamates, organophosphates, halogenated compounds, etc.):[120] $a=0.52$; $b=0.64$; $r=0.95$. This equation, correlating $\log K_{om}$ to $\log K_{ow}$, was obtained from only two soil series, but similar results can be derived from results with widely differing soils. Briggs[120] reported similar equations derived from the data obtained with 17 Australian soils,[558] with Iowa soils,[122] with Brazilian soils,[559] and with soils and a stream sediment from Eastern Canada,[264]

(iii) Nonionized phenols:[337] $a=0.82$; $b=0.02$; $r^2=0.98$, where the K_{oc} values were obtained from the K_d measured with three sorbents, lake sediment, river sediment, and aquifer material and the respective f_{oc} values (0.094, 0.026, 0.0084);

(iv) Nonionized phenols:[111] $a=0.75$; $b=0.62$ with a standard error of fit $s=0.19$ which allows predictions within a factor of 2.

Estimates of K_{doc} with this type of equations were obtained by Chin and Weber[206] who collected data of the association or binding constants with humic acids for 14 compounds (TCE, toluene, PAHs, PCBs, chlorobenzenes, α-chlordane, and DDT) and obtained a correlation with the respective K_{ow}[560] having $a=0.82$ and $b=0.1923$ with $r=0.96$. The experimental binding constants were consistently 0.2–1.5 log units lower than their respective K_{ow}; these differences appear to increase with increasing hydrophobicity. They concluded that humic polymers are more polar than octanol and thus comprise thermodynamically less favorable partitioning phases for nonpolar organic solutes, as already suggested by Chiou *et al.*[55]

Correlation between log association constants (K_{doc}s) with humic substances and $\log K_{ow}$ for PCB congeners[413] gave a relationship with $a=0.377$, $b=2.387$, and $r=0.974$.

Sabljić *et al.*[561] have recently carried out a systematic study to evaluate the quality and reliability of the quantitative $\log K_{oc}-\log K_{ow}$ relationships. A system of QSAR models has been derived which is based on a reliable set of experimental or estimated $\log K_{ow}$ data. Particular emphasis has been made to clearly define the boundaries for application of developed models as well as the quality of estimates. Thus, for each developed model its application domain has been uniquely defined by unambiguous description of its chemical (structural) domain, substituents domain, and X-variable domain. As a result of this study, a series of $\log K_{oc}-\log K_{ow}$ relationships has been obtained, which are specific for 20 compound types. Finally, the QSAR model with the first-order molecular connectivity indices has been incorporated in the derived system of QSAR models since the soil sorption estimates of the predominantly hydrophobic chemicals based on the $\log K_{ow}$ data have large uncertainties, particularly in the $\log K_{ow}$ data range from 4 to 7.5.

Gerstl[562] collected and analyzed sorption data for more than 400 compounds. He found that the equations $\log K_{oc}$ vs $\log K_{ow}$ for individual chemical groups were preferred over the general equation representing all data, which is

$$\log K_{oc}=0.679\log K_{ow}+0.663 \quad r^2=0.831.$$

The individual class curves are mostly not parallel to each other and intersect at a K_{ow} value of ~2. Both above and below this value of K_{ow} the lines diverge so that use of the "total" equation at extreme values of K_{ow} will result in very large errors. Furthermore, application of a polarity correction term (F_c) might improve the fit over a certain segment of the curve, but will at the same time increase the discrepancy along the rest of the curve so that overall no improvement will be noted. The correction term F_c can be obtained by the following expression:

$$F_c=1/n\sum_n(\log K_{oc}^{\text{pred}}-\log K_{oc}^{\text{obs}}),$$

where K_{oc}^{pred} is the K_{oc} value predicted from the general equation. This enables us to calculate an adjusted K_{oc} value

$$\log K_{oc}^{\text{adj}}=\log K_{oc}^{\text{pred}}-F_c.$$

F_c is related to the polar character of the compounds; the lower the value of F_c (non-negative) the more nonpolar the group; similarly, the greater the F_c, the more polar the compounds comprising that group.

12.2. Correlations with Water Solubility

Most of the $K_{oc}-S$ relationships were derived between 1979 and 1990. In some of them, derived for liquid and solid compounds, solubility of solid compounds was taken as such without including any correction term. This procedure did not take into consideration that solubility of solid compounds must be modified because of the melting point effect when it has to be examined together with solubility of liquid compounds.

Chiou *et al.*[195] determined the linear isotherms for seven chlorinated hydrocarbons onto a silt loam soil with 1.6% organic matter and collected from the literature the sorption data for several chlorinated compounds (PCBs and pesticides), which covered over seven orders of magnitude of solubilities (S). For all these 15 liquid compounds the $\log K_{\mathrm{om}}$ values were correlated to $\log S$, giving

$$\log K_{\mathrm{om}} = -0.557 \log S + 4.040 \quad r^2 = 0.988,$$

where S is in mmol m^{-3}. This result, together with the lack of isotherm curvature, is consistent with the idea that the uptake of neutral organic chemicals by soil is essentially a process of partitioning (dissolution) rather than physical adsorption, with a corresponding low enthalpy contribution.

Similar values of the slope were often obtained in this type of relationships:

(i) An equation with $a = -0.561$ and $b = 3.8$ was found by Gerstl and Mingelgrin[563] for seven pesticides of different chemical composition, spanning eight order of magnitude of solubility (μmol dm^{-3});

(ii) Felsot and Dahm[122] derived their equation ($a = -0.539$; $b = 8.012$; $r^2 = 0.950$) for five carbamate insecticides in five soils with various OM content. S was expressed in g m^{-3}.

(iii) Kenaga and Goring[217] and Kenaga[564] estimated the K_{oc} values for 358 compounds, mostly pesticides, using an equation, derived from 106 experimental literature data, having $a = -0.55$ and $b = 3.64$, where S was in g m^{-3}. This relationship gave values of $\log K_{\mathrm{oc}}$ ± 1.23 order of magnitude from the calculated values at 95% confidence limit.

(iv) Karickhoff *et al.*[108] found the same slope of the plots ($a = -0.54$; $b = 0.44$; $r^2 = 0.94$) in which the K_{oc} values were averages for isotherms run on the coarse silt fractions of two sediments with seven PAHs, benzene, methoxychlor and 2,4,6,2′,4′,6′-HCB and S was in mole fraction.

A slightly different equation was derived[97,180,210,565] ($a = -0.686$; $b = 4.273$; $r^2 = 0.933$) with the data for a total of 22 compounds including PAHs, chlorinated compounds, and few polar compounds on soil/sediment systems,[179] with S in g m^{-3}. The relationship between $\log K_{\mathrm{oc}}$ and $\log S$ (g m^{-3}) for benzene, naphthalene, and anthracene on estuarine colloids gave a slope of -0.693 and an intercept of 4.851 with $r^2 = 0.985$,[399] demonstrating that natural colloids and soils/sediments exhibit similar sorption characteristics to nonpolar organic compounds.

Correlation between $\log K_{\mathrm{doc}}$ s and $\log S$ (mg m^{-3}) for the association of PCBs[413] with humic substances allows to recognize the influence of the ortho-substitution because K_{doc} decreases within groups of isomers with increasing number of ortho-chlorines. This is due to the fact that solubility of PCB isomers increases with ortho-substitution. The relative equation has $a = -0.973$ and $b = 6.186$ ($r = -0.976$).

As we have seen, some of the $\log K_{\mathrm{oc}}$–$\log S$ equations shown so far were derived without taking into consideration any correction for the solubility of solid compounds. Briggs[120] observed that the solubility was not such a good predictor as K_{ow} for the K_{oc} values calculated by Kenaga and Goring[216] for organic pesticides, probably because the effect of melting point on solubility was not taken into account for solid compounds.

Karickhoff[52,96] reported the K_{oc} expression for nonpolar organic compounds as a function of the fugacity coefficients for water and soil (sediment) OM

$$K_{\mathrm{oc}} = \phi^{\mathrm{w}} / \phi^{\mathrm{oc}}. \tag{60}$$

In comparing K_{oc} for a series of hydrophobic solutes on a given soil or sediment, variations are expected to be dominated by variations in the aqueous phase coefficient, ϕ^{w}, due to solute–solvent dissimilarity, and can be related to solute solubility in the aqueous phase. For the series of compounds taken into consideration by the author (benzene, naphthalene, phenanthrene, anthracene, and pyrene), for which solubility goes from 1790 to 0.135 g m^{-3}, one would expect a 3–4 order of magnitude increase in activity coefficients, γ_{w}, in going from benzene to pyrene. On the other hand, for hydrophobic solutes in association with sediment or soil organic carbon, one would expect solute–sorbent adhesive interactions to be quite similar to solute–solute cohesive interactions with a much smaller range of variability from solute to solute. For a series of hydrophobic solutes, Eq. (60) becomes

$$K_{\mathrm{oc}} \propto \gamma_{\mathrm{w}},$$

where the reference fugacity state for the solute is taken to be the pure super-cooled liquid. For hydrophobic liquids, γ_{w} is equal to the reciprocal of the mole fraction solubility X_{sol}. For solutes that are solids at room temperature, a crystal energy term must be added

$$\log \gamma_{\mathrm{w}} = -\log X_{\mathrm{sol}} - \Delta S_{\mathrm{f}}(T_{\mathrm{m}} - T)/(2.303RT), \tag{61}$$

where T_{m} and T are the melting and equilibrium temperatures (K), ΔS_{f} is the enthropy of fusion, and R is the gas constant. The entropy of fusion ($\Delta H_{\mathrm{f}}/T_{\mathrm{m}}$) has been found[566–568] to be not highly variable for many aromatic compounds having "rigid" molecules (generally 12–15 eu), with an approximate value of 13.5 ± 3 cal mol^{-1} K^{-1} or 56.5 J mol^{-1} K^{-1}. With these assumptions, the crystal energy term in Eq. (61) becomes $-0.00953\,(T_{\mathrm{m}} - 298)$.

Thus, the dependence of K_{oc} on solubility can be expressed as

$$\log K_{\mathrm{oc}} = -a \log X_{\mathrm{sol}} - 0.00953(T_{\mathrm{m}} - 298) - b, \tag{62}$$

where b depends upon the fugacity coefficient, ϕ_{oc}; ideally, if ϕ_{oc} is relatively independent of solute, a approximates unity.

Commonly, the linear regression of $\log K_{\mathrm{oc}}$ vs $\log X_{\mathrm{sol}}$ has been used with no explicit crystal energy contribution.[108,195,211,217] For the five cited aromatic hydrocarbons,[96] the linear regression without this contribution gives

$$\log K_{\mathrm{oc}} = -0.594 \log X_{\mathrm{sol}} - 0.197 \quad r^2 = 0.945,$$

while linear regression including the crystal energy term gives the following form of Eq. (62):

$$\log K_{oc} = -0.921 \log X_{sol} - 0.009\,53(t_m - 25) - 1.405 \quad r^2 = 0.995. \tag{63}$$

This crystal energy term significantly improves the quality of fit to the experimental data. For solutes that are liquids at 25 °C, the melting point is "set" at 25 °C and the crystal term vanishes. Also, the fitted coefficient, a, for the solubility term much more closely approximates unity, thus supporting the assumed dominance of γ_w in K_{oc} variations between solutes. Equation (63) has been used to derive K_{oc} values for many compounds (triazines, carbamates, organophosphates, and chlorinated hydrocarbons), and was found to estimate K_{oc} usually within a factor of 2–3 of measured values.[52] Equation (63) worked well for low molecular weight compounds but tended to overestimate sorption coefficients of highly chlorinated, high molecular weight compounds, for which the a value may be in the range of 0.7–0.8. For 47 organic compounds the literature K_{oc} values allowed to obtain an a value of 0.83 and a b value of −0.93.

Briggs[120] derived the following relationship for a pool of several polar (mostly pesticides) and nonpolar compounds (chlorinated hydrocarbons):

$$\log K_{om} = -0.51[\log S + (0.01 t_m - 0.25)] + 0.8 \quad r = -0.88,$$

where S is the molar water solubility, t_m is the melting point in °C.

Following Chiou *et al.*,[55] to analyze the relative effects on partition coefficient of solute solubility in water, compatibility with soil organic phase, and alteration of water solubility by soil organic components dissolved in water, a reference ideal line relating sorption coefficient with water solubility is needed. The authors, by considering the major components of soil humus to be amorphous polymeric substances, applied the Flory–Huggins theory[200,201] to account for the solute activity in an amorphous polymer. They derived an equation describing a reference ideal line relating sorption coefficient to water solubility. The equation, after some approximations, is

$$\log K^0_{om} = -\log S V_m - 0.622, \tag{64}$$

where K^0_{om} is the theoretical K_{om}, S is the molar water solubility, and V_m is the molar volume of the solute.

The authors[55] investigated the sorption of 12 aromatic compounds (benzene derivatives and PCBs) from aqueous solutions on a soil having 1.9% organic matter content. They derived the following regression equation:

$$\log K_{om} = -0.813 \log S V_m - 0.993 \quad r^2 = 0.995, \tag{65}$$

where S is in moles/L and V_m in L/mole. The experimental $\log K_{om}$ values show a systematic deviation from the ideal line [Eq. (64)] making the slope of the experimental line significantly different from −1. Therefore, the effect of $\log S V_m$ is more important than the effect of solute incompatibility with soil organic phase, which was found greater than the corresponding effect for the same compounds with the octanol phase.[569] This indicates that soil organic matter is inferior to octanol as a partition phase for relatively nonpolar organic compounds in agreement with the generally more polar nature of the soil organic matter with respect to octanol. Finally, since variability of V_m is small compared to that of S, the correlation between $\log K_{om}$ and $\log S$ should be essentially linear. Omitting the molar volume term from Eq. (65), the present study leads to

$$\log K_{om} = -0.729 \log S + 0.001 \quad r^2 = 0.996. \tag{66}$$

The coefficient of $\log K_{ow}$ for a selected group of compounds should approximate the ratio of the change of $\log K_{om}$ with $\log S$ to that of $\log K_{ow}$ with $\log S$. The ratio of −0.729 in Eq. (66) to −0.799 in $\log K_{ow}$ vs $\log S$ for the 12 compounds yields 0.912, in good agreement with the coefficient (0.904) of Eq. (59).[55]

Vowles and Mantoura[128] obtained a good correlation between $\log K_d$ for 14 aromatic and polyaromatic hydrocarbons sorbed on a surface sediment and $-\log S V_m$, where S is the liquid or supercooled liquid molar solubility and V_m is the molar volume of hydrocarbon

$$\log K_d = -1.142 \log S V_m - 3.132 \quad r^2 = 0.955.$$

Alkylbenzenes are more closely correlated ($r^2 = 0.994$) with the PAHs showing enhanced sorption.

Lara and Ernst[182] found highly significant correlations between the experimental $\log K_{oc}$ values for 33 PCB congeners obtained with each of three sediments and the respective $\log S$ values. However, if the K_{oc}s of the three sediments were pooled, lower correlations were obtained. The correlations became significantly higher if a multiple regression analysis were adopted, taking the pooled $\log K_d$ values of the same PCB congeners for the three sediments as dependent variable and $\log f_{oc}$ and $\log S$ as independent variables. The regression equation obtained was:

$$\log K_d = 4.669 - 0.488 \log S + 0.785 \log f_{oc} \quad r = 0.976$$

where S was in g m^{-3}.

The sorption of three groups of polar organic compounds capable of H bonding with inorganic soil surfaces (ketones, alcohols, phenols) by three soils having different organic carbon contents was compared with the sorption of nonpolar compounds by the same soils.[570] A wide variation in K_{oc} values among the compounds and soils has been observed. The average range of K_{oc} for individual compounds among the three soils was a factor of 3–4 for all compound classes except phenols, for which the average range was of about a factor of 100. When phenols were excluded from consideration, the relationship observed between water solubility of subcooled liquid phase (g m^{-3}) and K_{oc} in this work showed a constant $a = -0.50$ and a constant $b = 3.94$.

Gerstl[562] derived $\log K_{oc} - \log S$ (molar) correlations for more than 400 compounds. It was observed that, like $K_{oc} - K_{ow}$ relationship, the equations for individual chemical groups were to be preferred over the general equation for all chemicals, but that a group correction term (F_c) added to the total equation gave similar results. Solubility of solid compounds was corrected (S_{corr}) for the crystal energy contribution. The results of this investigation showed that in general the correlation between K_{oc} and K_{ow} is better than that between K_{oc} and S or S_{corr}. In many cases the use of S_{corr} instead of S does not result in any significant improvement in correlations. In particular, the classes for which S_{corr} results in the greatest increase in correlation are amides, triazines, and dinitroanilines. For these compounds, which have a similar structural unit based on an aromatic ring, the solubility correction term, which was derived basically for rigid molecules, is more apt to reflect true changes in solubility. For any other classes (carbamates, organophosphorous pesticides, etc.) the combination of a large number of different structures makes any correction in S of secondary importance only. An interesting point is that the slopes for each individual class to more or less parallel for the K_{oc}–S relationship. Thus, the adjusted curves (calculated using F_c) would be shifted to more or less overlap the "total" curve, which is represented by the following equation:

$$\log K_{oc} = -0.508 \log S + 0.953 \quad r^2 = 0.757$$

or by

$$\log K_{oc} = -0.515 \log S_{corr} + 1.310 \quad r^2 = 0.716.$$

The fact that the K_{oc}–S curves for the different groups are nearly parallel would seem to indicate that the same interactions affecting a compound's aqueous solubility also affect its sorption by soil OM. The difference between groups (intercepts) might be indicative of differences in the nature of the sorbent OM or of basic solubility differences between the chemical classes.

12.3. Correlations with Capacity Factors in RPLC

The partition concept for sorption appears to parallel the theory for reversed-phase high-pressure liquid chromatography (RP-HPLC or RPLC).[55,571–573] Both processes involve partition of the solute into the polymeric (organic) phase. The mineral fraction of soil and the column support interact preferentially with the polar solvent (water) and are thus relatively inert to nonionic organic compounds.[55]

In RPLC the stationary phase is typically a nonpolar coating of a long chain hydrocarbon (e.g., C18) bonded to an inert support and the mobile phase is generally constituted by methanol/water (given as v/v) mixtures of various compositions. Woodburn *et al.*[574] have demonstrated the similarity in sorption energetics and, therefore, in solute retention mechanism for PAH retention by the RPLC sorbents (trichloroalkylsilanes: C2, C4, and C8) and by a soil from the binary mixed solvent (30/70 methanol/water). The RPLC method would allow us to overcome the difficulty with $\log K_d\,(K_{oc}) - \log K_{ow}$ relationships; first, the uncertainty in the K_{ow} values, and second, the necessity of using different equations changing substrate or compound types.

The fundamental expression associated with equilibrium sorption on chromatographic supports is

$$k' = rK,$$

where k' is the chromatographic retention factor or capacity factor, r is the volume phase ratio of the stationary and mobile phases, and K is the thermodynamic equilibrium binding constant.[574] The k' value is given by

$$k' = (t_r - t_0)/t_0,$$

where t_0 is the retention time of an unretained compound and t_r is the retention time of the solute under study.

McCall *et al.*[575] found a good linear correlation between $\log K_{oc}$ for nine pesticides and retention time with C18 reverse phase column, using 85/15 methanol/water mixture as the mobile phase. This allows us to predict K_{oc} values for any chemical from its retention time. Hamaker[576] showed that the distance a chemical moves through a soil column is inversely proportional to its sorption coefficient. Therefore, a plot of $1/(K_{oc} \times f_{oc})$ or $1/K_d$ versus distance moved should be linear. Such a plot has been obtained by McCall *et al.*[575] with the nine pesticides and each of the three soils they used. From these results they derived a classification system with general mobility classes for chemicals based on the retention time and K_{oc} values

Retention time relative to 2,4-D	K_{oc}	Mobility class
0–1	0–150	Very high
1–1.8	50–150	High
1.8–3.1	150–500	Medium
3.1–4.5	500–2000	Low
4.5–7.0	2000–5000	Slight
>7.0	>5000	Immobile

2,4-D and carbofuran leached completely through the column, therefore retention times were referred to that of 2,4-D. Chemicals which are more soluble in the organic stationary phase, more hydrophobic, will exhibit longer retention times which can be correlated with the different partition coefficients.[573,575] Linear regression analysis of a log–log plot of the measured K_{oc} values for the nine pesticides versus their RPLC retention times (t_r) gave the following linear regression equation:

$$\ln K_{oc} = 3.446 \ln t_r + 1.029 \quad r = 0.98.$$

Estimation of K_{oc} by this equation appeared to provide nearly as good a value as the actual measurement.

Vowles and Mantoura[128] determined for a series of hydrophobic compounds the K_d values for a sediment/water sistem and the capacity factors on RPLC using an octadecylsilane phase (ODS) (75/25 methanol/water) and an alkylcyano phase (CN) (55/45 methanol/water), respectively. They obtained a series of $\log K_d - \log k'$ relationships and concluded that the alkylcyano phase is behaving as a similar sorbent to sediment organic matter for all 14 hydrocarbons and that octanol and octadecylsilane show progressively larger divergences; thus an order may be generated

organic matter~alkyl CN>octanol>ODS.

The divergences in the behavior of these four phases are interpreted on the basis of different polarity, with organic matter being the most polar due to the presence of groups such as carboxyl, phenol, and amine in humic materials and octadecylsilane the least polar. Octanol and alkylcyano are intermediate. Aromatic hydrocarbons are more polar than aliphatic hydrocarbons; modification of the aromatic structure may then cause greater change in partition to a similar phase (organic matter) than to one that is not (octanol or ODS).

Therefore, ODS phase is not the most suitable for the prediction of K_{oc} values for polar compounds, due to nonhydrophobic interactions involved in sediment adsortion.[577] The correlation $\log K_{oc}-\log k'$ improves with increasing water content; one reason may be that the higher water content in the mobile phase more closely represents the conditions which prevail when measuring the real soil/water partition coefficients. However, the correlation coefficient is still low ($r^2=0.755$); it may be improved if two types of variables, which reflect polar interactions, are included. One is the $\Delta\chi$ term, which is derived from molecular connectivity indices[578] (Sec. 12.4), and the other is an indicator variable which expresses hydrogen-bonding actions (HA, the number of electron acceptor groups+HD, the number of electron donor groups). The regression equation obtained introducing the two independent variables are

$$\log K_{oc}=0.432+0.588\log k'_w+0.529\Delta^0\chi \quad (r^2=0.878)$$

$$\log K_{oc}=0.471+0.578\log k'_w+0.172(\mathrm{HA}+\mathrm{HD})$$

$$(r^2=0.863),$$

where k'_w is the capacity factor at 100% water in mobile phase. Therefore, using retention data from a nonpolar stationary phase can be a tool for estimating adsorption coefficients on soil for both nonpolar and polar chemicals by adding a second variable that takes nonhydrophobic interactions into account.

Hodson and Williams[579] found a great increase in correlation on changing from the octadecylsilane column to the cyanopropyl column. An increase of the water content of the mobile phase (water–methanol) from 25% to 45% results in an improvement in correlation. They used seven reference compounds (three benzene derivatives and four PAH) having reliable $\log K_{oc}$ values taken from the literature and measured their capacity factors (cyanopropyl column, mobile phase 45% water). A very high correlation was found with $a=2.70$, $b=2.04$, and $r^2=0.992$. Using this relationship, the value of $\log K_{oc}$ was determined from the measured k' values for 22 compounds of different types, including pesticides, benzene derivatives, and phenols. In most cases there was good agreement between the reported value ($\pm 0.1\log K_{oc}$) and that obtained by RPLC. In some cases (halogenated compounds and phenols) the $\log K_{oc}$ values obtained by RPLC were higher than the literature values obtained from soil adsorption measurements. Two possible causes of error have been suggested: (a) when measuring $\log K_{oc}$ values, using soil, insufficient time is allowed for equilibrium conditions to be reached; (b) the pH may be such that the chemical is measured in the ionized form.

Also Kördel *et al.*[580,581] reported that the cyanopropyl columns were the most suitable to predict K_{oc} values. The correlation equation for 48 compounds of various classes had[580] $a=1.8$, $b=2.4$, and $r=0.93$, using 55/45 methanol/citrate buffer as the mobile phase. This method was compared to other approaches based on $\log K_{ow}$, connectivity indices, molar refraction, and molecular fragment.[582] For the data set under consideration (66 compounds from different chemical classes) only the RPLC screening method and, to a lesser extent, the $\log K_{ow}$ method proved to be suitable for predictiong soil sorption coefficients with acceptable accuracy.

Gawlik *et al.*[583] tested the applicability of the same screening technique[580] to adsorption coefficients derived from classical batch experiments with five most frequent European soil types (EUROSOLS).[63] The adsorption data obtained for more than 40 nonionic organic chemicals belonging to different substance classes could be correlated successfully with the respective retention behavior in a liquid-chromatographic system, thus allowing the estimation of soil adsorption coefficients based on a single measurement of a chemical's HPLC capacity factor.

Relative retentions, k', of protonated and deprotonated chlorinated phenols were measured on C18 reversed-phase columns.[337] For the protonated phenols (2–4 chlorine substitution) the mobile phase was 50/50 methanol/water, acidified to pH~2. Correlation $\log k'-\log K_d$, where K_d values were measured by batch experiments with two sediments and one aquifer material, were allowed to obtain K_d values for 2,3,4,6-TeCP and PCP, for which the contribution of deprotonated species were large at the adopted experimental conditions. Similar correlations derived for the same compounds predominantly as phenolate anions (pH~11.5) showed that they are retained in the same sequence as the corresponding nonionized phenols, i.e., increasing retention with increasing octanol/water partition coefficient of the nonionized compound.

Szabo *et al.*[584] prepared an RPLC packing material bearing immobilized humic acid and studied the effect of changing the mobile phase water content on the correlation between log (capacity factor) and $\log K_{oc}$. In order to eliminate selective solute–solvent interactions, they used $\log k'_w$, the capacity factor obtained by extrapolation of retention data from binary eluents to 100% water instead of using $\log k'$, the capacity factor obtained from binary eluents. They constructed a calibration curve using the $\log K_{oc}$ values from the literature for ten compounds (benzene, five benzene derivatives, and four PAHs) and experimentally determined $\log k'_w$. By using this calibration curve they have redetermined $\log K_{oc}$ for the same compounds and for four other PAH compounds. By way of comparison they have also determined $\log K_{oc}$ on ethylsilica phase they have synthetized. The correlation equations for the ten reference compounds are the following:

$$\text{octanol phase:}\quad \log K_{\mathrm{oc}}=1.023\log K_{\mathrm{ow}}-0.578\quad r^2=0.922$$

$$\text{ethylsilica phase:}\quad \log K_{\mathrm{oc}}=1.370\log k'_{\mathrm{w}}+1.545\quad r^2=0.950$$

$$\text{humic acid phase:}\quad \log K_{\mathrm{oc}}=0.948\log k'_{\mathrm{w}}+1.781\quad r^2=0.986. \tag{67}$$

These equations indicate that it is more accurate to estimate $\log K_{\mathrm{oc}}$ from k'_{w}, determined from the humic acid phase, than via a single relationship between $\log K_{\mathrm{oc}}$ and $\log k'_{\mathrm{w}}$ on the ethyl phase or by a $\log K_{\mathrm{oc}}-\log K_{\mathrm{ow}}$ relationship. Thus, from the divergences for the ten chemicals, the following order can be generated:

organic matter on the soil

>immobilized humic acid>ethylsilica>octanol.

This is the order of decreasing polarity of the media. The $\log K_{\mathrm{oc}}$ values obtained by using the immobilized humic acid phase are in good agreement with the reported values for all the reference compounds. Finally by increasing the water content from 40% to 60% in the mobile phase improves the correlation; this is partially due to the reduction of errors in calculating the capacity factor when water content is higher. Also, the high water content of the mobile phase represents more closely the conditions of soil/water sorption in the environment.

Szabo *et al.*[585] have then used the same technique with two humic acid columns prepared with two different techniques. The first was the same already used in the previous work,[584] named chemically immobilized humic acid silica gel (CIHAC) and the second was named physically immobilized humic acid silica phase (PIHAC). The potential of the two columns for determining soil adsorption coefficients (K_{oc}) was compared; $\log K_{\mathrm{oc}}$ values were estimated from $\log K_{\mathrm{oc}}$ versus $\log k'_{\mathrm{w}}$ using the same reference compounds of the previous work.[584] While the CIHAC column gives Eq. (67), the PIHAC column gives the following equation:

$$\log K_{\mathrm{oc}}=0.963\log k'_{\mathrm{w}}+2.436\quad r^2=0.994. \tag{68}$$

From a comparison of Eqs. (67) and (68) it is evident that the physically immobilized humic acid phase is slightly superior to the chemically bonded humic acid. Perhaps this superiority reflects the nature of the association of humic acids with the mineral phase in the environment. The authors have then calculated the K_{d} values for the same compounds using the relationship

$$K_{\mathrm{d}}=k'_{\mathrm{w}}V_{\mathrm{v}}/V_{\mathrm{s}},$$

where V_{v} is the volume of the solvent required to elute a solute associated with the stationary phase in the RPLC column, corrected for the volume retained in the pore spaces, and V_{s} is the volume of the solid phase. These K_{d} values were then transformed to the K_{oc} values by using the carbon content of the humic acid on the phases. These K_{oc} values were in very good agreement with the literature values, showing that humic acid phases are useful to determine K_{oc} values without using calibration curves. It has been demonstrated that the mineral phase has little influence upon sorption of organic pollutants by humic acid, which is the principal organic component of soil.[586]

The same authors,[587] as part of the development of a liquid chromatographic procedure for predicting K_{oc} values of organic pollutants, evaluated two silica-derivatized phases, formed by immobilizing salicylic acid (SaA) and 8-hydroxyquinoline (HQ) on silica, to simulate the constituent groups of humic acids. The correlations between $\log K_{\mathrm{oc}}$ and $\log k'_{\mathrm{w}}$ were similar and appeared to be better than the correlation made between $\log K_{\mathrm{oc}}$ and $\log K_{\mathrm{ow}}$. The correlations are
for SaA:

$$\log K_{\mathrm{oc}}=1.037\log k'_{\mathrm{w}}+0.471\quad r^2=0.948$$

for HQ:

$$\log K_{\mathrm{oc}}=1.002\log k'_{\mathrm{w}}+0.201\quad r^2=0.931.$$

Then, it has been demonstrated[588] that the prediction of the soil adsorption factor $\log K_{\mathrm{oc}}$, by using K_{ow} or the retention factors determined by RPLC, can be improved by multilinear relations in which the Hildebrand parameter δ[589,590] represents the second independent variable. This parameter is related to the cohesion energy and the molar volume of a compound and the cohesion energy between liquid molecules is a function of polarizability, ionization potential, and dipole moment. The results indicate that the contribution of this variable is higher for more apolar stationary phases (octadecyl and phenyl silica phases). When the capacity factors obtained from the humic acid phase are considered, this contribution seems to be negative. This may be due to the fact that extracted humic acid may be somewhat more polar in nature than undisturbed soil organic matter.

12.4. Correlations with Molecular Descriptors

It has been observed that the experimental determination of $K_{\mathrm{om}}(K_{\mathrm{oc}})$ values is often a costly and time-consuming process and it is also very inaccurate for compounds of low water solubility (DDT, lindane, and PCBs).[591] The alternative methods based on correlations with solubility or octanol–water partition coefficients are inaccurate too, because it is impossible to determine these parameters accurately for compounds whose solubility is below 1 ppm. Therefore Sabljic[591] proposed applying molecular topology and quantitative structure–activity relationship (QSAR) analysis to this problem, with the aim of finding a parameter that will describe the relationship between the molecular structure of the compounds and their sorption by soil with an accuracy independent of its magnitude. The structural parameters used in this investigation are the molecular connectivity indices (MCIs), that were successfully applied to estimate both biological parameters (enzyme induction, biodegradation, toxicity, etc.)[592] and constants of environmental interest (solubility, Henry's law constant, partition coefficients, etc.).[11]

Another possibility of computing thermodynamic properties of organic compounds is the use of prediction methods based on the consideration that a molecule is a collection of molecular fragments. Each of them makes a distinct contribution to the thermodynamic property, which is relatively independent of the rest of the molecule.[52] This concept was introduced by Leo *et al.*[556] for the estimation of the K_{ow} values and was used to predict also sorption in soil.[96,116,108,211]

The concept of molecular connectivity was introduced by Randic[593] and further developed and extensively used by Kier and Hall.[594,595] MCIs are derived from the assignment of a numerical adjacency value to each atom other than hydrogen in the molecular skeleton. This value corresponds to the bond number or the valence of each atom. Simple indices (χ) are calculated by assigning to each nonhydrogen atom a delta value (δ) equal to the number of atoms to which it is bonded. Valence indices (χ^v) are calculated by assigning to each atom a δ value equal to the number of valence electrons not involved in bonds to hydrogen atoms. These indices may be identified by an order and a type. The order refers to the number of bonds in the molecular structure and the type refers to the structural fragment: path, chain, cluster, and path cluster. Different orders correspond to each type.

For instance, the first order valence MCI can be calculated by dissecting the skeleton structure into first order (one bond) fragments. Each fragment is defined by two delta valence values; for each fragment one can calculate a fragment index according to the algorithm

$$C_{i,j}=(\delta_i^v\delta_j^v)^{-0.5} \tag{69}$$

and sum of fragment index values to get first-order valence molecular connectivity index

$$^1\chi^v=\Sigma(\delta_i^v\delta_j^v)^{-0.5}. \tag{70}$$

On this basis Koch[596] found a good correlation between $\log K_{oc}$ and first order valence molecular connectivity index for a series of 18 hydrophobic organic compounds

$$\log K_{oc}=0.445+0.673(^1\chi^v) \quad r=0.974.$$

The simple first order MCI ($^1\chi$) can be calculated in the same way [Eqs. (69) and (70)], but by assigning to each nonhydrogen atom its δ value, which is equal to the number of adjacent nonhydrogen atoms.

Sabljic[591] derived the simple zero, first and second-order MCIs for 37 compounds: eight PAHs and their alkyl derivatives, seven chlorobenzenes, eight PCB's plus DDT and DDE, and 12 chloro- and bromoalkanes or alkenes. He also collected from the literature the respective experimental K_{om} values. The best linear relationship was obtained between $\log K_{om}$ and the first order molecular connectivity index

$$\log K_{om}=(0.55\pm0.02)\,^1\chi+(0.45\pm0.12) \quad r=0.973. \tag{71}$$

Statistically, Eq. (71) accounts for 95% of the variation in the $\log K_{om}$ data. This is as good as can be expected since the accuracy of the K_{om} data is approximately 10% for compounds with high water solubility (low K_{om}) and up to 1 order of magnitude poorer for weakly soluble compounds (high K_{om}).[217] The alternative correlations $\log S$ vs $\log K_{om}$ and $\log K_{ow}$ vs $\log K_{om}$ were also examined, and both were found to be inferior to Eq. (71).

Equation (71) was then[597] applied to other 31 compounds, including chlorobenzenes, PAHs, alkylbenzenes, chlorinated alkanes and alkenes, heterocyclic and substituted PAHs, and chlorophenols. Comparison of the observed and predicted soil sorption coefficients demonstrated that the molecular connectivity model is very accurate in predicting the soil sorption coefficients. The average difference between predicted and observed soil sorption coefficients is only 0.24 log unit, and more than 90% of the coefficients are predicted within 2 standard deviations. Only 1,2,3,4- and 1,2,4,5-TeCBz and 2,3,4,5-TeCP soil sorption coefficients are predicted outside the 2 standard deviation range. The author noted that the experimental soil sorption coefficients are from a laboratory which tends to report higher K_{om} values for chlorinated compounds than other investigators. Then all these compounds except the three outliers were combined with the compounds of the previous study[591] into a single regression model. The resulting molecular connectivity model for the quantitative description of soil sorption coefficients was

$$\log K_{om}=0.53\,^1\chi+0.54 \quad r=0.976. \tag{72}$$

Equations (71) and (72) are statistically significant above the 99% level and both have similar levels of accuracy. Thus, the range of applicability of the molecular connectivity model is extended to all the cited classes of compounds. The author then examined the predictive ability of empirical models based on the octanol/water partition coefficients or water solubility for the compounds used in this work. He found a surprisingly high variability in the experimental K_{ow} data (the ranges are varying between 0.5 and 3.3 log units). This variability and the wide variety of reported quantitative linear models describing the relationships used to predict soil sorption from K_{ow} values resulted in a range of predicted soil sorption coefficients over 1.5 log units. This result is far inferior to that obtained by the molecular connectivity model, for which the standard error and/or average difference between the predicted and observed soil sorption coefficients is below 0.3 log unit.

The problem of having a single correlation model relating $\log K_{oc}$ to MCIs for hydrophobic and polar compounds can be solved by introducing one index or a combination of indices to estimate the nonhydrophobic contribution to K_{oc}. Bahnick and Doucette[578] obtained a large improvement of the regression model of the type used by Sabljic[597] including a nondispersive force factor term to take into account organic chemicals with substantial hydrophilicity. This improvement was accomplished by replacing oxygen and nitrogen atoms with carbon atoms to compute MCIs related to molecular size. In this way the resulting molecule is largely nonpolar. The nondispersive force factor can be computed by

$$\Delta\chi=(\chi)_{\mathrm{np}}-\chi,$$

where $(\chi)_{\mathrm{np}}$ is the MCI for the nonpolar molecular structure and χ is the MCI for the corresponding polar structure. For testing the effects of inclusion of the $\Delta\chi$ values in the regression model, a subset of 56 organic compounds was used. Values for $\log K_{\mathrm{oc}}$ were obtained from the literature. When the values were given as $\log K_{\mathrm{om}}$, they were converted to $\log K_{\mathrm{oc}}$ by adding 0.24 log unit to the tabulated $\log K_{\mathrm{om}}$. The linear regression involving only $\log K_{\mathrm{oc}}$ and ${}^1\chi$ was

$$\log K_{\mathrm{oc}}=0.44\,{}^1\chi+0.34 \quad r=0.71,$$

while using ${}^1\chi$ and $\Delta{}^1\chi^{\mathrm{v}}$ the following equation was obtained:

$$\log K_{\mathrm{oc}}=0.53\,{}^1\chi-2.09\Delta{}^1\chi^{\mathrm{v}}+0.64 \quad r=0.969.$$

This model was then tested by choosing a different subset of 40 organic chemicals and their corresponding $\log K_{\mathrm{oc}}$ from the literature. Predicted $\log K_{\mathrm{oc}}$ values obtained in this way showed a standard deviation from the experimental values of 0.37. The largest difference between calculated and experimental values was 0.82.

Dobbs *et al.*[535] found that $\log K_{\mathrm{om}}$ obtained for ten compounds (alkylchlorides, chlorobenzene, pesticides) sorbed on wastewater solids correlated with the modified Randic indexes giving the relationship

$$\log K_{\mathrm{om}}=1.79+0.29\,{}^1\chi^{\mathrm{v}} \quad r=0.97.$$

Meylan *et al.*[598] developed a new estimation method based on ${}^1\chi$ and a series of statistically derived fragment contribution factors to predict soil sorption coefficients for nonpolar and polar compounds. The general equation used to estimate the $\log K_{\mathrm{oc}}$ of any compound is

$$\log K_{\mathrm{oc}}=0.53\,{}^1\chi+\Sigma P_f N,$$

where $\Sigma P_f N$ is the summation of the products of all applicable correction factors multiplied by the number of times (N) that fragment occurs in the structure. The combined training set includes 189 compounds. Summary statistics for the correlation of experimental versus calculated $\log K_{\mathrm{oc}}$ for the 189 compounds are correlation coefficient, $r=0.977$, standard deviation, SD=0.230, and mean error, ME=0.182.

Sabljic *et al.*[599] used first order MCIs to accurately describe the association of PCBs with dissolved marine humic substances. The association coefficients for 26 PCB congeners were those measured by Lara and Ernst.[413] The best correlation is obtained between K_{dom} coefficients and a quadratic function of the first-order MCI

$$\log K_{\mathrm{dom}}=-21.42+5.30\,{}^1\chi-0.25({}^1\chi)^2 \quad r=0.974.$$

Then, three additional indicator variables, the number of ortho, meta, and para chlorine substituents, were tested in multivariate regression analysis. The best two variable regression model is

$$\log K_{\mathrm{dom}}=-19.44+4.83\,{}^1\chi-0.22({}^1\chi)^2 -0.16(\mathrm{NoCl_0}) \quad r=0.995. \tag{73}$$

The introduction of the second variable, the number of ortho chlorine ($\mathrm{NoCl_0}$) made significant improvements to the model, and helped to explain all of the remaining variation in the $\log K_{\mathrm{dom}}$ data. Equation (73) accounts for almost 99% of the variation in the $\log K_{\mathrm{dom}}$ data. The $\mathrm{NoCl_0}$ variable seems to provide a good estimation for the extent of nonplanarity of PCBs, thus correcting imperfections of the ${}^1\chi$ index which is only a two dimensional descriptor. The authors observed that this model, when compared with existing models for PCBs association with humic substances (correlations with K_{ow}, S, and TSA),[413] shows superior performance in accuracy and future applications.

Lara and Ernst[182] measured sorption of 18 PCB congeners on three sediments. They used a multiple regression analysis between K_{d}, as the dependent variable, and the OC content (f_{oc}) of the sediments, the ${}^1\chi$ value, and the number of ortho-chlorines ($\mathrm{NoCl_0}$), as the independent variables. While the two combinations $\log K_{\mathrm{d}}-({}^1\chi,\log f_{\mathrm{oc}})$ and $\log K_{\mathrm{d}}-[{}^1\chi,({}^1\chi)^2,\log f_{\mathrm{oc}}]$ resulted in high significant correlations, the model developed using the quadratic function of ${}^1\chi$, $\mathrm{NoCl_0}$ and $\log f_{\mathrm{oc}}$

$$\log K_{\mathrm{d}}=-16.170+4.663\,{}^1\chi-0.246({}^1\chi)^2 -0.060(\mathrm{NoCl_0})+0.692\log f_{\mathrm{oc}} \quad r=0.964$$

was able to explain almost 93% of the observed variance and to predict $\log K_{\mathrm{d}}$ with an average difference between observed and predicted values of 0.056 log units.

The dependency of both equilibrium and nonequilibrium sorption coefficients with soil–solute systems on topological descriptors representing structural properties of the solutes was investigated.[600] For both equilibrium and nonequlibrium parameters, the first order valence molecular connectivity (${}^1\chi^{\mathrm{v}}$) was found to be the best topological descriptor. Most of the rate-limited sorption behavior could be explained by accounting for the size and structure of the solute molecule, as indicated by the good correlation between the rate coefficient and ${}^1\chi^{\mathrm{v}}$. This supports the contention that rate-limited sorption in these systems is controlled by a physical diffusion mechanism.

The characteristic root index (CRI) model was proposed as a valuable tool for estimating soil–sorption coefficients by the application of QSPR technique.[601] The model was applied to chlorinated benzenes, phenols, and biphenyls. The calculation of the CRI starts from the hydrogen suppressed skeleton of a molecule. First, each nonhydrogen atom is assigned a delta value, which is calculated from their electronic configuration by the following equation:

$$\delta^{\mathrm{v}}=(Z^{\mathrm{v}}-h)/(Z-Z^{\mathrm{v}}-1),$$

where Z^{v} is the number of valence electrons in an atom, Z is the atomic number, and h is the number of hydrogen atoms bound to the same atom. The CRI is the sum of the positive characteristic roots obtained from the characteristic polynomial of the matrix with the entries calculated from the electronic input information (atomic δ^v values) by the following equation:

$$wij=(\delta_i^v\delta_j^v.....\delta_n^v)^{-1/2},$$

where $i,j,.....,n$ correspond to the consecutive nonhydrogen atoms. The entries, wij, of the matrix are calculated by considering the shortest path to any other nonhydrogen atoms. In the case of equal paths $(wij=wji)$ clockwise direction was chosen. So, all possible orders of the connectivity index except zero order for each chemical are included in the constructed square matrix $(m*m)$. Diagonal entries (wii, wjj) of the matrix are zero assuming that there is no path bonding to the atom itself. The final equation, relating $\log K_{\mathrm{oc}}$ to CRI, was obtained from 36 literature data for K_{oc} and is

$$\log K_{\mathrm{oc}}=1.034\,\mathrm{CRI}+0.441 \quad r^2=0.964.$$

The average difference between predicted and observed soil sorption coefficients is only 0.17 log units.

Despite these often encouraging results, correlations of more than 400 K_{oc} data by Gerstl[562] with the respective MCIs demonstrated that the use of these indices alone were inadequate for predicting sorption values with the exception of a few homologous groups. Multivariate analysis of the entire data base failed to improve regressions. Simple and multiple regression analysis indicated that the use of S or K_{ow} for each individual group of compounds was highly preferable and use of MCIs for predictive purposes, based on 20 test compounds, does not provide adequate K_{oc} values.

12.5. Prediction Based on the Linear Solvation Energy Relationship (LSER)

Park and Lee[602] reported the use of the Kamlet–Taft solvatochromic parameters[603] in the linear solvation energy relationship (LSER)[604] to correlate and estimate bioconcentration factors in fish, adsorption coefficients on soil and sediments, and interfacial tensions of organic nonelectrolytes with water. The LSER equation for a property (SP) has the form

$$\mathrm{SP}=\mathrm{SP}_0+mV_{\mathrm{I}}/100+s\pi^*+d\delta+b\beta+a\alpha, \tag{74}$$

where V_{I} is the intrinsic solute molecular volume, scaled by 1/100 so that it should cover roughly the same range as the other independent variables, π^*, β, and α are the solvatochromic parameters that measure dipolarity/polarizability, hydrogen bond acceptor basicity, and donor acidity of the compound, respectively, and δ is a "polarizability correction" parameter. Equation (74) allows us to give quantitative information on the solute–target system interactions which determine the property of interest. The K_{oc} data were assembled for 42 compounds whose solvatochromic parameters were known or could be estimated. The coefficient a was found to be statistically zero and thus the term $(a\alpha)$ was removed in the correlation. The resulting multiple regression equation was

$$\log K_{\mathrm{oc}}=0.23+4.84V_{\mathrm{I}}/100-0.5\pi^*-0.59\delta-1.11\beta$$

$$r=0.968.$$

Increasing V_{I} leads to decreasing solubility in water and thereby increasing adsorption to soil/sediment organics. Increasing dipolarity and polarizability lead to increasing water solubility, which in turn decrease adsorption to the soil or sediment. Increasing hydrogen bond acceptor basicity of compound favors solubility in water over the soil organics and should lead to decreased adsorption. Accuracy of the LSER predictions is comparable to that of molecular connectivity models, while range of applicability of the LSER is less wide than molecular connectivity models, because solvatochromic parameters for complex molecules are not as easily found by the present parameter estimation rules. Calculated $\log K_{\mathrm{oc}}$ values are compared with the experimental values for 11 compounds. The average difference is 0.36 log units, which is the same as the standard error of estimate obtained from the LSER model.

12.6. Prediction from Vapor Sorption (LSC)

The sorption of compounds in vapor phase onto the dry vadose-zone soil HA is measured with a static sorption chamber.[363] Either water vapor or compound vapor are introduced into the sorption chamber containing 10–15 mg of vacuum-dried soil HA on an electrical microbalance at 23 °C. The mass of vapor sorbed to the HA is determined by the increase in the weight of the soil sample at equilibrium. The corresponding vapor pressure of compound or water in the system is measured with a Baratron pressure gauge.

The uptake of volatile compounds (mg g^{-1}) on soil HA is highly linear over a wide range of relative pressure (P/P^0), where P is the equilibrium partial pressure and P^0 is the saturation vapor pressure of the compound at the system temperature. Isotherms approaching $P/P^0=1$ show a general steep rise due to an induced vapor condensation onto the exterior surface of the humic sample. Extrapolating the linear portion of the vapor phase isotherms at $P/P^0=1$ the LSC is obtained. The values of LSC, converted to volume basis using the density of the sorbed liquid, gives the values of Q^0_{ha}s, which are strikingly similar among the relatively nonpolar organic liquids (the average Q^0_{ha} value is 0.018 $\mathrm{cm}^3\,\mathrm{g}^{-1}$ of humic acid). The relative invariance of LSCs suggests a means for assessing the sorption capacities of other relatively nonpolar compounds on HA and, consequently, the corresponding capacities on soil OM, if the relative sorption efficiency of HA and soil OM is known. The equation

$$Q^0_{\mathrm{om}}=K_{\mathrm{om}}S_{\mathrm{w}} \tag{75}$$

gives a means of calculating the limiting partition capacity of the solute on soil OM (Q^0_{om}) knowing the partition coefficient of the solute between soil OM and water (K_{om}) and the water solubility of the solute (S_{w}). It has been demonstrated that the ratios $Q^0_{\mathrm{om}}/Q^0_{\mathrm{ha}}$ for five compounds are fairly constant and their average value is about 2.3. This result suggests that the soil OM as a whole is about twice as effective as the HA isolated from soil OM in uptake of relatively nonpolar organic compounds. Given that $Q^0_{\mathrm{om}}/Q^0_{\mathrm{ha}}$ is approximately 2, one can predict the approximate K_{om} values for other relatively nonpolar compounds from Eq. (75). For organic liquids, the calculation is carried out first by assuming $Q^0_{om}(\mathrm{cm}^3\,\mathrm{g}^{-1}) = 2Q^0_{ha}(\mathrm{cm}^3\,\mathrm{g}^{-1})$ with Q^0_{ha} being 0.018 $\mathrm{cm}^3\,\mathrm{g}^{-1}$ and then converting $Q^0_{om}(\mathrm{cm}^3\,\mathrm{g}^{-1})$ to $Q^0_{om}(\mathrm{mg\,g}^{-1})$ by using the liquid density of the compound. The same procedure applies for solids except that the $Q^0_{ha}(\mathrm{cm}^3\,\mathrm{g}^{-1})$ value is to be corrected for the melting point effect on solid solubility, that is, the $Q^0_{ha}(\mathrm{cm}^3\,\mathrm{g}^{-1})$ is to be multiplied by the activity of the solid (in reference to its supercooled liquid) at the system temperature, which is defined (see also Sec. 12.2) as

$$\ln a = -(\Delta H_f/R)[(T_m - T)/(TT_m)],$$

where a is the solid activity at the system temperature T, ΔH_f is the enthalpy of fusion of the solid, R is the gas constant, and T_m is the melting point. The $Q^0_{om}(\mathrm{mg\,g}^{-1})$ so calculated is then divided by S_w to give the estimated K_{om} [Eq. (75)]. The K_{om} values estimated for a series of ten compounds with this procedure are only slightly greater, by less than a factor of 2, than the literature observed values. Only the estimated K_{om} for p,p′-DDT is about four times as large as the observed value. This difference may be due to a significant reduction in solubility, other than the melting point effect, in OM as the size of the organic compound increases. It is quite possible that the lower observed K_{om} for DDT results partly from an enhancement of the DDT water solubility by dissolved and suspended OM in soil–water systems. The small differences among K_{om} of the other compounds may be due to variations of OM composition between soils.

12.7. Prediction by Flory–Huggins Model (FH)

Chin and Weber[206] applied a modified Flory–Huggins model (Sec. 12.2) in conjunction with solute aqueous activity coefficients data to estimate the association of organic contaminants to humic and other organic polymers in aqueous phase. They used an expression similar to that derived by Chiou *et al.*[55]

$$\log K_d = \log(\gamma_i^w) + \log(V_w/V_i) - \log \rho - (1+\chi)/2.303, \tag{76}$$

where γ_i^w is the activity coefficient for the solute in the aqueous phase, V_w is the molar volume of water, V_i is the molar volume of the target compound, ρ the density of the polymer added to ultimately express K_d in terms of volume per unit mass, and χ is the Flory parameter. Equation (76) was applied to predict the equilibrium binding constants for 14 target compounds in Aldrich or Fluka humic acid/water system. The solubility parameters of "humic like" organic "surrogates" having well-defined physicochemical properties were used to calibrate the model. Predictions based on model calibrations to methyl salicylate agreed well with experimental values for the binding of the target compounds, exhibiting a wide range of properties, to commercial humic acid substrates. The predicted $\log K_d$ values were converted to $\log K_{oc}$ ones; these $\log K_{oc}$s agreed within less than 0.5 order of magnitude with observed values for all cases studied.

13. Analysis of the Data and Comments

13.1. Data Collection and Effects of the Experimental Procedure

The sorption coefficients in aqueous phase for organic pollutants belonging to different classes are collected in Tables 1–9 together with the sorbent characteristics [texture, organic carbon (OC) content, cation exchange capacity (CE), specific surface area (SA), etc.] and the presence of salt in the aqueous solution. When the presence of salt is not specified, sorption coefficients are intended to be measured in distilled water. The last columns are concerned with temperature, experimental method adopted, and literature reference. When temperature is not specified, room temperature is assumed. Sorption data obtained with prediction procedures are also listed.

The first column contains the sorption coefficients, expressed as $\log K_d(\mathrm{cm}^3\,\mathrm{g}^{-1})$ or $\log K_f$ values and their respective exponents $(1/n)$.

Taking into account that the empirical Freundlich coefficient K_f is equal to q when C equals unity [Eqs. (4) and (5)], its value depends on the units in which both the concentration in sorbent and the concentration in water are expressed. Thus, considering that most authors used the equilibrium concentration in sorbent, q in $\mu\mathrm{g\,g}^{-1}$, and the equilibrium concentration in water, C, in $\mu\mathrm{g\,cm}^{-3}$, all other K_f data were converted to $\mu\mathrm{g}^{1-1/n}\,\mathrm{cm}^{3/n}\,\mathrm{g}^{-1}$. This conversion appeared necessary to have a common basis of comparison of the sorption data, especially when the values of $1/n$ were not very close to 1. As a matter of fact, it was found that, when for instance the K_fs were given on a molar basis (q in μmol kg^{-1} and C in μmol dm^{-3})[149,158,403,643,668] and $1/n$ was on the order of 0.98 or 1.02, the difference between their values and those calculated on mass basis could be of few percent, but became as large as more than 10% if $1/n$ was 0.90 or 1.10. Many other K_f data were obtained with a great variety of different q and C units which, when converted using the appropriate equation, sometimes showed sensible differences increasing more and more by increasing the difference between $1/n$ and 1. When such conversions were completed, only the Freundlich data having the respective $1/n$ values in the range of ~0.9 and ~1.1 were used to calculate K_{oc} values, taking into account that the error involved assuming linear isotherm was acceptable.[87,105,562]

In the second column the $\log K_{oc}$ or $\log K_{doc}$ data ($\mathrm{cm}^3\,\mathrm{g}^{-1}$ of OC) are given as found in the literature or calculated using the OC fraction in sorbents. Sorption coefficients expressed as K_{om} were transformed to K_{oc} using the factor 1.724. The same factor was used to transform OM data to OC. Calculated values for $\log K_d$ or $\log K_{oc}$ are indicated in square parentheses. Only the $\log K_{oc}$ values obtained when the sorbent OC content was ≥0.1% were reported.

For single-point sorption data, K_d and K_{oc} values were reported only if the equilibrium solution concentration was

TABLE 1. Sorption coefficients for monoaromatic hydrocarbons

log K_d log K_f^0 ($1/n$)	log K_{oc}	Sorbent composition (%)				Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
						Benzene			
−0.86° (0.84)				100		Montmorillonite (<0.125 mm) treated with H_2O_2	22	BE	171
−0.86° (0.75)				100		Illite (<0.125 mm) treated with H_2O_2	22	BE	171
−1.58° (0.98)				100		Kaolinite (<0.125 mm) treated with H_2O_2	22	BE	171
1.73° (1.08)				100		Montmorillonite-Al;pH 4.2; CE=80 me/100 g	25	BE	170
0.61° (0.99)				100		Montmorillonite-Ca; pH 6.6; CE=80 me/100 g	25	BE	170
1.00	[1.74]				18	Muck (<1 mm)	22	GP	517
−1.10	[1.31]	95.5	3.2	1.3	0.39	Eustis soil (<1 mm)		MD	517
−0.15	1.58	49.8	30.7	19.4	1.84	Riddles soil top layer below corn residue; pH 5.0; CE=9.0 cmol/kg	20	BE	605
−0.54	1.49	49.8	26.0	24.2	0.94	Idem: below top layer; pH 5.3; CE=18.3 cmol/kg			605
−1.96	[0.58]	98	1	1	0.29	Borden soil; 0.01 N $CaCl_2$		MD	600
0.49	[1.39]	60.3	24.0	15.7	12.6	Mt. Lemmon soil; 0.01 N $CaCl_2$		MD	600
0.05° (0.89)	1.63	1		31	2.6	Hastings soil; pH 5.6; CE=17 me/100 g	25	BE	170
0.08° (0.94)	1.82	15		34	1.8	Overton soil; pH 7.8; CE=29 me/100 g	25	BE	170
−1.12	1.58	97.3	2.2	0.5	0.2	Forest soil; pH 5.6; CE=0.48 me/100 g		MD	344
−0.02	1.64	65.2	25.6	9.2	2.2	Agricultural soil; pH 7.4; CE=9.0 me/100 g		MD	344
0.30	1.73	69.5	20.5	10.1	3.7	Forest soil; pH 4.2; CE=2.9 me/100 g		MD	344
−0.09	1.74				1.49	Captina sil soil; pH 4.97; 0.01 M $CaNO_3$		BE	606
−0.37	1.81				0.66	Mc Laurin sl soil; pH 4.43; 0.01 M $CaNO_3$		BE	606
−0.24	[1.34]	56.6	22.0	21.4	5.18* 2.59	Marlette soil (A horizon); pH 6.4; CE=16.4 me/100 g	20	BE	222, 223
0.89	[2.08]				10.0* 6.48	Idem-HDTMA complex			222, 223
0.68	[2.04]				7.43* 4.37	Idem-DDTMA complex			222
1.22	[2.65]				4.85* 3.71	Marlette soil (Bt horizon)-HDTMA complex	20	BE	222, 223
0.89	[2.59]				2.73* 1.98	Idem-DDTMA complex			222
0.32	[2.25]				1.74* 1.18	Idem-NTMA complex			222
1.20	[2.69]				4.38* 3.25	St. Clair soil (Bt horizon)-HDTMA complex	20	BE	222
0.58	[2.66]				1.12* 0.83	Oshtemo soil (Bt horizon)-HDTMA complex	20	BE	222
[−0.46]	[1.50]	9	68	21	1.9* [1.1]	Woodburn soil; CE=14 me/100 g	20	BE	55
[1.32]	[1.51]				64.0	Peat extracted with 0.1 M NaOH; 0.005 M $CaCl_2$	24	BE	229
[1.10]	[1.34]				57.1	Peat; $SA(N_2)=1.5\ m^2/g$; 0.005 M $CaCl_2$	24	BE	229
[0.88]	[1.16]				53.1	Houghton muck soil; $SA(N_2)=0.8\ m^2/g$; 0.005 M $CaCl_2$	24	BE	229
1.83	[2.62]				16.44 20.5*	VSC; vermiculite-HDTMA; CE=80 cmol/kg		BE	225
1.59	[2.67]				8.46 10.5*	1 Mt-1; illite-HDTMA; CE=24 cmol/kg		BE	225

TABLE 1. Sorption coefficients for monoaromatic hydrocarbons—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%)				Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
2.26	[2.91]				23.00 28.7*	SAz-1; smectite (high-charge)-HDTMA; CE= 130 cmol/kg		BE	225
2.09	[2.78]				20.60 25.7*	SWa-1; smectite-HDTMA; CE= 107 cmol/kg		BE	225
1.72	[2.48]				17.46 21.8*	SWy-1; smectite (low charge)-HDTMA; CE=87 cmol/kg		BE	225
1.77	[2.52]				18.15 22.6*	SAC; smectite (low-charge)-HDTMA; CE=90 cmol/kg		BE	225
0.48	[2.44]				0.94 1.17*	KGa-2; kaolinite-HDTMA; CE= 4 cmol/kg		BE	225
	[0.10]				44.4	Cellulose; $SA(N_2)=2.3\ m^2/g$ 0.005 M $CaCl_2$	24	BE	229
1.79	[2.55]				21.6* 17.3	HDTMA-smectite complex		BE	224
1.71	[2.59]				16.2* 13.0	Idem			224
0.96	[2.11]				8.9* 7.1	Idem			224
−0.33	[1.89]	91	8	1	0.6	Aquifer material		LE	428
−1.05		95	3	2	0.071	Allerod-1 aquifer material (a. m.); $SA=1.7\ m^2/g$		BE	208
−0.92		96	4	0	0.048	Allerod-2 a.m.; $SA(N_2)=2.0\ m^2/g$		BE	208
−1.40		98	2	0	0.020	Borris a.m.; $SA(N_2)=0.3\ m^2/g$			
−1.30		97	2	1	0.010	Brande-1 a.m.; $SA(N_2)=1.7\ m^2/g$		BE	208
−1.15		97	2	1	0.020	Brande-2 a.m.		BE	208
−0.52	[2.15]	97	2	0	0.213	Finderup-2 a.m.; $SA(N_2)=2.5\ m^2/g$		BE	208
−1.40		99	0	1	0.009	Gunderup-1 a.m.; $SA(N_2)=1.0\ m^2/g$		BE	208
−1.00		96	4	0	0.021	Gunderup-2 a.m.; $SA(N_2)=2.5\ m^2/g$		BE	208
−0.19	[2.48]	98	2	0	0.213	Herborg a.m.; $SA(N_2)=0.5\ m^2/g$		BE	208
−0.89		99	0	1	0.016	Rabis a.m.; $SA(N_2)=0.4\ m^2/g$		BE	208
−0.92		96	2	3	0.048	Tirstrup-1 a.m.; $SA(N_2)=3.3\ m^2/g$		BE	208
−0.96		97	0	2	0.035	Tirstrup-2 a.m.; $SA(N_2)=1.9\ m^2/g$		BE	208
−0.74	[2.05]	94	2	4	0.159	Tylstrup a.m.; $SA(N_2)=3.3\ m^2/g$		BE	208
−1.22		97	2	1	0.012	Vasby a.m.; $SA(N_2)=0.8\ m^2/g$		BE	208
−1.15		98	1	1	0.029	Vejen-1 a.m.; $SA(N_2)=1.7\ m^2/g$		BE	208
−0.72		98	0	3	0.032	Vejen-2 a.m.; $SA(N_2)=2.6\ m^2/g$		BE	208
−1.30		99	0	1	0.006	Vorbasse-1 a.m.; $SA(N_2)=1.8\ m^2/g$		BE	208
−1.30		98	2	0	0.007	Vorbasse-2 a.m.; $SA(N_2)=0.3\ m^2/g$		BE	208
−0.64	[2.28]	98	1	1	0.122	Vorbasse-3 a.m.; $SA(N_2)=0.1\ m^2/g$		BE	208
	1.92av				2.78, 3.27	Coarse si fractions of Doe Run and Hickory Hill sediments	25	BE	108
0.02	[1.42]				4.02	Tamar estuary sediment (<60 μm)		BE	128
	2.96					Estuarine colloids (Chesapeake Bay) 42.0 mg/l	20	BE	399
	1.78av		7–75.6	1–69.1	0.11–2.38	17 sediments and soils	25	BE	96
	1.92					Soil; experimental (literature)			217
	1.82, 1.87					Humic acid-silica column	20–23	RPLC	584, 585
	1.57					Humic acid-silica column	20–23	RPLC	587
	1.62					Salicylic acid-silica column	20–23	RPLC	587
	1.74					8-Hydroxyquinoline-silica column	20–23	RPLC	587
	1.82					C18 column; correlation $\log K_{oc}$-$(\log k'+\Delta^0\chi)$		RPLC	577
	1.84					C18 column; correlation $\log K_{oc}$-($\log k'$+hydrogen bonding index)		RPLC	577
	1.72					Correlation $\log K_{oc}-\log K_{ow}$			96
	1.90					Correlation $\log K_{oc}-\log K_{ow}$			108
	2.01					Correlation $\log K_{oc}-\log K_{ow}$			207
	1.85					Correlation $\log K_{oc}-\log S$			564
	1.82					Correlation $\log K_{oc}-\log S$			96
	1.72					Correlation $\log K_{oc}-\log S$(mp)			96
	[2.33]					Correlation $\log K_{om}$–MCI			591

TABLE 1. Sorption coefficients for monoaromatic hydrocarbons—Continued

log K_d log K_f^0 (1/n)	log K_{oc}	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
	1.71					Correlation log k_{oc}–CRI			601
	1.60					Correlation log k_{oc}–LSER			602
						Toluene			
−0.72^c (0.79)				100		Montmorillonite (<0.125 mm) treated with H_2O_2	22	BE	171
−0.87^c (0.76)				100		Illite (<0.125 mm) treated with H_2O_2	22	BE	171
−0.94^c (0.90)				100		Kaolinite (<0.125 mm) treated with H_2O_2	22	BE	171
−1.30	[1.59]	97.1	2.3	0.6	0.13	Tampa aquifer; pH 8; 0.01 N $CaCl_2$		MD	521
−0.70	[1.71]	95.5	3.2	1.3	0.39	Eustis soil; 0.01 N $CaCl_2$		MD	522
−0.36	2.28				0.23	Offutt AFB soil (11-13 ft. depth)	25	HS	193
−0.50	1.89				0.41	Whiteman AFB soil (3–4.7 ft. depth)	25	HS	193
1.05	2.18				7.51	Sapsucker Woods (SW) soil	25	HS	194
1.06	2.21				7.05	SW soil, ethyl ether extracted	25	HS	194
0.37	2.43				0.88	SW soil humin	25	HS	194
1.00	1.91				12.4	SWsoil humic acid	25	HS	194
0.41	1.13				19.2	SW soil fulvic acid	25	HS	194
0.89	1.19				50.5	Tannic acid	25	HS	194
1.99	2.18				64.6	Lignin	25	HS	194
1.85	2.09				57.2	Zein	25	HS	194
−1.7	−1.3				45.3	Cellulose	25	HS	194
1.63	1.95				47.9	Aldrich humic acid	25	HS	194
−1.80	[0.74]	98	1	1	0.29	Borden soil; 0.01 N $CaCl_2$		MD	600
0.75	[1.65]	60.3	24.0	15.7	12.6	Mt. Lemmon soil; 0.01 N $CaCl_2$		MD	600
[−0.85]		92	5.9	2.1	0.09	Lincoln soil; fine sand; pH 6.4; CE=3.5 me/100g	20	LE	541
−0.43	[2.39]				0.15	KB 1H soil (63–125 μm); $SA(N_2)=4.9\ m^2/g$	20	LE	207
−0.21	[2.01]	91	8	1	0.6	Aquifer material		LE	428
−0.96	1.74	97.3	2.2	0.5	0.2	Forest soil; pH 5.6; CE=0.48 me/100 g		MD	344
0.32	1.98	65.2	25.6	9.2	2.2	Agricultural soil; pH 7.4; CE=9.0 me/100 g		MD	344
0.69	2.13	69.5	20.5	10.1	3.7	Forest soil; pH 4.2; CE=2.9 me/100 g		MD	344
0.40	2.22				1.49	Captina sil soil; pH 4.97; 0.01 M $CaNO_3$		BE	606
−0.02	2.16				0.66	Mc Laurin sl soil; pH 4.43; 0.01 M $CaNO_3$		BE	606
0.11	[1.70]	56.6	22.0	21.4	5.18* 2.59	Marlette soil (A horizon); pH 6.4; CE=16.4 me/100 g	20	BE	222
1.31	[2.50]				10.0* 6.48	Idem-HDTMA complex			222
1.03	[2.39]				7.43* 4.37	Idem-DDTMA complex			222
1.43	[2.86]				4.85* 3.71	Marlette soil (Bt horizon)-HDTMA complex	20	BE	222
1.16	[2.86]				2.73* 1.98	Idem-DDTMA complex			222
0.52	[2.45]				1.74* 1.18	Idem-NTMA complex			222
−0.77	[1.59]	21.0	34.9	44.1	0.88* 0.44	St. Clair soil (Bt horizon); pH 6.72; CE=18.3 me/100 g	20	BE	222
1.54	[3.03]				4.38* 3.25	Idem-HDTMA complex			222
0.82	[2.90]				1.12* 0.83	Oshtemo soil (Bt horizon)-HDTMA complex	20	BE	222
2.23	[3.02]				16.44 20.5*	VSC; vermiculite-HDTMA; CE=80 cmol/kg		BE	225
1.89	[2.96]				8.46	IM t-1; illite-HDTMA;		BE	225

TABLE 1. Sorption coefficients for monoaromatic hydrocarbons—Continued

log K_d log K_f^0 (1/n)	log K_{oc}	Sorbent composition (%)				Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
					10.5*	CE=24 cmol/kg			
2.50	[3.15]				23.00 28.7*	SAz-1; smectite (high-charge)-HDTMA; CE=130 cmol/kg		BE	225
2.29	[2.98]				20.60 25.7*	SWa-1; smectite-HDTMA; CE=107 cmol/kg		BE	225
1.87	[2.63]				17.46 21.8*	SWy-1; smectite (low charge)-HDTMA; CE=87 cmol/kg		BE	225
1.85	[2.60]				18.15 22.6*	SAC; smectite (low-charge)-HDTMA; CE=90 cmol/kg		BE	225
0.85	[2.86]				0.94 1.17*	KGa-2; kaolinite-HDTMA; CE=4 cmol/kg		BE	225
0.60	[2.00]				4.02	Tamar estuary sediment (<60 μm)		BE	128
	2.34				50.2	Aldrich and Fluka humic acid; predicted (Flory–Huggins Model)			206
1.80	2.27				33.5	ICN humic acid	25	HS	193
−0.40	1.87				0.54	ICN humic acid coated Al_2O_3	25	HS	193
	2.10, 2.26					Humic acid-silica column	20–23	RPLC	584, 585
	2.21					Humic acid-silica column	20–23	RPLC	587
	2.31					Salicylic acid-silica column	20–23	RPLC	587
	2.21					8-Hydroxyquinoline-silica column	20–23	RPLC	587
	[2.02]				58.0	Prediction by limiting vapor sorption on soil humic acid	23	LSC	363
	2.17					C18 column; correlation log K_{oc}-(log $k'+\Delta^0\chi$)		RPLC	577
	2.18					C18 column; correlation log K_{oc}-(log k'+hydrogen bonding index)		RPLC	577
	1.93					Correlation log K_{oc}– log S(180)			193
	2.43					Correlation log K_{oc}– log K_{ow} (207)			193
	2.49					Correlation log K_{oc}– log K_{ow} (108)			193
	2.32					Correlation log K_{oc}–MCI			597
	2.09					Correlation log K_{oc}–LSER			602
						o-Xylene			
−1.16° (1.08)				100		Montmorillonite (<0.125 mm) treated with H_2O_2	22	BE	171
−1.02° (0.88)				100		Illite (<0.125 mm) treated with H_2O_2	22	BE	171
−1.18° (0.99)				100		Kaolinite (<0.125 mm) treated with H_2O_2	22	BE	171
−0.68	[1.73]	95.5	3.2	1.3	0.39	Eustis soil; 0.01 N $CaCl_2$		MD	522
[0.33]	[2.33]				1.01	Narragansett sil soil		BE	607
0.95	[2.35]				4.02	Tamar estuary sediment (<60 μm)		BE	128
−0.60		>98			0.007	Rabis aquifer mat.	10	MD	166
	2.40, 2.37					Humic acid-silica column	20–23	RPLC	584, 585
	2.36					Humic acid-silica column	20–23	RPLC	587
	2.65					Salicylic acid-silica column	20–23	RPLC	587
	2.65					8-Hydroxyquinoline-silica column	20–23	RPLC	587
	2.73					Cyanopropyl column	20–25	RPLC	579
	2.45					C18 column; correlation log K_{oc}-(log $k'+\Delta^0\chi$)		RPLC	577
	2.45					C18 column; correlation log K_{oc}-(log k'+hydrogen bonding index)		RPLC	577
	2.65					Correlation log K_{oc}–MCI			598
						m-Xylene			
−0.90° (0.90)				100		Montmorillonite (<0.125 mm) treated with H_2O_2	22	BE	171
−0.88° (0.92)				100		Illite (<0.125 mm) treated with H_2O_2	22	BE	171
−1.46° (1.08)				100		Kaolinite (<0.125 mm) treated with H_2O_2	22	BE	171

TABLE 1. Sorption coefficients for monoaromatic hydrocarbons—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%)				Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
[0.32]	[2.32]				1.01	Narragansett sl soil		BE	607
−1.31	[1.23]	98	1	1	0.29	Borden soil; 0.01 N $CaCl_2$		MD	600
−0.60	2.11	97.3	2.2	0.5	0.2	Forest soil; pH 5.6; CE=4.8 me/100 g		MD	344
0.54	2.20	65.2	25.6	9.2	2.2	Agricultural soil; pH 7.4; CE=90 me/100 g		MD	344
1.03	2.46	69.5	20.5	10.1	3.7	Forest soil; pH 4.2; CE=29 me/100 g		MD	344
	2.62					C18 column; correlation $\log K_{oc}$-($\log k' + \Delta^0\chi$)		RPLC	577
	2.63					C18 column; correlation $\log K_{oc}$-($\log k'$+hydrogen bonding index)		RPLC	577
	2.53					Correlation $\log K_{oc}$–MCI			597
	2.48					Correlation $\log K_{oc}$–LSER			602
						p-Xylene			
−1.15° (0.79)				100		Montmorillonite (<0.125 mm) treated with H_2O_2	22	BE	171
−1.10° (0.78)				100		Illite (<0.125 mm) treated with H_2O_2	22	BE	171
−1.49° (1.07)				100		Kaolinite (<0.125 mm) treated with H_2O_2	22	BE	171
−0.31	[2.09]	95.5	3.2	1.3	0.39	Eustis soil; 0.01 N $CaCl_2$		MD	522
0.49	1.87	55.0	20.0	25.0	4.14	Webster soil; $SA(N_2)=2.6\ m^2/g$; 0.01 N $CaCl_2$		BE	375
0.01	2.66	55.0	20.0	25.0	0.23	Webster soil, oxidized with H_2O_2; $SA(N_2)=33.0\ m^2/g$; 0.01 N $CaCl_2$		BE	375
[0.32]	[2.32]				1.01	Narragansett sil soil		BE	607
0.90	2.72				1.49	Captina sil soil; pH 4.97; 0.01 M $CaNO_3$		BE	606
0.21	2.39				0.66	Mc Laurin sl soil; pH 4.43; 0.01 M $CaNO_3$		BE	606
0.02	[2.24]	91	8	1	0.6	Aquifer material		LE	428
−1.07		52.3	41.5	6.2	0.03	Barksdale aquifer; 0.005 M $CaSO_4$		MD	519
−0.85	[2.03]	97.1	2.3	0.6	0.13	Tampa aquifer; pH 8; 0.01 N $CaCl_2$		MD	521
−0.64		96			0.025	Borden aquifer; $SA(N_2)=0.3\ m^2/g$	22	HS	520
−0.32		93			0.034	Lula aquifer; $SA(N_2)=7.7\ m^2/g$	22	HS	520
−0.30	[2.52]				0.15	KB 1 H soil (63–125 μm) 20 $SA=4.9\ m^2/g$		LE	207
1.02	[2.42]				4.02	Tamar estuary sediment (<60 μm)		BE	128
	2.43					C18 column; correlation $\log K_{oc}$-($\log k' + \Delta^0\chi$)		RPLC	577
	2.44					C18 column; correlation $\log K_{oc}$-($\log k'$+hydrogen bonding index)		RPLC	577
	2.65					Correlation $\log K_{oc}$–MCI			578
	2.53					Correlation $\log K_{oc}$–MCI			597
	2.49					Correlation $\log K_{oc}$–LSER			602
						1,2,3-Trimethylbenzene			
−0.02	[2.80]				0.15	KB 1H soil (63–125 μm) $SA=4.9\ m^2/g$	20	LE	207
	2.89					Correlation $\log K_{oc}$–MCI			578
	2.77					Correlation $\log K_{oc}$–MCI			597
	2.97					Correlation $\log K_{oc}$–LSER			602
						1,2,4-Trimethylbenzene			
−0.51	[1.90]	95.5	3.2	1.3	0.39	Eustis soil; 0.01 N $CaCl_2$		MD	522
						1,3,5-Trimethylbenzene			
0.00	2.82				0.15	KB 1H soil (63–125 μm) $SA(N_2)=4.9\ m^2/g$	20	LE	207
	2.85					Correlation $\log K_{oc}$–MCI			578

TABLE 1. Sorption coefficients for monoaromatic hydrocarbons—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
	2.75					Correlation $\log K_{oc}$–MCI			597
	2.97					Correlation $\log K_{oc}$–LSER			602
						1,2,4,5-tetramethylbenzene			
0.29	[3.12]				0.15	KB 1H soil (63–125 μm) 20 $SA(N_2)=4.9\ m^2/g$		LE	207
0.53	[2.76]	91	8	1	0.6	Aquifer material		LE	428
	2.99					Correlation $\log K_{oc}$–MCI			597
	3.43					Correlation $\log K_{oc}$–LSER			602
						Ethylbenzene			
−0.66	[1.75]	95.5	3.2	1.3	0.39	Eustis soil; 0.01 N $CaCl_2$		MD	522
0.53	2.27	49.8	30.7	19.4	1.84	Riddles soil; top layer below corn residue; pH 5.0; CE=9.0 cmol/kg	20	BE	605
0.03	2.05	49.8	26.0	24.2	0.94	Idem; below top layer; pH 5.3; CE=18.3 cmol/kg			605
[0.26]	[2.22]	9	68	21	1.9* [1.1]	Woodburn soil; CE=14 me/100 g		BE	55
−1.44	[1.09]	98	1	1	0.29	Borden soil; 0.01 N $CaCl_2$		MD	600
[0.33]	[2.33]				1.01	Narragansett sil soil		BE	607
0.45	[2.03]	56.6	22.0	21.4	5.18* 2.59	Marlette soil (A horizon); pH 6.4; CE=16.4 me/100 g	20	BE	222
1.64	[2.83]				10.0* 6.48	Idem-HDTMA complex			222
1.25	[2.61]				7.43* 4.37	Idem-DDTMA complex			222
−0.39	[2.13]	38.8	31.6	29.6	0.60* 0.30	Marlette soil (Bt horizon); pH 5.4; CE=14.6 me/100 g	20	BE	222
1.80	[3.23]				4.85* 3.71	Idem-HDTMA complex			222
1.41	[3.12]				2.73* 1.98	Idem-DDTMA complex			222
0.66	[2.58]				1.74* 1.18	Idem-NTMA complex			222
−0.09	[2.26]	21.0	34.9	44.1	0.88* 0.44	St. Clair soil (Bt horizon); pH 6.72; CE=18.3 me/100 g	20	BE	222
1.88	[3.37]				4.38* 3.25	Idem-HDTMA complex			222
−0.68	[2.28]	89.3	4.4	6.3	0.22* 0.11	Oshtemo soil (Bt horizon); pH 5.84; CE=3.5 me/100 g	20	BE	222
1.11	[3.19]				1.12* 0.83	Idem-HDTMA complex			222
2.65	[3.44]				16.44 20.5*	VSC; vermiculite-HDTMA; CE=80 cmol/kg		BE	225
2.19	[3.27]				8.46 10.5*	IMt-1; illite-HDTMA; CE=24 cmol/kg		BE	225
2.77	[3.41]				23.00 28.7*	SAz-1; smectite (high-charge)-HDTMA; CE=130 cmol/kg		BE	225
2.58	[3.27]				20.60 25.7*	SWa-1; smectite-HDTMA; CE=107 cmol/kg		BE	225
2.10	[2.87]				17.46 21.8*	SWy-1; smectite (low charge)-HDTMA; CE=87 cmol/kg		BE	225
2.13	[2.88]				18.15 22.6*	SAC; smectite (low-charge)-HDTMA; CE=90 cmol/kg		BE	225
1.32	[3.35]				0.94 1.17*	KGa-2; kaolinite-HDTMA; CE=4 cmol/kg		BE	225
1.01	[2.40]				4.02	Tamar estuary sediment (<60 μm)		BE	128
	2.47, 2.52					Humic acid-silica column	20–23	RPLC	584, 585
	2.35					Humic acid-silica column	20–23	RPLC	587
	2.40					Salicylic acid-silica column	20–23	RPLC	587
	2.42					8-Hydroxyquinoline-silica column	20–23	RPLC	587
	2.38					Cyanopropyl column	20–25	RPLC	579

TABLE 1. Sorption coefficients for monoaromatic hydrocarbons—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%)				Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
	2.51					C18 column; correlation $\log K_{oc}$-($\log k'+\Delta^0\chi$)		RPLC	577
	2.51					C18 column; correlation $\log K_{oc}$-($\log k'$+hydrogen bonding index)		RPLC	577
	[2.55]				58.0	Prediction by limiting vapor sorption on soil humic acid	23	LSC	363
	[2.85]					Correlation $\log K_{om}$–MCI			591
						n-Propylbenzene			
−0.48	[1.93]	95.5	3.2	1.3	0.39	Eustis soil; 0.01 N $CaCl_2$		MD	522
−0.92	[1.62]	98	1	1	0.29	Borden soil; 0.01 N $CaCl_2$		MD	600
3.21	[4.00]				16.44 20.5*	VSC; vermiculite-HDTMA; CE=80 cmol/kg		BE	225
3.15	[3.79]				23.00 28.7*	SAz-1; smectite (high-charge)-HDTMA; CE=130 cmol/kg		BE	225
2.96	[3.65]				20.60 25.7*	SWa-1; smectite-HDTMA; CE=107 cmol/kg		BE	225
2.52	[3.28]				17.46 21.8*	SWy-1; smectite (low charge)-HDTMA; CE=87 cmol/kg		BE	225
2.60	[3.34]				18.15 22.6*	SAC; smectite (low-charge)-HDTMA; CE=90 cmol/kg		BE	225
1.47	[2.87]				4.02	Tamar estuary sediment (<60 μm)		BE	128
	2.98, 2.83					Humic acid-silica column	20–23	RPLC	584, 585
	2.81					Humic acid-silica column	20–23	RPLC	587
	2.84					Salicylic acid-silica column	20–23	RPLC	587
	2.87					8-Hydroxyquinoline-silica column	20–23	RPLC	587
	2.98					Correlation $\log K_{oc}$–MCI			598
						n-Butylbenzene			
−0.38	[2.03]	95.5	3.2	1.3	0.39	Eustis soil; 0.01 N $CaCl_2$		MD	522
−0.21	[2.32]	98	1	1	0.29	Borden soil; 0.01 N $CaCl_2$		MD	600
0.57	[3.39]				0.15	KB 1H soil (63–125 μm) SA=4.9 m^2/g	20	LE	207
3.41	[4.20]				16.44 20.5*	VSC; vermiculite-HDTMA; CE=80 cmol/kg		BE	225
3.01	[3.78]				17.46 21.8*	SWy-1; smectite (low charge)-HDTMA; CE=87 cmol/kg		BE	225
2.00	[3.40]				4.02	Tamar estuary sediment (<60 μm)		BE	128
	3.32, 3.15					Humic acid-silica column	20–23	RPLC	584, 585
	3.35					Humic acid-silica column	20–23	RPLC	587
	3.38					Salicylic acid-silica column	20–23	RPLC	587
	3.39					8-Hydroxyquinoline-silica column	20–23	RPLC	587
	3.51					Cyanopropyl column	20–25	RPLC	579
	3.25					Correlation $\log K_{oc}$–MCI			578
	3.16					Correlation $\log K_{oc}$–MCI			597
	3.53					Correlation $\log K_{oc}$–LSER			602
						sec-Buthylbenzene			
0.49	[2.71]	91	8	1	0.6	Aquifer material		LE	428
						3-Ethyltoluene			
0.20	[2.42]	91	8	1	0.6	Aquifer material		LE	428
						Nitrobenzene			
0.74° (0.90)	2.32		4	7	2.58	Gribskov soil; B-hor.; pH 3.59; CE=9.6 me/100 g; 0.01 M $CaCl_2$	5	BE	131
0.64° (0.92)	2.23		4	7	2.58	Gribskov soil; B-hor.; pH 3.59; CE=9.6 me/100 g; 0.01 M $CaCl_2$	21	BE	131
0.49° (0.82)			3	5	1.82	Gribskov soil; C hor.; pH 4.07; CE=7.0 me/100 g; 0.01 M $CaCl_2$	5	BE	131
0.83°			3	5	1.82	Gribskov soil; C hor.; pH 4.07;	21	BE	131

TABLE 1. Sorption coefficients for monoaromatic hydrocarbons—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
(0.66)						CE=7.0 me/100 g; 0.01 M $CaCl_2$			
−1.54°					0.12	Delta soil; pH 5;		BE	91
(0.86)						CE=5.0 me/100 g; 0.01 N $CaSO_4$			
−0.77	[2.15]					Idem			91
−0.66°					1.14	Ann Arbor soil; pH 8;		BE	91
(0.73)						CE=6.9 me/100 g; 0.01 N $CaSO_4$			
0.83	[2.77]					Idem			91
−1.21	1.49	97.3	2.2	0.5	0.2	Forest soil; pH 5.6; CE=4.8 me/100 g		MD	344
0.29	1.95	65.2	25.6	9.2	2.2	Agricultural soil; pH 7.4; CE=90 me/100 g		MD	344
0.58	2.01	69.5	20.5	10.1	3.7	Forest soil; pH 4.2; CE=29 me/100 g		MD	344
[0.16]		92	5.9	2.1	0.09	Lincoln fine s soil; pH 6.4; CE=3.5 me/100 g	20	MD	541
0.12	1.95				1.49	Captina sil soil; pH 4.97; 0.01 M $CaNO_3$		BE	606
−0.16	2.02				0.66	Mc Laurin sl soil; pH 4.43; 0.01 M $CaNO_3$		BE	606
	[1.94]av				1.09*–4.25*	4 arable sil soils;	20	BE	120
	2.05					Humic acid-silica column	20–23	RPLC	587
	2.16					Salicylic acid-silica column	20–23	RPLC	587
	2.15					8-Hydroxyquinoline-silica column	20–23	RPLC	587
	1.99					C18 column; correlation $\log K_{oc}$ - ($\log k' + \Delta^0\chi$)		RPLC	577
	1.84					C18 column; correlation $\log K_{oc}$ - ($\log k'$ +hydrogen bonding index)		RPLC	577
	1.85					Correlation $\log K_{oc}- \log S$			564
	2.17					Correlation $\log K_{oc}$ −MCI			578
	1.85					Correlation $\log K_{oc}$−LSER			602

Values in square parentheses have been calculated by the author.

*% OM content.

av: average value.

Idem refers to the sorbent reported just above; only the data (texture, OC, temperature, method) which were changed are specified.

TABLE 2. Sorption coefficients for polyaromatic hydrocarbons (PAHs)

log K_d log K_f^0 (1/n)	log K_{oc}	Sorbent composition (%)				Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
						Naphthalene			
1.16	3.29				0.74	Eustis soil (<250 μm); K_d extrapolated from log K_d–f_c plots (methanol-water); 0.01 M $CaCl_2$		BE, MD	457
−0.03	[2.38]	96.4	1.8	1.8	0.39	Eustis soil; 0.01 N $CaCl_2$		MD	526
0.90	[2.61]				1.94	Hagerstown sil soil; 0.01 N $CaCl_2$	23	BE	454
0.93	[2.48]				2.85	Berkeley sil soil; 0.01 N $CaCl_2$	23	BE	454
0.30	[2.60]				0.50	Tifton s soil; 0.01 N $CaCl_2$	23	BE	454
−1.31	[1.23]	98	1	1	0.29	Borden soil; 0.01 N $CaCl_2$		MD	600
2.58	[3.48]	60.3	24.0	15.7	12.6	Mt. Lemmon soil; 0.01 N $CaCl_2$		MD	600
1.42	3.21				1.6	Menlo Park soil; pH 5.7; 0.01 M $CaSO_4$	15	LE	132
1.36	3.15					Idem	25	BE, LE	132
1.30	3.10					Idem	35	LE	132
1.20	3.00					Idem	50	LE	132
0.38	2.76				0.42	Eustis s soil; pH 5.1; CE=1.8 me/100 g; 0.01 M $CaSO_4$	25	BE, LE	132
0.80° (0.91)	2.64				1.42	Soil; cl; (kaolinite); pH 5.91; CE=12.4 me/100 g	20	BE	214
1.10° (0.84)					1.51	Soil; light c; (montmorillonite); pH 5.18; CE=13.2 me/100 g	20	BE	214
1.38° (0.81)					3.23	Soil; light c; (montmorill.-illite); pH 5.26; CE=28.3 me/100 g	20	BE	214
1.52° (0.79)					7.91	Soil; sl; (allophane); pH 5.41; CE=26.3 me/100 g	20	BE	214
1.75° (1.0)	2.73				10.4	Soil; cl; (allophane); pH 4.89; CE=35.0 me/100 g	20	BE	214
1.26° (0.82)			6	3	1.41	Gribskov soil; A hor.; pH 3.23; CE=4.8 me/100 g; 0.01 M $CaCl_2$	6	BE	131
1.15° (0.76)			4	7	2.58	Idem; B hor.; pH 3.59; CE=9.6 me/100 g; 0.01 M $CaCl_2$			131
0.95° (0.84)			3	5	1.82	Idem (C hor.); pH 4.07; CE=7.0 me/100 g; 0.01 M $CaCl_2$			131
1.48° (0.88)	2.76		5	4	5.11	Strodam soil; AB hor.; pH 3.88; CE=13.0 me/100 g; 0.01 M $CaCl_2$	6	BE	131
0.28° (0.73)			3	3	0.09	Idem (C hor.); pH 4.95; CE=1.6 me/100 g; 0.01 M $CaCl_2$			131
0.38° (0.57)			1	2	0.15	Tisvilde soil; C hor.; pH 4.21; CE=1.3 me/100 g; 0.01 M $CaCl_2$	6	BE	131
1.15° (0.84)			18	12	1.64	Roskilde soil; agric.; pH 5.40; CE=14.0 me/100 g; 0.01 M $CaCl_2$	6	BE	131
−0.49° (0.77)			4	18	0.06	Esrum soil; subsurface; pH 4.71; CE=9.1 me/100 g; 0.01 M $CaCl_2$	6	BE	131
−0.04° (0.87)			7	3	0.05	Tirstrup soil; subsurf.; pH 6.14; CE=1.4 me/100 g; 0.01 M $CaCl_2$	6	BE	131
0.32° (0.72)			34	41	0.13	Bjodstrup soil; subsurf.; pH 7.64; CE=40.5 me/100 g; 0.01 M $CaCl_2$	6	BE	131
1.34° (1.04)	3.50				0.69	Speyer soil 2.1 (0.15–0.5 mm); pH 7.0	22	BE	181
2.79° (1.05)	4.43				2.24	Speyer soil 2.2 (0.15–0.5 mm); pH 5.8	22	BE	181
1.26° (0.97)	3.21				1.12	Speyer soil 2.3 (0.15–0.5 mm); pH 7.1	22	BE	181
0.99° (0.88)	3.11	12.9	64.3	19.6	0.76	Alfisol; pH 7.45 LE	22	BE	181
1.20° (0.61)		8.5	68.3	20.6	1.11	Entisol; pH 7.9	22	BE	181
2.10° (1.42)						Cellulose	22	BE	181
0.48						Silica gel	22	BE	181

TABLE 2. Sorption coefficients for polyaromatic hydrocarbons (PAHs)—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
0.00						Alumina	22	BE	181
0.75	[2.98]	33.6	45.3	21.1	1* [0.58]	Bosket loam soil	6.5	BE	392
0.92	[3.15]					Idem	15		392
0.81	[3.04]					Idem	25		392
0.64	[2.88]					Idem	37		392
[0.04]	3.00	4	10	86	0.11	Apison soil; pH 4.5; CE=76 me/100 g		BE	570
[−0.24]		11	21	68	0.05	Fullerton soil; pH 4.4; CE=64 me/100 g		BE	570
[0.68]	2.60	2	38	60	1.2	Dormont soil; pH 4.2; CE=129 me/100 g		BE	570
3.14	[3.93]				16.44 20.5*	VSC; vermiculite-HDTMA; CE=80 cmol/kg		BE	225
3.10	[4.18]				8.46 10.5*	IMt-1; illite-HDTMA; CE=24 cmol/kg		BE	225
3.68	[4.33]				23.00 28.7*	SAz-1; smectite (high-charge)-HDTMA; CE=130 cmol/kg		BE	225
3.05	[3.82]				17.46 21.8*	SWy-1; smectite (low charge)-HDTMA; CE=87 cmol/kg		BE	225
0.93	2.66	87	12	1	1.87	Aquifer		BE	199
−0.89		98	1	1	0.02	Aquifer		BE	199
−1.10		>98			0.025	Vejen aquifer mat.	10	MD	166
−0.66		91.0	5.6	3.4	0.02	Lula aquifer.0.005 M $CaSO_4$		MD	519
−1.12		52.3	41.5	6.2	0.03	Barksdale aquifer; 0.005M $CaSO_4$		MD	519
−0.66	[2.23]	97.1	2.3	0.6	0.13	Tampa aquifer; pH 8; 0.01 N $CaCl_2$		MD	521
−0.11		40.8	53.1	4.7	0.01	Tinker aquifer: $SA(N_2)=9.2$ m^2/g; CE=39.95 me/100 g; Fe=14 g/kg	22.5	BE	213
−0.33		74.8	18.2		0.027	Carswell aquifer; $SA(N_2)=9.5$ m^2/g; CE=13.91 me/100 g; Fe=9.0 g/kg	22.5	BE	213
−0.24	2.73	52.3	41.5		0.105	Barksdale aquifer; $SA(N_2)=7.5$ m^2/g; CE=64.36 me/100 g; Fe=10.0 g/kg	22.5	BE	213
−0.21		98.2	1.1		0.011	Traverse City aquifer; CE=28.11 me/100 g; $SA(N_2)=0.2$ m^2/g; Fe=3.0 g/kg	22.5	BE	213
−0.55		96.0	2.0	2.0	0.016	Borden aquifer; $SA(N_2)=0.3$ m^2/g; Fe=15.0 g/kg	22.5	BE	213
−0.57		91.0	5.6	3.4	0.020	Lula aquifer; CE=9.83 me/100 g; $SA(N_2)=11.8$ m^2/g; Fe=29.0 g/kg	22.5	BE	213
−0.12		95	3	2	0.071	Allerod-1 aquifer material (a. m.); $SA(N_2)=1.7$ m^2/g		BE	208
0.01		96	4	0	0.048	Allerod-2 a.m.; $SA(N_2)=2.0$ m^2/g		BE	208
−0.60		98	2	0	0.020	Borris a.m.; $SA(N_2)=0.3$ m^2/g			
−0.18		97	2	1	0.010	Brande-1 a.m.; $SA(N_2)=1.7$ m^2/g		BE	208
−0.04		97	2	1	0.020	Brande-2 a.m.		BE	208
0.45	[3.12]	97	2	0	0.213	Finderup-2 a.m.; $SA(N_2)=2.5$ m^2/g		BE	208
−0.92		99	0	1	0.009	Gunderup-1 a.m.; $SA(N_2)=1.0$ m^2/g		BE	208
−0.24		96	4	0	0.021	Gunderup-2 a.m.; $SA(N_2)=2.5$ m^2/g		BE	208
1.20	[3.87]	98	2	0	0.213	Herborg a.m.; $SA(N_2)=0.5$ m^2/g		BE	208
−0.10		99	0	1	0.016	Rabis a.m.; $SA(N_2)=0.4$ m^2/g		BE	208
−0.11		96	2	3	0.048	Tirstrup-1 a.m.; $SA(N_2)=3.3$ m^2/g		BE	208
−0.39		97	0	2	0.035	Tirstrup-2 a.m.; $SA(N_2)=1.9$ m^2/g		BE	208
0.30	[3.10]	94	2	4	0.159	Tylstrup a.m.; $SA(N_2)=3.3$ m^2/g		BE	208
−0.82		97	2	1	0.012	Vasby a.m.; $SA(N_2)=0.8$ m^2/g		BE	208
−1.00		98	1	1	0.029	Vejen-1 a.m.; $SA(N_2)=1.7$ m^2/g		BE	208
0.06		98	0	3	0.032	Vejen-2 a.m.; $SA(N_2)=2.6$ m^2/g		BE	208
−0.82		98	2	0	0.007	Vorbasse-2 a.m.; $SA(N_2)=0.3$ m^2/g		BE	208
0.78	[3.69]	98	1	1	0.122	Vorbasse-3 a.m.; $SA(N_2)=0.1$ m^2/g		BE	208
0.53	2.67			61	0.72	EPA-6 sediment; pH 8.2; CE=33.0 me/100 g		BE	132

TABLE 2. Sorption coefficients for polyaromatic hydrocarbons (PAHs)—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%)				Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
1.75	2.97				5.96	Idem modified by sorption of 85 mg/g of poly (N,N-dimethyl aminoethyl methacrylate)			132
1.30	3.12	1.6	42.91	55.4	1.5	Mississippi River sediment; pH 7.7; CE=20.9 me/100 g		BE	151
1.53	[2.93]				4.02	Tamar estuary sediment (<60 μm)		BE	128
[1.8]	3.3				2.9	Offshore Grand Haven sediment; (solute complexation model)		BE	464, 494
[2.1]	3.5				3.8	Benton Harbor sediment; (solute complexation model)		BE	464, 494
	3.11				2.07	Lake Oostvaardersplassen sediment	25	BE	58
	2.80				1.87	Lake Ketelmeer sediment	25	BE	58
3.04	3.59				28	Syntetic "sludge" of autoclaved yeast obtained by culturing bakers' yeast in sucrose solution	25	BE	608
2.18					27	Municipal sludge from Oak Ridge wastewater treatment plant	25	BE	608
2.88					14	Oily biosludge 913 from ORNL (4% oil content)	25	BE	608
3.56					25	Oily biosludge 969 from ORNL (14% oil content)	25	BE	608
3.35					33	Oily biosludge 972 from ORNL (24% oil content)	25	BE	608
	3.78					Oil extracted from waste 972	25	BE	608
	[2.62]av				1.09*–4.25*	5 soils; pH 6.1–7.5; 0.01 M $CaCl_2$	20	BE	120
	3.11					Soil: experimental (literature data)			217
	2.94av		7–75.6	1–69.1	0.11–2.38	17 sediments and soils	25	BE	96
	5.00av				3.38av	23 Brisbane River sediments		FM	544
	3.11av				2.78, 3.27	Coarse si fractions of Doe Run and Hickory Hill pond sediments	25	BE	108,
	3.16, 3.15					Humic acid-silica column	20–23	RPLC	584, 585
	3.16					Humic acid-silica column	20–23	RPLC	587
	3.05					Salicylic acid-silica column	20–23	RPLC	587
	3.06					8-Hydroxyquinoline-silica column	20–23	RPLC	587
	[3.04]				50.2	Aldrich humic acid (2.5 mg C/l)	23	ED	400
	2.89				50.2	Aldrich and Fluka humic acid		FH	206
	3.61					Estuarine colloids (Chesapeake Bay) 43.3 mg/l	20	BE	399
	2.97					Correlation $\log K_{oc} - \log K_{ow}$			96
	3.15					Correlation $\log K_{oc} - \log K_{ow}$			108
	2.91					Correlation $\log K_{oc} - \log K_{ow}$			207
	2.81					Correlation $\log K_{oc} - \log S$			564
	2.98					Correlation $\log K_{oc} - \log S$			96
	3.00					Correlation $\log K_{oc} - \log S$(mp)			96
	3.27					Correlation $\log K_{oc}$ −MCI			578
	[3.42]					Correlation $\log K_{om}$ −MCI			591
	3.11					Correlation $\log K_{oc}$ −LSER			602
						1-Methylnaphthalene			
−0.36		40.8	53.1	4.7	0.0096	Tinker aquifer; $SA(N_2)=9.2\ m^2/g$; CE=39.95 me/100 g; Fe=14 g/kg	22.5	BE	213, 609
−0.35		74.8	18.2		0.027	Carswell aquifer; $SA(N_2)=9.5\ m^2/g$; CE=13.91 me/100 g; Fe=9.0 g/kg	22.5	BE	213, 609
−0.02	2.96	52.3	41.5		0.105	Barksdale aquifer; $SA(N_2)=7.5\ m^2/g$; CE=64.36 me/100 g; Fe=10.0 g/kg	22.5	BE	213, 609

TABLE 2. Sorption coefficients for polyaromatic hydrocarbons (PAHs)—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
0.49	3.29	67.8	27.3	3.5	0.156	Blytheville aquifer; $SA(N_2)=8.0\ m^2/g$; CE=32.98 me/100 g; Fe=7.0 g/kg	22.5	BE	213, 609
−0.12		98.2	1.1		0.011	Traverse City aquifer; CE=28.11 me/100 g; $SA(N_2)=0.2\ m^2/g$; Fe=3.0 g/kg	22.5	BE	213
−0.19		96.0	2.0	2.0	0.016	Borden aquifer; $SA(N_2)=0.3\ m^2/g$; Fe=15.0 g/kg	22.5	BE	213, 609
−0.29		91.0	5.6	3.4	0.020	Lula aquifer; CE=9.83 me/100 g; $SA(N_2)=11.8\ m^2/g$; Fe=29.0 g/kg	22.5	BE	213, 609
1.96	[3.36]				4.02	Tamar estuary sediment ($<60\ \mu m$)		BE	128
	3.48					Correlation $\log K_{oc}-MCI$			598
2-Methylnaphthalene									
2.00	[3.40]				4.02	Tamar estuary sediment ($<60\ \mu m$)		BE	128
3.31					28	Syntetic "sludge" of autoclaved yeast obtained by culturing bakers' yeast in sucrose solution	25	BE	608
2.79					27	Municipal sludge from Oak Ridge wastewater treatment plant	25	BE	608
3.45					14	Oily biosludge 913 from ORNL (4% oil content)	25	BE	608
4.01					25	Oily biosludge 969 from ORNL (14% oil content)	25	BE	608
3.85					33	Oily biosludge 972 from ORNL (24% oil content)	25	BE	608
	4.21					Oil extracted from waste 972	25	BE	608
	3.93					Soil; experimental (literature data)			217
	3.87av				2.78, 3.27	Coarse si fractions of Doe Run and Hickory Hill sediments	25	BE	108
	2.87					Correlation $\log K_{oc}-\log S$			564
	3.48					Correlation $\log K_{oc}-MCI$			578
	[3.64]					Correlation $\log K_{om}-MCI$			591
	3.24					Correlation $\log K_{oc}-LSER$			602
1-Ethylnaphthalene									
2.37	[3.77]				4.02	Tamar estuary sediment ($<60\ \mu m$)		BE	128
	3.89					Cyanopropyl column		RPLC	579
	3.77					Correlation $\log K_{oc}-MCI$			598
2-Ethylnaphthalene									
2.36	[3.76]				4.02	Tamar estuary sediment ($<60\ \mu m$)		BE	128
	3.76					Correlation $\log K_{oc}-MCI$			598
Acenaphthene									
	5.38av				3.38av	23 Brisbane River sediments		FM	544
	3.79					Chemically immobilized humic ac.	20–23	RPLC	584, 585
	3.59					Physically immobilized humic ac.	20–23	RPLC	585
Acenaphthylene									
	3.83					Chemically immobilized humic ac.	20–23	RPLC	584, 585
	3.75					Physically immobilized humic ac.	20–23	RPLC	585
Fluorene									
	5.47av				3.38av	23 Brisbane River sediments		FM	544
	3.87				50.2	Aldrich and Fluka humic acid		FH	206
	3.95					Commercial humic acid		ED	610
	4.15					Chemically immobilized humic ac.	20–23	RPLC	584, 585
	4.21					Physically immobilized humic ac.	20–23	RPLC	585
	4.05					Correlation $\log K_{oc}-MCI$			598

TABLE 2. Sorption coefficients for polyaromatic hydrocarbons (PAHs)—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
Phenanthrene									
2.29	4.42				0.74	Eustis soil (<250 μm); K_d extrapolated from $\log K_d - f_c$ plots (methanol-water) 0.01 M $CaCl_2$		BE, MD	457
[0.81]	3.77	4	10	86	0.11	Apison soil; pH 4.5; CE=76 me/100 g		BE	570
[−0.07]		11	21	68	0.06	Fullerton soil; pH 4.4; CE=64 me/100 g		BE	570
[1.84]	3.76	2	38	60	1.2	Dormont soil; pH 4.2; CE=129 me/100 g		BE	570
2.40	4.37	80.5	11.2	8.3	1.08	Speyer soil (SP380; 2.3); pH 6.4; CE=8 me/100 g	25	BE	537
1.11	4.07	98.7	1.2(s+c)		0.4* 0.11	Quarry dark sand; pH 8.6		BE	430
	4.64					DOM from Rhinebeck soil		FQ	430
3.40	3.82				37.8	Leaves	25	BE	611
2.90	3.30				39.8	Thatch	25	BE	611
	4.48				2.07	Lake Oostvaardersplassen sediment	25	BE	58
	4.22				1.87	Lake Ketelmeer sediment	25	BE	58
2.40	4.22	1.6	42.91	55.4	1.5	Mississippi River sediment; pH 7.7; CE=20.9 me/100 g		BE	151
	4.5				4.60	Rotterdam Harbor sedim. (0.064–10.8 g/L); K_d extrapolated from water/methanol; 0–0.6 M NaCl	21	BE	461
2.04	3.77	87	12	1	1.87	Aquifer		BE	199
−0.05		98	1	1	0.02	Aquifer		BE	199
	4.30				5.23	Fort Point Channel (FPC) harbor sediments (25–29 cm); 0.6 M NaCl		BE	419
	4.43					FPC sediment porewater colloids (25–29 cm; 13 mg C/L); 0.6 M NaCl		FQ	419
	4.89				41.5	Fulvic acid from podzolic soil (from Lee, NH)		FQ	415
	4.70				54.1	Humic acid from podzolic soil (from Lee, NH)		FQ	415
	3.92					Aldrich humic acid ($\log K_{doc}$ is the zero intercept of the regression line of $\log K_{doc}$ vs DOC conc.)		RS	414
	4.08					Aldrich humic acid; pH 7.32 (DOC=0–16 mg/L)	6.6	RS	546
	4.36					DOC (11.7 mg/L) in interstitial water (Lake Michigan); pH 7.88	6.6	RS	546
	3.99					Aldrich humic acid (11.5 mg C/L); pH 7		RS	545
	6.12av				3.38av	23 Brisbane River sediments		FM	544
	4.59av					8 Eagle Harbor contaminated sediment-pore water systems		FM	612
	4.36av				2.78, 3.27	Coarse si fractions of Doe Run and Hickory Hill sediments	25	BE	108
	4.08av		7–75.6	1–69.1	0.11–2.38	17 sediments and soils	25	BE	96
	4.36					Soil; experimental (literature)			217
	4.28, 4.22					Humic acid-silica column	20–23	RPLC	584, 585
	4.28					Humic acid-silica column	20–23	RPLC	587
	4.12					Salicylic acid-silica column	20–23	RPLC	587
	4.23					8-Hydroxyquinoline-silica column	20–23	RPLC	587
	3.89				50.2	Aldrich and Fluka humic acid		FH	206
	4.10					Prediction from addition of ring fragments			96
	4.18					Correlation $\log K_{oc} - \log K_{ow}$			96
	3.58					Correlation $\log K_{oc} - \log S$			564
	3.90					Correlation $\log K_{oc} - \log S$			96

TABLE 2. Sorption coefficients for polyaromatic hydrocarbons (PAHs)—Continued

log K_d log K_f^0 (1/*n*)	log K_{oc}	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
	4.22					Correlation log K_{oc} – log S(mp)			96
	4.32					Correlation log K_{oc} – MCI			578
	[4.51]					Correlation log K_{om} – MCI			591
	3.92					Correlation log K_{oc} – LSER			602
						Anthracene			
1.53	[4.94]	96.4	1.8	1.8	0.39	Eustis soil; 0.01 N $CaCl_2$		MD	526
0.87	[3.41]	98	1	1	0.29	Borden soil; 0.01 N $CaCl_2$		MD	600
1.41	4.11				0.2	Fine sand soil; soil+dextran/water system		MD	429
	4.62				2.07	Lake Oostvaardersplassen sediment	25	BE	58
	4.20				53.1	Fulvic acid from podzolic soil (North Conway, NH)		FQ	415
	4.51				41.5	Fulvic acid from podzolic soil (Lee, NH)		FQ	415
	4.72				38.2	Aldrich humic acid		FQ	415
	4.57				54.1	Humic acid from podzolic soil (Lee, NH)		FQ	415
	4.93				54.1	Idem		FQ	415
	4.81				54.6	Humic acid from dark lignite soil		FQ	415
	3.95					Aldrich humic acid (DOC=9.4 mg/L); pH 5.8–6.8		RS	414
	4.46					Idem		ED	414
	4.15					Idem (log K_{doc} is the zero intercept of the regression line of log K_{doc} vs DOC concentration)		RS	414
	3.95					DOC in Lake Erie water (9.6 mg/L)		RS	414
	4.73					Idem		ED	414
	4.87					DOC in Huron River wat. (7.8 mg/L)		RS	414
	5.70					Idem		ED	414
1.63° (0.91)	[4.24]				0.25	Kaolinite coated with Phohokee peat humic acid; 0.1 M $NaClO_4$	25	BE	228
0.78° (0.82)					0.02	Idem	25	BE	228
213° (0.95)	[4.68]				0.28	Cecil/Pacolet clay coated with Pahokee humic acid; 0.1 M $NaClO_4$	25	BE	228
0.89° (0.84)					0.02	Idem	25	BE	228
	[4.20]				50.2	Aldrich humic acid (DOC=2.5 mg/L)	23	ED	400
	4.32					Aldrich humic acid; pH 7.32 (DOC=0–14.5 mg/L)	6.6	RS	546
	5.71					Estuarine colloids (Chesapeake Bay) 43.1 mg/L	20	BU	399
	4.20av	6–94	3–66	3–35	0.8–3.9	5 soils; 0.01 N $CaCl_2$	25	BE	455
	4.22					5 soils; extrapolated from log K_d – f_c plots (methanol–water)	25	BE	455
	4.23					5 soils; extrapolated from log K_d – f_c plots (acetone–water)	25	BE	455
	4.42					Soil; experimental (literature)			217
	4.20av		7–75.6	1–69.1	0.11–2.38	17 sediments and soils	25	BE	96
	4.41av				2.78, 3.27	Coarse si fractions of Doe Run and Hickory Hill pond sediments	25	BE	108
	5.76av				3.38av	23 Brisbane River sediments		FM	544
	4.42, 4.53					Humic acid-silica column	20–23	RPLC	584, 585
	4.34					Humic acid-silica column	20–23	RPLC	587
	4.38					Salicylic acid-silica column	20–23	RPLC	587
	4.32					8-Hydroxyquinoline-silica column	20–23	RPLC	587
	4.38					Cyanopropyl column	20–25	RPLC	579

TABLE 2. Sorption coefficients for polyaromatic hydrocarbons (PAHs)—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
	3.92				50.2	Aldrich and Fluka humic acid predicted (Flory–Huggins model)		FH	206
	4.10					Prediction from addition of ring fragments			96
	4.15					Correlation $\log K_{oc}$ – $\log K_{ow}$			96
	4.26					Correlation $\log K_{oc}$ – $\log S$			564
	4.63					Correlation $\log K_{oc}$ – $\log S$			96
	4.25					Correlation $\log K_{oc}$ – $\log S$(mp)			96
	4.31					Correlation $\log K_{oc}$ –MCI			578
	[4.50]					Correlation $\log K_{om}$ –MCI			591
	3.92					Correlation $\log K_{oc}$ –LSER			602
						Fluoranthene			
2.62	4.81	92.5	4.4	3.1	0.64	Speyer soil (Sp 180); pH 6.0	25	BE	388
3.00	4.65	89	4.9	6.1	2.24	Idem (Sp 280); pH 5.6	25	BE	388
2.83	4.80	80.5	11.2	8.3	1.08	Idem (Sp 380); pH 6.4	25	BE	388
2.93	4.90				1.08	Idem	15	BE	388
3.02	4.99				1.08	Idem	5	BE	388
2.79	4.82	54	24	22	0.93	Soil (Shenyang Ecol. Station, P.R. China); pH 7.0	25	BE	388
[1.86]	4.16	0.0	93.8	6.3	0.50	WES reference soil; 6 months incubation (m.i.)	25	BE	218
[2.43]	4.51	5	70	25	0.84	Brown's lake sedim.; 6 m.i.	25	BE	218
[3.73]	5.05	55	32.5	12.5	4.76	Hamlet City lake sedim.; 6 m.i.	25	BE	218
[3.31]	5.28				1.06	Oakland Harbor sedim./ interstitial saline water system; 15 d incubation; Nereis virens bioaccumulation (BA) study	15	BE	613
[2.70]	4.67					Idem; Macoma nasuta BA study			613
[2.94]	4.47				2.92	Red Hook sedim./interstitial saline water; 15 d incubation; Nereis virens BA study	15	BE	613
[3.08]	4.62					Idem; Macoma nasuta BA study			613
[4.11]	5.4				5.1	Lake Ketelmeer sedim.	20	GP	394
	4.93					DOC from Lake Ketermeer sedim.	45	GP	394
	5.05					Idem	35		394
	5.18					Idem	20		394
	5.25					Idem	16		394
	4.16–5.03					DOC in sediment interstitial water (from 11 harbors and lakes)		RS	411
	5.32				2.07	Lake Oostvaardersplassen sediment	25	BE	58
	4.89				1.87	Lake Ketelmeer sediment	25	BE	58
	6.38av				3.38av	23 Brisbane River sediments		FM	544
	4.79av					6 Eagle Harbor contaminated sediment-pore water systems		FM	612
	4.74					Chemically immobilized humic ac.	20–23	RPLC	584, 585
	4.62					Physically immobilized humic ac.	20–23	RPLC	585
	4.81					Correlation $\log K_{oc}$ – $\log K_{ow}$ (180)			388
	5.09					Correlation $\log K_{oc}$ – $\log K_{ow}$(96)			613
	4.73					Correlation $\log K_{oc}$ – $\log S$(180)			388
	4.85					Correlation $\log K_{oc}$ –MCI			598
						Pyrene			
1.64	[4.18]	98	1	1	0.29	Borden soil; 0.01 N $CaCl_2$		MD	600
1.62	4.51				0.13	Hickory Hill pond s sediment (>50 μm)	25	BE	108
3.48	4.96				3.27	Idem; coarse si (50–20 μm)			108
3.40	5.11				1.98	Idem; medium si (20–5 μm)			108
3.18	5.04				1.34	Idem; fine si (5–2 μm)			108
3.15	5.08				1.20	Idem; c (>2 μm)			108
0.97	4.04				0.086	Doe Run s sediment	25	BE	108
3.32	4.88				2.78	Idem; coarse si			108

TABLE 2. Sorption coefficients for polyaromatic hydrocarbons (PAHs)—Continued

log K_d log K_f^0 (1/n)	log K_{oc}	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
3.48	5.11				2.34	Idem; medium si			108
3.56	5.08				2.89	Idem; fine si			108
3.58	5.08				3.29	Idem; c			108
1.83	4.08				0.57	Oconee River s sediment	25	BE	108
3.51	5.04				2.92	Idem; coarse si			108
3.36	5.08				1.99	Idem; medium si			108
3.40	5.04				2.26	Idem; fine si			108
3.73	[5.13]				4.02	Tamar estuary sediment (<60 μm)		BE	128
3.10	4.92	1.6	42.91	55.4	1.5	Mississippi River sediment; pH 7.7; CE=20.9 me/100 g		BE	151
3.46	[4.98]		27.1	52.6	3.04	Ohio Riv. sediment (Ceredo, WV) (0.4 g/L); pH 6.90; equilibr. time=21 d		GP	156
3.11	[4.94]		55.4	37.1	1.48	Mississippi Riv. sed. (Mc Clure, IL) (0.5 g/L); pH 7.75; equilibr. time=15 d		GP	156
2.88	4.80	67.5	13.9	18.6	1.21	Sediment EPA-B2; pH 6.35; CE=3.72 me/100 g	25	BE	180
3.03	4.71	3.0	41.8	55.2	2.07	Sediment EPA-4; pH 7.79; CE=23.72 me/100 g	25	BE	180
3.06	4.70	33.6	35.4	31.0	2.28	Sediment EPA-5; pH 7.44; CE=19.0 me/100 g	25	BE	180
2.79	4.93	0.2	31.2	68.6	0.72	Sediment EPA-6; pH 7.83; CE=33.01 me/100 g	25	BE	180
2.00	4.83	82.4	10.7	6.8	0.15	Sediment EPA-8; pH 8.32; CE=3.72 me/100 g	25	BE	180
1.85	4.81	7.1	75.6	17.4	0.11	Soil EPA-9; pH 8.34; CE=12.4 me/100 g	25	BE	180
2.44	4.76	2.1	34.4	63.6	0.48	Soil EPA-14; pH 4.54; CE=18.86 me/100 g	25	BE	180
2.89	4.92	15.6	48.7	35.7	0.95	Sediment EPA-15; pH 7.79 ; CE=11.30 me/100 g	25	BE	180
2.70	4.88	34.6	25.8	39.5	0.66	Sediment EPA-18; pH 7.76; CE=15.43 me/100 g	25	BE	180
2.86	4.78	0.0	71.4	28.6	1.30	Soil EPA-20; pH 5.50; CE=8.50 me/100 g	25	BE	180
3.05	4.77	50.2	42.7	7.1	1.88	Sediment EPA-21; pH 7.60; CE=8.33 me/100 g	25	BE	180
2.91	4.68	26.1	52.7	21.2	1.67	Sediment EPA-22; pH 7.55; CE=8.53 me/100 g	25	BE	180
3.02	4.64	17.3	13.6	69.1	2.38	Sediment EPA-23; pH 6.70; CE=31.15 me/100 g	25	BE	180
3.00	4.83	1.6	55.4	42.9	1.48	Sediment EPA-26; pH 7.75; CE=20.86 me/100 g	25	BE	180
3.06	4.79	87	12	1	1.87	Aquifer		BE	199
0.72		98	1	1	0.02	Aquifer		BE	199
2.18	4.88				0.2	Fine s soil; soil+dextran/water system		MD	429
2.78	3.15				42	Dextran; soil+dextran/water system		MD	429
	5.20					Aldrich humic acid	25	RS	409
4.76av	5.65av					Great Lakes suspended matter (three phases distribution)	25	RS	409
	3.76av					Great Lakes DOC(same procedure)	25	RS	409
5.01av	5.79av				16	Green Bay suspended matter (same procedure)	25	RS	410
	4.14av					Green Bay DOC(same procedure)	25	RS	410
[3.94]	5.20				5.47	Fort Point Channel (FPC) harbor sediment (7–9 cm); 0.6 M NaCl		BE	419
[3.91]	5.19				5.19	Idem (15–17 cm)		BE	419
[3.72]	5.00				5.23	Idem (25–29 cm)		BE	419
[3.75]	5.23				3.34	Spectacle Island (SI) harbor sediment (14–16 cm); 0.6 M NaCl		BE	419

TABLE 2. Sorption coefficients for polyaromatic hydrocarbons (PAHs)—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
	5.05					FPC porewater organic colloids (7–9 cm; 7.3 mg C/L); 0.6 M NaCl		FQ	419
	5.00					Idem (15–17 cm; 7.7 mg C/L)		FQ	419
	4.88					Idem (25–29 cm; 13 mg C/L)		FQ	419
	4.71					SI sediment porewater organic colloids (14–16 cm; 21.5 mg C/L); 0.6 M NaCl		FQ	419
	5.23				54.1	Humic acid from podzolic soil (Lee, NH)		FQ	415
	5.08				41.5	Fulvic acid from podzolic soil (Lee, NH)		FQ	415
	4.74				53.1	Fulvic acid from podzolic soil (North Conway, NH)		FQ	415
	5.00				51.3	Suwannee River, GA, fulvic acid		FQ	415
	4.54				39.07	Marine sediment humic acid (MH-1)		FQ	188
	4.70				47.22	Idem (MH-2)			188
	4.46				47.76	Idem (MH-3)			188
	4.81				45.10	Estuarine sediment humic acid (MH-4)		FQ	188
	4.60				40.60	Idem (MH-5)			188
	4.74				48.58	Idem (MH-6)			188
	5.10				37.61	Soil humic acid (SH-1)		FQ	188
	4.94				47.23	Podzolic soil humic acid (SH-2)		FQ	188
	5.21				54.15	Idem (SH-3)			188
	5.51				54.66	Dark lignite soil humic acid (SH-4)		FQ	188
	5.38				57.53	Idem (SH-5)			188
	4.82				41.52	Podzolic soil fulvic acid (SF-1)		FQ	188
	4.73				53.1	Idem (SF-2)			188
	5.02				51.3	Suwannee River fulvic acid (SF-3)		FQ	188
	5.02				38.23	Aldrich humic acid		FQ	188
	5.15					Aldrich humic acid; pH 7.32 (DOC=0–16.7 mg/L)	6.6	RS	546
	4.55–5.64					DOC in porewater of Lake Michigan (LM) sediment after filtration		RS	547
	5.54–5.92					DOC in porewater of LM sediment after centrifugation		RS	547
	4.79–5.68					DOC in elutriate of LM sediment after filtration		RS	547
	4.65–5.18					DOC in elutriate of LM sediment after centrifugation		RS	547
	4.67av					8 Eagle Harbor contaminated sediment-pore water systems		FM	612
	4.92					Soil; experimental (literature)			217
	4.85av					33 literature data			562
	4.83av		7–75.6	1–69.1	0.11–2.38	17 sediments and soils	25	BE	96
	6.51av				3.38av	23 Brisbane River sediments		FM	544
	4.77, 4.82					Humic acid-silica column	20–23	RPLC	584, 585
	4.80					Humic acid-silica column	20–23	RPLC	587
	4.81					Salicylic acid-silica column	20–23	RPLC	587
	4.72					8-Hydroxyquinoline-slicia column	20–23	RPLC	587
	4.79					Correlation $\log K_{oc} - \log K_{ow}$			96
	4.97					Correlation $\log K_{oc} - \log K_{ow}$			108
	4.22					Correlation $\log K_{oc} - \log K_{ow}$			207
	4.11					Correlation $\log K_{oc} - \log S$			564
	4.51					Correlation $\log K_{oc} - \log S$			96
	4.64					Correlation $\log K_{oc} - \log S(\text{mp})$			96
	4.84					Correlation $\log K_{oc}$–MCI			578
	[5.05]					Correlation $\log K_{om}$–MCI			591
	4.50					Correlation $\log K_{oc}$–LSER			602

TABLE 2. Sorption coefficients for polyaromatic hydrocarbons (PAHs)—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%)				Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
Benzo(a)anthracene									
	5.77				2.07	Lake Oostvaardersplassen sediment	25	BE	58
	5.47				1.87	Lake Ketelmeer sediment	25	BE	58
	6.30av				3.38av	23 Brisbane River sediments		FM	544
	5.49av					8 Eagle Harbor contaminated sediment-pore water systems		FM	612
	5.30					Aldrich humic acid ($\log K_{doc}$ is the zero intercept of the regression line of $\log K_{doc}$ vs DOC conc.)		RS	414
	5.92					Aldrich humic acid; pH 7.32 (DOC=0–1.9 mg/L)	6.6	RS	546
	[5.23]				50.2	Aldrich humic acid (DOC=2.5 mg/L)	23	ED	400
	5.36					Correlation $\log K_{oc}$ –MCI			598
Benzo(a)pyrene									
	7.0				4.60	Rotterdam Harbor sedim. (0.064–10.8 g/L); K_0 extrapolated from water/methanol; 0–0.6 M NaCl	21	BE	461
	6.4				5.1	Lake Ketelmeer sedim.	20	GP	394
	6.08					DOC from Lake Ketelmeer sedim.	45	GP	394
	6.14					Idem	35		394
	6.52					Idem	20		394
	6.54					Idem	16		394
	5.99				2.07	Lake Oostvaardersplassen sediment	25	BE	58
	5.53				1.87	Lake Ketelmeer sediment	25	BE	58
	5.73av				58.1	Humic acid from Arno River sediments; pH 5.0–8.0	20	ED	425
	4.76av				51.7	Fulvic acid from Arno River sediments; pH 5.0–8.0	20	ED	425
	5.74av				64.1	Humic acid from Tyrrenhian Sea sediments; pH 5.0–8.0	20	ED	425
	4.88av				45.6	Fulvic acid from Tyrrenhian Sea sediments; pH 5.0–8.0	20	ED	425
	5.37av				53.3	Humic acid from Arno River water; pH 5.0–8.0	20	ED	425
	4.66av				54.6	Fulvic acid from Arno River water; pH 5.0–8.0	20	ED	425
5.78av	6.66av					Great Lakes suspended matter (three phases distribution)	25	RS	409
	4.57av					Great Lakes DOC(same procedure)	25	RS	409
5.60av	6.38av				16	Green Bay suspended matter (same procedure)	25	RS	410
	4.77av					Green Bay DOC(same procedure)	25	RS	410
	5.95					Aldrich humic acid ($\log K_{doc}$ is the zero intercept of the regression line of $\log K_{doc}$ vs DOC conc.)		RS	414
	6.42					Aldrich humic acid; pH 7.32 (DOC=0–0.47 mg/L)	6.6	RS	546
	5.81					DOC (11.7 mg/L) in interstitial water (Lake Michigan); pH 7.88	6.6	RS	546
	5.53					Lake Maridalsvannet; water DOC (3.5 mg C/L); pH 6.6	20	ED	440
	5.35					Lake Louhilampi: water DOC (18.0 mg C/L); pH 4.6	20	ED	440
	4.88					Hellerudmyra bog; water DOC (20.6 mg C/L); pH 4.4	20	ED	440
	4.89					Nordic fulvic acid (19.4 mg C/L); pH 4.31	20	ED	440
	4.96					"NIVA-concentrate;" water humic sample (19.4 mg C/L); pH 4.42	20	ED	440
	5.18–					DOC in porewater of Lake		RS	547

TABLE 2. Sorption coefficients for polyaromatic hydrocarbons (PAHs)—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%)				Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
	6.07					Michigan (LM) sediment after filtration			
	6.40–6.41					DOC in porewater of LM sediment after centrifugation		RS	547
	4.72–6.73					DOC in elutriate of LM sediment after filtration		RS	547
	6.02–6.99					DOC in elutriate of LM sediment after centrifugation		RS	547
	6.26				50.2	Aldrich humic acid (2.5 mg C/L)	23	ED	400
	6.21					Aldrich humic acid (5 mg C/L)	23	ED	434
	6.56					Aldrich humic acid		ED	435
	6.26av				3.38av	23 Brisbane River sediments		FM	544
	5.81av					8 Eagle Harbor contaminated sediment-pore water systems		FM	612
	5.90					Correlation $\log K_{oc}$ –MCI			598
						Tetracene			
	5.81					Soil; experimental (literature data)			217
	5.81av				2.78, 3.27	Coarse si fractions of Doe Run and Hickory Hill sediments	25	BE	108
	5.26					Prediction from addition of ring fraction			96
	4.74					Correlation $\log K_{oc} - \log K_{ow}$			207
	5.69					Correlation $\log K_{oc} - \log K_{ow}$			108
	5.51					Correlation $\log K_{oc} - \log K_{ow}$			96
	5.25					Correlation $\log K_{oc} - \log S(\mathrm{mp})$			96
	[5.58]					Correlation $\log K_{om}$ –MCI			591
	5.36					Correlation $\log K_{oc}$ –MCI			578
	5.09					Correlation $\log K_{oc}$ –LSER			602

Values in square parentheses have been calculated by the author.

*% OM content.

av: average value.

Idem refers to the sorbent reported just above; only the data (texture, OC, temperature, method) which were changed are specified.

TABLE 3. Sorption coefficients for halogenated alkyl hydrocarbons

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%)				Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
						Dichloromethane			
	2.06*av				65*–85*	Three municipal wastewater solids	22.5	BE	535
	1.44					Correlation $\log K_{oc}$ – MCI			596
	1.39					Correlation $\log K_{oc}$ – MCI			578
	[1.47]					Correlation $\log K_{om}$ – MCI			591
	1.03					Correlation $\log K_{oc}$ – LSER			602
						Trichloromethane			
−0.25	1.57				1.49	Captina sil soil; pH 4.97; 0.01 M $CaNO_3$		BE	606
−0.72	1.46				0.66	Mc Laurin sl soil; pH 4.43; 0.01 M $CaNO_3$		BE	606
	1.44av					Soil, sand, loess	20	HS	226
	1.98av					Weathered shale, mudrock	20	HS	226
	2.79av					Unweathered shale, mudrock	20	HS	226
	2.15*av				65*–85*	Three municipal wasterwater solids	22.5	BE	535
[−1.16]		92	5.9	2.1	0.09	Lincoln soil; fine s; pH 6.4 CE = 3.5 me/100 g	20	MD	541
	1.65					Correlation $\log K_{oc}$ – MCI			596
	1.56					Correlation $\log K_{oc}$ – MCI			578
	[1.64]					Correlation $\log K_{om}$ – MCI			591
	1.59					Correlation $\log K_{oc}$ – LSER			602
						Tetrachloromethane (TeCM)			
	2.65*av				65*–85*	Three municipal wastewater solids	22.5	BE	535
0.13	1.26	3.6	7.3	89.1	7.56	DTMA-Wyoming bentonite	20	BE	93
0.18	1.34	3.6	7.3	89.1	6.97	TTMA-Wyoming bentonite	20	BE	93
0.49	1.70	3.6	7.3	89.1	6.16	HTMA-Wyoming bentonite	20	BE	93
0.82	1.96	3.6	7.3	89.1	7.13	BDHA-Wyoming bentonite	20	BE	93
0.88	2.07	3.6	7.3	89.1	6.57	DDPA-Wyoming bentonite	20	BE	93
1.97° (0.64)		3.6	7.3	89.1	2.6	30% DTMDA-Wyoming bentonite	20	BE	92
2.03° (0.68)					4.5	61% Idem	20		92
2.20° (0.71)					5.8	80% Idem	10		92
2.16° (0.71)					5.8	80% Idem	20		92
2.07° (0.72)					5.8	80% Idem	35		92
0.65	1.69	3.6	7.3	89.1	9.0	80% DTMA-Wyoming bentonite	10–35	BE	92
[0.10]	1.72				2.40	U.S. EPA ref soil 2; $SA(N_2) = 7.85/m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[−0.12]	1.72				1.43	U.S. EPA ref soil 3; 0.005 M $CaCl_2$	24	BE	230
[0.14]	1.80				2.21	U.S. EPA ref soil 7; $SA(N_2) = 22.4\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[0.07]	1.76				2.04	U.S. EPA ref soil 10; $SA(N_2) = 8.84\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[0.11]	1.76				2.25	U.S. EPA ref soil 12; $SA(N_2) = 9.38\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[0.07]	1.83				1.73	U.S. EPA ref soil 19; $SA(N_2) = 3.75\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[−0.18]	1.79				1.08	Anoka soil; $Sa(N_2) = 1.07\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[−0.11]	1.72				1.49	Piketon soil; $SA(N_2) = 7.77\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230

TABLE 3. Sorption coefficients for halogenated alkyl hydrocarbons—Continued

log K_d log K_f^0 (1/n)	log K_{oc}	Sorbent composition (%)				Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
[−0.09]	1.65				1.80	Marlette soil; SA(N_2)=3.99 m^2/g; 0.005 M $CaCl_2$	24	BE	230
[−0.18]	1.81				1.03	Spinks soil; SA(N_2)=1.51 m^2/g; 0.005 M $CaCl_2$	24	BE	230
[0.15]	1.69				2.90	Elliot (IHSS ref soil); 0.005 M $CaCl_2$	24	BE	230
[−0.09]	1.81				1.26	Woodburn soil; SA(N_2)=11.2 m^2/g; 0.005 M $CaCl_2$	24	BE	230
[0.15]	1.77				2.40	Renslow soil; SA(N_2)=11.6 m^2/g; 0.005 M $CaCl_2$	24	BE	230
[0.61]	1.83				6.09	Sanhedrin soil; SA(N_2)=7.88 m^2/g; 0.005 M $CaCl_2$	24	BE	230
[0.36]	1.87				3.12	Cathedral soil; SA(N_2)=5.58 m^2/g; 0.005 M $CaCl_2$	24	BE	230
[0.37]	1.83				3.47	Wellsboro soil; SA(N_2)=5.73 m^2/g; 0.005 M $CaCl_2$	24	BE	230
[0.48]	1.73				5.61	Fangshan District Beijing, China (C.); SA(N_2)=4.96 m^2/g;	24	BE	230
[0.28]	1.83				2.83	Anda, Heilongjiang, China; 0.005 M $CaCl_2$	24	BE	230
[−0.75]	1.72				0.34	Jinxian County, Jiangxi, (C.); 0.005 M $CaCl_2$	24	BE	230
[−0.18]	1.79				1.08	Nanjing, Jiangsu, (C.); 0.005 M $CaCl_2$	24	BE	230
[0.01]	1.74				1.77	Changshu, Jiangsu, (C.); 0.005 M $CaCl_2$	24	BE	230
[−0.45]	1.72				0.67	Xuyi County, Jiangsu, (C.); SA(N_2)=54.0 m^2/g; 0.005 M $CaCl_2$	24	BE	230
[0.41]	1.81				4.02	Jinhu County, Jiangsu, (C.); 0.005 M $CaCl_2$	24	BE	230
[−0.24]	1.85				0.81	Hongze County, Jiangsu, (C.); SA(N_2)=22.8 m^2/g; 0.005 M $CaCl_2$	24	BE	230
[0.19]	1.79				2.54	Dushan County, Guizhou, (C.); SA(N_2)=8.20 m^2/g; 0.005 M $CaCl_2$	24	BE	230
[−0.16]	1.79				1.12	Gangcha County, Qinghai, (C.); SA(N_2)=4.21 m^2/g; 0.005 M $CaCl_2$	24	BE	230
[−1.03]	1.77				0.16	Xinghai County, Qinghai, (C.); SA(N_2)=2.8 m^2/g; 0.005 M $CaCl_2$	24	BE	230
[−0.52]	1.82				0.46	Luochuan County, Shanxi, (C.); 0.005 M $CaCl_2$	24	BE	230
[−0.36]	1.82				0.66	Yishan County, Guangxi, (C.); SA(N_2)=40.2 m^2/g; 0.005 M $CaCl_2$	24	BE	230
[−0.27]	1.81				0.83	Yangchun County, Guangdong, (C.); 0.005 M $CaCl_2$	24	BE	230
[−0.45]	1.74				0.64	Xuwen County, Guangdong, (C.); 0.005 M $CaCl_2$	24	BE	230
[−0.68]	1.79				0.34	Qiongzhong County, Hainan, (C.); SA(N_2)=4.85 m^2/g; 0.005 M $CaCl_2$	24	BE	230
[1.87]	[2.06]				64.0	Peat extracted with 0.1 M NaOH; 0.005 M $CaCl_2$	24	BE	229
[1.65]	[1.89]				57.1	Peat; SA(N_2)=1.5 m^2/g; 0.005 M $CaCl_2$	24	BE	229

TABLE 3. Sorption coefficients for halogenated alkyl hydrocarbons—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%)				Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
[1.45]	[1.72]				53.1	Houghton muck soil; $SA(N_2)=0.8\ m^2/g$; 0.005 M $CaCl_2$	24	BE	229
	[0.60]				44.4	Cellulose; $SA(N_2)=2.3\ m^2/g$; 0.005 M $CaCl_2$	24	BE	229
0.33	2.16				1.49	Captina sil soil pH 4.97; 0.01 M $CaNO_3$		BE	606
−0.49	1.69				0.66	Mc Laurin sl soil; pH 4.43; 0.01 M $CaNO_3$		BE	606
[0.00]	1.82				1.50	U.S. EPA ref sediment 11; $SA(N_2)=20.2\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[−0.09]	2.01				0.79	U.S. EPA ref sediment 18; $SA(N_2)=22.1\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[0.40]	2.06				2.20	U.S. EPA ref sediment 22; $SA(N_2)=3.39\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[−0.05]	1.95				0.99	U.S. EPA ref sediment 25; $SA(N_2)=7.60\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[0.15]	1.97				1.50	Mississippi River sed. (pool 2); $SA(N_2)=5.90\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[−0.01]	1.94				1.13	Mississippi River sed. (pool 11); $SA(N_2)=4.86\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[0.11]	1.96				1.40	Mississippi River sed. (pool 26); $SA(N_2)=15.5\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[0.24]	2.04				1.60	Mississippi River sediment; $SA(N_2)=12.8\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[−0.16]	2.08				0.58	Yazoo River sediment; $SA(N_2)=19.7\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[−0.32]	2.08				0.40	Mississippi River sediment; $SA(N_2)=8.09\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[0.34]	2.05				1.97	Lake Charles sediment; $SA(N_2)=13.3\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[0.09]	2.02				1.17	Suisin Bay marine sediment; $SA(N_2)=15.7\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[0.20]	2.03				1.48	Suisin Bay marine sediment; $SA(N_2)=21.6\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[0.28]	2.03				1.78	Suisin Bay marine sediment; $SA(N_2)=21.3\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[0.70]	2.03				4.73	Tangwang River sed., China (C.); $SA(N_2)=12.8\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[0.12]	2.07				1.12	Sonhuajiang River sed. (C.) 0.005 M $CaCl_2$	24	BE	230
[0.27]	1.97				1.99	Tumen River sediment (C.); $SA(N_2)=4.93\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[0.62]	2.01				4.12	Xuanwu Lake sediment (C.); 0.005 M $CaCl_2$	24	BE	230
[0.06]	1.97				1.24	Guchen Lake sediment (C.); 0.005 M $CaCl_2$	24	BE	230
[0.02]	2.00				1.04	Lake Hongze sediment (C.); $SA(N_2)=29.9\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[0.51]	1.98				3.37	Zhujiang River sediment (C.); 0.005 M $CaCl_2$	24	BE	230
[−0.91]	2.05				0.11	Yellow River sediment (C.); 0.005 M $CaCl_2$	24	BE	230
[−0.96]	2.00				0.11	Yinghe River sediment (C.); $SA(N_2)=1.85\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[0.37]	2.03				2.19	Ziya River sediment (C.); $SA(N_2)=5.83\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[−0.11]	2.05				0.70	Ganjiang River sediment (C.); $SA(N_2)=5.32\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[0.41]	1.96				2.82	Zishui River sediment (C.); $SA(N_2)=8.97\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[−0.35]	2.06				0.29	Liuyanghe River sediment (C.); 0.005 M $CaCl_2$	24	BE	230

TABLE 3. Sorption coefficients for halogenated alkyl hydrocarbons—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
[0.05]	1.96				1.22	Youshui River sediment (C.); $SA(N_2)=11.9\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[−0.43]	1.98				0.39	Niqu River sediment (C.); $SA(N_2)=4.84\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[−0.25]	2.05				0.50	Huaihe River sediment (C.); $SA(N_2)=17.6\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[−0.39]	1.96				0.45	Huaihe River sediment (C.); $SA(N_2)=8.21\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[−0.11]	2.03				0.73	Jinghe River sediment (C.); $SA(N_2)=12.1\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[−0.41]	2.01				0.38	Sangonghe River sediment (C.); $SA(N_2)=4.00\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[−0.32]	2.03				0.45	Yaluzangbu River sediment (C.); $SA(N_2)=4.94\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[0.29]	2.00				1.94	Lake Pumo sediment (C.); $SA(N_2)=3.87\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[−0.30]	1.97				0.54	Niyanghe River sediment (C.); $SA(N_2)=3.12\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
−0.77					0.02	Borden aquifer mat.; CE=0.52 me/100 g; $SA(N_2)=0.8\ m^2/g$	21	BE	614
−0.97		>98			0.007	Rabis aquifer mat.	10	MD	166
	2.04					Correlation $\log K_{oc}-\log S$			564
	1.85					Correlation $\log K_{oc}-MCI$			596
	1.70					Correlation $\log K_{oc}-MCI$			578
	[1.79]					Correlation $\log K_{om}-MCI$			591
	2.17					Correlation $\log K_{oc}-LSER$			602
						1,2-Dichloroethane (−DCA)			
[−0.52]	[1.51]	3.3	69	26	1.6* [0.93]	Willamette soil; pH 6.8	20	BE	195
[−1.16]		92	5.9	2.1	0.09	Lincoln soil; fine s; pH 6.4; CE=3.5 me/100 g	20	MD	541
	1.06					Correlation $\log K_{oc}-\log K_{ow}$			96
	1.48					Correlation $\log K_{oc}-\log S$			96
	1.19					Correlation $\log K_{oc}-\log S$ (mp)			96
	[1.74]					Correlation $\log K_{om}-MCI$			591
	1.54					Correlation $\log K_{oc}-LSER$			602
						1,2-Dibromoethane (Ethylene dibromide, ED)			
[−0.24]	[1.79]	3.3	69	26	1.6* [0.93]	Willamette soil; pH 6.8	20	BE	195
[0.31]	[1.06]	29.1	14.3	56.6	30.6* [17.7]	Whittlesey soil; $SA=197.0\ m^2/g$	20	BE	615
[−0.40]	[1.22]	84.1	8.1	7.8	4.15* [2.41]	Ashurst soil; $SA=28.1\ m^2/g$; analysis by a catalytic combustion method	20	BE	615
[−0.60]	[1.02]					Idem; analysis by a radiotracer method			615
0.17	2.13				1.11	Lockwood fine sl soil; 0.01 M $CaCl_2$	25	BE	380
0.32	2.11				1.61	Warehouse Point fine sl soil; 0.01 M $CaCl_2$	25	BE	380
0.23	2.01				1.65	Broad Brook fine sl soil; 0.01 M $CaCl_2$	25	BE	380
−0.93	1.76				1.49	Captina sil soil; pH 4.97; 0.01 M $CaNO_3$		BE	606
−0.52	1.66				0.66	Mc Laurin sl soil; pH 4.43; 0.01 M $CaNO_3$		BE	606
	1.64					Soil; experimental (literature)			217
<−1.0	[<1.86]				0.24* [0.14]	Aquifer fines (<100 μm)		BE	504

TABLE 3. Sorption coefficients for halogenated alkyl hydrocarbons—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%)				Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
	2.08					Cyanopropyl column	20–25	RPLC	579
	1.65					Correlation $\log K_{oc}$–MCI			578
	[1.74]					Correlation $\log K_{om}$–MCI			591
	1.70					Correlation $\log K_{oc}$–$\log S$			564
	2.05					Correlation $\log K_{oc}$–LSER			602
1,1,1-Trichloroethane (–TCA)									
0.80° (1.03)						Acid peat		BE	472
0.74° (1.01)						Acid humic topsoil		BE	472
0.11° (1.00)						Calcareous humic topsoil		BE	472
−0.14° (0.81)						Subsoil rich in iron oxides		BE	472
	1.65av					Soil, sand, loess	20	HS	226
	2.22av					Weathered shale, mudrock	20	HS	226
	3.02av					Unweathered shale, mudrock	20	HS	226
[0.22]	[2.26]	3.3	69	26	1.6* [0.93]	Willamette soil; pH 6.8	20	BE	195
−1.52	[1.36]	97.1	2.3	0.6	0.13	Tampa aquifer; pH 8. 0.01 N $CaCl_2$		MD	521
−1.00		95	3	2	0.071	Allerod-1 aquifer material (a.m.); $SA(N_2)=1.7\ m^2/g$		BE	208
−0.82		96	4	0	0.048	Allerod-2 a.m.; $SA(N_2)=2.0\ m^2/g$		BE	208
−1.30		98	2	0	0.020	Borris a.m.; $SA(N_2)=0.3\ m^2/g$			
−0.82		97	2	1	0.010	Brande-1 a.m.; $SA(N_2)=1.7\ m^2/g$		BE	208
−0.52		97	2	1	0.020	Brande-2 a.m.		BE	208
−1.40		95	1	1	0.006	Finderup-1 a.m.; $SA(N_2)=0.9\ m^2/g$		BE	208
−0.52	[2.15]	97	2	0	0.213	Finderup-2 a.m.; $SA(N_2)=2.5\ m^2/g$		BE	208
−0.89		96	4	0	0.021	Gunderup-2 a.m.; $SA(N_2)=2.5\ m^2/g$		BE	208
−0.26	[2.41]	98	2	0	0.213	Herborg a.m.; $SA(N_2)=0.5\ m^2/g$		BE	208
−0.80		99	0	1	0.016	Rabis a.m.; $SA(N_2)=0.4\ m^2/g$		BE	208
−0.72		96	2	3	0.048	Tirstrup-1 a.m.; $SA(N_2)=3.3\ m^2/g$		BE	208
−0.82		97	0	2	0.035	Tirstrup-2 a.m.; $SA(N_2)=1.9\ m^2/g$		BE	208
−0.54	[2.26]	94	2	4	0.159	Tylstrup a.m.; $SA(N_2)=3.3\ m^2/g$		BE	208
−0.68		97	2	1	0.012	Vasby a.m.; $SA(N_2)=0.8\ m^2/g$		BE	208
−0.85		98	1	1	0.029	Vejen-1 a.m.; $SA(N_2)=1.7\ m^2/g$		BE	208
−0.70		98	0	3	0.032	Vejen-2 a.m.; $SA(N_2)=2.6\ m^2/g$		BE	208
−0.80		99	0	1	0.006	Vorbasse-1 a.m.; $SA(N_2)=1.8\ m^2/g$		BE	208
−0.85		98	2	0	0.007	Vorbasse-2 a.m.; $SA(N_2)=0.3\ m^2/g$		BE	208
−0.40	[2.52]	98	1	1	0.122	Vorbasse-3 a.m.; $SA(N_2)=0.1\ m^2/g$		BE	208
	[2.03]av					17 soils		BE	472
	2.11					Cyanopropyl column	20–25	RPLC	579
	2.08					Correlation $\log K_{oc}$–$\log K_{ow}$			96
	2.02					Correlation $\log K_{oc}$–$\log S$			96
	2.04					Correlation $\log K_{oc}$–$\log S$ (mp)			96
	1.70					Correlation $\log K_{oc}$–MCI			578
	[1.79]					Correlation $\log K_{om}$–MCI			591
	2.08					Correlation $\log K_{oc}$–LSER			602
1,1,2-Trichloroethane (–TCA)									
−0.92	1.78	97.3	2.2	0.5	0.2	Forest soil; pH 5.6; CE=0.48 me/100 g		MD	344
0.15	1.80	65.2	25.6	9.2	2.2	Agricultural soil; pH 7.4; CE=9.0 me/100 g		MD	344
0.60	2.03	69.5	20.5	10.1	3.7	Forest soil; pH 4.2; CE=2.9 me/100 g		MD	344
[−1.16]		92	5.9	2.1	0.09	Lincoln soil; pH 6.4; CE=3.5 me/100 g	20	MD	541
	1.84					Correlation $\log K_{oc}$–MCI			578
	1.70					Correlation $\log K_{oc}$–MCI			597

TABLE 3. Sorption coefficients for halogenated alkyl hydrocarbons—Continued

log K_d log K_f^0 (1/*n*)	log K_{oc}	Sorbent composition (%)				Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
	1.99					Correlation log K_{oc}–LSER			602
						1,1,2,2-Tetrachloroethane (—TeCA)			
[−0.13]	[1.90]	3.3	69	26	1.6* [0.93]	Willamette soil; pH 6.8	20	BE	195
	2.00					Correlation log K_{oc}–log K_{ow}			96
	1.87					Correlation log K_{oc}–log S			96
	1.80					Correlation log K_{oc}–log S (mp)			96
	2.04					Correlation log K_{oc}–MCI			578
	[2.14]					Correlation log K_{om}–MCI			591
	2.33					Correlation log K_{oc}–LSER			602
						1,1-Dichloroethylene			
	2.23*av				65*– 85*	Three municipal wastewater solids	22.5	BE	535
						1,2-trans-Dichloroethylene			
−1.30	[1.59]	97.1	2.3	0.6	0.13	Tampa aquifer; pH 8; 0.01 N $CaCl_2$		MD	521
						Trichloroethylene (TCE)			
	2.09av					Soil, sand, loess	20	HS	226
	2.56av					Weathered shale, mudrock	20	HS	226
	3.43av					Unweathered shale, mudrock	20	HS	226
	2.63				26.8	Shale (tertiary)	20	HS	226
	3.19				9.7	Shale (jurassic)	20	HS	226
	2.23				33.4	Peat	20	HS	226
	2.43				18.5	Lignite	20	HS	226
	3.24				83.6	Bitominous coal	20	HS	226
	3.64				80.1	Anthracite	20	HS	226
0.90	2.03				7.51	Sapsucker Woods (SW) soil	25	HS	194
0.94	2.09				7.05	SW soil; ether extracted	25	HS	194
0.11	2.16				0.88	SW soil humin	25	HS	194
0.85	1.76				12.4	SW soil humic acid	25	HS	194
−0.10	0.62				19.2	SW soil fulvic acid	25	HS	194
0.94	1.24				50.5	Tannic acid	25	HS	194
1.89	2.08				64.6	Lignin	25	HS	194
1.80	2.05				57.2	Zein	25	HS	194
−0.04	0.30				45.3	Cellulose	25	HS	194
1.51	1.83				47.9	Aldrich humic acid	25	HS	194
1.61	[2.36]				18	Muck (<1 mm)	22	GP	517
0.04	[2.37]	92	6.2	1.8	0.47	Grayling soil (<1 mm)	22	GP	517
0.07	[2.14]	87.6	10.1	2.3	0.85	Keweenaw soil (<1 mm)	22	GP	517
−0.64	[1.77]	95.5	3.2	1.3	0.39	Eustis soil (<1 mm)	22	GP	517
−0.60	[1.81]	95.5	3.2	1.3	0.39	Eustis soil; 0.01 N $CaCl_2$		MD	522
−1.96	[0.58]	98	1	1	0.29	Borden soil; 0.01 N $CaCl_2$		MD	600
0.80	[1.70]	60.3	24.0	15.7	12.6	Mt. Lemmon soil; 0.01 N $CaCl_2$		MD	600
−0.06	[1.53]	56.6	22.0	21.4	5.18* 2.59	Marlette soil (A horizon); pH 6.4; CE=16.4 me/100 g	20	BE	222
1.43	[2.61]				10.0* 6.48	Idem-HDTMA complex	20	BE	222
0.76	[2.12]				7.43* 4.37	Idem-DDTMA complex	20	BE	222
1.47	[2.90]				4.85* 3.71	Marlette soil (Bt horizon)– HDTMA complex	20	BE	222
0.80	[2.50]				2.73* 1.98	Idem-DDTMA complex	20	BE	222
1.06° (1.08)						Acid peat		BE	472
0.96° (1.16)						Acid humic top soil		BE	472
0.09° (0.93)						Calcareous humic top soil		BE	472

TABLE 3. Sorption coefficients for halogenated alkyl hydrocarbons—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
−0.25° (0.88)						Subsoil rich in iron oxides		BE	472
−0.62° (0.70)						Clay subsoil		BE	472
−0.69° (0.71)						Sandy subsoil		BE	472
0.45	[2.04]		36	8	2.57	Agawam soil; 0.01 M $CaCl_2$	20–22	BE	381
−0.85	1.86	97.3	2.2	0.5	0.2	Forest soil; pH 5.6; CE=0.48 me/100 g		MD	344
0.32	1.98	65.2	25.6	9.2	2.2	Agricultural soil; pH 7.4; CE=9.0 me/100 g		MD	344
0.72	2.15	69.5	20.5	10.1	3.7	Forest soil; pH 4.2; CE=2.9 me/100 g		MD	344
[0.40]	1.80	60	26.5	13.5	4.02	Soil from a vadose zone	25	BE	370
[1.24]	1.86				24	Soil; composite sample from a peat layer	20	BE	616
[−1.05]		92	5.9	2.1	0.09	Lincoln soil; pH 6.4; CE=3.5 me/100 g	20	MD	541
−0.28		94	4	2	<0.1	Aquifer mat.; pH 8.2; SA(E)=18.7 m^2/g; CE=2.3 me/100 g	25	HS	372
−0.24	[1.74]	33	49	18	1.05	Yolo soil; pH 7.9; SA(E)=80.6 m^2/g; CE=21.1 me/100 g	25	HS	372
0.08	[1.93]	57.5	26.4	13.7	1.41	Ødum soil; pH 7.1; SA(E)=40.1 m^2/g; CE=13.97 me/100 g	25	HS	372
−0.16	[1.79]	80.2	13.2	4.8	1.12	Lundgaard soil; pH 6.1; SA(E)=10.84 m^2/g; CE=8.78 me/100 g	25	HS	372
−1.96					0.02	Alumina; pH 4.5	25	HS	371
−0.61					0.06	Iron oxide; pH 6.5	25	HS	371
−1.3					0.02	Montmorillonite; pH 8.3	25	HS	371
−0.57					0.01	Kaolinite; pH 4.2–5.2	25	HS	371
−0.51	[1.83]				0.45	Humic acid coated alumina; pH 7.18	25	HS	371
−1.05	[1.84]	97.1	2.3	0.6	0.13	Tampa aquifer; pH 8; 0.01 N $CaCl_2$		MD	521
−0.97		>98			0.007	Rabis aquifer mat.	10	MD	166
−1.00		96			0.025	Borden aquifer; $SA(N_2)=0.3\ m^2/g$	22	HS	520
−0.77		93			0.034	Lula aquifer; $SA(N_2)=7.7\ m^2/g$	22	HS	520
−0.74	2.03	23	42	35	0.169	Upper aquitard layer (OSCL); CE=15.5 me/100 g		BE	617
0.79	2.63	17	65	18	1.49	Lower aquitard layer (DGSL); CE=29 me/100 g		BE	617
−0.54	1.79				0.48	Porous alumina coated with humic acid; 0.1 M NaCl	25	HS	364
−0.42	[1.90]				0.48	Idem	25	MD	364
	[2.01]av					18 soils		BE	472
	2.28				50.2	Aldrich and Fluka humic acid		FH	206
1.72	2.20				33.5	ICN humic acid	25	HS	193
−0.64	1.76				0.40	ICN humic acid coated Al_2O_3	25	HS	193
1.64	[2.41]				21.6* 17.3	HDTMA-smectite complex		BE	224
1.52	[2.40]				16.2* 13.0	Idem		BE	224
0.64	[1.79]				8.9* 7.1	Idem		BE	224
	2.11					Cyanopropyl column	20–25	RPLC	579
	1.66					Correlation $\log K_{oc}-\log S(180)$			193
	2.14					Correlation $\log K_{oc}-\log K_{ow}(207)$			193
	2.09					Correlation $\log K_{oc}-\log K_{ow}(108)$			193
	1.70					Correlation $\log K_{oc}$−MCI			597

TABLE 3. Sorption coefficients for halogenated alkyl hydrocarbons—Continued

log K_d log K_f^0 (1/n)	log K_{oc}	Sorbent composition (%)				Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
	1.84					Correlation log K_{oc}–MCI			578
						Tetrachloroethylene (TeCE)			
−0.06	[2.35]	95.5	3.2	1.3	0.39	Eustis soil; 0.01 N $CaCl_2$		MD	522
1.23° (1.04)						Acid peat		BE	472
1.38° (1.12)						Acid humic topsoil		BE	472
0.49° (0.91)						Calcareous humic topsoil		BE	472
0.30° (0.98)						Subsoil rich in iron oxides		BE	472
−0.45° (0.95)						Clay subsoil		BE	472
−1.25° (0.60)						Sand subsoil		BE	472
	2.64av					Soil, sand, loess	20	HS	226
	3.29av					Weathered shale, mudrock	20	HS	226
	4.03av					Unweathered shale, mudrock	20	HS	226
[0.53]	[2.56]	3.36	70.2	26.4	1.6* [0.93]	Willamette soil; pH 6.8	20	BE	195
−0.13	[2.28]	95.5	3.2	1.3	0.39	Eustis Soil (<1 mm)	22	GP	517
−1.28	[1.26]	98	1	1	0.29	Borden soil; 0.01 N $CaCl_2$		MD	600
1.35	[2.25]	60.3	24.0	15.7	12.6	Mt. Lemmon soil; 0.01 N $CaCl_2$		MD	600
−0.77	[1.75]	38.8	31.6	29.6	0.60* 0.30	Marlette soil (Bt horizon); pH 5.4; CE=14.6 me/100 g	20	BE	222
1.44	[2.87]				4.85* 3.71	Idem-HDTMA complex	20	BE	222, 223
1.08	[2.78]				2.73* 1.98	Idem-DDTMA complex	20	BE	222
0.42	[2.00]	56.6	22.0	21.4	5.18* 2.59	Marlette soil (A horizon); pH 6.4; CE=16.4 me/100 g	20	BE	222, 223
1.57	[2.76]				10.0* 6.48	Idem-HDTMA complex	20	BE	222, 223
1.17	[2.53]				7.43* 4.37	Idel-DDTMA complex	20	BE	222
	3.00*av				65*–85*	Three municipal wastewater solids	22.5	BE	535
0.86	[2.45]		36	8	2.57	Agawam soil; 0.01 M $CaCl_2$	20–22	BE	381
−0.46	2.25	97.3	2.2	0.5	0.2	Forest soil; pH 5.6; CE=0.48 me/100 g		MD	344
0.65	2.31	65.2	25.6	9.2	2.2	Agricultural soil; pH 7.4; CE=9.0 me/100 g		MD	344
−0.25	[2.57]				0.15	KB 1H soil (63–125 μm); SA(N_2)=4.9 m^2/g	20	LE	207
[−0.65]		92	5.9	2.1	0.09	Lincoln fine s soil; pH 6.4; CE=3.5 me/100 g	20	MD	541
−0.34° (1.20)					0.03	Augusta subsurface soil (Spinks); median grain size=0.13 mm; SA(N_2)=1.2 m^2/g		BE	54
−0.17° (0.93)	[2.62]				0.16	Delta subsurface soil (Ottokee); median grain size=0.20 mm; SA(N_2)=1.6 m^2/g		BE	54
0.20° (1.06)	[2.44]				0.58	Ann Arbor II subsurface soil (Bookston); median grain size=0.16 mm; SA(N_2)=4.2 m^2/g		BE	54
1.12° (0.78)					2.49	Wagner subsurface soil (Miami); median grain size=0.53 mm; SA(N_2)=1.3 m^2/g		BE	54
1.09° (0.79)					1.24	Ypsilanti subsurface soil (Wasepi); median grain size=0.31 mm; SA(N_2)=1.2 m^2/g		BE	54
1.59°					1.29	Ann Arbor I subsurface soil		BE	54

TABLE 3. Sorption coefficients for halogenated alkyl hydrocarbons—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
(0.78)						(Brookston); SA(N_2)=2.4 m^2/g			
−0.66	2.06	60.9	37.7	1.6	0.19	Simsbury subsurface aquifer sed.; 0.01 M $CaCl_2$		BE	473
−0.13					0.021	Borden sandy aquifer material		BE	88
−0.46					0.02	Idem; SA(N_2)=0.23 m^2/g; 0.005 M $CaSO_4$	20	BE	113
−0.60		91.0	5.6	3.4	0.02	Lula aquifer; 0.005 M $CaSO_4$		MD	519
−0.62		52.3	41.5	6.2	0.03	Barksdale aquifer; 0.005 M $CaSO_4$		MD	519
−0.46	[2.43]	97.1	2.3	0.6	0.13	Tampa aquifer; pH 8; 0.01 N $CaCl_2$		MD	521
−0.64		>98			0.007	Rabis aquifer mat.	10	MD	166
−0.72		78	5	2	0.007	Gravely orange sand; CE=0.8 me/100 g		BE	617
−0.37	2.40	23	42	35	0.169	Upper aquitard layer (OSCL); CE=15.5 me/100 g		BE	617
1.34	3.17	17	65	18	1.49	Lower aquitard layer (DGSL); CE=29 me/100 g		BE	617
−0.32					0.02	Borden aquifer mat.; CE=0.52 me/100 g; SA(N_2)=0.8 m^2/g	21	BE	614
	[2.38]av					18 soils		BE	472
	2.39					Correlation $\log K_{oc}-\log K_{ow}$			108
	2.14					Correlation $\log K_{oc}-\log K_{ow}$			96
	2.78					Correlation $\log K_{oc}-\log K_{ow}$			217
	2.28					Correlation $\log K_{oc}-\log K_{ow}(180)$			88
	2.50					Correlation $\log K_{oc}-\log K_{ow}(87)$			88
	2.26					Correlation $\log K_{oc}-\log K_{ow}(120)$			88
	2.44					Correlation $\log K_{oc}-\log K_{ow}(130)$			88
	1.81					Correlation $\log K_{oc}-\log K_{ow}(55)$			88
	2.36					Correlation $\log K_{oc}-\log K_{ow}$			207
	2.35, 2.57					Correlation $\log K_{oc}-\log S$			96
	2.54, 2.89					Correlation $\log K_{oc}-\log S$ (mp)			96
	2.38					Correlation $\log K_{oc}-\log S$			564
	[2.14]					Correlation $\log K_{om}$−MCI			591
	2.52					Correlation $\log K_{oc}$−LSER			602
1,2-Dichloropropane									
[−0.36]	[1.67]	3.3	69	26	1.6* [0.93]	Willamette soil; pH 6.8	20	BE	195
−0.17	[1.42]		36	8	2.57	Agawam soil; 0.01 M $CaCl_2$	20–22	BE	381
	[1.94]					Correlation $\log K_{om}$−MCI			591
1,2,3-Trichloropropane									
0.15	1.98				1.49	Captina soil; silt loam; pH 4.97; 0.01 M $CaNO_3$		BE	606
−0.29	1.89				0.66	Mc Laurin soil; sandy loam; pH 4.43; 0.01 M $CaNO_3$		BE	606
1,3-Dichloropropene									
	1.36 (cis) 1.42 (trans)					Soil; experimental (literature data)			217
	1.91					Correlation $\log K_{oc}$−MCI			598
	[2.02]					Correlation $\log K_{om}$−MCI			591

Values in square parentheses have been calculated by the author.

*$\log K_{om}$ in column 2 and % OM content in column 6.

av average value.

Idem refers to the sorbent reported just above; only the data (texture, OC, temperature, method) which were changed are specified.

TABLE 4. Sorption coefficients for halogenated benzenes

log K_d log K_f^0 (1/n)	log K_{oc}	Sorbent composition (%)				Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
						Chlorobenzene (MCBz)			
[−0.04]	[1.92]	9	68	21	1.9* [1.1]	Woodburn soil; CE=14 me/100 g	20	BE	55
[−1.05]		92	5.9	2.1	0.09	Lincoln fine s soil; pH 6.4; CE=3.5 me/100 g	20	MD	541
−1.85	[0.68]	98	1	1	0.29	Borden soil; 0.01 N $CaCl_2$		MD	600
1.01	[1.91]	60.3	24.0	15.7	12.6	Mt. Lemmon soil; 0.01 N $CaCl_2$		MD	600
−0.41	[2.42]				0.15	KB 1H soil (63–125 μm); $SA(N_2)=4.9\ m^2/g$	20	LE	207
0.08	[2.21]				0.73	KS 1 soil (<125 μm); $SA(N_2)=4.4\ m^2/g$	20	LE	207
−0.40					0.08	KB 1H soil (<125 μm); $SA(N_2)=3.2\ m^2/g$	20	LE	207
−0.22					0.06	Kaolin; $SA(N_2)=12\ m^2/g$	20	LE	207
−0.22					<0.01	γ-Al_2O_3; $SA(N_2)=120\ m^2/g$	20	LE	207
0.62					<0.01	SiO_2; $SA(N_2)=500\ m^2/g$	20	LE	207
0.67	2.50				1.49	Captina sil soil; pH 4.97; 0.01 M $CaNO_3$		BE	606
−0.01	2.17				0.66	Mc Laurin sl soil; pH 4.43; 0.01 M $CaNO_3$		BE	606
1.35	[2.10]				18	Muck (<1 mm); 0.01 N $CaCl_2$	22	GP	517
−0.52	[1.89]	95.5	3.2	1.3	0.39	Eustis soil (<1 mm); 0.01 N $CaCl_2$		MD	517
−1.05	[1.84]	97.1	2.3	0.6	0.13	Tampa aquifer; pH 2; 0.01 N $CaCl_2$		MD	521
	2.64*av				65*–85*	Three municipal wastewater solids	22.5	BE	535
[1.1]	2.6				2.9	Offshore Grand Haven sediment; (solute complexation model)		BE	464, 494
[1.7]	3.1				3.8	Benton Harbor sediment; (solute complexation model)		BE	464, 494
	[2.15]				58.03	Prediction by limiting vapor sorption on soil humic acid	23	LSC	363
	2.19					C18 column; correlation log K_{oc}-(log $k'+\Delta^0\chi$)		RPLC	577
	2.20					C18 column; correlation log K_{oc}-(log k'+hydrogen bonding index)		RPLC	577
	2.44					Correlation log K_{oc}−log K_{ow}			207
	2.50					Correlation log K_{oc}−log K_{ow}			108
	2.18					Correlation log K_{oc}−log S			564
	2.44					Correlation log K_{oc}−MCI			578
	[2.56]					Correlation log K_{om}−MCI			591
	2.26					Correlation log K_{oc}−CRI			601
	2.01					Correlation log K_{oc}−LSER			602
						Bromobenzene			
	2.18					Soil; experimental (literature)			217
	2.65					Cyanopropyl column	20–25	RPLC	579
	2.65					Correlation log K_{oc}−MCI			578
	2.18					Correlation log K_{oc}−log S			564
	[2.56]					Correlation log K_{om}−MCI			591
						1,2-Dichorobenzene (-DCBz)			
[0.55]	[2.51]	9	68	21	1.9* [1.1]	Woodburn soil; CE=14 me/100 g	20	BE	55
[0.46]	[2.50]	3.3	69	26	1.6* [0.93]	Willamette soil; pH 6.8	20	BE	195
1.95	[2.73]				29* [16.8]	Peaty soil		BE	472
1.27	3.10				1.49	Captina sil soil; pH 4.97; 0.01 M $CaNO_3$		BE	606
0.72	2.90				0.66	Mc Laurin sl soil; pH 4.43; 0.01 M $CaNO_3$		BE	606

Table 4. Sorption coefficients for halogenated benzenes—Continued

log K_d log K_f^0 $(1/n)$	log K_{oc}	Sorbent composition (%)				Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
[0.80]	2.42				2.40	U.S. EPA ref soil 2; SA(N_2)=7.85 m^2/g; 0.005 M $CaCl_2$	24	BE	230
[0.59]	2.44				1.43	U.S. EPA ref soil 3; 0.005 M $CaCl_2$	24	BE	230
[0.84]	2.50				2.21	U.S. EPA ref soil 7; SA(N_2)=22.4 m^2/g; 0.005 M $CaCl_2$	24	BE	230
[0.70]	2.39				2.04	U.S. EPA ref soil 10; SA(N_2)=8.84 m^2/g; 0.005 M $CaCl_2$	24	BE	230
[0.71]	2.36				2.25	U.S. EPA ref soil 12; SA(N_2)=9.38 m^2/g; 0.005 M $CaCl_2$	24	BE	230
[0.73]	2.49				1.73	U.S. EPA ref soil 19; SA(N_2)=3.75 m^2/g; 0.005 M $CaCl_2$	24	BE	230
[0.45]	2.42				1.08	Anoka soil; Sa(N_2)=1.07 m^2/g; 0.005 M $CaCl_2$	24	BE	230
[0.59]	2.42				1.49	Pikcton soil; SA(N_2)=7.77 m^2/g; 0.005 M $CaCl_2$	24	BE	230
[0.61]	2.35				1.80	Marlette soil; SA(N_2)=3.99 m^2/g; 0.005 M $CaCl_2$	24	BE	230
[0.51]	2.50				1.03	Spinks soil; SA(N_2)=1.51 m^2/g; 0.005 M $CaCl_2$	24	BE	230
[0.86]	2.40				2.90	Elliot (IHSS ref soil); 0.005 M $CaCl_2$	24	BE	230
[0.57]	2.47				1.26	Woodburn soil; SA(N_2)=11.2 m^2/g; 0.005 M $CaCl_2$	24	BE	230
[0.91]	2.53				2.40	Renslow soil; SA(N_2)=11.6 m^2/g; 0.005 M $CaCl_2$	24	BE	230
[1.32]	2.54				6.09	Sanhedrin soil; SA(N_2)=7.88 m^2/g; 0.005 M $CaCl_2$	24	BE	230
[1.10]	2.61				3.12	Cathedral soil; SA(N_2)=5.58 m^2/g; 0.005 M $CaCl_2$	24	BE	230
[1.12]	2.58				3.47	Wellsboro soil; SA(N_2)=5.73 m^2/g; 0.005 M $CaCl_2$	24	BE	230
[1.17]	2.42				5.61	Fangshan District, Beijing, China (C.); SA(N_2)=4.96 m^2/g;	24	BE	230
[0.91]	2.46				2.83	Anda, Heilongjiang, China; 0.005 M $CaCl_2$	24	BE	230
[0.04]	2.51				0.34	Jinxian County, Jiangxi, (C.); 0.005 M $CaCl_2$	24	BE	230
[0.40]	2.37				1.08	Nanjing, Jiangsu, (C.); 0.005 M $CaCl_2$	24	BE	230
[0.65]	2.40				1.77	Changshu, Jiangsu, (C.); 0.005 M $CaCl_2$	24	BE	230
[0.24]	2.41				0.67	Xuyi County, Jiangsu, (C.); SA(N_2)=54.0 m^2/g; 0.005 M $CaCl_2$	24	BE	230
[1.09]	2.49				4.02	Jinhu County, Jiangsu, (C.); 0.005 M $CaCl_2$	24	BE	230
[0.41]	2.50				0.81	Hongze County, Jiangsu, (C.); SA(N_2)=22.8 m^2/g; 0.005 M $CaCl_2$	24	BE	230
[0.90]	2.50				2.54	Dushan County, Guizhou, (C.); SA(N_2)=8.20 m^2/g; 0.005 M $CaCl_2$	24	BE	230

Table 4. Sorption coefficients for halogenated benzenes—Continued

log K_d log K_f^0 ($1/n$)	log K_{oc}	Sorbent composition (%)				Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
[0.52]	2.47				1.12	Gangcha County, Qinghai, (C.); $SA(N_2)=4.21\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[−0.38]	2.42				0.16	Xinghai County, Qinghai, (C.); $SA(N_2)=2.86\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[0.16]	2.50				0.46	Luochuan County, Shanxi, (C.); 0.005 M $CaCl_2$	24	BE	230
[0.26]	2.44				0.66	Yishan County, Guangxi, (C.); $SA(N_2)=40.2\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[0.39]	2.47				0.83	Yangchun County, Guangdong, (C.); 0.005 M $CaCl_2$	24	BE	230
[0.21]	2.41				0.64	Xuwen County, Guangdong, (C.); 0.005 M $CaCl_2$	24	BE	230
[0.01]	2.48				0.34	Qiongzhong County, Hainan, (C.); $SA(N_2)=4.85\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
−0.1	[2.43]	38.8	31.6	29.6	0.60* 0.30	Marlette soil (Bt horizon); pH 5.4; CE=14.6 me/100 g	20	BE	222, 223
2.21	[3.64]				4.85* 3.71	Idem-HDTMA complex	20	BE	222, 223
1.82	[3.52]				2.73* 1.98	Idem-DDTMA complex	20	BE	222
0.86	[2.45]	56.6	22.0	21.4	5.18* 2.59	Marlette soil (A horizon); pH 6.4; CE=16.4 me/100 g	20	BE	222, 223
2.08	[3.27]				10.0* 6.48	Idem-HDTMA complex	20	BE	222, 223
1.68	[3.04]				7.43* 4.37	Idem-DDTMA complex	20	BE	222
[0.66]	2.48				1.50	U.S. EPA ref sediment 11; $SA(N_2)=20.2\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[0.58]	2.68				0.79	U.S. EPA ref sediment 18; $SA(N_2)=22.1\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[1.10]	2.76				2.20	U.S. EPA ref sediment 22; $SA(N_2)=3.39\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[0.65]	2.65				0.99	U.S. EPA ref sediment 25; $SA(N_2)=7.60\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[0.83]	2.64				1.50	Mississippi River sed. (pool 2); $SA(N_2)=5.90\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[0.62]	2.57				1.13	Mississippi River sed. (pool 11); $SA(N_2)=4.86\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[0.74]	2.59				1.40	Mississippi River sed. (pool 26); $SA(N_2)=15.5\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[0.93]	2.73				1.60	Mississippi River sediment; $SA(N_2)=12.8\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[0.46]	2.70				0.58	Yazoo River sediment; $SA(N_2)=19.7\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[0.34]	2.74				0.40	Mississippi River sediment; $SA(N_2)=8.09\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[1.02]	2.73				1.97	Lake Charles sediment; $SA(N_2)=13.3\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230

Table 4. Sorption coefficients for halogenated benzenes—Continued

log K_d log K_f^0 ($1/n$)	log K_{oc}	Sorbent composition (%)				Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
[0.78]	2.71				1.17	Suisin Bay marine sediment; $SA(N_2)=15.7\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[0.90]	2.73				1.48	Suisin Bay marine sediment; $SA(N_2)=21.6\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[0.98]	2.73				1.78	Suisin Bay marine sediment; $SA(N_2)=21.3\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[1.42]	2.74				4.73	Tangwang River sed., China (C.); $SA(N_2)=12.8\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[0.79]	2.74				1.12	Sonhuajiang River sed. (C.); 0.005 M $CaCl_2$	24	BE	230
[0.92]	2.62				1.99	Tumen River sediment (C.); $SA(N_2)=4.93\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[1.37]	2.75				4.12	Xuanwu Lake sediment (C.); 0.005 M $CaCl_2$	24	BE	230
[0.83]	2.74				1.24	Guchen Lake sediment (C.); 0.005 M $CaCl_2$	24	BE	230
[0.68]	2.66				1.04	Lake Hongze sediment (C.); $SA(N_2)=29.9\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[1.27]	2.74				3.37	Zhujiang River sediment (C.); 0.005 M $CaCl_2$	24	BE	230
[−0.19]	2.77				0.11	Yellow River sediment (C.); 0.005 M $CaCl_2$	24	BE	230
[−0.28]	2.68				0.11	Yinghe River sediment (C.); $SA(N_2)=1.85\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[1.12]	2.78				2.19	Ziya River sediment (C.); $SA(N_2)=5.83\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[0.58]	2.73				0.70	Ganjiang River sediment (C.); $SA(N_2)=5.32\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[1.09]	2.64				2.82	Zishui River sediment (C.); $SA(N_2)=8.97\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[0.20]	2.74				0.29	Liuyanghe River sediment (C.); 0.005 M $CaCl_2$	24	BE	230
[0.74]	2.65				1.22	Youshui River sediment (C.); $SA(N_2)=11.9\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[0.27]	2.68				0.39	Niqu River sediment (C.); $SA(N_2)=4.84\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[0.43]	2.73				0.50	Huaihe River sediment (C.); $SA(N_2)=17.6\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[0.32]	2.67				0.45	Huaihe River sediment (C.); $SA(N_2)=8.21\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[0.63]	2.77				0.73	Jinghe River sediment (C.); $SA(N_2)=12.1\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[0.28]	2.70				0.38	Sangonghe River sediment (C.); $SA(N_2)=4.00\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[0.37]	2.72				0.45	Yaluzangbu River sediment (C.); $SA(N_2)=4.94\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230

Table 4. Sorption coefficients for halogenated benzenes—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%)				Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
[1.02]	2.73				1.94	Lake Pumo sediment (C.); $SA(N_2)=3.87\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[0.43]	2.69				0.54	Niyanghe River sediment (C.); $SA(N_2)=3.12\ m^2/g$; 0.005 M $CaCl_2$	24	BE	230
[3.21]	4.6				4.1	Lake Ontario sediment trap material		FM	49
	4.6				50	Niagara River organic matter		FM	49
−0.08		>98			0.007	Rabis aquifer mat.	10	MD	166
−1.00		40.8	53.1	4.7	0.0096	Tinker aquifer; Fe=14 g/kg; $SA(N_2)=9.2\ m^2/g$; CE=39.95 me/100 g	22.5	BE	213, 609
−0.74		74.8	18.2		0.027	Carswell aquifer; Fe=9.0 g/kg; $SA(N_2)=9.5\ m^2/g$; CE=13.91 me/100 g	22.5	BE	213, 609
−0.52	2.45	52.3	41.5		0.105	Barksdale aquifer; Fe=10.0 g/kg; $SA(N_2)=7.5\ m^2/g$; CE=64.36 me/100 g	22.5	BE	213, 609
0.11	2.91	67.8	27.3	3.5	0.156	Blythsville aquifer; Fe=7.0 g/kg; $SA(N_2)=8.0\ m^2/g$; CE=32.98 me/100 g	22.5	BE	213, 609
−0.44		98.2	1.1		0.011	Traverse City aquifer; Fe=3.0 g/kg; $SA(N_2)=0.2\ m^2/g$; CE=28.11 me/100 g	22.5	BE	213
−0.52		96.0	2.0	2.0	0.016	Borden aquifer; Fe=15.0 g/kg $SA(N_2)=0.3\ m^2/g$;	22.5	BE	213, 609
−0.85		91.0	5.6	3.4	0.020	Lula aquifer; Fe=29.0 g/kg; $SA(N_2)=11.8\ m^2/g$; CE=9.83 me/100 g	22.5	BE	213, 609
−0.09					0.02	Borden aquifer mat.; CE=0.52 me/100 g; $SA(N_2)=0.8\ m^2/g$	21	BE	614
	[2.72]				58.03	Prediction by limiting vapor sorption on soil humic acid	23	LSC	363
	2.39					C18 column; correlation $\log K_{oc}$-($\log k'+\Delta^0\chi$)		RPLC	577
	2.40					C18 column; correlation $\log K_{oc}$-($\log k'$+hydrogen bonding index)		RPLC	577
	3.00					Correlation $\log K_{oc}-\log K_{ow}$			96
	2.66					Correlation $\log K_{oc}$−MCI			578
	[2.78]					Correlation $\log K_{om}$−MCI			591
	2.79					Correlation $\log K_{oc}$−CRI			601
	2.44					Correlation $\log K_{oc}$−LSER			602
						1,3-Dichlorobenzene (-DCBz)			
1.70	[2.44]				18	Muck (<1 mm)	22	GP	517
−0.03	[2.38]	95.5	3.2	1.3	0.39	Eustis soil (<1 mm); 0.01 N $CaCl_2$		MD	517
1.90	[2.68]				29* [16.8]	Peaty soil		BE	472
	[2.47]	9	68	21	1.9* [1.1]	Woodburn soil; CE=14 me/100 g	20	BE	55
−0.42	[2.47]	97.1	2.3	0.6	0.13	Tampa aquifer; pH 2; 0.01 N $CaCl_2$		MD	521
[3.11]	4.5				4.1	Lake Ontario sediment trap material		FM	49
	4.1				50	Niagara River organic matter		FM	49
	[2.78]				58.03	Prediction by limiting vapor sorption on soil humic acid	23	LSC	363
	2.43					Humic acid-silica column	20–23	RPLC	587
	2.58					Salicylic acid-silica column	20–23	RPLC	587

Table 4. Sorption coefficients for halogenated benzenes—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
	2.88					8-Hydroxyquinoline-silica column	20–23	RPLC	587
	2.60					C18 column; correlation $\log K_{oc}$-($\log k'+\Delta^0\chi$)		RPLC	577
	2.60					C18 column; correlation $\log K_{oc}$-($\log k'$+hydrogen bonding index)		RPLC	577
	3.0					Correlation $\log K_{oc}-\log K_{ow}$(96)			49
	2.65					Correlation $\log K_{oc}$–MCI			578
	[2.77]					Correlation $\log K_{om}$–MCI			591
	2.81					Correlation $\log K_{oc}$–CRI			601
	2.47					Correlation $\log K_{oc}$–LSER			602
						1,4-Dichlorobenzene (-DCBz)			
[0.48]	[2.44]	9	68	21	1.9* [1.1]	Woodburn soil; CE=14 me/100 g	20	BE	55
[−0.14]	2.82	4	10	86	0.11	Apison soil; pH 4.5; CE=76 me/100 g		BE	570
[−0.29]		11	21	68	0.06	Fullerton soil; pH 4.4; CE=64 me/100 g		BE	570
[0.53]	2.45	2	38	60	1.2	Dormont soil; pH 4.2; CE=129 me/100 g		BE	570
1.86	[2.64]				29** [16.8]	Peaty soil		BE	472
0.04	[2.87]				0.15	KB 1H soil (63–125 μm); $SA(N_2)=4.9\ m^2/g$	20	LE	207
0.64	[2.78]				0.73	KS 1 soil (<125 μm); $SA(N_2)=4.4\ m^2/g$	20	LE	207
0.04					0.08	KB 1H soil (<125 μm); $SA(N_2)=3.2\ m^2/g$	20	LE	207
0.04					0.06	Kaolin; $SA(N_2)=12\ m^2/g$	20	LE	207
−0.05					<0.01	γ-Al_2O_3; $SA(N_2)=120\ m^2/g$	20	LE	207
0.78					<0.01	SiO_2; $SA(N_2)=500\ m^2/g$	20	LE	207
[−0.45]		92	5.9	2.1	0.09	Lincoln fine s soil; pH 6.4; CE=3.5 me/100 g	20	MD	541
−0.12° (0.76)					0.03	Augusta subsurface soil (Spinks); median grain size=0.13 mm; $SA(N_2)=1.2\ m^2/g$		BE	54
−0.01° (0.89)	[2.79]				0.16	Delta subsurface soil (Ottokee); median grain size=0.20 mm; $SA(N_2)=1.6\ m^2/g$		BE	54
0.30° (0.88)	[2.54]				0.58	Ann Arbor II subsurface soil (Brookston); median grain size=0.16 mm; $SA(N_2)=4.2\ m^2/g$		BE	54
1.26° (0.77)					2.49	Wagner subsurface soil (Miami); median grain size=0.53 mm; $SA(N_2)=1.3\ m^2/g$		BE	54
1.23° (0.78)					1.24	Ypsilanti subsurface soil (Wasepi); median grain size=0.31 mm; $SA(N_2)=1.2\ m^2/g$		BE	54
1.78° (0.69)					1.29	Ann Arbor I subsurface soil (Brookston); median grain size=0.21 mm; $SA(N_2)=2.4\ m^2/g$		BE	54
−0.12		>98			0.007	Rabis aquifer mat.	10	MD	166
[3.41]	4.8				4.1	Lake Ontario sediment trap material		FM	49
	5.0				50	Niagara River organic matter		FM	49
1.94	[2.95]				17* [9.86]	Charles River sediment	22	GP	155
	2.92				50.2	Aldrich humic acid; pH 8.0; 0.1 M $NaHCO_3$	22	ED	206
	2.91				50.2	Aldrich and Fluka humic acid		FH	206
	[2.76]				58.03	Prediction by limiting vapor sorption (LSC) on soil humic acid	23	LSC	363

Table 4. Sorption coefficients for halogenated benzenes—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
	2.60					C18 column; correlation $\log K_{oc}$-($\log k'+\Delta^0\chi$)		RPLC	577
	2.61					C18 column; correlation $\log K_{oc}$-($\log k'$+hydrogen bonding index)		RPLC	577
	3.0					Correlation $\log K_{oc}-\log K_{ow}$(96)			49
	2.59					Correlation $\log K_{oc}-\log S$			564
	2.65					Correlation $\log K_{oc}$–MCI			578
	[2.77]					Correlation $\log K_{om}$–MCI			591
	2.79					Correlation $\log K_{oc}$–CRI			601
	2.50					Correlation $\log K_{oc}$–LSER			602
						1,2,3-Trichlorobenzene (-TCBz)			
1.48	3.21	49.8	30.7	19.4	1.84	Riddles soil; top layer below corn residue; pH; 5.0; CE=9.0 mol/kg	20	BE	605
1.11	3.14	49.8	26.0	24.2	0.94	Idem; below top layer; pH 5.3; CE=18.3 cmol/kg	20	BE	605
1.32° (0.85)					1.42	Soil; cl; (kaolinite); pH 5.91; CE=12.4 me/100 g	20	BE	214
1.56	3.38				1.51	Soil; light c; (montmorillonite); pH 5.18; CE=13.2 me/100 g	20	BE	214
1.93° (0.97)	3.43				3.23	Soil; light c; (montmorillite); pH 5.26; CE=28.3 me/100 g	20	BE	214
2.16° (0.98)	3.26				7.91	Soil; sl; (allophane); pH 5.41; CE=26.3 me/100 g2	20	BE	214
2.26	3.23				10.4	Soil; cl; (allophane); pH 4.89; CE=35.0 me/100 g	20	BE	214
1.40		99.3	0.20	0.55	0.03	Ispra soil (C2 horizon); pH 5.1	22	BE	153
1.57	[4.36]	95.5	3.4	1.6	0.16	Idem (C4 horizon); pH 4.8	22	BE	153
2.25	3.91	91.8	6.4	1.8	1.87	Idem (A2 horizon); pH 4.8	22	BE	153
0.60	[3.42]				0.15	KB 1H soil (63–125 μm); SA(N_2)=4.9 m^2/g	20	LE	207
2.20	3.81				2.5	Lake sediment from The Netherlands	21	BE	530
[3.31]	4.7				4.1	Lake Ontario sediment trap material		FM	49
	4.1				50	Niagara River organic matter		FM	49
	3.0				58.0	Sanhedron soil humic acid; pH 6.5	24	SE	220
	2.3				48.7	Sanhedron soil fulvic acid; pH 6.5	24	SE	220
	2.0				54.2	Suwannee River humic acid; pH 6.5	24	SE	220
	2.0				53.8	Suwannee River fulvic acid: pH 6.5	24	SE	220
	3.7					Correlation $\log K_{oc}-\log K_{ow}$(95)			49
	2.77					Correlation $\log K_{oc}$–MCI			597
	3.28					Correlation $\log K_{oc}$–CRI			601
	2.88					Correlation $\log K_{oc}$–LSER			602
						1,2,4-Trichlorobenzene (-TCBz)			
1.98	[2.73]				18	Muck (<1 mm)	22	GP	517
0.48	[2.89]	95.5	3.2	1.3	0.39	Eustis soil (<1 mm); 0.01 N $CaCl_2$		MD	517
−0.14	[2.75]	97.1	2.3	0.6	0.13	Tampa aquifer; pH 8; 0.01 N $CaCl_2$		MD	521
−0.58	[1.95]	98	1	1	0.29	Borden soil; 0.01 N $CaCl_2$		MD	600
0.75	[3.27]	38.8	31.6	29.6	0.60* 0.30	Marlette soil (Bt horizon); pH 5.4; CE=14.6 me/100 g	20	BE	222
2.48	[3.91]				4.85* 3.71	Idem-HDTMA complex	20	BE	222
1.94	[3.64]				2.73* 1.9	Idem-DDTMA complex	20	BE	222
1.11	[3.04]				1.74*	Idem-NTMA complex	20	BE	222

Table 4. Sorption coefficients for halogenated benzenes—Continued

log K_d log K_f^0 ($1/n$)	log K_{oc}	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
1.61	[3.19]	56.6	22.0	21.4	1.18 5.18* 2.59	Marlette soil (A horizon); pH 6.4; CE=16.4 me/100 g	20	BE	222
2.47	[3.66]				10.0* 6.48	Idem-HDTMA complex	20	BE	222
2.04	[3.40]				7.43* 4.37	Idem-DDTMA complex	20	BE	222
[0.36]	3.32	4	10	86	0.11	Apison soil; pH 4.5; CE=76 me/100 g		BE	570
[−0.11]		11	21	68	0.06	Fullerton soil; pH 4.4; CE=64 me/100 g		BE	570
[1.03]	2.95	2	38	60	1.2	Dormont soil; pH 4.2; CE=129 me/100 g		BE	570
[0.98]	[2.94]	9	68	21	1.9* [1.1]	Woodburn soil; CE=14 me/100 g	20	BE	55
2.38	[3.16]				29* [16.8]	Peaty soil		BE	472
1.61		99.3	0.20	0.55	0.03	Ispra soil (C2 horizon); pH 5.1	22	BE	153
1.59		95.5	3.4	1.6	0.16	Idem (C4 horizon); pH 4.8	22	BE	153
2.35	4.02	91.8	6.4	1.8	1.87	Idem (A2 horizon); pH 4.8	22	BE	153
0.55	[3.37]				0.15	KB 1H soil (63 mm–125 μm); $SA(N_2)=4.9\ m^2/g$	20	LE	207
1.16	[3.30]				0.73	KS 1 soil (<125 μm); $SA(N_2)=4.4\ m^2/g$	20	LE	207
0.40					0.08	KB 1H soil (<125 μm); $SA(N_2)=3.2\ m^2/g$	20	LE	207
0.38					0.06	Kaolin; $SA(N_2)=12\ m^2/g$	20	LE	207
0.18					<0.01	γ-Al_2O_3; $SA(N_2)=120\ m^2/g$	20	LE	207
0.88					<0.01	SiO_2; $SA(N_2)=500\ m^2/g$	20	LE	207
[0.05]		92	5.9	2.1	0.09	Lincoln soil; fine sand; pH 6.4; CE=3.5 me/100 g	20	MD	541
0.41° (0.84)					0.03	Augusta subsurface soil (Spinks); median grain size=0.13 nm; $SA(N_2)=1.2\ m^2/g$		BE	54
0.69° (0.85)					0.16	Delta subsurface soil (Ottokee); median grain size=0.20 mm; $SA(N_2)=1.6\ m^2/g$		BE	54
0.98° (0.89)	[3.22]				0.58	Ann Arbor II subsurface soil (Brookstan); median grain size=0.16 mm; $SA(N_2)=4.2\ m^2/g$		BE	54
1.65° (0.77)					2.49	Wagner subsurface soil (Miami); median grain size=0.53 mm; $SA(N_2)=1.3\ m^2/g$		BE	54
1.72° (0.75)					1.24	Ypsilanti subsurface soil (Wasepi); median grain size=0.31 mm; $SA(N_2)=1.2\ m^2/g$		BE	54
2.04° (0.68)					1.29	Ann Arbor I subsurface soil (Brookston); median grain size=0.21 mm; $SA(N_2)=2.4\ m^2/g$		BE	54
2.22	2.65				37.8	Leaves	25	BE	611
1.28	1.68				39.8	Thatch	25	BE	611
2.42	[3.43]				17* [9.86]	Charles River sediment	24	GP	155
[3.31]	4.7				4.1	Lake Ontario sediment trap material		FM	49
	4.4				50	Niagara River organic matter		FM	49
	3.11				50.2	Aldrich humic acid; pH 8.0; 0.01 M $NaHCO_3$	22	ED	206
	3.32				50.2	Aldrich and Fluka humic acid		FH	206

Table 4. Sorption coefficients for halogenated benzenes—Continued

log K_d log K_f^0 (1/n)	log K_{oc}	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
	[3.27]				58.03	Prediction by limiting vapor sorption by soil humic acid	23	LSC	363
	2.71					C18 column; correlation log K_{oc}–(log $k'+\Delta^0\chi$)		RPLC	577
	2.71					C18 column; correlation log K_{oc}–(log k'+hydrogen bonding index)		RPLC	577
	3.6					Correlation log K_{oc}–log K_{ow}(96)			49
	2.83					Correlation log K_{oc}–log S			564
	2.86					Correlation log K_{oc}–MCI			578
	[3.00]					Correlation log K_{om}–MCI			591
	3.32					Correlation log K_{oc}–CRI			601
	2.94					Correlation log K_{oc}–LSER			602
						1,3,5-Trichlorobenzene (-TCBz)			
2.48	[3.26]				29* [16.8]	Peaty soil		BE	472
1.59		99.3	0.20	0.55	0.03	Ispra soil (C2 horizon); pH 5.1	22	BE	153
1.71	[4.51]	95.5	3.4	1.6	0.16	Idem (C4 horizon); pH 4.8	22	BE	153
2.46	4.13	91.8	6.4	1.8	1.87	Idem (A2 horizon); pH 4.8	22	BE	153
0.15	2.85	97.3	2.2	0.5	0.2	Forest soil; pH 5.6; CE=0.48 me/100 g		MD	344
2.36	3.96				2.5	Lake sediment from The Netherlands	21	BE	530
	5.1				4.1	Lake Ontario sediment trap material		FM	49
	4.2				50	Niagara River organic matter		FM	49
	3.8					Correlation log K_{oc}–log K_{ow}(96)			49
	2.85					Correlation log K_{oc}–MCI			578
	2.75					Correlation log K_{oc}–MCI			597
	3.35					Correlation log K_{oc}–CRI			601
	2.96					Correlation log K_{oc}–LSER			602
						1,2,3,4-Tetrachlorobenzene(-TeCBz)			
0.74	[3.15]	95.5	3.2	1.3	0.39	Eustis soil. 0.01 N $CaCl_2$		MD	522
1.67° (0.89)	3.52				1.42	Soil; cl; (kaolinite); pH 5.91; CE=12.4 me/100 g	20	BE	214
2.09° (1.00)	3.91				1.51	Soil; light c; (montmorillonite); pH 5.18; CE=13.0 me/100 g	20	BE	214
2.26° (0.87)	3.75				3.23	Soil; light c; (montmorillite) pH 5.26; CE=28.3 me/100 g	20	BE	214
2.50° (0.88)	3.48				7.91	Soil; sl; (allophane); pH 5.41; CE=26.3 me/100 g	20	BE	214
2.53° (1.00)	3.52				10.4	Soil; cl; (allophane); pH 4.89; CE=35.0 me/100 g	20	BE	214
1.56		99.3	0.20	0.55	0.03	Ispra soil (C2 horizon); pH 5.1	22	BE	153
1.73	[4.53]	95.5	3.4	1.6	0.16	Idem (C4 horizon); pH 4.8	22	BE	153
2.58	4.28	91.8	6.4	1.8	1.87	Idem (A2 horizon); pH 4.8	22	BE	153
[1.67]	[3.49]				2.64* [1.53]	Batcombe sil soil; pH 5.9; 0.01 M $CaCl_2$	20	BE	120
1.02	[3.84]				0.15	KB 1H soil (63–125 μm); SA(N_2)=4.9 m^2/g	20	LE	207
1.76	[3.19]				6.5* [3.77]	Iowa EPA-10 soil	22	GP	155
3.09	[4.10]				17* [9.86]	Charles River sediment; mixed particle size (<28–840 μm)	24	GP	155
3.01	[4.02]					Idem	40		155
2.84	[3.85]					Idem	55		155
3.18	[4.19]					Idem; particle size=96 μm	23		155
3.14	[4.15]					Idem; particle size=232 μm	28		155
2.62	[3.92]				8.8* [5.10]	North River sediment	23	GP	155

Table 4. Sorption coefficients for halogenated benzenes—Continued

log K_d log K_f^0 (1/n)	log K_{oc}	Sorbent composition (%)				Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
2.66	4.26				2.5	Lake sediment from The Netherlands	21	BE	530
[2.85]	4.26				3.86	Sediment (three phase model)		BE	493
	3.90					DOC from the same sediment (three phase model)			493
[3.61]	5.0				4.1	Lake Ontario sediment trap material		FM	49
	4.9				50	Niagara River organic matter		FM	49
	4.1					Correlation log K_{oc}–log K_{ow}(96)			49
	3.09					Correlation log K_{oc}–MCI			578
	3.00					Correlation log K_{oc}–MCI			597
	3.75					Correlation log K_{oc}–CRI			601
	3.35					Correlation log K_{oc}–LSER			602
1,2,3,5-Tetraclorobenzene (-TeCBz)									
1.43		99.3	0.20	0.55	0.03	Ispra soil (C2 horizon); pH 5.1	22	BE	153
1.66	[4.46]	95.5	3.4	1.6	0.16	Idem (C4 horizon); pH 4.8	22	BE	153
2.54	4.25	91.8	6.4	1.8	1.87	Idem (A2 horizon); pH 4.8	22	BE	153
	3.20					Correlation log K_{oc}–MCI			596
	3.08					Correlation log K_{oc}–MCI			578
	[3.22]					Correlation log K_{om}–MCI			591
	3.80					Correlation log K_{oc}–CRI			601
	3.35					Correlation log K_{oc}–LSER			602
1,2,4,5-Tetrachlorobenzene (-TeCBz)									
0.69					0.06	Kaolin; SA(N_2)=12 m^2/g	20	LE	207
0.34					<0.01	γ-Al_2O_3; SA(N_2)=120 m^2/g	20	LE	207
1.08					<0.01	SiO_2; SA(N_2)=500 m^2/g	20	LE	207
1.11	[3.93]				0.15	KB 1H soil (63–125 μm); SA(N_2)=4.9 m^2/g	20	LE	207
1.58	[3.72]				0.73	KS 1 soil (<125 μm); SA(N_2)=4.4 m^2/g	20	LE	207
0.79					0.08	KB 1H soil (<125 μm); SA(N_2)=3.2 m^2/g	20	LE	207
0.61	2.79				0.66	Mc Laurin sl soil; pH 4.43; 0.01 M $CaNO_3$		BE	606
1.48					0.021	Borden sandy aquifer material		BE	88
[3.71]	5.1				4.1	Lake Ontario sediment trap material		FM	49
	4.7				50	Niagara River organic matter		FM	49
	4.39					Correlation log K_{oc}–log K_{ow}(108)			88
	3.86					Correlation log K_{oc}–log K_{ow}(217)			88
	4.28					Correlation log K_{oc}–log K_{ow}(180)			88
	4.42					Correlation log K_{oc}–log K_{ow}(87)			88
	3.32					Correlation log K_{oc}–log K_{ow}(120)			88
	4.32					Correlation log K_{oc}–log K_{ow}(130)			88
	4.20					Correlation log K_{oc}–log K_{ow}(96)			88
	3.80					Correlation log K_{oc}–log K_{ow}(207)			88
	3.61					Correlation log K_{oc}–log K_{ow}(55)			88
	4.1					Correlation log K_{oc}–log K_{ow}(96)			49
	3.20					Correlation log K_{oc}–log S			564
	2.99					Correlation log K_{oc}–MCI			597
	3.80					Correlation log K_{oc}–CRI			601
	3.38					Correlation log K_{oc}–LSER			602
Pentachlorobenzene (PCBz)									
1.57		99.3	0.20	0.55	0.03	Ispra soil (C2 horizon); pH 5.1	22	BE	153
2.05	[5.30]	95.5	3.4	1.6	0.16	Idem (C4 horizon); pH 4.8	22	BE	153
2.79	4.49	91.8	6.4	1.8	1.87	Idem (A2 horizon); pH 4.8	22	BE	153
2.38	[3.81]				6.5* [3.77]	Iowa EPA 10 soil	25	GP	155
3.19	[4.49]				8.8* [5.10]	North River sediment	26	GP	155

Table 4. Sorption coefficients for halogenated benzenes—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
3.67	[4.38]				17* [9.86]	Charles River sediment	23	GP	155
3.08	4.68				2.5	Lake sediment from The Netherlands	21	BE	530
3.91	[5.42]		27.1	52.6	3.04	Ohio Riv. sed. (Ceredo, WV) (2.5 g/L); pH 6.90; equilibr. time=28 d		GP	156
3.85	[5.37]					Idem (3.5 g/L); equilibr. time=15 d		GP	156
3.34	[5.17]		55.4	37.1	1.48	Mississippi Riv. sed. (Mc Clure, IL) (7.5 g/L); pH 7.75; equilibr. time=28 d		GP	156
[3.91]	5.3				4.1	Lake Ontario sediment trap material		FM	49
	5.4				50	Niagara River organic matter		FM	49
	3.50					Correlation $\log K_{oc}$–MCI			596
	4.5					Correlation $\log K_{oc}$–$\log K_{ow}$(96)			49
	4.11					Correlation $\log K_{oc}$–$\log S$			564
	3.31					Correlation $\log K_{oc}$–MCI			578
	[3.46]					Correlation $\log K_{om}$–MCI			591
	4.18					Correlation $\log K_{oc}$–CRI			601
	3.81					Correlation $\log K_{oc}$–LSER			602
						Hexachlorobenzene (HCBz)			
0.91° (1.56)					2.24	Speyer soil 2.2(0.15–0.5 mm); pH 5.8	22	BE	181
0.58° (0.99)	2.70	12.9	64.3	19.6	0.76	Alfisol soil; pH 7.45	22	BE	181
[2.67]	[4.49]				2.64* [1.53]	Batcombe sil soil; pH 5.9; 0.01 M $CaCl_2$	20	BE	120
1.41	3.23				1.49	Captina sil soil; pH 4.97; 0.01 M $CaNO_3$		BE	606
2.55	4.73				0.66	Mc Laurin sl soil; pH 4.43; 0.01 M $CaNO_3$		BE	606
3.04	[6.00]		75.6	17.4	0.11	Loess soil (Turin, IA) (10 g/L); pH 8.34; equilibr. time=18 d		GP	156
1.96	4.66				0.2	Fine s soil; soil-dextran/water system		BE,MD	429
2.70	3.08				42	Dextran; soil-dextran/water system		BE,MD	429
2.21	4.91				0.2	Fine a soil; soil-humic acid/ water system		BE	429
3.38	4.98				2.5	Lake sediment from The Netherlands	21	BE	530
3.04	[5.87]		10.7	6.8	0.15	Missouri Riv. sed. (Onawa, IA) (32 g/L); pH 8.32; equilibr. time=18 d		GP	156
3.86	[5.55]		41.8	55.2	2.07	Missouri Riv. sed. (Stanton, ND) (5 g/L); pH 7.79; equilibr. time=20 d		GP	156
4.51	[6.02]		27.1	52.6	3.04	Ohio Riv. sed. (Ceredo, WV) (3 g/L); pH 6.90; equilibr. time=28 d		GP	156
4.45	[5.96]					Idem (2.5 g/L); equilibr. time=25 d		GP	156
3.42	[5.25]		55.4	37.1	1.48	Mississippi Riv. sed. (Mc Clure, IL); pH 7.75; equilibr. time=28 d		GP	156
3.54	[5.46]		13.9	18.6	1.21	Small stream sed. (Watkinsville, GA) (13 g/L); pH 6.35; equilibr. time=20 d		GP	156
3.42	[5.23]		31.1	37.1	1.52	Oconee Riv. susp. sed. (Athens, GA) (3.5 g/L); pH 6.47; equilibr. time=22 d		GP	156

Table 4. Sorption coefficients for halogenated benzenes—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%)				Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
[4.51]	5.9				4.1	Lake Ontario sediment trap material		FM	49
	5.5				50	Niagara River organic matter		FM	49
	5.98				48	Fluka humic acid; soil-humic acid/water system		BE	429
	5.65					Groundwater DOC		ED	429
	4.77					Cyanopropyl column	20–25	RPLC	579
	3.59					Soil; experimental (literature)			217
	5.1					Correlation $\log K_{oc}-\log K_{ow}(96)$			49
	3.53					Correlation $\log K_{oc}$–MCI			578
	4.45					Correlation $\log K_{oc}-\log S$			564
	[3.70]					Correlation $\log K_{om}$–MCI			591
	4.67					Correlation $\log K_{oc}$–CRI			601
	4.27					Correlation $\log K_{oc}$–LSER			602

Values in square parentheses have been calculated by the author.

*$\log K_{om}$ in column 2 and % OM content in column 6.

av average value.

Idem refers to the sorbent reported just above; only the data (texture, OC, temperature, method) which were changed are specified.

TABLE 5. Sorption coefficients for phenol and substituted phenols

log K_d log K_f^0 (1/*n*)	log K_{oc}	Sorbent composition (%)				Other sorbent and solution data: prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
						Phenol (pK_a=9.8, Ref. 675)			
−2.0– −1.27				100		Kaolinite; pH 5.6; SA 10 m^2/g; CE=2.0 cmol/kg		MD	469
[0.02]	[0.77]	29.1	14.3	56.6	30.6* [17.7]	Whittlesey soil; SA=197.0 m^2/g	20	BE	615
[−0.63]	[0.99]	84.1	8.1	7.8	4.15* [2.41]	Ashurst soil; SA=28.1 m^2/g	20	BE	615
[−0.75]	[0.97]	72.0	10.4	17.6	3.28* [1.90]	Kirton soil; SA=41.2 m^2/g	20	BE	615
[0.77]	[1.72]				2.51* [1.46]	Batcombe sil soil; pH 6.7; 0.01 M $CaCl_2$	20	BE	120
0.094° (0.79)					5.1* 2.68	Brookston cl soil; pH 5.7; CE=22.22 me/100 g; 0.0025 M $CaCl_2$	20	BE	335
−0.33	1.56			75	1.3	Eurosol-1; c; pH 5.1; 0.01 M $CaCl_2$		BE	583
0.12	1.56			22.6	3.7	Eurosol-2; sil; pH 7.4; 0.01 M $CaCl_2$		BE	583
−0.21	1.26			17.0	3.45	Eurosol-3; l; pH 5.2; 0.01 M $CaCl_2$		BE	583
−0.50	1.31			20.3	1.55	Eurosol-4; si; pH 6.5; 0.01 M $CaCl_2$		BE	583
0.49	1.52			6.0	9.25	Eurosol-5; ls; pH 3.2; 0.01 M $CaCl_2$		BE	583
[−1.22]	1.74	4	10	86	0.11	Apison soil; pH 4.5; CE=70 me/100 g		BE	570
[−0.37]		11	21	68	0.05	Fullerton soil; pH 4.4; CE=64 me/100 g		BE	570
[−1.08]	0.85	2	38	60	1.2	Dormont soil; pH 4.2; CE=129 me/100 g		BE	570
−0.24° (0.96)	[1.95]	33	55	12	1.1* [0.64]	Captina soil; SA=14 m^2/g; pH 5.4; CE=6 me/100 g; 0.01 M $CaCl_2$; phenol conc.=E-9 to E-2M	25	BE	489, 532
0.08° (0.76)		17	59	24	3.6* [2.09]	Palouse soil; SA=90 m^2/g; pH 5.4; CE=22 me/100 g; 0.01 M $CaCl_2$ phenol conc.=E-5 to E-2M	25	BE	489
−0.09° (1.00)	[1.59]					Idem; phenol conc.=E-9 to E-6M			
[2.47]	3.46				10.2	Lake Zoar surface sediment (<2 μm); pH 6.21–6.35		FE	100
[2.11]	3.49				4.2	Lake surface sediment (>2 μm); pH 6.21–6.35		FE	100
	1.35					Cyanopropyl column; pH 3	20–25	RPLC	579
	1.42					Humic acid-silica column	20–23	RPLC	587
	1.00					Salicylic acid-silica column	20–23	RPLC	587
	1.24					8-Hydroxyquinoline-silica column	20–23	RPLC	587
	1.59					C18 column; correlation log K_{oc}–(log $k'+\Delta^0\chi$)		RPLC	577
	1.67					C18 column; correlation log K_{oc}–(log k'+hydrogen bonding index)		RPLC	577
	1.43					Soil; experimental (literature)			217
	2.17					Correlation log K_{oc}–log K_{ow}			618
	0.86					Correlation log K_{oc}–log $S(180)$			335
	0.95					Correlation log K_{oc}–log S			564
	1.86					Correlation log K_{oc}–MCI			578
	2.43					Correlation log K_{oc}–MCI			598
	1.85					Correlation log K_{oc}–CRI			601
	1.50					Correlation log K_{oc}–LSER			602
						2-Chlorophenol(-MCP; pK_a=8.5, Ref. 675)			
0.562°					5.1*	Brookston soil; cl; pH 5.7;	20	BE	335

TABLE 5. Sorption coefficients for phenol and substituted phenols—Continued

log K_d log K_f^0 $(1/n)$	log K_{oc}	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
(0.80)					2.68	CE=22.22 me/100 g; 0.0025 M $CaCl_2$			
[2.70]	3.69				10.2	Lake Zoar surface sediment (<2 μm); untreated; pH 6.21–6.35		FE	100
[2.50]	3.98				3.3	Idem; treated (H_2O_2); pH 6.21–6.35		FE	100
[2.22]	3.60				4.2	Lake Zoar surface sediment (>2 μm); untreated; pH 6.21–6.35		FE	100
[2.21]	4.37				0.7	Idem; treated (H_2O_2); pH 6.21–6.35		FE	100
	1.21					Correlation log K_{oc}–log S(180)			335
	2.65					Correlation log K_{oc}–MCI			598
	2.36					Correlation log K_{oc}–CRI			601
						3-Chlorophenol (-MCP; pK_a=9.37, Ref. 676)			
0.609°					5.1*	Brookston soil; cl; pH 5.7;	20	BE	335
(0.83)					2.68	CE=22.22 me/100 g; 0.0025 M $CaCl_2$			
0.3° (0.8)				1.2	1.7	Soil (Kootwijk); humic s; pH 3.4; 0.01 M $CaCl_2$	10	BE	111
0.6° (0.8)				1.5	2.2	Soil (Rolde); humic s; pH 4.9; 0.01 M $CaCl_2$	10	BE	111
0.9° (0.8)				3.7	3.2	Soil (Holten); humic-rich s; pH 4.7; 0.01 M $CaCl_2$	10	BE	111
1.6° (0.7)					29.8	Soil (Schipluiden); peat; pH 4.6; 0.01 M $CaCl_2$	10	BE	111
−0.1° (0.6)				8.7	0.9	Soil (Maasdijk); light l; pH 7.5; 0.01 M $CaCl_2$	10	BE	111
0.1° (0.7)				18	1.7	Soil (Opijnen); heavy l; pH 7.1; 0.01 M $CaCl_2$	10	BE	111
0.6° (0.8)					2.7	Humus "soil" (syntetic); pH 3.7; 0.01 M $CaCl_2$	10	BE	111
0.5° (0.8)					2.8	Humus "soil" (syntetic); pH 6.0; 0.01 M $CaCl_2$	10	BE	111
0.6° (1.0)	[2.1]				2.8	Humus "soil" (syntetic); pH 7.3; 0.01 M $CaCl_2$	10	BE	111
	1.24					Correlation log K_{oc}–log S(180)			335
	2.64					Correlation log K_{oc}–MCI			598
	2.37					Correlation log K_{oc}–CRI			601
						4-Chlorophenol (-MCP; pK_a=9.37, Ref. 677)			
0.903°					5.1*	Brookston soil; cl; pH 5.7;	20	BE	335
(0.70)					2.68	CE=22.22 me/100 g; 0.0025 M $CaCl_2$			
−1.15	[1.73]	97.1	2.3	0.6	0.13	Tampa aquifer; pH 2; 0.01 N $CaCl_2$		MD	521
0.49	2.38			75	1.3	Eurosol-1; c; pH 5.1; 0.01 M $CaCl_2$		BE	583
1.25	2.69			22.6	3.7	Eurosol-2; sil; pH 7.4; 0.01 M $CaCl_2$		BE	583
0.42	2.03			17.0	3.45	Eurosol-3; l; pH 5.2; 0.01 M $CaCl_2$		BE	583
0.41	2.22			20.3	1.55	Eurosol-4; si; pH 6.5; 0.01 M $CaCl_2$		BE	583
1.30	2.33			6.0	9.25	Eurosol-5; ls; pH 3.2; 0.01 M $CaCl_2$		BE	583
−0.72	[1.69]	96.4	1.8	1.8	0.39	Eustis soil; pH 6.8; CE=3.37 me/100 g; 0.01 N KCl		BE	460
	1.23					Correlation log K_{oc}–log S(180)			335
	2.35					Correlation log K_{oc}–CRI			601
						4-Bromophenol (MBP)			
[1.57]	[2.41]				2.51*	Batcombe sil soil; pH 6.7;	20	BE	120

TABLE 5. Sorption coefficients for phenol and substituted phenols—Continued

log K_d log K_f^0 (1/n)	log K_{oc}	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
					[1.46]	0.01 M $CaCl_2$			
	2.08					Correlation log K_{oc}–MCI			578
	2.53					Correlation log K_{oc}–MCI			597
	2.64					Correlation log K_{oc}–MCI			598
	2.22					Correlation log K_{oc}–LSER			602
2,3-Dichlorophenol (-DCP; pK_a=7.61, Ref. 337)									
1.18° (0.79)		45.12	28.08	26.80	4.74* [2.75]	Brookston soil (aerobic); pH 5.5; CE=22.74 me/100 g; 0.0025 M $CaCl_2$	20	BE	531
1.09° (0.83)						Idem (anaerobic)			531
1.22° (0.78)						Idem (autoclaved)			531
1.32u	2.35u				9.4	Lake sediment (<63 μm); pH 6.5–8.5; SA(N_2)=3.8 m^2/g; $CaCO_3/CO_2$ buffer	20	BE	337
1.08u	2.66u				2.6	River sediment (<63 μm); pH 6.5–8.5; SA(N_2)=4.8 m^2/g; $CaCO_3/CO_2$	20	BE	337
0.70u	2.77u				0.84	Aquifer material (<63 μm); pH 6.5–8.5; SA(N_2)=6.4 m^2/g; $CaCO_3/CO_2$ buffer	20	BE	337
	2.77					Correlation log K_{oc}–MCI			597
	2.94					Correlation log K_{oc}–log K_{ow}(108)			597
	3.08					Correlation log K_{oc}–log K_{ow}(217)			597
	2.28					Correlation log K_{oc}–log K_{ow}(120)			597
	2.83					Correlation log K_{oc}–log K_{ow}(180)			597
	2.05					Correlation log K_{oc}–log K_{ow}(55)			597
	2.86					Correlation log K_{oc}–CRI			601
2,4-Dichlorophenol (-DCP; pK_a=7.85, Ref. 337)									
1.26° (0.73)		45.12	28.08	26.80	4.74* [2.75]	Brookston soil (aerobic); pH 5.5; CE=22.74 me/100 g; 0.0025 M $CaCl_2$	20	BE	531
1.17° (0.79)						Idem (anaerobic)			531
1.29° (0.76)						Idem (autoclaved)			531
0.82	2.70			75	1.3	Eurosol-1; c; pH 5.1; 0.01 M $CaCl_2$		BE	583
0.80	2.23			22.6	3.7	Eurosol-2; sil; pH 7.4; 0.01 M $CaCl_2$		BE	583
0.99	2.45			17.0	3.45	Eurosol-3; l; pH 5.2; 0.01 M $CaCl_2$		BE	583
0.54	2.35			20.3	1.55	Eurosol-4; si; pH 6.5; 0.01 M $CaCl_2$		BE	583
1.91	2.95			6.0	9.25	Eurosol-5; ls; pH 3.2; 0.01 M $CaCl_2$		BE	583
−0.15	[2.25]	96.4	1.8	1.8	0.39	Eustis soil; CE=3.37 me/100 g pH 6.1; 0.01 N KCl		BE	460
−0.21	[2.20]					Idem; pH 5.5; 0.015 N $CaCl_2$			460
1.26° (0.67)					5.1* 2.68	Brookston cl soil; pH 5.7; CE=22.22 me/100 g; 0.0025 M $CaCl_2$	20	BE	335
0.14	2.84	97.3	2.2	0.5	0.2	Forest soil; pH 5.6; CE=0.48 me/100 g		MD	344
−0.31	[2.39]					Idem		BE	344
1.05	[2.71]	65.2	25.6	9.2	2.2	Agricultural soil; pH 7.4; CE=9.0 me/100 g		BE	344
1.45	[2.88]	69.5	20.5	10.1	3.7	Forest soil; pH 4.2; CE=2.9 me/100 g		BE	344

TABLE 5. Sorption coefficients for phenol and substituted phenols—Continued

log K_d log K_f^0 $(1/n)$	log K_{oc}	Sorbent composition (%)				Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
−1.00	[1.89]	97.1	2.3	0.6	0.13	Tampa aquifer pH 2; 0.01 N $CaCl_2$		MD	521
[2.61]	3.60				10.2	Lake Zoar surface sediment (<2 μm); untreated; pH 6.21–6.35		FE	100
[2.23]	3.71				3.3	Idem; treated (H_2O_2);			100
[2.12]	3.50				4.2	Lake Zoar surface sediment (>2 μm); untreated; pH 6.21–6.35		FE	100
[1.82]	3.98				0.7	Idem; treated (H_2O_2)			100
1.40u	2.42u				9.4	Lake sediment (<63 μm); pH 6.5–8.5; SA(N_2)=3.8 m^2/g; $CaCO_3/CO_2$ buffer	20	BE	337
1.23u	2.82u				2.6	River sediment (<63 μm); pH 6.5–8.5; SA(N_2)=4.8 m^2/g; $CaCO_3/CO_2$ buffer	20	BE	337
0.78u	2.85u				0.84	Aquifer material (<63 μm); pH 6.5–8.5; SA(N_2)=6.4 m^2/g; $CaCO_3/CO_2$ buffer	20	BE	337
	2.47					C18 column; correlation log K_{oc}–(log $k'+\Delta^0\chi$)		RPLC	577
	2.53					C18 column; correlation log K_{oc}–(log k'+hydrogen bonding index)		RPLC	577
	1.76					Correlation log K_{oc}–log $S(180)$			335
	2.29					Correlation log K_{oc}–MCI			578
	2.76					Correlation log K_{oc}–MCI			597
	2.89					Correlation log K_{oc}–CRI			601
3,4-Dichlorophenol (-DCP; pK_a=8.62, Ref. 676)									
1.1° (0.9)	[2.9]			1.2	1.7	Soil (Kootwijk); humic s; pH 3.4; 0.01 M $CaCl_2$	10	BE	111
1.4° (0.9)	[3.1]			1.5	2.2	Soil (Rolde); humic s; pH 4.9; 0.01 M $CaCl_2$	10	BE	111
1.3° (0.8)				3.7	3.2	Soil (Holten); humic-rich s; pH 4.7; 0.01 M $CaCl_2$	10	BE	111
1.6° (0.7)					29.8	Soil (Schipluiden); peat; pH 4.6; 0.01 M $CaCl_2$	10	BE	111
0.5° (0.8)				8.7	0.9	Soil (Maasdijk); light 1; pH 7.5; 0.01 M $CaCl_2$	10	BE	111
0.6° (0.7)				18	1.7	Soil (Opijnen); heavy 1; pH 7.1; 0.01 M $CaCl_2$	10	BE	111
1.4° (0.9)	[3.0]				2.7	Humus ''soil'' (syntetic); pH 3.7; 0.01 M $CaCl_2$	10	BE	111
1.5° (1.0)	[3.1]				2.8	Humus ''soil'' (syntetic); pH 6.0; 0.01 M $CaCl_2$	10	BE	111
1.2° (1.0)	[2.8]				2.8	Humus ''soil'' (syntetic); pH 7.3; 0.01 M $CaCl_2$	10	BE	111
	2.86					Correlation log K_{oc}–MCI			598
	2.88					Correlation log K_{oc}–CRI			601
2,4,6-Trichlorophenol (-TCP; pK_a=6.15, Ref. 337)									
−0.62	[2.27]	97.1	2.3	0.6	0.13	Tampa aquifer; pH 2; 0.01 N $CaCl_2$		MD	521
0.05	2.75	97.3	2.2	0.5	0.2	Forest soil; pH 5.6; CE=0.48 me/100 g		MD	344
−0.14	[2.56]	97.3	2.2	0.5	0.2	Idem		BE	344
0.30	1.96	65.2	25.6	9.2	2.2	Agricultural soil; pH 7.4; CE=9.0 me/100 g		MD	344
0.38	[2.04]	65.2	25.6	9.2	2.2	Idem		BE	344
1.86	[3.29]	69.5	20.5	10.1	3.7	Forest soil; pH 4.2; CE=2.9 me/100 g		BE	344
	3.34°av (0.78)				1.7, 5.2	2 soils; pH 6		BE BE	341 341
	2.79°av (0.78)					Idem; pH 7			341

TABLE 5. Sorption coefficients for phenol and substituted phenols—Continued

log K_d log K_f^0 $(1/n)$	log K_{oc}	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
	2.23°av (0.78)					Idem; pH 7.7			341
	3.56°u (0.78)					Idem; calculated value			341
0.95u	3.03u				0.84	Aquifer material (<63 μm); pH 6.5–8.5; SA(N_2)=6.4 m^2/g; $CaCO_3/CO_2$ buffer	20	BE	337
1.89u	2.92u				9.4	Lake sediment (<63 μm); pH 6.5–8.5; SA(N_2)=3.8 m^2/g; $CaCO_3/CO_2$ buffer	20	BE	337
1.53u	3.12u				2.6	River sediment (<63 μm); pH 6.5–8.5; SA(N_2)=4.8 m^2/g; $CaCO_3/CO_2$ buffer	20	BE	337
	2.50					Correlation log K_{oc}–MCI			578
	2.99					Correlation log K_{oc}–MCI			597
	3.39					Correlation log K_{oc}–CRI			601
2,4,5-Trichlorophenol (-TCP; **pK_a=6.94**, Ref. 337)									
1.66° (0.71)					5.1* 2.68	Brookston soil; cl; pH 5.7; CE=22.22 me/100 g; 0.0025 M $CaCl_2$	20	BE	335
1.5° (0.9)	[3.3]			1.2	1.7	Soil (Kootwijk); humic s; pH 3.4; 0.01 M $CaCl_2$	10	BE	111
1.7° (0.9)	[3.4]			1.5	2.2	Soil (Rolde); humic s; pH 4.9; 0.01 M $CaCl_2$	10	BE	111
1.7° (0.8)				3.7	3.2	Soil (Holten); humic-rich s; pH 4.7; 0.01 M $CaCl_2$	10	BE	111
2.5° (0.8)					29.8	Soil (Schipluiden); peat; pH 4.6; 0.01 M $CaCl_2$	10	BE	111
0.5° (0.8)				8.7	0.9	Soil (Maasdijk); light l; pH 7.5; 0.01 M $CaCl_2$	10	BE	111
0.9° (0.8)				18	1.7	Soil (Opijnen); heavy l; pH 7.1; 0.01 M $CaCl_2$	10	BE	111
1.7° (0.9)	[3.3]				2.7	Humus "soil" (syntetic); pH 3.7; 0.01 M $CaCl_2$	10	BE	111
1.6° (0.9)	[3.2]				2.8	Humus "soil" (syntetic); pH 6.0; 0.01 M $CaCl_2$	10	BE	111
1.2° (1.0)	[2.8]				2.8	Humus "soil" (syntetic); pH 7.3; 0.01 M $CaCl_2$	10	BE	111
0.27	[2.68]	96.4	1.8	1.8	0.39	Eustis soil; CE=3.37 me/100 g; pH 5.9; 0.01 N KCl		BE	460
−0.85	[1.55]					Idem; pH>10; 0.0155 N $CaCl_2$		BE	460
1.30u	3.38u				0.84	Aquifer material (<63 μm); pH 6.5–8.5; SA(N_2)=6.4 m^2/g; $CaCO_3/CO_2$ buffer	20	BE	337
2.22u	3.25u				9.4	Lake sediment (<63 μm); pH 6.5–8.5; SA(N_2)=3.8 m^2/g; $CaCO_3/CO_2$ buffer	20	BE	337
1.87u	3.45u				2.6	River sediment (<63 μm); pH 6.5–8.5; SA(N_2)=4.8 m^2/g; $CaCO_3/CO_2$ buffer	20	BE	337
	2.01					Correlation log K_{oc}–log S(180)			335
	2.99					Correlation log K_{oc}–MCI			597
	3.37					Correlation log K_{oc}–CRI			601
3,4,5-Trichlorophenol (-TCP; **pK_a=7.73**, Ref. 337)									
2.44u	3.47u				9.4	Lake sediment (<63 μm); pH 6.5–8.5; SA(N_2)=3.8 m^2/g; $CaCO_3/CO_2$ buffer	20	BE	337
2.06u	3.64u				2.6	River sediment (<63 μm); pH 6.5–8.5; SA(N_2)=4.8 m^2/g; $CaCO_3/CO_2$ buffer	20	BE	337

TABLE 5. Sorption coefficients for phenol and substituted phenols—Continued

log K_d log K_f^0 (1/*n*)	log K_{oc}	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
1.49u	3.57u				0.84	Aquifer material (<63 μm); pH 6.5–8.5; SA(N_2)=6.4 m^2/g; $CaCO_3/CO_2$ buffer	20	BE	337
	2.99					Correlation log K_{oc}–MCI			597
	3.36					Correlation log K_{oc}–CRI			601
2,3,4,5-Tetrachlorophenol (-TeCP; pK_a=6.35, Ref. 337)									
−0.03	[2.86]u	97.1	2.3	0.6	0.13	Tampa aquifer; pH 2; 0.01 N $CaCl_2$		MD	521
0.62	[3.03]	96.4	1.8	1.8	0.39	Eustis soil; CE=3.37 me/100 g; pH 6.3; 0.01 N KCl		BE	460
−0.58	[1.82]d					Idem; pH>10; 0.0155 N $CaCl_2$		BE	460
2.02u	4.10u				0.84	Aquifer material (<63 μm); pH 6.5–8.5; SA(N_2)=6.4 m^2/g; $CaCO_3/CO_2$ buffer	20	BE	337
3.09u	4.12u				9.4	Lake sediment (<63 μm); pH 6.5–8.5; SA(N_2)=3.8 m^2/g; $CaCO_3/CO_2$ buffer	20	BE	337
2.56u	4.14u				2.6	River sediment (<63 μm); pH 6.5–8.5; SA(N_2)=4.8 m^2/g; $CaCO_3/CO_2$ buffer	20	BE	337
	3.32					Correlation log K_{oc}–MCI			597
	3.82					Correlation log K_{oc}–CRI			601
2,3,4,6-Tetrachlorophenol (-TeCP; pK_a=5.40, Ref. 337)									
0.18	2.88	97.3	2.2	0.5	0.2	Forest soil; pH 5.6; CE=0.48 me/100 g		MD	344
0.12	[2.82]	97.3	2.2	0.5	0.2	Idem		BE	344
0.53	2.19	65.2	25.6	9.2	2.2	Agricultural soil; pH 7.4; CE=9.0 me/100 g		MD	344
0.60	[2.26]	65.2	25.6	9.2	2.2	Idem		BE	344
2.37	[3.80]	69.5	20.5	10.1	3.7	Forest soil; pH 4.2; CE=2.9 me/100 g		BE	344
1.9° (1.0)	[3.7]			1.2	1.7	Soil (Kootwijk); humic s; pH 3.4; 0.01 M $CaCl_2$	10	BE	111
1.7° (0.9)	[3.4]			1.5	2.2	Soil (Rolde); humic s; pH 4.9; 0.01 M $CaCl_2$	10	BE	111
2.4° (1.0)	[3.9]			3.7	3.2	Soil (Holten); humic-rich s; pH 4.7; 0.01 M $CaCl_2$	10	BE	111
2.5° (0.8)					29.8	Soil (Schipluiden); peat; pH 4.6; 0.01 M $CaCl_2$	10	BE	111
0.1° (0.9)	[2.2]			8.7	0.9	Soil (Maasdijk); light l; pH 7.5; 0.01 M $CaCl_2$	10	BE	111
	2.45d					Idem; calculated value			111
0.4° (0.8)				18	1.7	Soil (Opijnen); heavy l; pH 7.1; 0.01 M $CaCl_2$	10	BE	111
	2.70d					Idem; calculated value			111
0.9° (0.6)					2.7	Humus "soil" (syntetic); pH 3.7; 0.01 M $CaCl_2$	10	BE	111
1.4° (0.9)	[3.0]				2.8	Humus "soil" (syntetic); pH 6.0; 0.01 M $CaCl_2$	10	BE	111
0.1° (0.7)					2.8	Humus "soil" (syntetic); pH 7.3; 0.01 M $CaCl_2$	10	BE	111
1.72u	3.79u				0.84	Aquifer material; estimated by a C18 column at pH~2		RPLC	337
2.75u	3.78u				9.4	Lake sediment; estimated by a C18 column at pH~2		RPLC	337
2.30u	3.89u				2.6	River sediment; estimated by a C18 column at pH~2		RPLC	337
	3.90u					Correlation log K_{oc}–log K_{ow}			111
	2.72					Correlation log K_{oc}–MCI			578
	3.32					Correlation log K_{oc}–MCI			597
	4.21					Correlation log K_{oc}–log K_{ow}(108)			597

TABLE 5. Sorption coefficients for phenol and substituted phenols—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%)				Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
	3.77					Correlation $\log K_{oc}-\log K_{ow}(217)$			597
	2.94					Correlation $\log K_{ow}-\log K_{ow}(120)$			597
	4.11					Correlation $\log K_{oc}-\log K_{ow}(180)$			597
	3.2					Correlation $\log K_{oc}-\log K_{ow}(55)$			597
	3.83					Correlation $\log K_{oc}-$CRI			601
						Pentachlorophenol (PCP; pK_a=4.74, Ref. 676)			
−0.35	[2.06]	96.4	1.8	1.8	0.39	Eustis soil; CE=3.37 me/100 g; pH>10; 0.0038 N $CaCl_2$		BE	460
−0.09	[2.32]					Idem; 0.0155 N $CaCl_2$			460
1.94	[4.40]					Idem; pH<2; K_d value extrapolated at $f_c=0$ (methanol/water solutions)		BE, MD	460
0.26	2.96	97.3	2.2	0.5	0.2	Forest soil; pH 5.6; CE=0.48 me/100 g		MD	344
0.32	[3.02]					Idem		BE	344
1.08	[2.74]	65.2	25.6	9.2	2.2	Agricultural soil; pH 7.4; CE=9.0 me/100 g		BE	344
2.27	[3.70]	69.5	20.5	10.1	3.7	Forest soil; pH 4.2; CE=2.9 me/100 g		BE	344
1.55	[3.96]	96.4	1.8	1.8	0.39	Eustis (1) soil; pH<3; $\mu=0.0015$ ($CaCl_2$)	22–25	BE	339
1.55	[3.96]					Idem; pH<3; $\mu=0.015$			339
1.59	[4.00]					Idem; pH<3; $\mu=0.15$			339
1.66	[4.07]					Idem; pH<3; $\mu=1.5$			339
0.10	[2.51]					Idem; pH>7; $\mu=0.01$			339
0.31	[2.72]					Idem; pH>7; $\mu=0.08$			339
0.45	[2.86]					Idem; pH>7; $\mu=0.15$			339
0.88	[3.28]					Idem; pH>7; $\mu=1.4$			339
1.21	[3.32]	91.6	4.2	4.2	0.78	Eustis (2) soil; pH 5.3; $\mu=0.00315$ ($CaCl_2$)	22–25	BE	339
1.37	[3.48]					Idem; pH 5.08; $\mu=0.015$			339
1.57	[3.68]					Idem; pH 4.83; $\mu=0.145$			339
1.31	[2.78]	29.6	40.9	29.5	3.41	Webster (1) soil; pH 7.5; $\mu=0.00315$ ($CaCl_2$)	22–25	BE	339
1.46	[2.92]					Idem; pH 7.3; $\mu=0.015$			339
1.72	[3.19]					Idem; pH 6.86; $\mu=0.145$			339
2.04	[3.51]					Idem; pH 6.37, $\mu=1.49$			339
−0.19	[2.46]	88.6	9.4	2.0	0.22	Lincoln soil; pH 6.84; $\mu=0.00015$ ($CaCl_2$)	22–25	BE	339
0.16	[2.82]					Idem; pH 6.69; $\mu=0.0132$			339
0.29	[2.95]					Idem; pH 6.65; $\mu=0.015$			339
0.38	[3.04]					Idem; pH 6.43; $\mu=0.1352$			339
0.80	[3.46]					Idem; pH 5.65; $\mu=1.575$			339
1.57	3.88	99.9	0.1 (si+c)		0.5	Sandy soil; pH 5.2; DOC<0.1 mg/L; $PCP_{equil.}<0.4$ nmol/mL	21	BE	106
1.59	3.89					Idem; DOC=15 mg/L			106
1.63	3.73	99.9	0.1 (si+c)		0.8	Sandy soil; pH 5.4; DOC<0.1 mg/L; $PCP_{equil.}<3$ nmol/mL	21	BE	106
1.74	3.84					Idem; DOC=15 mg/mL			106
1.08	3.17	99.9	0.1 (si+c)		0.8	Sandy soil; pH 6.1; DOC<0.1 mg/L; $PCP_{equil.}<3$ nmol/mL	21	BE	106
1.22	3.32					Idem; DOC=15 mg/L	21	BE	106
	4.44u					Calculated in the DOM poor fraction; $\mu=0.02$; pH 5.4			106
	2.48d					Idem; pH 6.1			106
1.9° (0.9)	[3.7]			1.2	1.7	Soil (Kootwijk); humic s; pH 3.4; 0.01 M $CaCl_2$	10	BE	111
1.9° (0.9)	[3.6]			1.5	2.2	Soil (Rolde); humic s; pH 4.9; 0.01 M $CaCl_2$	10	BE	111
2.6°	[4.1]			3.7	3.2	Soil (Holten); humic-rich s;	10	BE	111

TABLE 5. Sorption coefficients for phenol and substituted phenols—Continued

log K_d log K_f^0 (1/n)	log K_{oc}	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
(1.0)						pH 4.7; 0.01 M $CaCl_2$			
2.7° (0.8)					29.8	Soil (Schipluiden); peat; pH 4.6; 0.01 M $CaCl_2$	10	BE	111
0.8° (0.9)	[2.9]			8.7	0.9	Soil (Maasdijk); light 1; pH 7.5; 0.01 M $CaCl_2$	10	BE	111
	3.10d					Idem; calculated value			111
0.9° (0.8)				18	1.7	Soil (Opijnen); heavy 1; pH 7.1; 0.01 M $CaCl_2$	10	BE	111
	3.26d					Idem; calculated value			111
1.4° (0.7)					2.7	Humus "soil" (syntetic); pH 3.7; 0.01 M $CaCl_2$	10	BE	111
1.4° (0.8)					2.8	Humus "soil" (syntetic); pH 6.0; 0.01 M $CaCl_2$	10	BE	111
0.8° (1.0)	[2.4]				2.8	Humus "soil" (syntetic); pH 7.3; 0.01 M $CaCl_2$	10	BE	111
−0.70° (0.76)					0.12	Bluepoint soil; pH 7.8	25	BE	338
0.68° (0.94)	3.06				0.42	Idem+municipal sewage sludge (MSS) (45 Mg/ha); pH 7.4			338
	5.71u					Idem; calculated value			338
0.85 (0.89)	3.03				0.65	Glendale soil; pH 7.3	25	BE	338
	5.58u					Idem; calculated value			338
1.15 (0.95)	3.17				0.95	Idem+MSS (45 Mg/ha); pH 7.1			338
	5.52u					Idem; calculated value			338
1.40° (0.93)	3.35				1.10	Norfolk soil; pH 4.3			338
	3.49u					Idem; calculated value			338
1.56° (0.96)	3.41				1.40	Idem+MSS (45 Mg/ha); pH 4.4			338
	3.57u					Idem; calculated value			338
0.20° (0.83)					1.10	Norfolk limed soil; pH 6.9	25	BE	338
0.64° (0.89)	2.50				1.40	Idem+MSS (45 Mg/ha); pH 6.9			338
	4.65u					Idem; calculated value			338
0.56	[3.45]	97.1	2.3	0.6	0.13	Tampa aquifer; pH 2; 0.01 N $CaCl_2$		MD	521
3.56u	4.59u				9.4	Lake sediment; estimated by a C18 column at pH~2		RPLC	337
2.97u	4.55u				2.6	River sediment; estimated by a C18 column at pH~2		RPLC	337
2.30u	4.38u				0.84	Aquifer material; estimated by a C18 column at pH~2		RPLC	337
	3.67				58.1	Humic acid from Arno River sediments; pH 5.0	20	ED	425
	3.45				58.1	Idem; pH 6.5	20	ED	425
	3.90				64.1	Humic acid from Tyrrenhian Sea sediments; pH 5.0	20	ED	425
	3.53					Idem; pH 6.5	20	ED	425
	3.28					Idem; pH 8.0	20	ED	425
	3.15				53.3	Humic acid from Arno River water; pH 5.0	20	ED	425
	4.04					Cyanopropyl column; pH 3	20–25	RPLC	579
	2.95					Soil; experimental (literature)			217
	4.40u					Correlation log K_{oc}−log K_{ow}			111
	3.00					Correlation log K_{oc}−log S			564
	2.95					Correlation log K_{oc}−MCI			578
	3.46					Correlation log K_{oc}−MCI			597
	4.27					Correlation log K_{oc}−CRI			601

TABLE 5. Sorption coefficients for phenol and substituted phenols—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%)				Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
						2-nitrophenol (-NP; log pK$_a$=7.21, Ref. 678)			
0.54	2.42			75	1.3	Eurosol-1; c; pH 5.1; 0.01 M $CaCl_2$		BE	583
0.08	1.51			22.6	3.7	Eurosol-2; sil; pH 7.4; 0.01 M $CaCl_2$		BE	583
0.39	1.85			17.0	3.45	Eurosol-3; 1; pH 5.2; 0.01 M $CaCl_2$		BE	583
−0.05	1.76			20.3	1.55	Eurosol-4; si; pH 6.5; 0.01 M $CaCl_2$		BE	583
1.30	2.33			6.0	9.25	Eurosol-5; 1s; pH 3.2; 0.01 M $CaCl_2$		BE	583
0.725° (0.89)	[2.30]				5.1* 2.68	Brookston cl soil; pH 5.7; CE=22.22 me/100 g; 0.0025 M $CaCl_2$	20	BE	335
	1.99					Correlation $\log K_{oc}-\log S$(179)			335
						3-nitrophenol (-NP)			
0.728° (0.73)					5.1* 2.68	Brookston soil; cl; pH 5.7; CE=22.22 me/100 g; 0.0025 M $CaCl_2$	20	BE	335
	1.44					Correlation $\log K_{oc}-\log S$(179)			335
						4-nitrophenol (-NP; pK$_a$=7.15, Ref. 678)			
0.769° (0.72)					5.1* 2.684	Brookston soil; cl; pH 5.7; CE=22.22 me/100 g; 0.0025 M $CaCl_2$	20	BE	335
0.19° (0.93)	2.04		6	3	1.41	Gribskov soil; A hor.; pH 3.23; CE=4.8 me/100 g; 0.01 M $CaCl_2$	20	BE	131
0.43° (0.91)	2.00		4	7	2.58	Idem; B hor.; pH 3.59; CE=9.6 me/100 g; 0.01 M $CaCl_2$			131
0.01° (0.86)	1.75		3	5	1.82	Idem; C hor.; pH 4.07; CE=7.0 me/100 g; 0.01 M $CaCl_2$			131
0.52° (0.91)	1.81		5	4	5.11	Strodam soil; AB hor.; pH 3.88; CE=13.0 me/100 g; 0.01 M $CaCl_2$	20	BE	131
−0.40° (0.99)	2.45		3	3	0.09	Idem; C hor.; pH 4.95; CE=1.6 me/100 g; 0.01 M $CaCl_2$			131
−0.80° (0.73)			1	2	0.15	Tisvilde soil; C hor.; pH 4.21; CE=1.3 me/100 g; 0.01 M $CaCl_2$	20	BE	131
0.31° (0.91)	2.11		18	12	1.64	Roskilde soil; agric.; pH 5.40; CE=14.0 me/100 g; 0.01 M $CaCl_2$	20	BE	131
−0.49° (0.96)			4	18	0.06	Esrum soil; subsurf.; pH 4.71; CE=9.1 me/100 g; 0.01 M $CaCl_2$	20	BE	131
−0.92° (0.79)			7	3	0.05	Tirstrup soil; subsurf.; pH 6.14; CE=1.4 me/100 g; 0.01 M $CaCl_2$	20	BE	131
−0.17° (0.99)	2.72		34	41	0.13	Bjodstrup soil; subsurf; pH 7.64; CE=40.5 me/100 g; 0.01 M $CaCl_2$	20	BE	131
	2.18					Cyanopropyl column; pH 3	20–25	RPLC	579
	2.16					C18 column; correlation $\log K_{oc}-(\log k'+\Delta^0\chi)$		RPLC	577
	2.07					C18 column; correlation $\log K_{oc}-$(log k'+hydrogen bonding index)		RPLC	577
	1.37					Correlation $\log K_{oc}-\log S$(180)			335
	2.49					Correlation $\log K_{oc}-$MCI			598

Values in square parentheses have been calculated by the author.

*% OM content.

av average value.

d: Totally dissociated compound calculated following the procedure in Sec. 4.2.

u: Totally undissociated compound calculated following the procedure in Sec. 4.2.

Idem refers to the sorbent reported just above; only the data (texture, OC, temperature, method) which were changed are specified.

TABLE 6. Sorption coefficients for polychlorobiphenyls (PCBs)

log K_d log K_f^0 (1/n)	log K_{oc}	Sorbent composition (%)				Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
Biphenyl (0)									
−0.48	[2.06]	98	1	1	0.29	Borden soil. 0.01 N $CaCl_2$		MD	600
1.19° (1.00)	3.04				1.42	Soil; cl; (kaolinite); pH 5.91; CE=12.4 me/100 g	20	BE	214
1.50° (1.00)	3.32				1.51	Soil; light c; (montmorillonite); pH 5.18; CE=13.2 me/100 g	20	BE	214
1.75° (0.98)	3.26				3.23	Soil; light c; (montmorillite); pH 5.26; CE=28.3 me/100 g	20	BE	214
1.95° (1.00)	3.04				7.91	Soil sl; (allophane); pH 5.41; CE=26.3 me/100 g	20	BE	214
2.09° (0.78)					10.4	Soil; cl; (allophane); pH 4.89; CE=35 me/100 g	20	BE	214
[0.56]	3.52	4	10	86	0.11	Apison soil; pH 4.5; CE=76 me/100 g		BE	570
[−0.27]		11	21	68	0.05	Fullerton soil; pH 4.4; CE=64 me/100 g		BE	570
[1.02]	2.94	2	38	60	1.2	Dormont soil; pH 4.2; CE=129 me/100 g		BE	570
3.57	[4.36]				16.44 20.5*	VSC; vermiculite-HDTMA; CE=80 cmol/kg		BE	225
3.51	[4.27]				17.46 21.8*	SWy-1; smectite (low charge)-HDTMA; CE=87 cmol/kg		BE	225
3.56	4.12				28	Syntetic "sludge" of autoclaved yeast obtained by culturing bakers' yeast in sucrose solution	25	BE	608
2.66					27	Municipal sludge from Oak Ridge wastewater treatment plant	25	BE	608
3.53					14	Oily biosludge 913 from ORNL (4% oil content)	25	BE	608
3.35					25	Oily biosludge 969 from ORNL (14% oil content)	25	BE	608
3.90					33	Oily biosludge 972 from ORNL (24% oil content)	25	BE	608
	4.26					Oil extracted from waste 972	25	BE	608
−0.56		>98			0.025	Vejen aquifer mat.	10	MD	166
	3.00					Aldrich humic acid (DOC=9.4 mg/l); pH 5.8–6.8		RP	414
	3.27					Idem (zero intercept of the regression line of log K_{doc} vs DOC concentration)		RP	414
	3.57					DOC in Lake Erie water (9.6 mg/L)		RP	414
	3.77					Idem		ED	414
	5.58					DOC in Huron River wat. (7.8 mg/L)		RP	414
	4.04					Idem		ED	414
	3.67				50.2	Aldrich and Fluka humic acid		FH	206
	3.15					Correlation log K_{oc}−log S			564
	3.80					Correlation log K_{oc}−MCI			598
	2.93					Correlation log K_{oc}−CRI			601
2-(1)									
[1.51]	[3.47]	9	68	21	1.9* [1.1]	Woodburn soil; CE=14 me/100 g	20	BE	55
0.06	[2.59]	98	1	1	0.29	Borden soil. 0.01 N $CaCl_2$		MD	600
	[4.2]					Correlation log K_{om}−MCI			591
	3.43					Correlation log K_{oc}−CRI			601
4-(3)									
3.83av	4.71av					Great Lakes suspended matter (three phases distribution)	25	RS	409
	4.02av					Great Lakes DOC (same procedure)	25	RS	409
3.92av	4.70av				16	Green Bay suspended matter (same procedure)	25	RS	410
	4.61av					Green Bay DOC (same procedure)	25	RS	410

TABLE 6. Sorption coefficients for polychlorobiphenyls (PCBs)—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%)				Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
	3.52					Correlation $\log K_{oc}-\log S$			564
	3.49					Correlation $\log K_{oc}$–CRI			601
						2,2′-(4)			
[1.96]	[3.92]	9	68	21	1.9* [1.1]	Woodburn soil; CE=14 me/100 g	20	BE	55
	[4.42]					Correlation $\log K_{oc}$–CRI			591
	3.96					Correlation $\log K_{oc}$–MCI			601
						2,4′-(8)			
	[4.13]	9	68	21	1.9* [1.1]	Woodburn soil; CE=14 me/100 g	20	BE	55
0.40^{o} (0.85)				16.2	3.1* [1.8]	Woodburn soil; sil	24	BE	178
1.87^{o} (1.19)						Illite clay	24	BE	178
5.8						Lake Superior suspended sol. (1980)		FM	50
4.5						Idem (1983)			50
	4.08^{o}* (1.16)					Aldrich humic acid	24	BE	178
	[4.41]					Correlation $\log K_{om}$–MCI			591
	3.99					Correlation $\log K_{oc}$–CRI			601
	3.38					Correlation $\log K_{oc}$–LSER			602
						4,4′-(15)			
	4.30					Correlation $\log K_{oc}-\log S$			564
	4.03					Correlation $\log K_{oc}$–CRI			601
						2,2′,3-(16)			
6.0						Lake Superior suspended sol. (1980)		FM	50
4.8						Idem (1983)			50
	4.52					Correlation $\log K_{oc}$–CRI			601
						2,2′,4-(17)			
6.5						Lake Superior suspended sol. (1980)		FM	50
4.6						Idem (1983)			50
	4.44					Correlation $\log K_{oc}$–MCI			598
	4.51					Correlation $\log K_{oc}$–CRI			601
						2,2′,5-(18)			
7.2						Lake Superior suspended sol. (1980)		FM	50
4.6						Idem (1983)			50
[2.96]	4.5				2.9	Offshore Grand Haven sediment; (solute complexation model)		BE	464, 494
[3.03]	4.5				3.4	Nearshore Grand Haven sediment; (solute complexation model)		BE	464, 494
[3.58]	5.0				3.8	Benton Harbor sediment; (solute complexation model)		BE	464, 494
	4.57				50.2	Aldrich humic acid; pH 8.0; 0.1 M $NaHCO_3$	22	ED	206
	4.85				50.2	Aldrich and Fluka humic acid		FH	206
[4.01]	5.4				4.1	Lake Ontario sediment trap material		FM	49
	5.5				50	Niagara River organic matter		FM	49
	5.2					Correlation $\log K_{oc}-\log K_{ow}$(96)			49
	4.23					Correlation $\log K_{oc}-\log S$			564
	4.44					Correlation $\log K_{oc}$–MCI			598
	4.53					Correlation $\log K_{oc}$–CRI			601

TABLE 6. Sorption coefficients for polychlorobiphenyls (PCBs)—Continued

log K_d log K_f^0 (1/n)	log K_{oc}	Sorbent composition (%)				Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
2,3,4′-(22)									
5.7						Lake Superior suspended sol. (1980)		FM	50
4.9						Idem (1983)			50
	4.54					Correlation log K_{oc}–CRI			601
2,4,4′-(28)									
[2.66]	[4.62]	9	68	21	1.9* [1.1]	Woodburn soil; CE=14 me/100 g	20	BE	55
	4.40				58.0	Sanhedron soil humic acid; pH 6.5	24	SE	220
	3.89				4.87	Sanhedron soil fulvic acid; pH 6.5	24	SE	220
	3.54				54.2	Suwannee River humic acid; pH 6.5	24	SE	220
	3.57				53.8	Suwannee River fulvic acid; pH 6.5	24	SE	219
	3.53					Suwannee River water; pH 6.5; DOC=37 mg/L	24	SE	219
	3.57					Sopchoppy River water; pH 6.5; DOC=44 mg/L	24	SE	219
	4.84				65.8	Fluka-Tridom humic acid; pH 6.5	24	SE	219
	4.24				56.7	Calcasieu River Humic extr.; pH 6.5	24	SE	219
5.5						Lake Superior suspended sol. (1980)		FM	50
4.66	5.28					Idem (1983)			50
	5.30					Correlation log K_{oc}–log K_{ow}(96)			50
	4.59					Correlation log K_{oc}–log K_{ow}(207)			50
	4.23					Correlation log K_{oc}–log S			564
	[4.61]					Correlation log K_{om}–MCI			591
	4.46					Correlation log K_{oc}–CRI			601
2,4′,5-(31)									
5.9						Lake Superior suspended sol. (1980)		FM	50
4.8						Idem (1983)			50
	4.51					Correlation log K_{oc}–CRI			601
2,3,3′-(33)									
4.8						Lake Superior suspended sol. (1983)		FM	50
	4.50					Correlation log K_{oc}–CRI			601
3,4,4′-(37)									
5.7						Lake Superior suspended sol. (1980)		FM	50
4.8						Idem (1983)			50
	4.46					Correlation log K_{oc}–CRI			601
2,2′,3,3′-(40)									
[4.11]	5.5				4.1	Lake Ontario sediment trap material		FM	49
	5.5				50	Niagara River organic matter		FM	49
	5.2					Correlation log K_{oc}–log K_{ow}(K8)			49
	5.00					Correlation log K_{oc}–CRI			601
2,2′,3,4-(41)									
5.8						Lake Superior suspended sol. (1980)		FM	50
4.8						Idem (1983)			50
	5.01					Correlation log K_{oc}–CRI			601
2,2′,3,5′-(44)									
5.6						Lake suspended solids, 1980		FM	50
4.7						Idem (1983)			50
	5.05					Correlation log K_{oc}–CRI			601
2,2′,4,4′-(47)									
5.3						Lake Superior suspended sol. (1980)		FM	50
4.9						Idem (1983)			50
	4.61					Correlation log K_{oc}–log S			564
	5.04					Correlation log K_{oc}–CRI			601

TABLE 6. Sorption coefficients for polychlorobiphenyls (PCBs)—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%)				Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
						2,2′,5,5′-(52)			
3.70	6.15				0.36	Composite Condie silt soil	22	BE	619
2.28		99.3	0.20	0.55	0.03	Ispra soil (C2 horizon); pH 5.1	22	BE	153
2.52	[5.31]	95.5	3.4	1.6	0.16	Idem (C4 horizon); pH 4.8			153
3.68	5.41	91.8	6.4	1.8	1.87	Idem (A2 horizon); pH 4.8			153
1.60° (1.09)						Illite clay	24	BE	178
1.69	[3.43]			16.2	3.1* [1.8]	Woodburn soil; silt loam	24	BE	178
5.6						Lake Superior suspended sol. (1980)		FM	50
4.87	5.35					Idem (1983)			50
	5.90				7–13	River sediments		BE	620
[4.21]	5.6				4.1	Lake Ontario sediment trap material		FM	49
	5.5				50	Niagara River organic matter		FM	49
[2.94]	5.02	5	70	25	0.84	Brown's lake sedim.; 6 months incubation (m.i.)	25	BE	218
[4.72]	6.04	55	32.5	12.5	4.76	Hamlet City lake sedim.; 6 m.i.	25	BE	218
[2.50]	4.80	0.0	93.8	6.3	0.50	WES reference soil; 6 m.i.	25	BE	218
	5.00					Aldrich humic acid	25	RS	409
4.93av	5.83av					Great Lakes suspended matter (three phases distribution)	25	RS	409
	3.88av					Great Lakes DOC (same procedure)	25	RS	409
4.96av	5.74av				16	Green Bay suspended matter (same procedure)	25	RS	410
	3.66av					Green Bay DOC (same procedure)	25	RS	410
	4.85					Aldrich humic acid; pH 6.4		GP	416
	4.76					Aldrich humic acid		ED	435
	4.54					Aldrich humic acid (DOC=9.4 mg/L); pH 5.8–6.8		RS	414
	4.42					Idem		ED	414
	4.40					Idem (zero intercept of the regression line of $\log K_{doc}$ vs DOC concentration)		RS	414
	3.87					DOC in Huron River wat.(7.8 mg/L)		RS	414
	4.36					Idem		ED	414
	2.42 °* (0.26)					Aldrich humic acid	24	BE	178
	4.94					Aldrich humic acid; pH 7.32 (DOC=0–7.5 mg/L)	6.6	RS	546
	5.06				50.2	Aldrich and Fluka humic acid; predicted (Flory-Huggins Model)		FH	206
	5.70					Correlation $\log K_{oc}-\log K_{ow}(96)$			50
	4.87					Correlation $\log K_{oc}-\log K_{ow}(207)$			50
	5.7					Correlation $\log K_{oc}-\log K_{ow}(96)$			49
	4.61					Correlation $\log K_{oc}-\log S$			564
	4.65					Correlation $\log K_{oc}-$MCI			578
	[4.86]					Correlation $\log K_{om}-$MCI			591
	5.09					Correlation $\log K_{oc}-$CRI			601
	4.49					Correlation $\log K_{oc}-$LSER			602
						2,2′,6,6′-(54)			
3.10	[4.72]	55.0	45.0	<1.0	2.4	Hickory Hill Pond sed.; pH 6.3		BE	621
3.03	[4.89]	56.0	44.0	<1.0	1.4	Doe Run Pond sed.; pH 6.1		BE	621
2.81	[4.91]				0.8	USDA Pond sed.; pH 6.4		BE	621
2.71	[5.11]	93.0	6.0	2.0	0.4	Oconee River sed.; pH 6.5		BE	621
	5.01					Correlation $\log K_{oc}-$CRI			601
						2,3,4,4′-(60)			
6.2						Lake Superior suspended sol. (1980)		FM	50
5.0						Idem (1983)			50
	5.03					Correlation $\log K_{oc}-$CRI			601

TABLE 6. Sorption coefficients for polychlorobiphenyls (PCBs)—Continued

log K_d log K_f^0 $(1/n)$	log K_{oc}	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
						2,3′,4,4′-(66)			
5.8						Lake Superior suspended sol. (1980)		FM	50
4.9						Idem (1983)			50
	4.90					Correlation log K_{oc}–CRI			601
						2,3′,4′,5-(70)			
5.7						Lake Superior suspended sol. (1980)		FM	50
5.1						Idem (1983)			50
3.07	[4.69]	55.0	45.0	<1.0	2.4	Hickory Hill Pond sed.; pH 6.3		BE	621
3.00	[4.85]	56.0	44.0	<1.0	1.4	Doe Run Pond sed.; pH 6.1		BE	621
2.76	[4.86]				0.8	USDA Pond sed.; pH 6.4		BE	621
2.62	[5.02]	93.0	6.0	2.0	0.4	Oconee River sed.; pH 6.5		BE	621
	5.07					Correlation log K_{oc}–CRI			601
						2,4,4′,5-(74)			
5.8						Lake Superior suspended sol. (1980)		FM	50
4.9						Idem (1983)			50
	5.00					Correlation log K_{oc}–CRI			601
						2,2′,3,4,5′-(87)			
2.87		99.3	0.20	0.55	0.03	Ispra soil (C2 horizon); pH 5.1	22	BE	153
3.11	[5.91]	95.5	3.4	1.6	0.16	Idem (C4 horizon); pH 4.8			153
4.03	5.73	91.8	6.4	1.8	1.87	Idem (A2 horizon); pH 4.8			153
	4.76					Marine water DHS (5 mg C/L)	20	AG	413
	4.87					Idem (10 mg C/L)			413
	4.85					Idem (20 mg C/L)			413
	3.75					Idem (40 mg C/L)			413
5.6						Lake Superior suspended sol. (1980)		FM	50
5.1						Idem (1983)			50
	4.88					Correlation log K_{oc}–MCI			578
	4.75					Correlation log K_{doc}–MCI (doc=dissol. marine humic subst.)			599
	[5.09]					Correlation log K_{om}–MCI			591
	5.54					Correlation log K_{oc}–CRI			601
	4.88					Correlation log K_{oc}–LSER			602
						2,2′,3,4′,5-(90)			
	4.66					Marine water DHS (5 mg C/L)	20	AG	413
	4.68					Idem (10 mg C/L)			413
	4.75					Idem (20 mg C/L)			413
	3.75					Idem (40 mg C/L)			413
	4.73					Correlation log K_{doc}–MCI (doc=dissol. marine humic subst.)			599
						2,2′,3,5′,6-(95)			
2.64		99.3	0.20	0.55	0.03	Ispra soil (C2 horizon); pH 5.1	22	BE	153
2.94	[5.74]	95.5	3.4	1.6	0.16	Idem (C4 horizon); pH 4.8			153
3.84	5.55	91.8	6.4	1.8	1.87	Idem (A2 horizon); pH 4.8			153
3.38	5.68	76.66	4.59	18.75	0.50	North Sea sediment No. 125	20	BE	182
3.87	5.70	36.70	36.15	27.15	1.47	North Sea sediment No. 106	20	BE	182
4.10	5.64	3.29	57.82	38.89	2.33	North Sea sediment No. 99	20	BE	182
	4.60					Marine water DHS (5 mg C/L)	20	AG	413
	4.66					Idem (10 mg C/L)			413
	4.61					Idem (20 mg C/L)			413
	3.70					Idem (40 mg C/L)			413
	4.59					Correlation log K_{doc}–MCI (doc=dissol. marine humic subst.)			599
	5.57					Correlation log K_{oc}–CRI			601
						2,2′,3′,4,5-(97)			
3.40		99.3	0.20	0.55	0.03	Ispra soil (C2 horizon); pH 5.1	22	BE	153
3.52	[6.32]	95.5	3.4	1.6	0.16	Idem (C4 horizon); pH 4.8			153

TABLE 6. Sorption coefficients for polychlorobiphenyls (PCBs)—Continued

log K_d log K_f^0 (1/*n*)	log K_{oc}	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
4.06	5.69	91.8	6.4	1.8	1.87	Idem (A2 horizon); pH 4.8			153
3.53	5.83	76.66	4.59	18.75	0.50	North Sea sediment No. 125	20	BE	182
4.05	5.89	36.70	36.15	27.15	1.47	North Sea sediment No. 106	20	BE	182
4.15	5.78	3.29	57.82	38.89	2.33	North Sea sediment No. 99	20	BE	182
5.4						Lake Superior suspended sol. (1980)		FM	50
5.1						Idem (1983)			50
	4.75					Correlation log K_{doc}–MCI (doc=dissol. marine humic subst.)			599
	5.50					Correlation log K_{oc}–CRI			601
2,2′,4,4′,5-(99)									
5.7						Lake Superior suspended sol. (1980)		FM	50
5.1						Idem (1983)			50
	4.73					Correlation log K_{doc}–MCI (doc=dissol. marine humic subst.)			599
	5.54					Correlation log K_{oc}–CRI			601
2,2′,4,5,5′-(101)									
3.97	6.41				0.36	Composite Condie si soil	22	BE	619
2.91		99.3	0.20	0.55	0.03	Ispra soil (C2 horizon); pH 5.1	22	BE	153
3.13	[5.93]	95.5	3.4	1.6	0.16	Idem (C4 horizon); pH 4.8			153
3.98	5.67	91.8	6.4	1.8	1.87	Idem (A2 horizon); pH 4.8			153
3.51	5.81	76.66	4.59	18.75	0.50	North Sea sediment No. 125	20	BE	182
4.00	5.83	36.70	36.15	27.15	1.47	North Sea sediment No. 106	20	BE	182
4.15	5.78	3.29	57.82	38.89	2.33	North Sea sediment No. 99	20	BE	182
	4.87				58.0	Sanhedron soil humic acid; pH 6.5	24	SE	220
	4.12				48.7	Sanhedron soil fulvic acid; pH 6.5	24	SE	220
	4.07				54.2	Suwannee River humic acid; pH 6.5	24	SE	220
	4.10				53.8	Suwannee River fulvic acid; pH 6.5	24	SE	220
	4.09					Suwannee River water; pH 6.5; DOC=37 mg/L	24	SE	219
	4.01					Sopchoppy River water; pH 6.5; DOC=44 mg/L	24	SE	219
	5.41				69.4	Aldrich humic acid Na salt; pH 6.5	24	SE	219
	5.41				65.8	Fluka-Tridom humic acid; pH 6.5	24	SE	219
	4.81				56.7	Calcasieu River humic extr.; pH 6.5	24	SE	219
	4.77					Marine water DHS (5 mg C/L)	20	AG	413
	4.86					Idem (10 mg C/L)			413
	4.80					Idem (20 mg C/L)			413
	3.86					Idem (40 mg C/L)			413
5.7						Lake Superior suspended sol. (1980)		FM	50
5.09	5.65					Idem (1983)			50
[4.21]	5.6				4.1	Lake Ontario sediment trap material		FM	49
	5.5				50	Niagara River organic matter		FM	49
	5.45					C18 column		RPLC	573
	4.63					Soil; experimental (literature)			217
	6.6					Correlation log K_{oc}–log K_{ow}(96)			49
	6.68					Correlation log K_{oc}–log K_{ow}(96)			50
	5.58					Correlation log K_{oc}–log K_{ow}(207)			50
	4.74					Correlation log K_{oc}–log S			564
	4.87					Correlation log K_{oc}–MCI			578
	4.73					Correlation log K_{doc}–MCI (doc=dissol. marine humic subst.)			599
	[5.08]					Correlation log K_{om}–MCI			591
	5.58					Correlation log K_{oc}–CRI			601
	4.91					Correlation log K_{oc}–LSER			602
2,3,3′,4,4′-(105)									
3.23		99.3	0.20	0.55	0.03	Ispra soil (C2 horizon); pH 5.1	22	BE	153
3.41	[6.20]	95.5	3.4	1.6	0.16	Idem (C4 horizon); pH 4.8			153
4.13	5.81	91.8	6.4	1.8	1.87	Idem (A2 horizon); pH 4.8			153

TABLE 6. Sorption coefficients for polychlorobiphenyls (PCBs)—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
	4.91					Correlation $\log K_{doc}$–MCI (doc=dissol. marine humic subst.)			599
	5.50					Correlation $\log K_{oc}$–CRI			601
						2,3,3′,4′,6-(110)			
2.86		99.3	0.20	0.55	0.03	Ispra soil (C2 horizon); pH 5.1	22	BE	153
3.10	[5.90]	95.5	3.4	1.6	0.16	Idem (C4 horizon); pH 4.8			153
4.00	5.71	91.8	6.4	1.8	1.87	Idem (A2 horizon); pH 4.8			153
	4.72					Marine water DHS (5 mg C/L)	20	AG	413
	4.80					Idem (10 mg C/L)			413
	4.77					Idem (20 mg C/L)			413
	3.79					Idem (40 mg C/L)			413
5.6						Lake Superior suspended sol. (1980)		FM	50
5.1						Idem (1983)			50
	4.75					Correlation $\log K_{doc}$–MCI (doc=dissol. marine humic subst.)			599
	5.50					Correlation $\log K_{oc}$–CRI			601
						2,3′,4,4′,5-(118)			
3.10		99.3	0.20	0.55	0.03	Ispra soil (C2 horizon); pH 5.1	22	BE	153
3.30	[6.10]	95.5	3.4	1.6	0.16	Idem (C4 horizon); pH 4.8			153
4.12	5.81	91.8	6.4	1.8	1.87	Idem (A2 horizon); pH 4.8			153
5.7						Lake Superior susp. solids (1980)		FM	50
5.1						Idem (1983)			50
	4.88					Correlation $\log K_{doc}$–MCI (doc=dissol. marine humic subst.)			599
	5.52					Correlation $\log K_{oc}$–CRI			601
						2,2′,3,3′,4,4′-(128)			
3.97	6.28	76.66	4.59	18.75	0.50	North Sea sediment No. 125	20	BE	182
4.34	6.17	36.70	36.15	27.15	1.47	North Sea sediment No. 106	20	BE	182
4.38	6.01	3.29	57.82	38.89	2.33	North Sea sediment No. 99	20	BE	182
	5.05					Correlation $\log K_{oc}$–MCI			596
	5.06					Correlation $\log K_{oc}$–MCI			578
	[5.33]					Correlation $\log K_{om}$–MCI			591
	5.26					Correlation $\log K_{doc}$–MCI (doc=dissol. marine humic subst.)			599
	5.93					Correlation $\log K_{oc}$–CRI			601
	5.25					Correlation $\log K_{oc}$–LSER			602
						2,2′,3,3′,5,6-(134)			
	5.18					Marine water DHS (5 mg C/L)	20	AG	413
	5.16					Idem (10 mg C/L)			413
	5.15					Idem (20 mg C/L)			413
	4.41					Idem (40 mg C/L)			413
	5.10					Correlation $\log K_{doc}$–MCI (doc=dissol. marine humic subst.)			599
						2,2′,3,3′,6,6′-(136)			
3.71	6.01	76.66	4.59	18.75	0.50	North Sea sediment No. 125	20	BE	182
4.23	6.06	36.70	36.15	27.15	1.47	North Sea sediment No. 106	20	BE	182
4.26	5.90	3.29	57.82	38.89	2.33	North Sea sediment No. 99	20	BE	182
6.17	6.53				43.2	Lake suspended solids (0.7 mg/L)		FM	494
4.85	5.68				14.8	Idem (6.5 mg/L)		FM	494
	4.95					Marine water DHS (5 mg C/L)	20	AG	413
	5.05					Idem (10 mg C/L)			413
	4.95					Idem (20 mg C/L)			413
	4.27					Idem (40 mg C/L)			413
	4.94					Correlation $\log K_{doc}$–MCI (doc=dissol. marine humic subst.)			599
	6.02					Correlation $\log K_{oc}$–CRI			601

TABLE 6. Sorption coefficients for polychlorobiphenyls (PCBs)—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%)				Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
						2,2′,3,4,4′,5-(138)			
3.38		99.3	0.20	0.55	0.03	Ispra soil (C2 horizon); pH 5.1	22	BE	153
3.53	[6.33]	95.5	3.4	1.6	0.16	Idem (C4 horizon); pH 4.8			153
4.26	5.93	91.8	6.4	1.8	1.87	Idem (A2 horizon); pH 4.8			153
3.92	6.22	76.66	4.59	18.75	0.50	North Sea sediment No. 125	20	BE	182
4.29	6.12	36.70	36.15	27.15	1.47	North Sea sediment No. 106	20	BE	182
4.35	5.99	3.29	57.82	38.89	2.33	North Sea sediment No. 99	20	BE	182
5.8						Lake Superior susp. solids (1980)		FM	50
5.3						Idem (1983)			50
	5.21					Marine water DHS (5 mg C/L)	20	AG	413
	5.22					Idem (10 mg C/L)			413
	5.17					Idem (20 mg C/L)			413
	4.60					Idem (40 mg C/L)			413
	5.24					Correlation $\log K_{doc}$–MCI (doc=dissol. marine humic subst.)			599
	5.94					Correlation $\log K_{oc}$–CRI			601
						2,2′,3,4,5,5′-(141)			
3.40		99.3	0.20	0.55	0.03	Ispra soil (C2 horizon); pH 5.1	22	BE	153
3.52	[6.32]	95.5	3.4	1.6	0.16	Idem (C4 horizon); pH 4.8			153
4.36	6.05	91.8	6.4	1.8	1.87	Idem (A2 horizon); pH 4.8			153
5.8						Lake Superior suspended sol. (1980)		FM	50
5.1						Idem (1983)			
	5.24					Correlation $\log K_{doc}$–MCI (doc=dissol. marine humic subst.)			599
	6.02					Correlation $\log K_{oc}$–CRI			601
						2,2′,3,4′,5,5′-(146)			
3.37		99.3	0.20	0.55	0.03	Ispra soil (C2 horizon); pH 5.1	22	BE	153
3.52	[6.32]	95.5	3.4	1.6	0.16	Idem (C4 horizon); pH 4.8			153
4.20	5.86	91.8	6.4	1.8	1.87	Idem (A2 horizon); pH 4.8			153
5.8						Lake Superior suspended sol. (1980)		FM	50
5.40	5.88					Idem (1983)			50
	5.18					Marine water DHS (5 mg C/L)	20	AG	413
	5.22					Idem (10 mg C/L)			413
	5.14					Idem (20 mg C/L)			413
	4.58					Idem (40 mg C/L)			413
	6.92					Correlation $\log K_{oc}$–$\log K_{ow}$(96)			50
	5.75					Correlation $\log K_{oc}$–$\log K_{ow}$(207)			50
	5.22					Correlation $\log K_{doc}$–MCI (doc=dissol. marine humic subst.)			599
	6.01					Correlation $\log K_{oc}$–CRI			601
						2,2′,3,4′,5,6′-(148)			
3.05		99.3	0.20	0.55	0.03	Ispra soil (C2 horizon); pH 5.1	22	BE	153
3.32	[6.11]	95.5	3.4	1.6	0.16	Idem (C4 horizon); pH 4.8			153
4.03	5.71	91.8	6.4	1.8	1.87	Idem (A2 horizon); pH 4.8			153
	5.06					Correlation $\log K_{doc}$–MCI (doc=dissol. marine humic subst.)			599
						2,2′,3,4′,5′,6-(149)			
3.21		99.3	0.20	0.55	0.03	Ispra soil (C2 horizon); pH 5.1	22	BE	153
3.39	[6.18]	95.5	3.4	1.6	0.16	Idem (C4 horizon); pH 4.8			153
4.12	5.79	91.8	6.4	1.8	1.87	Idem (A2 horizon); pH 4.8			153
	5.08					Correlation $\log K_{doc}$–MCI (dom=dissol. marine humic subst.)			599
						2.2′,3,5,5′,6-(151)			
3.16		99.3	0.20	0.55	0.03	Ispra soil (C2 horizon); pH 5.1	22	BE	153
3.35	[6.15]	95.5	3.4	1.6	0.16	Idem (C4 horizon); pH 4.8			153
4.11	5.79	91.8	6.4	1.8	1.87	Idem (A2 horizon); pH 4.8			153
[2.55]	4.85	0.0	93.8	6.3	0.50	WES reference soil; 6 m.i.	25	BE	218

TABLE 6. Sorption coefficients for polychlorobiphenyls (PCBs)—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
3.75	6.05	76.66	4.59	18.75	0.50	North Sea sediment No. 125	20	BE	182
4.22	6.05	36.70	36.15	27.15	1.47	North Sea sediment No. 106	20	BE	182
4.30	5.93	3.29	57.82	38.89	2.33	North Sea sediment No. 99	20	BE	182
	5.03					Marine water DHS (5 mg C/L)	20	AG	413
	5.11					Idem (10 mg C/L)			413
	5.09					Idem (20 mg C/L)			413
	4.41					Idem (40 mg C/L)			413
	4.99	5	70	25	0.84	Brown's lake sedim.; 6 months incubation (m. i.)	25	BE	218
	4.82	55	32.5	12.5	4.76	Hamlet City lake sedim.; 6 m. i.	25	BE	218
	5.08					Correlation $\log K_{doc}$–MCl (doc=dissol. marine humic subst.)			599
						2,2′,4,4′,5,5′-(153)			
4.03				100	<0.1*	Montmorillonite; pH 6.5; $SA(N_2)=12.6\ m^2/g$; clay clay conc.=50 mg/L	24	BE	467
3.83						Idem; pH 6.6; clay conc.=200 mg/L			467
3.46						Idem; pH 6.8; clay conc.=1000 mg/L			467
4.21						Idem; pH 8.0; 2 mM $NaHCO_3$; clay conc.=55 mg/L:			467
3.32						Idem; pH 8.4; 2 mM $NaHCO_3$; clay conc.=1100 mg/L			467
1:67° (0.79)						Illite clay	24	BE	178
1.91° (0.80)				16.2	3.1* [1.8]	Woodburn soil; silt loam	24	BE	178
4.41	6.86				0.36	Composite Condie silt soil	22	BE	619
3.40		99.3	0.20	0.55	0.03	Ispra soil (C2 horizon); pH 5.1	22	BE	153
3.54	[6.34]	95.5	3.4	1.6	0.16	Idem (C4 horizon); pH 4.8			153
4.20	5.86	91.8	6.4	1.8	1.87	Idem (A2 horizon); pH 4.8			153
2.39		83.7	6.8	9.5	0.039	Aquifer (155–210 cm); 0.7 mg Fe/g; 0.025 M KCl; pH 6.0	22	BE, MD	431
3.88	6.18	76.66	4.59	18.75	0.50	North Sea sediment No. 125	20	BE	182
4.30	6.13	36.70	36.15	27.15	1.47	North Sea sediment No. 106	20	BE	182
4.36	5.99	3.29	57.82	38.89	2.33	North Sea sediment No. 99	20	BE	182
	5.09					DOC from a stream channel; aquifer+DOC/water system; pH 6.0 0.025 M KCl	22	BE	431
4.17	[6.81]	91	9(si+c)		0.4* [0.23]	Saginaw Bay (SB) sed. 19 (<75 μm); $SA(N_2)=17\ m^2/g$		BE	491
4.09	[5.60]	7	93(si+c)		5.4* [3.1]	SB 31; $SA(N_2)=17.8\ m^2/g$		BE	491
4.03	[5.58]	9	91(si+c)		4.9* [2.8]	SB 43; $SA(N_2)=15.9\ m^2/g$		BE	491
3.85	[5.42]	15	85(si+c)		4.6* [2.7]	SB 50; $SA(N_2)=12.8\ m^2/g$		BE	491
4.05	[6.20]	85	15(si+c)		1.2* [0.70]	SB 53; $SA(N_2)=7.0\ m^2/g$		BE	491
1.56		95	5(si+c)		0.1* [0.06]	SB 69; $SA(N_2)=0.2\ m^2/g$		BE	491
3.98	[5.54]	18	82(si+c)		4.9* [2.8]	SB S. River; $SA(N_2)=8.4\ m^2/g$		BE	491
[4.18]	6.15				1.06	Oakland Harbor sedim./interstitial saline water system; 15 d incubation; Nereis virens bioaccumulation (BA) study	15	BE	613
[3.73]	5.70				1.06	Idem; Macoma nasuta BA study			613
[4.01]	5.54				2.92	Red Hook sedim./interstitial saline water system; 15 d incubation; Nereis virens BA study	15	BE	613

TABLE 6. Sorption coefficients for polychlorobiphenyls (PCBs)—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
3.73	5.26				2.92	Idem; Macoma nasuta BA study			613
4.23	[5.82]				4.5* [2.61]	Saginaw Bay sediment 50; pH 7.0; SA(N_2)=12.8 m^2/g; sed. conc.=55 mg/L	24	BE	467
4.09	[5.67]					Idem; pH 6.8; sed. conc.=220 mg/L			467
4.00	[5.58]					Idem; pH 6.9; sed. conc.=1100 mg/L			467
5.06	6.61				2.8	Saginaw Bay sediment 50; sediment-interstitial water	24	DF	466
	6.60				7–13	River sediment		BE	620
[4.21]	5.6				4.1	Lake Ontario sediment trap material		FM	49
	5.5				50	Niagara River organic matter		FM	49
5.3						Lake Superior suspended sol. (1983)		FM	50
5.74av	6.76av					Great Lakes suspended matter (three phases distribution)	25	RS	409
	4.42av					Great Lakes DOC(same procedure)	25	RS	409
[4.0]	5.5				2.9	Offshore Grand Haven sediment; (solute complexation model)		BE	464, 494
[4.2]	5.7				3.4	Nearshore Grand Haven sediment; (solute complexation model)		BE	464, 494
[4.7]	6.1				3.8	Benton Harbor sediment; (solute complexation model)		BE	464, 494
	5.26					Marine water DHS (5 mg C/L)	20	AG	413
	5.25					Idem (10 mg C/L)			413
	5.19					Idem (20 mg C/L)			413
	4.62					Idem (40 mg C/L)			413
	5.51					Aldrich humic acid; pH 7.32 (DOC=0–11 mg/L)	6.6	RS	546
	7.31 °* (0.26)					Aldrich humic acid	24	BE	178
	6.08					Soil; experimental (literature)			217
	7.3					Correlation $\log K_{oc}-\log K_{ow}$(96)			49
	6.43					Correlation $\log K_{oc}-\log K_{ow}$			96
	5.33					Correlation $\log K_{oc}-\log K_{ow}$			207
	6.51					Correlation $\log K_{oc}-\log K_{ow}$			108
	5.95					Correlation $\log K_{oc}-\log S$			96
	6.42					Correlation $\log K_{oc}-\log S$(mp)			96
	5.29					Correlation $\log K_{oc}-\log S$			564
	5.22					Correlation $\log K_{doc}-$MCI (doc=dissol. marine humic subst.)			599
	[5.31]					Correlation $\log K_{om}-$MCI			591
	6.02					Correlation $\log K_{oc}-$CRI			601
	5.32					Correlation $\log K_{oc}-$LSER			602
						2,2′,4,4′,6,6′-(155)			
	6.08av				2.78, 3.27	Coarse si fractions of Doe Run and Hickory Hill sediments	25	BE	108
	5.95					Correlation $\log K_{oc}-\log K_{ow}$			96
	5.95					Correlation $\log K_{oc}-\log S$			96
	7.28					Correlation $\log K_{oc}-\log S$(mp)			96
	4.91					Correlation $\log K_{doc}-$MCI (doc=dissol. marine humic subst.)			599
	6.17					Correlation $\log K_{oc}-$CRI			601
						2,2′,3,3′,4,4′,5-(170)			
	5.63					Marine water DHS (5 mg C/L)	20	AG	413
	5.48					Idem (10 mg C/L)			413
	5.42					Idem (20 mg C/L)			413
	4.99					Idem (40 mg C/L)			413
	5.68					Correlation $\log K_{doc}-$MCI (doc=dissol. marine humic subst.)			599

TABLE 6. Sorption coefficients for polychlorobiphenyls (PCBs)—Continued

log K_d log K_f^0 (1/n)	log K_{oc}	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
2,2′,3,3′,4,5,5′-(172)									
	5.71					Marine water DHS (5 mg C/L)	20	AG	413
	5.44					Idem (10 mg C/L)			413
	5.38					Idem (20 mg C/L)			413
	4.97					Idem (40 mg C/L)			413
	5.66					Correlation log K_{doc}–MCI (doc=dissol. marine humic subst.)			599
2,2′,3,3′,4,5,6′-(174)									
3.58		99.3	0.20	0.55	0.03	Ispra soil (C2 horizon); pH 5.1	22	BE	153
3.71	[6.51]	95.5	3.4	1.6	0.16	Idem (C4 horizon); pH 4.8			153
4.18	5.82	91.8	6.4	1.8	1.87	Idem (A2 horizon); pH 4.8			153
	5.52					Correlation log K_{doc}–MCI (doc=dissol. marine humic subst.)			599
2,2′,3,3′,4′,5,6-(177)									
3.62		99.3	0.20	0.55	0.03	Ispra soil (C2 horizon); pH 5.1	22	BE	153
3.77	[6.57]	95.5	3.4	1.6	0.16	Idem (C4 horizon); pH 4.8			153
4.21	5.81	91.8	6.4	1.8	1.87	Idem (A2 horizon); pH 4.8			153
	5.54					Marine water DHS (5 mg C/L)	20	AG	413
	5.39					Idem (10 mg C/L)			413
	5.35					Idem (20 mg C/L)			413
	4.90					Idem (40 mg C/L)			413
	5.52					Correlation log K_{doc}–MCI (doc=dissol. marine humic subst.)			599
2,2′,3,4,4′,5,5′-(180)									
3.67		99.3	0.20	0.55	0.03	Ispra soil (C2 horizon); pH 5.1	22	BE	153
3.80	[6.60]	95.5	3.4	1.6	0.16	Idem (C4 horizon); pH 4.8			153
4.20	5.78	91.8	6.4	1.8	1.87	Idem (A2 horizon); pH 4.8			153
4.06	6.36	76.66	4.59	18.75	0.50	North Sea sediment No. 125	20	BE	182
4.40	6.23	36.70	36.15	27.15	1.47	North Sea sediment No. 106	20	BE	182
4.47	6.10	3.29	57.82	38.89	2.33	North Sea sediment No. 99	20	BE	182
	5.73					Marine water dissolved humic substances (5 mg C/L)	20	AG	413
	5.54					Idem (10 mg C/L)			413
	5.50					Idem (20 mg C/L)			413
	5.09					Idem (40 mg C/L)			413
	5.66					Correlation log K_{doc}–MCI (doc=dissol. marine humic subst.)			599
2,2′,3,4,4′,5′,6-(183)									
3.56		99.3	0.20	0.55	0.03	Ispra soil (C2 horizon); pH 5.1	22	BE	153
3.74	[6.54]	95.5	3.4	1.6	0.16	Idem (C4 horizon); pH 4.8			153
4.21	5.82	91.8	6.4	1.8	1.87	Idem (A2 horizon); pH 4.8			153
4.06	6.36	76.66	4.59	18.75	0.50	North Sea sediment No. 125	20	BE	182
4.41	6.25	36.70	36.15	27.15	1.47	North Sea sediment No. 106	20	BE	182
4.45	6.09	3.29	57.82	38.89	2.33	North Sea sediment No. 99	20	BE	182
	5.53					Marine water DHS (5 mg C/L)	20	AG	413
	5.40					Idem (10 mg C/L)			413
	5.35					Idem (20 mg C/L)			413
	4.92					Idem (40 mg C/L)			413
	5.50					Correlation log K_{doc}–MCI (doc=dissol. marine humic subst.)			599
2,2′,3,4,5,5′,6-(185)									
3.99	6.29	76.66	4.59	18.75	0.50	North Sea sediment No. 125	20	BE	182
4.24	6.08	36.70	36.15	27.15	1.47	North Sea sediment No. 106	20	BE	182
4.49	6.13	3.29	57.82	38.89	2.33	North Sea sediment No. 99	20	BE	182
	5.33					Correlation log K_{oc}–log K_{ow}			578
	5.52					Correlation log K_{doc}–MCI (doc=dissol. marine humic subst.)			599

TABLE 6. Sorption coefficients for polychlorobiphenyls (PCBs)—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%)				Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
	[5.55]					Correlation $\log K_{dom}$–MCI			591
	5.80					Correlation $\log K_{oc}$–LSER			602
						2,2′,3,4′,5,5′,6-(187)			
	5.51					Marine water DHS (5 mg C/L)	20	AG	413
	5.40					Idem (10 mg C/L)			413
	5.33					Idem (20 mg C/L)			413
	4.90					Idem (40 mg C/L)			413
	5.50					Correlation $\log K_{doc}$–MCI (doc=dissol. marine humic subst.)			599
						2,2′,3,3′,4,4′,5,5′-(194)			
4.10	6.41	76.66	4.59	18.75	0.50	North Sea sediment No. 125	20	BE	182
4.37	6.20	36.70	36.15	27.15	1.47	North Sea sediment No. 106	20	BE	182
4.43	6.06	3.29	57.82	38.89	2.33	North Sea sediment No. 99	20	BE	182
	5.94					Marine water DHS (5 mg C/L)	20	AG	413
	5.72					Idem (10 mg C/L)			413
	5.68					Idem (20 mg C/L)			413
	5.36					Idem (40 mg C/L)			413
	6.02					Correlation $\log K_{doc}$–MCI (doc=dissol. marine humic subst.)			599
	6.96					Correlation $\log K_{oc}$–CRI			601
						2,2′,3,3′,4,4′,5,6-(195)			
4.11	6.42	76.66	4.59	18.75	0.50	North Sea sediment No. 125	20	BE	182
4.42	6.25	36.70	36.15	27.15	1.47	North Sea sediment No. 106	20	BE	182
4.51	6.13	3.29	57.82	38.89	2.33	North Sea sediment No. 99	20	BE	182
	5.78					Marine water DHS (5 mg C/L)	20	AG	413
	5.59					Idem (10 mg C/L)			413
	5.55					Idem (20 mg C/L)			413
	5.22					Idem (40 mg C/L)			413
	5.87					Correlation $\log K_{doc}$–MCI (doc=dissol. marine humic subst.)			599
						2,2′,3,3′,4,5,5′,6-(198)			
4.13	6.44	76.66	4.59	18.75	0.50	North Sea sediment No. 125	20	BE	182
4.43	6.26	36.70	36.15	27.15	1.47	North Sea sediment No. 106	20	BE	182
4.52	6.15	3.29	57.82	38.89	2.33	North Sea sediment No. 99	20	BE	182
	5.91					Marine water DHS (5 mg C/L)	20	AG	413
	5.63					Idem (10 mg C/L)			413
	5.56					Idem (20 mg C/L)			413
	5.23					Idem (40 mg C/L)			413
	5.86					Correlation $\log K_{doc}$–MCI (doc=dissol. marine humic subst.)			599
						2,2′,3,3′,4,5,6,6′-(199)			
4.14	6.44	76.66	4.59	18.75	0.50	North Sea sediment No. 125	20	BE	182
4.35	6.18	36.70	36.15	27.15	1.47	North Sea sediment No. 106	20	BE	182
4.39	6.02	3.29	57.82	38.89	2.33	North Sea sediment No. 99	20	BE	182
	5.68					Marine water DHS (5 mg C/L)	20	AG	413
	5.50					Idem (10 mg C/L)			413
	5.46					Idem (20 mg C/L)			413
	5.10					Idem (40 mg C/L)			413
	5.70					Correlation $\log K_{doc}$–MCI (doc=dissol. marine humic subst.)			599
						2,2′,3,3′,4,5′,6,6′-(200)			
	5.91					Marine water DHS (5 mg C/L)	20	AG	413
	5.65					Idem (10 mg C/L)			413
	5.60					Idem (20 mg C/L)			413
	5.31					Idem (40 mg C/L)			413
	5.86					Correlation $\log K_{doc}$–MCI (doc=dissol. marine humic subst.)			599

TABLE 6. Sorption coefficients for polychlorobiphenyls (PCBs)—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%)				Other sorbent and solution data: prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
	7.05					Correlation $\log K_{oc}$–CRI			601
2,2′,3,3′,5,5′,6,6′-(202)									
4.05	6.36	76.66	4.59	18.75	0.50	North Sea sediment No. 125	20	BE	182
4.30	6.13	36.70	36.15	27.15	1.47	North Sea sediment No. 106	20	BE	182
4.38	6.01	3.29	57.82	38.89	2.33	North Sea sediment No. 99	20	BE	182
	5.61					Marine water DHS (5 mg C/L)	20	AG	413
	5.46					Idem (10 mg C/L)			413
	5.41					Idem (20 mg C/L)			413
	4.99					Idem (40 mg C/L)			413
	5.70					Correlation $\log K_{doc}$–MCI (doc=dissol. marine humic subst.)			599
	7.04					Correlation $\log K_{oc}$–CRI			601
2,2′,3,3′,4,4′,5,5′,6-(206)									
4.16	6.46	76.66	4.59	18.75	0.50	North Sea sediment No. 125	20	BE	182
4.44	6.27	36.70	36.15	27.15	1.47	North Sea sediment No. 106	20	BE	182
4.56	6.19	3.29	57.82	38.89	2.33	North Sea sediment No. 99	20	BE	182
	6.15					Marine water DHS (5 mg C/L)	20	AG	413
	5.92					Idem (10 mg C/L)			413
	5.83					Idem (20 mg C/L)			413
	5.69					Idem (40 mg C/L)			413
	6.13					Correlation $\log K_{doc}$–MCI (doc=dissol. marine humic subst.)			599
2,2′,3,3′,4,4′,5,6,6′-(207)									
4.09	6.39	76.66	4.59	18.75	0.50	North Sea sediment No. 125	20	BE	182
4.34	6.17	36.70	36.15	27.15	1.47	North Sea sediment No. 106	20	BE	182
4.56	6.19	3.29	57.82	38.89	2.33	North Sea sediment No. 99	20	BE	182
	5.98					Marine water DHS (5 mg C/L)	20	AG	413
	5.77					Idem (10 mg C/L)			413
	5.67					Idem (20 mg C/L)			413
	5.44					Idem (40 mg C/L)			413
	5.97					Correlation $\log K_{doc}$–MCI (doc=dissol. marine humic subst.)			599
Decachlorobiphenyl (209)									
	6.19					Marine water DHS (5 mg C/L)	20	AG	413
	5.99					Idem (10 mg C/L)			413
	5.83					Idem (20 mg C/L)			413
	5.61					Idem (40 mg C/L)			413
	6.17					Correlation $\log K_{doc}$–MCI (doc=dissol. marine humic subst.)			599
Aroclor-1016									
3.11	[4.73]	55.0	45.0	<1.0	2.4	Hickory Hill Pond sed.; pH 6.3		BE	621
3.11	[4.96]	56.0	44.0	<1.0	1.4	Doe Run Pond sed.; pH 6.1		BE	621
3.14	[5.23]				0.8	USDA Pond sed.; pH 6.4		BE	621
2.79	[5.19]	93.0	6.0	2.0	0.4	Oconee River sed.; pH 6.5		BE	621
Aroclor-1242									
2.73	[4.05]	11.9	60.9	27.2	4.73	Catlin soil; $SA(CO_2)=26.5\ m^2/g$; pH 7.1; CE=18.1 me/100 g	25	BE	175, 215
2.67	[4.03]				4.37	Idem; 6 h low temp. ashed (LTA); $SA(CO_2)=25.4\ m^2/g$			175, 215
2.49	[3.93]				3.64	Idem; 12 h LTA; $SA(CO_2)=24.5\ m^2/g$			175, 215
2.38	[4.11]				1.84	Idem; 336 h LTA; $SA(CO_2)=23.8\ m^2/g$			175, 215
2.24	[4.27]			100	0.93	Montmorillonite; pH 7.0; $SA(CO_2)=20.1\ m^2/g$; CE=85.0 me/100 g	25	BE	175, 215

TABLE 6. Sorption coefficients for polychlorobiphenyls (PCBs)—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
2.16	[5.05]				0.13	Idem; LTA; SA(CO_2)=20.2 m^2/g			175, 215
1.34		100			<0.01	Ottawa silica sand; pH 5.2; SA(CO_2)=0.4 m^2/g	25	BE	175, 215
2.48	[3.68]	85.8	8.9	5.3	6.34	Ispra soil; A1 horizon; pH 4.3	22	BE	153
2.64	[4.37]	91.8	6.4	1.8	1.87	Idem; A2 horizon; pH 4.8			153
2.23	[4.53]	97.5	1.4	1.1	0.50	Idem; A3 horizon; pH 5.1			153
1.71	[4.48]	99.5	0.25	0.25	0.17	Idem; C1 horizon; pH 5.1			153
1.23		99.3	0.20	0.55	0.03	Idem; C2 horizon; pH 5.1			153
1.59	[4.51]	93.3	3.0	3.7	0.12	Idem; C3 horizon; pH 5.0			153
1.73	[4.53]	95.5	3.4	1.6	0.16	Idem; C4 horizon; pH 4.8			153
	4.17				0.7-3.8	Lake sediments			622
3.10	[4.72]	55.0	45.0	<1.0	2.4	Hickory Hill Pond sed.; pH 6.3		BE	621
3.04	[4.89]	56.0	44.0	<1.0	1.4	Doe Run Pond sed.; ph 6.1		BE	621
3.08	[5.18]				0.8	USDA Pond sed.; pH 6.4		BE	621
2.73	[5.13]	93.0	6.0	2.0	0.4	Oconee River sed.; pH 6.5		BE	621
						Aroclor-1254			
4.15						Illite clay; SA(N_2)=19.9 m^2/g		BE	624
4.00						Chlorite clay; SA(N_2)=2.1 m^2/g		BE	624
4.04						Fithian illite		BE	623
4.06	5.59				3	Fithian illite (95%)+heat-killed Thalassiosira pseudonana (5%)		BE	623
4.12	5.36				5.8	Fithian illite (90%)+heat-killed Thalassiosira pseudonana (10%)		BE	623
4.69	5.93				58	Thalassiosira pseudonana (100%)		BE	623
1.53° (0.91)						Illite clay		BE	30
2.11° (1.24)				16.2	3.1* [1.8]	Woodburn soil; silt loam		BE	30
4.23° (1.45)				57	0.9	Glendale soil; field; pH 7.57; SA(E)=177 m^2/g; CE=35.2 me/100 g; 0.005 M $CaCl_2$		BE	474
4.09° (1.47)						Idem; greenhouse			474
3.90° (1.53)				13.7	0.7	Harvey soil; field; pH 7.42; SA(E)=64.9 m^2/g; CE=14.0 me/100 g; 0.005 M $CaCl_2$		BE	474
4.05° (1.55)				13.7	0.8	Idem; greenhouse			474
3.02° (1.22)				14.5	0.9	Lea soil; field; pH 7.62; SA(E)=65.6 m^2/g; CE=14.1 me/100 g; 0.005 M $CaCl_2$		BE	474
3.08° (1.23)				14.5	0.7	Idem; greenhouse			474
3.21	[6.17]				0.11	Montmorillonite	22	BE	465
3.22						Kaolinite	22	BE	465
4.42	[6.16]				1.82	Blue clay	22	BE	465
3.56	[5.89]				0.47	Idem; treated with H_2O_2			465
4.38	[5.84]				3.45	Saginaw River 1 sedim.	22	BE	465
3.06	[5.04]				1.05	Idem; treated with H_2O_2			465
4.73	[6.31]				2.61	Saginaw River 2 sedim.	22	BE	465
4.50	[6.09]					Idem	12		465
5.18	[6.88]				1.98	Idem; NaOH extr.	22		465
4.55	[6.29]				1.84	Idem; benzene/MeOH extr.			465
5.01	[6.19]				0.67	Idem; treated with H_2O_2			465
4.89	[6.34]				3.51	Idem (<75 μm)			465
4.05					0.07	Saginaw Bay sedim.	22	BE	465
5.06	[6.10]				9.25	Huron River suspended solids	22	BE	465

TABLE 6. Sorption coefficients for polychlorobiphenyls (PCBs)—Continued

log K_d log K_f^0 (1/*n*)	log K_{oc}	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
4.95	[5.97]				9.48	Saginaw River 1 suspended solids	22	BE	465
5.07	[6.15]				8.30	Saginaw River 2 suspended solids	22	BE	465
	5.44				0.7- 3.8	Lake sediments			622
	6.0				2.0	Pond sediments			625
5.97	6.22				56	Lake suspended solids (Rice)		FM	494
3.72	5.88				0.7	Pore water/sediment (Rice)		FM	494
3.85	5.61				1.7	Idem (Rice)		FM	494
3.40	4.82				3.8	Idem (Rice)		FM	494

PCB congeners are identified by the chlorine substitution and B & Z number (Ref. 626).

Values in square parentheses have been calculated by the author.

*% OM content.

^{0}*Freundlich log nonlinear K_{om} with the respective value of (1/*n*) in below.

av average value.

Idem refers to the sorbent reported just above: only the data (texture, OC, temperature, method) which were changed are specified.

TABLE 7. Sorption coefficients for polychlorodibenzo-p-dioxins (PCDDs)

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
1,2,3,7-									
	5.39					Fulvic acid from a Manitoba soil (Brandon Caroll cl); 8.50 mg/L	20	SE	418
	5.45					Idem	30		418
	5.59					Idem; 8.08 mg/L	40		418
	5.98					Humic acid from water from a Manitoba peat bog (Piney peat); 1.95 mg/L	20	SE	418
	5.97					Idem	30		418
	5.91					Idem	40		418
	6.55					Aldrich humic acid, Na salt; 0.68 mg/L	20	SE	418
	6.42					Idem	30		418
	6.33					Idem	40		418
2,3,7,8-									
4.26	6.44	44	42	14	0.66	Soil n. 91, EPA site n. 04114B; pH 6.8; CE=5.4 me/100 g; 2 d isotherm		BE	109
4.48	6.66					Idem, prewashed five times; 10 d isotherm			109
	6.6					Idem; K_{oc} extrapolated from the data obtained with water-methanol mixtures			456
	6.6	38	40	22	7.7	Soil n. 96, EPA site n. 06126B; pH 5.8; CE=15.3 me/100 g; K_{oc} extrapolated from the data obtained with water–methanol mixtures		BE	456
	⩾6.3				2.45	Lake Ontario sediment	10	BE	498
	7.59					Idem (solid concentration data)			498
	7.25					Idem (DOC data)			498
6.6	6.8					Particulate from Baltic Sea		FM	627
	5					DOC from Baltic Sea (predicted)			627
	6.04					Correlation $\log K_{oc}-\log S$			628
	6.7					Correlation $\log K_{oc}-\log S(195)$			456
	7.0					Correlation $\log K_{oc}-\log S(108)$			456
	6.90					Correlation $\log K_{oc}-\log K_{ow}$			628
1,2,3,4,7-									
	4.85					Fulvic acid from a Manitoba soil (Brandon Caroll cl); 8.50 mg/L	20	SE	418
	4.60					Idem	30		418
	4.50					Idem	40		418
	5.80					Humic acid from water from a Manitoba peat bog (Piney peat); 1.95 mg/L	20	SE	418
	5.67					Idem	30		418
	5.90					Idem	40		418
	6.38					Aldrich humic acid, Na salt; 0.68 mg/L	20	SE	418
	6.39					Idem	30		418
	6.46					Idem	40		418
1,2,3,4,7,8-									
6.7	7.1					Particulate from Baltic Sea		FM	627
	5					DOC from Baltic Sea (predicted)			627
	5.41					Fulvic acid from a Manitoba soil (Brandon Caroll cl) 3.95 mg/L	20	SE	418
	5.31					Idem	30		418

TABLE 7. Sorption coefficients for polychlorodibenzo-p-dioxins (PCDDs)—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
	5.13					Idem	40		418
	6.02					Humic acid from water from a Manitoba peat bog (Piney peat) 1.95 mg/L	20	SE	418
	6.15					Idem	30		418
	5.95					Idem	40		418
	6.32					Aldrich humic acid, Na salt 0.86 mg/L	20	SE	418
	6.27					Idem	30		418
	6.15					Idem	40		418

Idem refers to the sorbent reported just above: only the data (texture, OC, temperature, method) which were changed are specified.

TABLE 8. Sorption coefficients for pesticides

log K_d log K_f^0 $(1/n)$	log K_{oc}	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data: prediction procedure	Temp. (°C)	Meth.	Ref.
						Alachlor			
2.85° (0.70)				100		Wyoming Li–montmorillonite <2 μm fraction	5	BE	395
2.60° (0.85)						Idem	22		395
2.99° (1.64)				100		Wyoming Na–montmorillonite <2 mm fraction	5	BE	395
1.46° (1.18)						Idem	22		395
3.92° (1.40)				100		Wyoming K–montmorillonite <2 mm fraction	5	BE	395
1.80° (1.65)						Idem	22		395
3.41° (0.81)				100		Wyoming Rb–montmorillonite <2 mm fraction	5	BE	395
3.51° (0.82)						Idem	22		395
3.32° (0.87)				100		Wyoming Cs–montmorillonite <2 mm fraction	5	BE	395
3.44° (0.85)						Idem	22		395
3.35° (0.99)				100		Wyoming HN_4–montmorillonite <2 mm fraction	5	BE	395
3.15° (0.99)						Idem	22		395
3.21° (0.94)				100		Wyoming Ca–montmorillonite <2 mm fraction	5	BE	395
2.97° (0.94)						Idem	22		395
3.10° (0.99)				100		Wyoming Mg–montmorillonite <2 mm fraction	5	BE	395
3.02° (0.99)						Idem	22		395
3.25° (0.98)				100		Wyoming Cu–montmorillonite <2 mm fraction	5	BE	395
3.22° (0.96)						Idem	22		395
1.99° (0.88)				100		Wyoming Al–montmorillonite <2 mm fraction	5	BE	395
3.40° (0.85)						Idem	22		395
0.48° (0.85)			60	23	2.64	Waukegan soil; pH 5.8; CE=23 cmol/kg		BE	158
0.61° (0.80)			30	27	2.77	Ves soil; pH 4.8; Ce=20 cmol/kg		BE	158
−0.52° (0.98)	1.58				0.79	Plainfield s soil, unamended; pH 6.8–7.0	25	BE	282
0.20° (1.09)	2.29				0.81	Idem; amended with waste activated carbon (WAC) at 0.5 t C/ha			282
0.40° (0.97)	2.48				0.84	Idem; amended with WAC at 1.0 t C/ha			282
0.62° (0.97)	2.67				0.88	Idem; amended with WAC at 2.1 t C/ha			282
−0.09° (0.81)					0.88	Idem; amended with digested munic. sewage sludge (DMS) at 2.1 t C/ha			282
0.00° (1.00)	2.01				0.98	Idem; amended with DMS at 4.2 t C/ha			282
0.20° (1.00)	2.14				1.16	Idem; amended with DMS at 8.4 t C/ha			282
−0.01° (0.97)	2.05				0.88	Idem; amended with animal manure (AM) at 2.1 t C/ha			282

TABLE 8. Sorption coefficients for pesticides—Continued

log K_d log K_f^0 (1/n)	log K_{oc}	Sorbent composition (%) Sand	 Silt	 Clay	 OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
0.03° (1.00)	2.04				0.98	Idem; amended with AM at 4.2 t C/ha			282
0.09° (0.95)	2.03				1.16	Idem; amended with AM at 8.4 t C/ha			282
0.54	2.53	25	49	26	1.02	Dundee tilled soil (0–5 cm); pH 5.76; 0.01 M $CaCl_2$	25	BE	159
0.73	2.51	20	51	29	1.67	Idem; no-tilled; pH 5.54			159
−0.23	[2.31]	80	15	5	0.5* [0.29]	Augusta soil; pH 5.7; CE=3.2 me/100 g; SA(E)=3.3 m^2/g	28	BE	280
−0.28	[2.25]	89	9	2	0.5* [0.29]	Norfolk soil; pH 5.4; CE=2.3 me/100 g; SA(E)=4.4 m^2/g	28	BE	280
0.19	[2.34]	72	23	5	1.2* [0.70]	Goldsboro soil; pH 5.3; CE=3.3 me/100 g; SA(E)=7.0 m^2/g	28	BE	280
−0.03	[2.06]	82	10	8	1.4* [0.81]	Appling soil; pH 6.8; CE=6.9 me/100 g; SA(E)=12.8 m^2/g	28	BE	280
0.42	[2.26]	70	22	8	2.5* [1.45]	Lynchburg soil; pH 5.5; CE=6.6 me/100 g; SA(E)=13.6 m^2 g	28	BE	280
0.01	[2.01]	76	16	8	1.7* [0.99]	Cecil soil; pH 5.4; CE=3.1 me/100 g; SA(E)=16.3 m^2/g	28	BE	280
0.40	[2.41]	26	64	10	1.7* [0.99]	Rains soil; pH 6.0; CE=7.1 me/100 g; SA(E)=18.8 m^2/g	28	BE	280
0.62	[2.22]	61	26	12	4.4* [2.55]	Portsmouth soil; pH 5.4; CE=10.6 me/100 g; SA(E)=20.6 m^2/g	28	BE	280
1.13	[2.41]	52	36	13	8.7* [5.05]	Cape Fear soil; pH 5.1; CE=10.3 me/100 g; SA(E)=77.2 m^2/g	28	BE	280
0.031° (0.61)		22	66	12	1.45*	Gigger soil, no-tilled; pH 5.37; 0.05 M $CaCl_2$		BE	161
−0.327° (0.66)		22	66	12	0.81*	Idem, tilled; pH 5.23		BE	161
−0.85	[2.03]	97.1	2.3	0.6	0.13	Tampa aquifer; pH 8. 0.01 N $CaCl_2$		BE	521
	[2.43]				63.36	Humic acid from municipal sewage sludge; pH 4.0	20	BU	160
	[2.44]				55.75	Humic acid from a control soil; pH 4.0	20	BU	160
	[2.34]				53.56	Humic acid from a soil amended with sewage sludge; pH 4.0	20	BU	160
	2.28					Soil; experimental (literature)			217
	2.32					Correlation log K_{oc}−log S			564
						Aldicarb			
−0.77° (0.93)	[1.52]	77	15	8	0.51	Sarpy soil; pH 7.3; CE=5.7 me/100 g; 0.01 M $CaCl_2$	24	BE	122
−0.70° (0.95)	[1.27]	83	9	8	1.07	Thurman soil; pH 6.83; CE=6.1 me/100 g; 0.01 M $CaCl_2$	24	BE	122
−0.21° (0.86)		37	42	21	2.64	Clarion agricol. soil; pH 5.00; CE=21 me/100 g; 0.01 M $CaCl_2$	24	BE	122
0.06° (0.85)		21	55	24	3.80	Harps agricol. soil; pH 7.30; CE=37.8 me/100 g; 0.01 M $CaCl_2$	24	BE	122
0.54° (0.89)	[1.28]	42	39	19	18.36	Peat; pH 6.98; CE=77.3 me/100 g; 0.01 M $CaCl_2$	24	BE	122
	[1.63]				3.53* [2.05]	Batcombe sil soil; pH 6.1; 0.01 M $CaCl_2$	20	BE	120
−0.82	1.11	53	37	10	1.17	Palmira soil; pH 4.9; CE=8.2 cmol/kg	15	BE	629
−1.15	0.78	53	37	10	1.17	Idem	25	BE	629
−1.22	0.71	53	37	10	1.17	Idem	35	BE	629

TABLE 8. Sorption coefficients for pesticides—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
	1.51					Correlation $\log K_{oc}$– $\log S$			564
						Aldrin			
[3.00]	[4.69]				3.53* [2.05]	Batcombe sil soil; pH 6.1; 0.01 M $CaCl_2$	20	BE	120
3.64	5.38	25	40	35	1.8	Taichung soil; pH 6.8	25	BE	407
	5.05					Aldrich humic acid	25	SE	407
	2.61					Soil; experimental (literature)			217
	4.68					Correlation $\log K_{oc}$–$\log S$			564
	5.02					Correlation $\log K_{oc}$ –MCI			598
	[5.22]					Correlation $\log K_{om}$ –MCI			591
						Ametryne (pK_a=3.93, Ref. 679)			
T.A.				100		H–montmorillonite; pH 3.6		BE	212
1.34				100		Na–montmorillonite; pH 7.9		BE	212
1.77				100		Ca–montmorillonite; pH 7.9		BE	212
1.38				100		Mg–montmorillonite; pH 8.2		BE	212
0.49	[2.33]	74.4	19.5	6.1	2.5* [1.45]	Aguadilla soil; pH 7.4; CE=10 me/100 g; 0.01 M $CaCl_2$		BE	256
0.44	[2.57]	27.6	35.6	36.8	1.3* [0.75]	Aguirre soil; pH 9.0; CE=14.3 me/100 g; 0.01 M $CaCl_2$		BE	256
0.85	[2.58]	14.9	39.3	45.8	3.2* [1.86]	Alonso soil; pH 5.1; CE=13.8 me/100 g; 0.01 M $CaCl_2$		BE	256
0.41	[2.08]	49.2	28.8	22.0	3.7* [2.15]	Altura soil; pH 8.0; CE=27.6 me/100 g; 0.01 M $CaCl_2$		BE	256
0.51	[2.51]	68.1	4.4	27.5	1.7* [0.99]	Bayamòn soil; pH 4.7; CE=5.0 me/100 g; 0.01 M $CaCl_2$		BE	256
2.22	[2.91]	36.0	36.0	28.0	36.0* [20.8]	Cano Tiburones soil; pH 5.5; CE=86.0 me/100 g; 0.01 M $CaCl_2$		BE	256
0.44	[2.40]	6.6	28.9	64.5	1.9* [1.10]	Catalina soil; pH 4.7; CE=11.8 me/100 g; 0.01 M $CaCl_2$		BE	256
0.32	[2.23]	89.0	7.3	2.08	2.1* [1.22]	Catano soil; pH 7.9; CE=6.9 me/100 g; 0.01 M $CaCl_2$		BE	256
0.60	[2.53]	58.8	23.4	17.8	2.0* [1.16]	Cayaguà soil; pH 5.2; CE=7.3 me/100 g; 0.01 M $CaCl_2$		BE	256
1.12	[2.67]	13.3	34.8	51.9	4.9* [2.84]	Cialitos soil; pH 5.4; CE=18.6 me/100 g; 0.01 M $CaCl_2$		BE	256
0.96	[2.63]	22.7	37.4	39.9	3.7* [2.15]	Coloso soil; pH 5.7; CE=23.0 me/100 g; 0.01 M $CaCl_2$		BE	256
0.40	[2.13]	23.4	24.8	51.8	3.2* [1.86]	Coto soil; pH 7.7; CE=14.0 me/100 g; 0.01 M $CaCl_2$		BE	256
0.57	[2.28]	39.1	29.7	32.2	3.4* [1.97]	Fe soil; pH 7.5; CE=27.6 me/100 g; 0.01 M $CaCl_2$		BE	256
1.26	[2.98]	15.0	50.7	34.3	3.3* [1.91]	Fortuna soil; pH 5.4; CE=23.3 me/100 g; 0.01 M $CaCl_2$		BE	256
0.52	[2.44]	15.5	32.5	52.0	2.1* [1.22]	Fraternidad soil; pH 6.3; CE=36.0 me/100 g; 0.01 M $CaCl_2$		BE	256
0.91	[2.52]	11.1	23.8	65.1	4.2* [2.44]	Fraternidad (Lajas) soil; pH 5.9; CE=58.0 me/100 g; 0.01 M $CaCl_2$		BE	256
0.61	[2.16]	6.4	19.6	74.0	4.8* [2.78]	Guànica soil; pH 8.1; CE=52.1 me/100 g; 0.01 M $CaCl_2$		BE	256
0.67	[2.68]	10.1	50.9	39.0	1.7* [0.99]	Humata soil; pH 4.5; CE=10.1 me/100 g; 0.01 M $CaCl_2$		BE	256
0.85	[2.57]	26.6	53.5	20.9	3.3* [1.91]	Josefa soil; pH 6.0; CE=16.8 me/100 g; 0.01 M $CaCl_2$		BE	256
1.04	[2.84]	15.2	41.6	43.2	2.7* [1.57]	Juncos soil; pH 6.2; CE=13.4 me/100 g; 0.01 M $CaCl_2$		BE	256
0.81	[2.46]	19.9	33.4	46.7	3.9* [2.26]	Mabì soil; pH 7.0; CE=55.2 me/100 g; 0.01 M $CaCl_2$		BE	256
0.75	[2.29]	22.7	40.7	36.6	4.9* [2.84]	Mabì soil; pH 5.7; CE=31.0 me/100 g; 0.01 M $CaCl_2$		BE	256
0.38	[2.23]	14.9	42.8	2.38	2.4*	Mercedita soil; pH 8.1;		BE	256

TABLE 8. Sorption coefficients for pesticides—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data: prediction procedure	Temp. (°C)	Meth.	Ref.
					[1.39]	CE=19.9 me/100 g; 0.01 M $CaCl_2$			
1.13	[2.79]	26.3	27.7	46.0	3.8* [2.20]	Moca soil; pH 5.8; CE=31.0 me/100 g; 0.01 M $CaCl_2$		BE	256
1.02	[2.74]	28.0	47.0	25.0	3.3* [1.91]	Mùcara soil; pH 5.8; CE=19.6 me/100 g; 0.01 M $CaCl_2$		BE	256
0.98	[2.49]	22.8	49.2	28.0	5.3* [3.07]	Nipe soil; pH 5.7; CE=11.9 me/100 g; 0.01 M $CaCl_2$		BE	256
0.56	2.50	59.4	28.2	12.4	2.0* [1.16]	Pandura soil; pH 5.7; CE=7.7 me/100 g; 0.01 M $CaCl_2$		BE	256
0.51	[2.20]	13.4	43.6	43.0	3.5* [2.03]	Rio Piedras soil; pH 4.9; CE=11.5 me/100 g; 0.01 M $CaCl_2$		BE	256
0.64	[2.44]	24.3	49.7	26.0	2.7* [1.57]	San Antòn soil; pH 6.7; CE=26.1 me/100 g; 0.01 M $CaCl_2$		BE	256
0.79	[2.88]	73.4	19.4	7.2	1.4* [0.81]	Talante soil; pH 5.1; CE=4.0 me/100 g; 0.01 M $CaCl_2$		BE	256
0.99	[2.92]	41.5	38.3	20.2	2.0* [1.16]	Toa soil; pH 5.3; CE=13.0 me/100 g; 0.01 M $CaCl_2$		BE	256
0.32	[2.77]	60.9	25.1	14.0	0.6* [0.35]	Toa soil; pH 6.0; CE=8.0 me/100 g; 0.01 M $CaCl_2$		BE	256
0.71	[2.40]	73.7	12.6	13.7	3.5* [2.03)	Vega Alta soil; pH 5.0; CE=5.6 me/100 g; 0.01 M $CaCl_2$		BE	256
0.93	[2.80]	45.2	36.8	18.0	2.3* [1.33]	Via soil; pH 5.1; CE=39.9 me/100 g; 0.01 M $CaCl_2$		BE	256
	2.59					Soil; experimental (literature)			217
	2.59av					32 soils (literature)			87
	2.40					Correlation $\log K_{oc}-\log S$			564
						Asulam (**pK_a=4.82**, Ref. 674)			
2.37	[2.64]				94* [54.5]	OM from peaty muck (Histosol) soil; pH 5.5	24	BE	121
	2.48					Soil; experimental (literature data)			217
	2.52					Correlation $\log K_{oc}$ −MCI			598
	1.60					Correlation $\log K_{oc}-\log S$			564
						Atratone (**pK_a=4.20**, Ref. 247)			
TA				100		H–montmorillonite (1–0.2 μm); pH 3.35; CE=73.5 me/100 g	25	BE	250
2.64° (0.48)				100		Na–montmorillonite (1–0.2 μm); pH–6.80; CE=87.0 me/100 g	25	BE	250
TA				100		H–montmorillonite; pH 8.6		BE	212
1.08				100		Na–montmorillonite; pH 7.9		BE	212
1.15				100		Ca–montmorillonite; pH 7.9		BE	212
1.00				100		Mg–montmorillonite; pH 8.2		BE	212
						Atrazine (**pK_a=1.68**, Ref. 679)			
TA				100		H–montmorillonite (1–0.2 μm); pH 3.35; CE=73.5 me/100 g	25	BE	250
1.18° (0.85)				100		Na–montmorillonite (1–0.2 μm); pH 6.80; CE=87.0 me/100 g	25	BE	250
TA				100		H–montmorillonite; pH 3.6		BE	212
0.78				100		Na–montmorillonite; pH 7.9		BE	212
1.11				100		Ca–montmorillonite; pH 7.9		BE	212
1.00				100		Mg–montmorillonite; pH 8.2		BE	212
1.54				100		Mississippi bentonite; pH 8.5	0	BE	251
0.83						Idem	50		251
1.03° (0.92)						Bentonite; 0.1 M $CaCl_2$	22	BE	144
1.56	[1.91]				77* [44.7]	Houghton muck; pH 5.6	0	BE	251
1.52	[1.87]					Idem	50		251
[1.30]	[1.74]				63* [36.5]	Mesic peat (acid treated); 0.01 M $CaCl_2$		BE	477

TABLE 8. Sorption coefficients for pesticides—Continued

log K_d log K_f^0 (1/n)	log K_{oc}	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
−0.96	[1.93]	97.1	2.3	0.6	0.13	Tampa aquifer; pH 8; 0.01 N $CaCl_2$		BE	521
0.46° (0.92)	1.95	57.8	19.6	22.6	5.6* [3.25]	Vetroz soil; pH 6.7	20	BE	630
0.30° (0.93)	1.98	38.4	49.4	12.2	3.6* [2.09]	Evouettes soil; pH 6.1	20	BE	630
−0.07° (0.89)	1.83	87.0	10.2	2.8	2.2* [1.28]	Collombey soil; pH 7.8	20	BE	630
0.45° (0.80)			73	21	2.6	Plano soil; pH 6.1; CE=17 cmol/kg; 0.01 M $CaCl_2$	23	BE	480
0.63° (0.81)						Idem; pH 4.5			480
0.46° (0.85)			59	22	2.8	Waukegan soil; pH 6.1; CE=21 cmol/kg; 0.01 M $CaCl_2$	23	BE	480
0.70° (0.83)						Idem; pH 4.0			480
0.44° (0.83)			60	23	2.64	Waukegan soil; pH 5.8; CE=23 cmol/kg		BE	158
0.63° (0.83)			30	27	2.77	Ves soil; pH 4.8; Ce=20 cmol/kg		BE	158
0.41	[1.80]	2.9	68.7	28.4	7.1* [4.12]	Lanton soil; pH 6.4; CE=32.8 me/100 g		BE	631
0.72	[2.28]		59	22	2.8	Waukegan soil; pH 4.1; CE=21 cmol/kg; 0.01 M $CaCl_2$	23	BE	323
0.46	[2.02]					Idem; pH 6.2			323
0.56	[2.14]		73	21	2.6	Plano soil; pH 4.7; CE=17 cmol/kg; 0.01 M $CaCl_2$	23	BE	323
0.54	[2.13]					Idem; pH 5.8			323
0.38	[1.97]					Idem; pH 6.3			323
0.23	[2.19]		62	15	1.1	Walla Walla soil; pH 5.0; CE=20 cmol/kg; 0.01 M $CaCl_2$	23	BE	323
0.08	[2.04]					Idem; pH 5.5			323
0.04	[2.00]					Idem; pH 6.0			323
0.60° (0.83)				33	3.8* [2.2]	Sharpsburg soil; pH 5.2; Water:soil(w/s)=0.4:1; 0.01 M $CaCl_2$	30	BE	241
0.58° (0.83)						Idem; w/s=5:1			241
	[2.37]								
0.27° (0.86)				28	2.9* [1.7]	Monona soil; pH 5.8; w/s=0.4:1; 0.01 M $CaCl_2$	30	BE	241
0.29° (0.84)						Idem; w/s=5:1			241
	[2.18]								
0.13° (0.84)				13	2.9* [1.7]	Keith soil; pH 6.3; w/s=0.4:1; 0.01 M $CaCl_2$	30	BE	241
0.20° (0.79)						Idem; w/s=5:1			241
	[2.08]								
0.12° (0.81)				6	1.4* [0.81]	Valentine soil; pH 5.9; w/s=0.4:1; 0.01 M $CaCl_2$	30	BE	241
0.14° (0.74)						Idem; w/s=5:1			241
	[2.10]								
0.87	[3.76]				0.22* [0.13]	Holdrege 1 soil; pH 5.6; conventional till (C.T.); 0–2.5 cm depth (d.)		BE BE	632
0.88	[3.77]					Idem; pH 5.2; C.T.; 2.5–5 cm d.			632
0.88	[3.82]				0.20* [0.12]	Idem; pH 5.7; C.T.; 5–10 cm d.			632
0.83	[3.76]				0.19* [0.11]	Idem; pH 6.2; C.T.; 10–15 cm d.			632

TABLE 8. Sorption coefficients for pesticides—Continued

log K_d log K_f^0 (1/n)	log K_{oc}	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
0.81	[3.80]				0.18* [0.10]	Idem; pH 6.3; C.T.; 15–20 cm d.			632
0.81					0.14* [0.08]	Idem; pH 6.6; C.T.; 20–25 cm d.			632
0.78					0.12* [0.07]	Idem; pH 6.7; C.T.; 25–30 cm d.			632
0.76					0.09* [0.05]	Idem; pH 6.9; C.T.; 30–35 cm d.			632
0.74					0.08* [0.05]	Idem; pH 7.0; C.T.; 35–40 cm d.			632
0.89	[3.61]				0.33* [0.19]	Idem; no till (N.T.); pH 5.2; 0–2.5 cm d.			632
0.85	[3.67]				0.26* [0.15]	Idem; N.T.; pH 5.0; 2.5–5 cm d.			632
0.85	[3.83]				0.18* [0.10]	Idem; N.T.; pH 5.8; 5–10 cm d.			632
0.86	[3.85]				0.18* [0.10]	Idem; N.T.; pH 6.2; 10–15 cm d.			632
0.85	[3.83]				0.18* [0.10]	Idem; N.T.; pH 6.3; 15–20 cm d.			632
0.79					0.14* [0.08]	Idem; N.T.; pH 6.5; 20–25 cm d.			632
0.79					0.12* [0.07]	Idem; N.T.; pH 6.7; 25–30 cm d.			632
0.79					0.11* [0.06]	Idem; N.T.; pH 6.8; 30–35 cm d.			632
0.76					0.10* [0.06]	Idem; N.T.; pH 6.9; 35–40 cm d.			632
0.30	[2.08]	30.1	55.2	14.7	1.64	Valois soil; pH 5.9; 0.005 M $CaSO_4$	23–27	BE	527
0.50	[2.00]	12.2	52.3	35.5	3.13	Rhinebeck soil; pH 6.7; 0.005 M $CaSO_4$	23–27	BE	527
0.68° (0.98)	2.57	3.31	21.9	75.0	1.30	Eurosol-1; c; pH 5.1; 0.01 M $CaCl_2$		BE	583
0.94	2.83					Idem; EEC laboratory ringtest			62
0.29° (0.88)	1.72	3.4	64.1	22.6	3.70	Eurosol-2; sil; pH 7.4; 0.01 M $CaCl_2$		BE	583
0.39	1.83					Idem; EEC laboratory ringtest			62
0.28° (0.99)	1.75	46.4	36.8	17.0	3.45	Eurosol-3; l; pH 5.2; 0.01 M $CaCl_2$		BE	583
0.45	1.91					Idem; EEC laboratory ringtest			62
−0.30° (1.05)	1.51	4.1	75.7	20.3	1.55	Eurosol-4; si; pH 6.5; 0.01 M $CaCl_2$		BE	583
−0.07	1.74					Idem; EEC laboratory ringtest			62
1.36 (0.87)		81.6	12.6	6.0	9.25	Eurosol-5; ls; pH 3.2; 0.01 M $CaCl_2$		BE	583
1.64	2.67					Idem; EEC laboratory ringtest			62
−0.91	1.69	1.7	82.4	16.0	0.25	Eurosol-6; EEC laboratory ringtest; pH 7.2; 0.01 M $CaCl_2$		BE	62
0.00^{b} (0.85)				18	3.3* [1.91]	Lakeland sl soil; pH 6.2; CE=2.9 me/100 g; 0.01 M $CaCl_2$	26	BE	633
0.26° (0.84)				43	1.9* [1.10]	Wehadkee sil soil pH 5.6; CE=10.2 me/100 g; 0.01 M $CaCl_2$	26	BE	633
0.60° (0.87)				38	4.4* [2.55]	Chillum sl soil; pH 4.6; CE=7.6 me/100 g; 0.01 M $CaCl_2$	26	BE	633
0.57° (0.87)				48	4.3* [2.49]	Hagerstown sicl soil; pH 5.5; 26 CE=12.5 me/100 g; 0.01 M $CaCl_2$		BE	633
0.23	[1.95]				3.31* [1.92]	Battrum sc soil; pH 5.6; Al=2031 ppm; Fe=6868 ppm	25	BE	296
0.28	[2.06]				2.85* [1.65]	Swift Current 1 soil; pH 6.0 Al=1794 ppm; Fe=5361 ppm	25	BE	296
1.25° (0.93)	[2.17]	45.5	15.9	6.6	12	Great House E.H.F. soil; pH 6.3; CE=18 me/100 g; 0.1 M $CaCl_2$	22	BE	144

TABLE 8. Sorption coefficients for pesticides—Continued

log K_d log K_f^0 (1/n)	log K_{oc}	Sorbent composition (%)				Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
0.35° (0.85)		66.0	18.4	15.6	1.93	Weed Res. Orgn. soil; pH 7.1: CE=11 me/100 g; 0.1 M $CaCl_2$	22	BE	144
2.16° (0.90)	[2.52]				76* [44]	OM from peat soil; 0.1 M $CaCl_2$	22	BE	144
2.14	[2.50]				76* [44]	OM from peat soil; 0.1 M $BaCl_2$		BE	270
	1.91*					Peat humic acid; 0.1 M $BaCl_2$		BE	270
0.62° (0.86)		17	56	27	0.24	Brandt soil; pH 5.74; 0.01 M $CaCl_2$; no incubation (N.I.)	25	BE	403
0.37° (0.86)						Idem; pH 7.81; +NH_3 (1.4 mg N/g soil); N.I.			403
0.25° (0.88)						Idem; pH 8.92; +NH_3 (2.8 mg N/g soil); N.I.			403
0.45° (0.85)						Idem; pH 5.69; 0.01 M $CaCl_2$; 8 d incubation (8 d I.)			403
0.35° (0.85)						Idem; pH 7.70; +NH_3 (1.4 mg N/g soil); 8 d I.			403
0.32° (0.86)						Idem; pH 8.17; +NH_3 (2.8 mg N/g soil); 8 d I.			403
0.66° (0.84)		43	27	27	0.22	Ves soil; pH 5.61; 0.01 M $CaCl_2$; N.I.	25	BE	403
0.52° (0.85)						Idem; pH 7.60; +NH_3 (1.4 mg N/g soil); N.I.			403
0.28° (0.88)						Idem; pH 8.88; +NH_3 (2.8 mg N/g soil); N.I.			403
0.53° (0.81)						Idem; pH 5.39; 0.01 M $CaCl_2$; 8 d I.			403
0.41° (0.83)						Idem; pH 7.10; +NH_3 (1.4 mg N/g soil); 8 d I.			403
0.29° (0.85)						Idem; pH 7.97; +NH_3 (2.8 mg N/g soil); 8 d I.			403
−0.57° (0.79)		67.1	25.8	7.1	0.43	Hanford soil; pH 6.05; CE=5.95 cmol/kg; 0.01 M $CaCl_2$	25	BE	528
−0.82° (0.83)		82.0	13.5	4.5	0.33	Tuiunga soil; pH 6.30; CE=0.45 cmol/kg; 0.01 M $CaCl_2$	25	BE	528
1.11	[2.55]	25	45	30	6.3* [3.65]	Drummer soil; CE=40 me/100 g; pH 3.9	0.5	BE	286
1.10	[2.54]					Idem	20		286
1.02	[2.46]					Idem	40		286
1.06	[2.49]					Idem; pH 4.7	0.5		286
1.03	[2.47]					Idem	20		286
0.93	[2.37]					Idem	40		286
1.03	[2.47]					Idem; pH 5.3	0.5		286
0.91	[2.35]					Idem	20		286
0.84	[2.28]					Idem	40		286
0.83	[2.27]					Idem; pH 6.0	0.5		286
0.81	[2.25]					Idem	20		286
0.73	[2.17]					Idem	40		286
0.78	[2.21]					Idem; pH 8.0	0.5		286
0.80	[2.24]					Idem	20		286
0.66	[2.10]					Idem	40		286
	2.63*					Humic acid from Leonardite; pH 2.5	0.5	BE	286
	2.80*					Idem; pH 2.5	20		286
	2.92*					Idem; pH 2.5	40		286
	1.64*					Idem; pH 7.0	0.5		286
	1.79*					Idem; pH 7.0	20		286
	1.90*					Idem; pH 7.0	40		286
0.55° (0.90)	[2.56]	3	36	61	1.7* [0.99]	Sharkey soil; Ap horizon; pH 6.48; 0.01 N $Ca(NO_3)_2$		BE	483
	1.98av	6–94	3–66	3–35	0.8–3.9	5 soils. 0.01 N $CaCl_2$	25	BE	455

TABLE 8. Sorption coefficients for pesticides—Continued

log K_d log K_f^0 ($1/n$)	log K_{oc}	Sorbent composition (%)				Other sorbent and solution data: prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
	1.95av					5 soils; extrapolated from lof K_d-f_c plots (methanol-water)	25	BE	455
	1.95av					5 soils; extrapolated from log K_d-f_c plots (acetone–water)	25	BE	455
−0.82	[1.88]	93.8	3.0	3.2	0.2	Eustis soil; pH 5.7; 0.01 N $CaCl_2$	25	BE	452
0.48– 0.56 0.53av	2.07– 2.12 2.10av	39.4– 43.1	36.6– 38.7	20.3– 21.9	2.58– 2.97 2.72av	Clarion soil; 6 aggregate sizes from 0 to 5 mm; 0.01 M $CaCl_2$	21–23	BE	634
0.55– 0.61 0.59av	2.16– 2.25 2.21av	2.2– 4.3	72.6– 74.6	23.0– 23.8	2.31– 2.47 2.42av	Edina soil; 6 aggregate sizes from 0 to 5 mm; 0.01 M $CaCl_2$	21–23	BE	634
0.38av	2.33av			10.5av	0.81av	109 soil horizons from 24 soil profiles; CE_{av}= 15.3 me/100 g; pH 5.8	22	BE	227
0.34	[1.96]		32.8	13.7	2.37	CVa, Merrimac f_{sl} soil (0–15 cm); 0.01 M $CaCl_2$	21	BE	481
0.12	[1.90]		42.7	8.7	1.65	CVb, Merrimac f_{sl} soil (5–30 cm); 0.01 M $CaCl_2$	21	BE	481
0.24	[2.09]		21.5	15.9	1.43	W3, Merrimac sl soil (0–15 cm); 0.01 M $CaCl_2$	21	BE	481
0.037° (0.95)	[2.33]		2	3	0.5	Zimmerman fine sand (0–15 cm); pH 5.8; 0.01 M $CaCl_2$		BE	635
−0.01° (0.93)	[2.39]		4	3	0.4	Idem (35–50 cm); pH 4.4; 0.01 M $CaCl_2$		BE	635
−0.43° (1.02)	[2.58]		1	1	0.1	Idem (175–190 cm); pH 6.1; 0.01 M $CaCl_2$		BE	635
−0.68° (1.00)	[1.92]	77	18	5	0.44* [0.26]	Mohave soil; pH 6.5; CE=5.1 me/100 g; 0.01 M $CaCl_2$	25	BE	127
0.42° (0.85)		16	68	16	2.58* [1.50]	Walla Walla soil; pH 6.8; CE=20 me/100 g; 0.01 M $CaCl_2$	25	BE	127
−0.22	[1.78]				1.7* [0.99]	Simeon sl soil; (0–60 cm depth)		BE	636
−0.34	[2.43]				0.3* [0.17]	Simeon ls soil; (60–90 cm depth)		BE	636
−0.35					0.1* [0.06]	Simeon s soil; (90–180 cm depth)		BE	636
0.19° (0.88)	[2.06]		40	21	1.35	Rambouillet soil (0–20 cm); pH 6.0; CE=11.4 cmol/kg; 0.01 M $CaCl_2$	25	BE	637
−0.19° (0.87)		26	63	11	0.63	Taloka soil; pH 5.6; 0.01 M $CaCl_2$	22	BE	234
0.49° (0.87)		38	50	12	2.41	Mountainburg soil; pH 5.5; 0.01 M $CaCl_2$	22	BE	234
0.78° (0.73)		18.4	45.3	38.3	3.87	Webster soil; CE=54.7 me/100 g; pH 7.3; 0.01 N $CaCl_2$	23	BE	102
−0.05° (1.04)	2.00	65.8	19.5	14.7	0.90	Cecil soil; CE=6.8 me/100 g; pH 5.6; 0.01 N $CaCl_2$	23	BE	102
−0.21° (0.79)		93.8	3.0	3.2	0.56	Eustis soil; CE=5.2 me/100 g; pH 5.6; 0.01 N $CaCl_2$	23	BE	102
0.32° (~0.9)	[2.04]	66.0	18.4	15.6	1.93	Begbroke soil; pH 7.1; 1:10 soil:water	22	BE	462
0.00	[1.71]					Idem	22	BE	638
−0.10° (~0.9)	[1.62]					Begbroke soil; pH 7.1; 4:1 soil:water	22	BE	462
0.09° (0.84)		3.6	64.7	31.7	1.11	Agricultural soil; pH 8.2; 1.9% $CaCO_3$	20	BE	347
0.08° (0.86)		29.2	19.5	51.3	1.50	Agricultural soil; pH 8.0; 26.4% $CaCO_3$	20	BE	347
−0.02° (0.82)		24.5	13.0	62.5	1.08	Agricultural soil; pH 8.0; 3.2% $CaCO_3$	20	BE	347
0.28	[2.24]	6	74	20	1.9* [1.1]	Putnam soil; pH 5.3; CE=12.3 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.65	[2.27]	4	66	30	4.2* [2.4]	Marshall soil; pH 5.4; CE=21.3 me/100 g; 0.01 M $CaCl_2$	20	BE	145

TABLE 8. Sorption coefficients for pesticides—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%)				Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
0.68	[2.36]	3	67	30	3.6* [2.1]	Grundy soil; pH 5.6; CE=13.5 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.34	[2.43]	9	74	17	1.4* [0.81]	Marian soil; pH 4.6; CE=9.9 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.56	[2.33]	4	72	24	2.9* [1.7]	Knox soil; pH 5.4; CE=18.8 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.51	[2.18]	26	43	31	3.6* [2.1]	Shelby soil; pH 4.3; CE=20.1 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.42	[2.48]	30	44	26	1.5* [0.87]	Lindley soil; pH 4.7; CE=6.9 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.57	[2.46]	1	36	63	2.2* [1.3]	Wabash soil; pH 5.7; CE=40.3 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.36	[2.28]	32	50	18	2.1* [1.2]	Salix soil; pH 6.3; CE=17.9 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.34	[2.47]	40	41	19	1.3* [0.75]	Sarpy soil; pH 7.1; CE=14.3 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.75	[2.29]	5	48	47	4.9* [2.8]	Summit soil; pH 4.8; CE=35.1 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.43	[2.21]	5	67	28	2.9* [1.7]	Oswego soil; pH 6.4; CE=21.0 me/100 g; 0.01 M $CaCl_2$	20	BE	145
−0.10	[1.99]	1	76	23	1.4* [0.81]	Bates soil; pH 6.5; CE=9.3 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.51	[2.31]	1	76	23	2.7* [1.6]	Gerald soil; pH 4.7; CE=11.0 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.26	[2.29]	11	75	14	1.6* [0.93]	Newtonia soil; pH 5.2; CE=8.8 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.40	[2.16]	8	72	20	3.0* [1.7]	Eldon soil; pH 5.9; CE=12.9 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.36	[2.28]	9	72	19	2.1* [1.2]	Baxter soil; pH 6.0; CE=11.2 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.23	[2.09]	4	85	11	2.4* [1.4]	Menfro soil; pH 5.3; CE=9.1 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.61	[2.60]	2	79	19	1.8* [1.04]	Union soil; pH 5.4; CE=6.8 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.34	[2.33]	13	70	17	1.8* [1.04]	Labanon soil; pH 4.9; CE=7.7 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.23	[2.32]	20	67	13	1.4* [0.81]	Clarksville soil; pH 5.7; CE=5.7 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.15	[2.30]	20	63	17	1.2* [0.70]	Cumberland soil; pH 6.4; CE=6.5 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.49	[2.33]	25	30	45	2.5* [1.5]	Sharkey soil; pH 5.0; CE=28.2 me/100 g; 0.01 M $CaCl_2$	20	BE	145
−0.22	[2.23]	84	11	5	0.6* [0.35]	Lintonia soil; pH 5.3; CE=3.2 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.48	[2.41]	14	66	20	2.0* [1.2]	Waverley soil; pH 6.4; CE=12.8 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.72						Illite; pH 7; CE=24 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.76						Idem; pH 5	20	BE	145
0.18						Putnam clay; pH 5; CE=42 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.63						Montmorillonite; pH 7; CE=105 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.78						Idem; pH 5	20	BE	145
1.33						Wisconsin peat; pH 7; CE=118 me/100 g; 0.01 M $CaCl_2$	20	BE	145
1.33						Idem; pH 5	20	BE	145
1.96						Peat moss; pH 7; CE=106 me/100 g; 0.01 M $CaCl_2$	20	BE	145
−0.17	[2.16]	86.4	9.1	4.5	0.46	Plainfield soil (0–20 cm); pH 6.4; CE=2.5 cmol/kg; 0.01 M $CaCl_2$	12.5	BE	639

TABLE 8. Sorption coefficients for pesticides—Continued

log K_d log K_f^0 ($1/n$)	log K_{oc}	Sorbent composition (%)				Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
−0.42	[2.01]	95.0	3.2	1.8	0.37	Sparta soil (0–20 cm); pH 5.5; CE=2.0 cmol/kg; 0.01 M $CaCl_2$	12.5	BE	639
−1.10		94.7	3.2	2.2	0.07	Plainfield (50–80 cm); pH 6.0; CE=1.0 cmol/kg; 0.01 M $CaCl_2$	12.5	BE	639
−1.05	[1.78]	95.7	2.0	2.3	0.15	Sparta soil (50–80 cm); pH 5.8; CE=1.0 cmol/kg; 0.01 M $CaCl_2$	12.5	BE	639
−0.17° (0.81)		66.4	15.5	18.1	0.77* [0.45]	Eutric Cambisol (Ah hor.); pH 7.5; CE=9.4 me/100 g	20	BE	350
0.53	1.92	12.3	31.4	56.3	4.30	Brimstone soil (Ap hor.; <2 mm); pH 6.1	20–24	BE	298
0.53	1.93				4.2	Idem (<250 μm)			298
0.72	2.42				1.9	Idem; oxidized by H_2O_2			298
−0.24	2.17	95.7	2.7	1.6	0.39	Sparta agricolt soil (Ap horizon); pH 6.4; 0.01 M $CaCl_2$		BE	292
−0.22	2.03	96.2	2.2	1.6	0.56	Idem (A horizon); pH 6.0			292
−0.46	2.01	96.2	2.3	1.5	0.34	Idem (AB horizon); pH 5.4			292
−0.52	2.05	96.5	2.5	1.0	0.27	Idem (Bw1 horizon); pH 5.5			292
−0.92	1.90	96.9	2.0	1.2	0.15	Idem (Bw2 horizon); pH 5.3			292
−1.00–−1.60		99.0–99.7	0.1–0.4	0.2–0.6	0.01–0.08	Idem (Bw3, BC, C horizons); pH 5.6–5.8			292
	2.00av				0.40–0.86	Idem (six surface samples); pH 5.0–6.6			292
0.01	2.22	87.7	8.2	4.1	0.62	Plainfield forest soil (Ap horizon); pH 6.4; 0.01 M $CaCl_2$		BE	292
−0.74	2.18	86.8	8.3	4.9	0.12	Idem (Bw1 horizon); pH 5.6			292
−0.80	2.20	90.8	5.4	3.7	0.10	Idem (Bw2 horizon); pH 5.4			292
−0.51–−1.15		88.9–99.2	0.3–5.4	0.5–5.8	0.01–0.07	Idem (seven horizons, from Bw3 to C2); pH 6.2–4.6			292
	2.49av				0.40–0.70	Idem (five surface samples); pH 6.0–6.6			292
−0.05	2.14	91.7	4.4	3.9	0.65	Tarr agricolt. soil (Ap horizon); pH 6.0; 0.01 M $CaCl_2$		BE	292
−0.33	1.96	89.7	5.3	5.0	0.51	Idem (A horizon); pH 6.3			292
−0.43	1.94	91.4	4.6	4.0	0.42	Idem (AB horizon); pH 6.1			292
−0.48	2.09	92.4	3.7	4.0	0.27	Idem (Bw1 horizon); pH 5.7			292
−0.89–0.57		97.7–98.9	0.4–1.0	0.7–1.4	0.05–0.08	Idem (Bw2, BC, C horizons); pH 5.7–5.6			292
0.67	2.41	89.8	5.7	4.5	1.83	Shawano forest soil (A horizon); pH 6.2; 0.01 M $CaCl_2$		BE	292
−0.39	2.12	90.3	5.2	4.6	0.31	Idem (Bw1 horizon); pH 5.5			292
−0.55	2.10	91.7	4.6	3.7	0.22	Idem (Bw2 horizon); pH 5.8			292
−0.70	2.26	97.0	2.9	0.1	0.11	Idem (Bw3 horizon); pH 5.6			292
−0.74–−1.05		72.3–98.6	1.0–24.6	0.4–3.1	0.03–0.07	Idem (E, Bw′, C1, C2 horizons); pH 5.6–5.8			292
−0.36	2.15	87.0	11.3	1.7	0.31	Rousseau forest soil (E horizon); pH 4.8; 0.01 M $CaCl_2$		BE	292
−0.57	1.86	82.0	6.4	11.6	0.37	Idem (Bt horizon); pH 5.6			292
−1.22	1.60	93.7	3.6	2.7	0.15	Idem (Bs1 horizon); pH 5.9			292
−1.22–−0.89		72.7–97.4	2.1–26.4	0.5–0.9	0.04–0.08	Idem (Bs2, BC, C horizons); pH 5.7–6.4			292
0.18	2.27			26	0.8	Agricultural soil; pH 7.4; CE=31 cmol/kg; 0.01 M $CaCl_2$	20	BE	297
0.49	2.42			54	1.2	Idem; pH 7.8; CE=24 cmol/kg			297
0.20	2.59			11	0.4	Idem; pH 8.0; CE=11 cmol/kg			297
1.04	2.16			6	7.6	Idem; pH 4.4; CE=27 cmol/kg			297
−0.70	2.05	88.0	4.0	8.0	0.18	Soil; s (Embarras River, ILL) (172–183 cm); pH 7.53; SA(N_2)=11.5 m^2/g	25	BE	479
−0.50	2.42	89.0	6.0	5.0	0.12	Idem; s (191–204 cm); pH 7.10; SA(N_2)=11.6 m^2/g			479
−0.14	2.72	87.0	11.0	2.0	0.14	Idem; s (204–248 cm); pH 7.20; SA(N_2)=10.3 m^2/g			479

TABLE 8. Sorption coefficients for pesticides—Continued

log K_d log K_f^0 (1/*n*)	log K_{oc}	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
0.41	2.91	31.0	52.0	17.0	0.32	Idem; till (350–364 cm); pH 8.15; $SA(N_2) = 17.3\ m^2/g$			479
0.23	3.23	88.0	6.0	6.0	0.10	Idem; s (78–117 cm); pH 5.58; $SA(N_2) = 13.0\ m^2/g$			479
0.45	2.93	33.0	56.0	11.0	0.33	Idem; till (409–427 cm): pH 7.65; $SA(N_2) = 17.8\ m^2/g$			479
−0.05	2.95	85.0	8.0	7.0	0.10	Idem; s (102–156 cm); pH 6.05; $SA(N_2) = 13.0\ m^2/g$			479
−0.46	2.59	88.0	4.0	8.0	0.09	Idem; s (156–208 cm); pH 6.91; $SA(N_2) = 8.1\ m^2/g$			479
−0.69	2.35	93.0	6.0	1.0	0.09	Idem; alluvium (0–6 cm); pH 7.61; $SA(N_2) = 2.0\ m^2/g$			479
−0.73	2.09	92.0	7.0	1.0	0.15	Idem; alluvium (0–6 cm); pH 7.61; $SA(N_2) = 2.6\ m^2/g$			479
0.85	2.33				3.27	Hickory Hill coarse si sediment; fraction (20–50 μm)	25	BE	129
0.66	2.62		27.4	72.1	1.1	Bear Creek 5290 sedim.; pH 5.7	25	BE	478
1.32	2.73		21.5	77.2	3.9	Bear Creek 5356 sedim.; pH 4.4	25	BE	478
0.53	2.42		37.6	59.7	1.3	Lake Chicot 5636 sedim.; pH 6.3	25	BE	478
0.36	2.62		48.1	30.9	0.55	Lake Chicot 5643 sedim.; pH 7.3	25	BE	478
−0.22	1.63		14.2	85.3	1.4	Lake Chicot 5700 sedim.; pH 6.2	25	BE	478
1.40	3.28		18.6	80.9	1.3	Wolf Lake 6262 sedim.; pH 4.5	25	BE	478
0.64	2.81		54.4	25.6	0.69	Wolf Lake 6268 sedim.; pH 7.7	25	BE	478
0.88	2.73		45.0	49.6	1.4	Wolf Lake 6272 sedim.; pH 5.7	25	BE	478
0.83	2.92		47.8	51.8	0.81	McWilliams Pond 1 sedim.; pH 5.8	25	BE	478
0.51	2.67		67.3	30.8	0.69	McWilliams Pond 2 sedim.; pH 6.8	25	BE	478
0.96	2.50		42.6	57.2	2.9	Beaver Pond sedim.; pH 5.2	25	BE	478
0.08	2.37		88.6	9.9	0.51	Lake Washington sedim.; pH 7.7	25	BE	478
	4.13					Choptank River colloidal fraction; TOC=98.6 mg/L; salinity=1.24‰	20	BE	406
	3.69					Idem; TOC=108.5 mg/L; salinity=9.92‰			406
	3.84					Idem; TOC=104.6 mg/L; salinity=14.2‰			406
	3.93					Idem; TOC=65.5 mg/L; salinity=1.50‰			406
	3.90					Idem; TOC=74.2 mg/L; salinity=5.71‰			406
	3.68					Idem; TOC=59.3 mg/L; salinity=17.0‰			406
	3.23					Patuxent River colloidal fraction; TOC=33.5 mg/L; salinity=19.1‰	20	BE	406
	3.27					Idem; TOC=44.0 mg/L; salinity=14.6‰			406
1.09° (0.92)						Ca-Wyoming smectite; pH 7.9; $SA(N_2) = 23\ m^2/g$; 0.01 M $CaCl_2$	20	BE	640
3.39° (0.78)						Fe-Wyoming smectite; pH 2.9; $SA(N_2) = 36\ m^2/g$; 0.01 M $CaCl_2$	20	BE	640
2.07° (0.92)	[2.36]				50.16	Soil humic acid; pH 2.9; 0.01 M $CaCl_2$	20	BE	640
2.29° (0.86)	[2.60]				49.83	Fluka humic acid; pH 4.6; 0.01 M $CaCl_2$	20	BE	640
	2.91*					Humic acid from Alberta black Chernozem soil (Ah hor.); pH 6.5	25	HT	548
	1.92					Cyanopropyl column	20–25	RPLC	579
	1.89					Idem; ring test		RPLC	581
	2.28					Soil; experimental (literature)			217
	2.17av					56 soils (literature)			87
	2.19av					217 literature data			562
	1.94, 2.42					Correlation log K_{oc}–log K_{ow}			96
	3.28					Correlation log K_{oc}–log K_{ow}(87)			528
	3.20					Correlation log K_{oc}–log K_{ow}(217)			528

TABLE 8. Sorption coefficients for pesticides—Continued

log K_d log K_f^0 ($1/n$)	log K_{oc}	Sorbent composition (%)				Other sorbent and solution data: prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
	3.18					Correlation log K_{oc}–log S(180)			528
	3.11					Correlation log K_{oc}–log S			96
	2.31					Correlation log K_{oc}–log S(mp)			96
	2.81					Correlation log K_{oc}–log S			564
	2.34					Correlation log K_{oc}–MCI			578
						Benefin			
[2.51]	[4.14]	6	71	23	4.0* [2.32]	Plano soil (soil/solut.=1 g/100 mL) pH 6.3; CE=20 me/100 g;	25	BE	351
[2.36]	[4.00]	6	71	23	4.0* [2.32]	Idem (soil/solut.=2 g/100 mL)	25	BE	351
[2.31]	[3.94]	6	71	23	4.0* [2.32]	Idem (soil/solut.=4 g/100 mL)	25	BE	351
[2.53]	[4.16]	6	71	23	4.0* [2.32]	Idem (soil/solut.=2 g/100 mL)	5	BE	351
1.44	[2.87]	17	64	19	6.5* [3.77]	Adolph soil; pH 6.2; CE=22.5 me/100 g	22	BE	345
0.82	[2.71]	9	78	13	2.2* [1.28]	Fayette soil; pH 6.5; CE=7.7 me/100 g	22	BE	345
1.04	[2.98]	23	42	35	2.0* [1.16]	Kewaunee soil; pH 7.8; CE=19.2 me/100 g	22	BE	345
1.30	[2.97]	12	61	27	3.7* [2.15]	Ontonagon soil; pH 6.6; CE=13.8 me/100 g	22	BE	345
1.08	[3.01]	27	12	61	2.0* [1.16]	Peebles soil; pH 7.4; CE=23.4 me/100 g	22	BE	345
0.62	[2.96]	89	6	5	0.8* [0.46]	Plainfield soil; pH 6.6; CE=3.7 me/100 g	22	BE	345
1.06	[2.62]	17	66	17	4.8* [2.78]	Plano soil; pH 6.7; CE=17.4 me/100 g	22	BE	345
1.46	[2.72]	23	62	15	9.5* [5.51]	Poigan soil; pH 7.0; CE=33.6 me/100 g;	22	BE	345
1.48	[2.65]	59	30	11	11.7* [6.79]	Sebewa soil; pH 6.8; CE=28.4 me/100 g	22	BE	345
1.18	[2.80]	17	73	10	4.1* [2.38]	Withee soil; pH 6.5; CE=10.9 me/100 g	22	BE	345
1.80	[3.18]	2.9	68.7	28.4	7.1* [4.12]	Lanton soil; pH 6.4; CE=32.8 me/100 g		BE	631
	4.03					Soil; experimental (literature)			217
						Bromacil (pK_a=9.3, Ref. 312)			
0.68° (0.8)						Silica gel (0.59–0.07 mm)(Grace Div. Chem., Baltimore, Md.); pH 4.6	25	BE	99
1.03° (0.8)						Idem	0	BE	99
0.42° (0.9)				100		Illite No. 35 (0.83 mm)(Fithian, Ill.); pH 7.0	25	BE	99
0.48° (0.9)						Idem	0		99
−0.14° (1.3)				100		Montmorillonite No. 25 (0.83 mm) (J.C. Lane Track, Upton, Wyo.) pH 6–7	25	BE	99
−0.03° (1.3)						Idem	0		99
0.18° (0.85)					2.1* [1.22]	Keyport sil soil; pH 5.4; aver. particle size=5.6 μm		BE	641
−1.10° (0.58)					0.7* [0.41]	Cecil ls soil; pH 5.8; aver. particle size=10.5 μm		BE	641
1.29° (0.93)	1.82				29.9	Hula-1 soil; peat; pH 6.3; SA(E)=132 m^2/g; CE=95 cmol/kg	28	BE	312
0.70°	1.81				7.85	Hula-2 soil; peat; pH 6.9;	28	BE	312

TABLE 8. Sorption coefficients for pesticides—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%)				Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
(1.04)						SA(E) = 98 m^2/g; CE = 74 cmol/kg			
0.23° (1.05)	1.74				3.08	Oxidized Hula-2 soil; pH 6.9; SA(E) = 66 m^2/g; CE = 30 cmol/kg	28	BE	312
0.05° (0.78)		20	25	55	1.22	Newe Ya'ar soil; pH 7.3; SA(E) = 360 m^2/g; CE = 72 cmol/kg	28	BE	312
−0.22° (1.15)	2.10				0.47	Idem; oxidized; pH 7.3; SA(E) = 356 m^2/g; CE = 64 cmol/kg			312
−0.20° (0.79)		36	31	33	0.56	Sa'ad soil; pH 7.6; CE = 18 cmol/kg; SA(E) = 160 m^2/g	28	BE	312
−1.52				7.5	0.06	Miytachim agric. surface soil; pH 8.5; 3.5% $CaCO_3$		BE	277
−1.00	1.40			13.7	0.40	Bet Degan I agric. surface soil; pH 7.9; 2.3% $CaCO_3$		BE	277
−0.80	1.46			23.1	0.55	Gilat agric. surface soil; pH 7.8; 12.9% $CaCO_3$		BE	277
−0.49	1.51			42.5	1.01	Bet Degan II agric. surface soil; pH 7.8; 2.6% $CaCO_3$		BE	277
−0.62	1.52			70.0	0.72	Shefer agric. surface soil; pH 7.2; 0.2% $CaCO_3$		BE	277
−0.41	1.52			70.0	1.18	Neve. Yaar agric. surface soil; pH 7.7; 8.9% $CaCO_3$		BE	277
0.30	1.34			35	9.1	Eversham soil; clay (0–0.02 m depth); pH 7.8; 0.005 M $CaCl_2$		BE	137
0.24	1.37			>35	7.3	Idem(0.02–0.22 m depth)			137
−1.46	1.55			11.2	0.17* [0.10]	Netanya agricolt. surface soil	25	BE	563
−1.46	1.06			6.9	0.45* [0.26]	Mivtahim agricult. surface soil	25	BE	563
−0.80	1.37			63.1	1.18* [0.68]	Golan agricult. surface soil	25	BE	563
−0.89	1.25			23.8	1.25* [0.73]	Gilat agricult. surface soil	25	BE	563
−0.68	1.41			72.5	1.42* [0.82]	Shefer agricult. surface soil	25	BE	563
−0.96	1.12			10.6	1.45* [0.84]	Bet Degan agricult. surface soil	25	BE	563
−0.40	1.39			71.2	2.82* [1.64]	Neve Yaar agricult. surface soil	25	BE	563
−0.18	1.29			76.2	5.82* [3.38]	Malkiya agricult. surface soil	25	BE	563
−0.39	1.36				3.08* [1.79]	Kinneret Lake sediment	25	BE	563
0.10	1.44			60.5	7.85* [4.55]	Kinneret A Lake sediment	25	BE	563
0.05	1.42			63.2	7.43* [4.31]	Kinneret F Lake sediment	25	BE	563
−0.10	1.49			63.8	4.39* [2.55]	Kinneret G Lake sediment	25	BE	563
	1.0°* (0.7)					Humic acid (0.59–0.2 mm) extracted from soil; pH 6–7	25	BE	99
	2.1°* (0.7)					Idem	0		99
	1.86					Soil; experimental (literature)			217
	1.86av					2 soils (literature)			87
	1.63					Correlation $\log K_{oc}-\log K_{ow}$			96
	2.33					Correlation $\log K_{oc}-\log S$			96
	1.34					Correlation $\log K_{oc}-\log S$(mp)			96
	3.13					Correlation $\log K_{oc}-\log S$			564
	2.56					Correlation $\log K_{oc}-$MCI			578

TABLE 8. Sorption coefficients for pesticides—Continued

log K_d log K_f^0 ($1/n$)	log K_{oc}	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
						Butralin			
2.70				100		Ca–montmorillonite; pH 6	24	BE	121
3.48	[3.74]				94* [54.5]	OM from peaty muck (Histosol) soil; pH 5.5	24	BE	121
	3.91					Soil; experimental (literature)			217
	3.64					Correlation log K_{oc}–log S			564
						Carbaryl			
	[2.11]av			1.4*-	72*	5 soils od different composition; pH 5.2–7.8	25	BE	590
[0.33]	[2.02]				3.53* [2.05]	Batcombe sil soil; pH 6.1; 0.01 M $CaCl_2$	20	BE	120
[0.39]	[1.97]				4.54* [2.63]	Warwick, Qld, soil; pH 6.3; 0.01 M $CaCl_2$		BE	558
[0.31]	[1.94]				4.07* [2.36]	Rutherglen, Vic., soil; pH 4.8; 0.01 M $CaCl_2$		BE	558
[0.10]	[2.07]				1.86* [1.08]	Wagga, N.S.W., soil; pH 5.1; 0.01 M $CaCl_2$		BE	558
[0.30]	[2.09]				2.81* [1.63]	Turretfield, S.A., soil; pH 5.2; 0.01 M $CaCl_2$		BE	558
[0.15]	[2.35]				1.09* [0.63]	Warracknabeal, Vic., soil; pH 8.0; 0.01 M $CaCl_2$		BE	558
[0.24]	[1.97]				3.20* [1.86]	Warracknabeal, Vic., soil; pH 8.4; 0.01 M $CaCl_2$		BE	558
−0.10	[1.88]				1.77* [1.03]	Cecil soil; pH 6.3; SA(W)=15 m^2/g		BE	73
2.24° (0.97)	[2.60]	52	34	14	75.3* [43.7]	Soil: organic; pH 6.1		BE	264
0.90° (0.96)	[2.69]	71	22	7	2.8* [1.62]	Big Creek sediment; pH 6.6		BE	264
0.60° (0.98)	[2.44]	56	30	14	2.5* [1.45]	Beverly soil; pH 6.8		BE	264
0.00° (1.08)	[2.39]	91.5	1.5	7	0.7* [0.41]	Plainfield soil; pH 7.0		BE	264
	2.49av (three soils)	38	48	14	0.68	Commerce soil; pH 6.7		BE	575
		56	30	14	1.12	Tracy soil; pH 6.2		BE	575
		12	56	32	2.01	Catlin soil; pH 6.2		BE	575
	2.36					Soil; experimental (literature)			217
	2.30					Cyanopropyl column	20–25	RPLC	579
	2.57					C18 column		RPLC	573
	2.42					Correlation log K_{oc}–log K_{ow}			96
	3.04					Correlation log K_{oc}–log S			96
	2.50					Correlation log K_{oc}–log S(mp)			96
	2.76					Correlation log K_{oc}–log S			564
	2.23					Correlation log K_{oc}–MCI			578
						Carbofuran			
−0.60	[1.80]				0.4	Plainfield-Bloomfield s soil; CE=1.7 me/100 g; 0.01 M $CaCl_2$	25	BE	265
−0.13	[1.79]				1.2	Gilford-Hoopeston-Ade sl soil; CE=7.5 me/100 g; 0.01 M $CaCl_2$	25	BE	265
0.15	[1.72]				2.7	Bryce-Swygert sic soil; CE=34.4 me/100 g; 0.01 M $CaCl_2$	25	BE	265
0.05	[1.56]				3.1	Drummer sicl soil; CE=24.8 me/100 g; 0.01 M $CaCl_2$	25	BE	265
0.14	[1.60]				3.5	Flanagan sil soil; CE=27.7 me/100 g; 0.01 M $CaCl_2$	25	BE	265
0.35	[1.47]				7.5	Bryce sicl soil; CE=55.5 me/100 g; 0.01 M $CaCl_2$	25	BE	265
0.94	[1.72]				16.8	Houghton soil; muck; CE=72.4 me/100 g; 0.01 M $CaCl_2$	25	BE	265
1.48°		15	63.5	21.5	79.5*	Peat; pH 3.8; CE=64.3 me/100 g	20	BE	266

TABLE 8. Sorption coefficients for pesticides—Continued

log K_d log K_f^0 (1/n)	log K_{oc}	Sorbent composition (%) Sand	 Silt	 Clay	 OC	Other sorbent and solution data: prediction procedure	Temp. (°C)	Meth.	Ref.
(0.85)					46.2				
0.54°	[1.50]	56.9	23.5	19.6	19.0*	Soil; 1; pH 6.8;	20	BE	266
(0.91)					11.04	CE=33.3 me/100 g			
0.22°	[1.60]	30.5	52.6	16.9	7.18*	Soil; 1; pH 6.5;	20	BE	266
(0.99)					4.18	CE=16.7 me/100 g			
−0.14°	[1.54]	10.8	31.2	58.0	3.57*	Soil (Limagne); pH 8.0;	20	BE	266
(1.03)					2.08	CE=31.8 me/100 g			
−0.21°	[1.57]	2.0	14.9	8.7	2.82*	Soil (Chalons); pH 8.1;	20	BE	266
(0.97)					1.64	CE=7.9 me/100 g; 74.4% $CaCO_3$			
−0.58°	[1.36]	15.2	63.8	20.5	1.94*	Soil (Versailles); pH 6.4;	20	BE	266
(0.88)					1.13	CE=10 me/100 g; 0.5% $CaCO_3$			
−0.48°	[1.34]	46.6	45.7	7.7	2.58*	du Val pond sediment; pH 7.7;	20	BE	266
(1.06)					1.50	CE=5.6 me/100 g			
−0.52°	[1.21]	21.8	64.1	14.1	3.16*	St-Quentin pond sediment; pH 7.1;	20	BE	266
(0.90)					1.84	CE=9.7 mc/100 g			
−0.80°		93.4	2.0	4.6	0.03*	Fontainebleau sand; pH 5.0;	20	BE	266
(0.59)					0.02	CE=1.4 me/100 g			
	[1.38]av			1.4*-		5 soils od different composition;	25	BE	590
					72*	pH 5.2–7.8			
1.43°	[1.79]	52	34	14	75.3*	Soil; organic; pH 6.1		BE	264
(1.08)					[43.7]				
0.30°	[2.09]	71	22	7	2.8*	Big Creek sediment; pH 6.6		BE	264
(0.98)					[1.62]				
0.20°	[2.04]	56	30	14	2.5*	Beverly soil; pH 6.8		BE	264
(1.07)					[1.45]				
−1.0°	[1.39]	91.5	1.5	7	0.7*	Plainfield soil; pH 7.0		BE	264
(0.88)					[0.41]				
	2.02av	38	48	14	0.68	Commerce soil; pH 6.7		BE	575
	(three	56	30	14	1.12	Tracy soil; pH 6.2		BE	575
	soils)	12	56	32	2.01	Catlin soil; pH 6.2		BE	575
	1.47av					5 soils (literature)			87
	1.63av					52 literature data			562
	2.11					C18 column		RPLC	573
	1.68					Correlation log K_{oc}–log K_{ow}			96
	2.46					Correlation log K_{oc}–log S			96
	1.51					Correlation log K_{oc}–log S(mp)			96
	2.20					Correlation log K_{oc}–log S			564
						Chlorbromuron			
[0.93]	[2.51]				4.54*	Warwick, Qld, soil; pH 6.3;		BE	558
					[2.63]	0.01 M $CaCl_2$			
[0.96]	[2.59]				4.07*	Rutherglen, Vic., soil; pH 4.8;		BE	558
					[2.36]	0.01 M $CaCl_2$			
[0.60]	[2.57]				1.86*	Wagga, N.S.W., soil; pH 5.1;		BE	558
					[1.08]	0.01 M $CaCl_2$			
[0.65]	[2.44]				2.81*	Turretfield, S.A., soil; pH 5.2;		BE	558
					[1.63]	0.01 M $CaCl_2$			
[0.51]	[2.71]				1.09*	Warracknabeal, Vic., soil; pH 8.0;		BE	558
					[0.63]	0.01 M $CaCl_2$			
[0.77]	[2.50]				3.20*	Warracknabeal, Vic., soil; pH 8.4;		BE	558
					[1.86]	0.01 M $CaCl_2$			
[0.77]	[2.19]				6.62*	Balkuling soil; pH 5.6;		BE	558
					[3.84]	0.01 M $CaCl_2$			
[0.75]	[2.66]				2.14*	Kojonup soil; pH 5.5;		BE	558
					[1.24]	0.01 M $CaCl_2$			
[0.44]	[2.53]				1.42*	Warranine soil; pH 6.5;		BE	558
					[0.82]	0.01 M $CaCl_2$			
[0.71]	[2.23]				5.17*	Yalanbee soil; pH 6.4;		BE	558
					[3.00]	0.01 M $CaCl_2$			
[0.76]	[2.54]				2.85*	Avondale soil; pH 5.9;		BE	558
					[1.65]	0.01 M $CaCl_2$			
[0.74]	[2.78]				1.58*	Badgingarra soil; pH 6.3;		BE	558
					[0.92]	0.01 M $CaCl_2$			

TABLE 8. Sorption coefficients for pesticides—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data: prediction procedure	Temp. (°C)	Meth.	Ref.
[−0.61]	[2.35]				0.19* [0.11]	Badgingarra soil; pH 6.3; 0.01 M $CaCl_2$		BE	558
[0.82]	[2.59]				2.92* [1.69]	Beverley soil; 0.01 M $CaCl_2$		BE	558
[1.02]	[2.68]				3.78* [2.19]	Gabalong soil; pH 5.9; 0.01 M $CaCl_2$		BE	558
[0.38]	[2.56]				1.13* [0.66]	Perth soil; pH 5.9; 0.01 M $CaCl_2$		BE	558
[0.75]	[2.72]				1.86* [1.08]	Tammin soil; pH 5.9; 0.01 M $CaCl_2$		BE	558
[2.07°] (0.45)		47.5	33.2	20.3	10.5* [6.09]	Melfort soil; pH 5.9	25	BE	260
1.31° (0.83)		53.3	27.5	19.2	6.46* [3.75]	Weyburn soil; pH 6.5	25	BE	260
1.25° (0.71)		5.3	25.3	69.5	4.15* [2.41]	Regina soil; pH 7.7	25	BE	260
1.36° (0.68)		69.3	12.3	18.5	4.07* [2.36]	Indian Head soil; pH 7.8	25	BE	260
0.90° (0.73)		81.6	10.4	8.0	1.77* [1.03]	Asquith soil; pH 7.5	25	BE	260
0.26° (0.86)				9.8	0.1* [0.06]	Soil; s, mesic; pH 7.0; SA(W)=14.8 m^2/g		BE	72
0.84° (0.70)				15.0	1.0* [0.58]	Soil; s, mixed, mesic; pH 7.6; SA(W)=18.1 m^2/g		BE	72
0.90° (0.67)				13.0	1.4* [0.81]	Soil; s, mixed, mesic; pH 7.3; SA(W)=30.3 m^2/g		BE	72
1.15° (0.59)				6.8	1.5* [0.87]	Soil; s, mixed, mesic; pH 7.1; SA(W)=15.2 m^2/g		BE	72
1.28° (0.80)				31.5	1.6* [0.93]	Soil; sc, mesic; pH 6.6; SA(W)=72.4 m^2/g		BE	72
1.45° (0.80)				10.6	1.9* [1.10]	Soil; s, mesic; pH 4.2; SA(W)=38.6 m^2/g		BE	72
1.60° (0.63)				18.3	1.2* [0.70]	Soil; s, mesic; pH 6.9; SA(W)=55.8 m^2/g		BE	72
2.11° (0.50)				4.5	4.6* [2.67]	Soil; s, mesic; pH 3.7; SA(W)=22.4 m^2/g		BE	72
0.96° (0.60)		30.1	43.4	26.5	1.89* [1.10]	Dundee sl soil (Tunica Co., MS); pH 6.2; 37% moisture content (soil moisture tension=0 bar)	27	BE	274
0.73° (0.75)		46.5	40.7	12.8	0.90* [0.52]	Dundee sl soil (Washington Co., MS); pH 6.2; 34% moisture content (soil moisture tension=0 bar)	27	BE	274
0.91° (0.71)		66.5	16.4	17.1	0.34* [0.20]	Dundee sl soil (Sharkey Co., MS); pH 6.2; 28% moisture content (soil moisture tension=0 bar)	27	BE	274
0.62° (0.82)		12.4	75.7	11.9	1.98* [1.15]	Memphis sil soil (Yazoo Co., MS); pH 5.1; 46% moisture content (soil moisture tension=0 bar)	27	BE	274
0.63° (0.81)		3.1	78.5	18.4	1.12* [0.65]	Memphis sil soil (Warren Co., MS); pH 4.4; 42% moisture content (soil moisture tension=0 bar)	27	BE	274
0.81° (0.48)		6.6	77.8	15.6	2.53* [1.47]	Memphis sil soil (Craighead Co., AR); pH 5.8; 40% moisture content (soil moisture tension=0 bar)	27	BE	274
0.75° (0.40)		4.7	29.8	65.5	2.11* [1.22]	Alligator C soil (Leflore Co., MS); pH 6.2; 49% moisture content (soil moisture tension=0 bar)	27	BE	274
	2.66					Soil; experimental (literature)			217
	3.00av					5 soils (literature)			87
	2.71					Correlation $\log K_{oc}-\log S$			564

TABLE 8. Sorption coefficients for pesticides—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data: prediction procedure	Temp. (°C)	Meth.	Ref.
α-Chlordane									
	4.77				50.2	Aldrich humic acid; pH 8.0; 22 0.1 M $NaHCO_3$		ED	206
	4.38				50.2	Aldrich and Fluka humic acid		FH	206
[4.11]	5.5				4.1	Lake Ontario sediment trap material		FM	49
	5.6					Correlation $\log K_{oc}-\log K_{ow}$(96)			49
	4.33					Correlation $\log K_{oc}-\log S$			564
	4.94					Correlation $\log K_{oc}-$MCI			598
Chlorfenvinphos									
[0.78]	[2.47]				3.53* [2.05]	Batcombe sil soil; pH 6.1; 0.01 M $Cacl_2$	20	BE	120
	2.77					Correlation $\log K_{oc}-$MCI			598
	2.45					Correlation $\log K_{oc}-\log S$			564
Chloroxuron									
2.68°		45.5	15.9	6.6	12.0	Great House E.H.F. soil; pH 6.3; CE=18 me/100 g	22	BE	259
2.52°		23	24.4	28.6	11.7	Toll Farm heavy peat; pH 7.4; CE=41 me/100 g	22	BE	259
2.24°		34.0	33.4	32.6	3.69	Trawscoed E.H.F. soil; pH 6.2; CE=12 me/100 g	22	BE	259
2.08°		66.0	18.4	15.6	1.93	Weed Res. soil; pH 7.1; CE=11 me/100 g	22	BE	259
1.85°		36.0	40.4	23.6	1.76	Rosemaunde E.H.F. soil; pH 6.7; CE=14 me/100 g	22	BE	259
	3.51					Soil; experimental (literature)			217
	3.64av					5 soils (literature)			87
	3.11					Correlation $\log K_{oc}-$MCI			598
	3.40					Correlation $\log K_{oc}-\log S$			564
Chlorpropham (CIPC)									
1.48° (1.09)				100		H-montmorillonite (1–0.2 μm); pH 3.35; CE=73.5 me/100 g	25	BE	250
1.43° (0.93)				100		Na-montmorillonite (1–0.2 μm); pH=6.80; CE=87.0 me/100 g	25	BE	250
1.61						Bentonite; 0.1 M $CaCl_2$	22	BE	144
[0.82]	[2.67]			22.4	2.42* [1.40]	Beltsville sil soil; pH 4.3; CE=4.2 me/100 g; 0.01 M $CaCl_2$	26	BE	38
[0.84]	[2.61]			23.9	2.90* [1.68]	Chester l soil; pH 4.9; CE=5.2 me/100 g; 0.01 M $CaCl_2$	26	BE	38
[0.63]	[2.53]			35.7	2.18* [1.26]	Thurlow cl soil; pH 7.7; CE=21.6 me/100 g; 0.01 M $CaCl_2$	26	BE	38
[0.95]	[2.35]			34.4	6.90* [4.00]	Barnes cl soil; pH 7.4; CE=33.8 me/100 g; 0.01 M $CaCl_2$	26	BE	38
[0.88]	[2.59]			18.0	3.30* [1.91]	Crosby sil soil; pH 4.8; CE=11.5 me/100 g; 0.01 M $CaCl_2$	26	BE	38
[0.89]	[2.50]			30.0	4.31* [2.50]	Hagerstown sicl soil; pH 5.5; CE=12.5 me/100 g; 0.01 M $CaCl_2$	26	BE	38
[0.95]	[2.50]			52.5	4.85* [2.81]	Toledo sic soil; pH 5.5; CE=29.8 me/100 g; 0.01 M $CaCl_2$	26	BE	38
[0.99]	[2.58]			22.1	4.40* [2.55]	Chillum sil soil; pH 4.6; CE=7.6 me/100 g; 0.01 M $CaCl_2$	26	BE	38
[1.11]	[2.62]			23.2	5.27* [3.06]	Iredell sil (topsoil); pH 5.4; CE=17.0 me/100 g; 0.01 M $CaCl_2$	26	BE	38
[0.82]	[2.47]			67.1	3.90* [2.26]	Sharkey c soil; pH 6.2; CE=40.2 me/100 g; 0.01 M $CaCl_2$	26	BE	38
[1.07]	[2.40]			50.5	8.02* [4.65]	Berkley sic (topsoil); pH 7.1; CE=33.7 me/100 g; 0.01 M $CaCl_2$	26	BE	38
[0.75]	[2.32]			43.6	4.68* [2.71]	Benevola sic (topsoil); pH 7.7; CE=19.5 me/100 g; 0.01 M $CaCl_2$	26	BE	38

TABLE 8. Sorption coefficients for pesticides—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%) Sand	 Silt	 Clay	 OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
2.12	[3.04]	45.5	15.9	6.6	12	Great House E.H.F. soil; pH 6.3; CE=18 me/100 g; 0.1 M $CaCl_2$	22	BE	144
1.32	[3.03]	66.0	18.4	15.6	1.93	Weed Res. Orgn. soil; pH 7.1; CE=11 me/100 g; 0.1 M $CaCl_2$	22	BE	144
2.82	[3.18]				76* [44]	OM from peat soil; 0.1 M $CaCl_2$	22	BE	144
1.12	[2.51]	2.9	68.7	28.4	7.1* [4.1]	Lanton soil; pH 6.4; CE=32.8 me/100 g		BE	631
	2.77					Soil; experimental (literature)			217
	2.54av					57 literature data			562
	2.67					Correlation $\log K_{oc}-\log K_{ow}$			96
	2.85, 2.80					Correlation $\log K_{oc}-\log S$			96
	3.17, 3.08					Correlation $\log K_{oc}-\log S$(mp)			96
	2.57					Correlation $\log K_{oc}-\log S$			564
						Chlorpyrifos			
1.39° (0.86)		77	15	8	0.51	Sarpy soil; pH 7.3; CE=5.7 me/100 g; 0.01 M $CaCl_2$	24	BE	122
1.56° (0.77)		83	9	8	1.07	Thurman soil; pH 6.83; CE=6.1 me/100 g; 0.01 M $CaCl_2$	24	BE	122
2.17° (0.91)	[3.75]	37	42	21	2.64	Clarion agric. soil; pH 5.00; CE=21.0 me/100 g; 0.01 M $CaCl_2$	24	BE	122
2.59° (0.98)	[4.01]	21	55	24	3.80	Harps agric. soil; pH 7.30; CE=37.8 me/100 g; 0.01 M $CaCl_2$	24	BE	122
2.06	3.44	18.9	26.3	54.8	4.24	Tsukuba soil; pH 6.5; 0.01 M $CaCl_2$	25	BE	642
2.68° (1.23)						Idem			642
1.13	3.00	23.1	15.4	61.5	1.35	Kanuma soil; pH 5.7; 0.01 M $CaCl_2$	25	BE	642
1.16° (1.01)						Idem			642
3.27° (1.09)	[3.63]	52	34	14	75.3* [43.7]	Soil; organic; pH 6.1		BE	264
2.14° (0.98)	[3.93]	71	22	7	2.8* [1.62]	Big Creek sediment; pH 6.6		BE	264
2.07° (0.99)	[3.91]	56	30	14	2.5* [1.45]	Beverly soil; pH 6.8		BE	264
1.26° (0.98)	[3.64]	91.5	1.5	7	0.7* [0.41]	Plainfield soil; pH 7.0		BE	264
	3.78av (three soils)	38	48	14	0.68	Commerce soil; pH 6.7		BE	575
		56	30	14	1.12	Tracy soil; pH 6.2		BE	575
		12	56	32	2.01	Catlin soil; pH 6.2		BE	575
	4.13					Soil; experimental (literature)			217
	4.00					C18 column		RPLC	573
	2.92, 4.43, 4.72					Correlation $\log K_{oc}-\log K_{ow}$			96
	3.96					Correlation $\log K_{oc}-\log S$			96
	4.87					Correlation $\log K_{oc}-\log S$(mp)			96
	3.93					Correlation $\log K_{oc}-\log S$			564
						Chlorthiamid			
	2.03					Soil; experimental (literature)			217
	1.99av					6 soils (literature)			87
	2.00					Correlation $\log K_{oc}-\log S$			564
						Chlortoluron			
[0.55]	[2.13]				4.54* [2.63]	Warwick, Qld, soil; pH 6.3; 0.01 M $CaCl_2$		BE	558

TABLE 8. Sorption coefficients for pesticides—Continued

log K_d log K_f^0 (1/n)	log K_{oc}	Sorbent composition (%)				Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
[0.37]	[2.00]				4.07* [2.36]	Rutherglen, Vic.. soil; pH 4.8; 0.01 M $CaCl_2$		BE	558
[0.06]	[2.03]				1.86* [1.08]	Wagga, N.S.W.. soil; pH 5.1; 0.01 M $CaCl_2$		BE	558
[0.18]	[1.97]				2.81* [1.63]	Turretfield, S.A., soil; pH 5.2; 0.01 M $CaCl_2$		BE	558
[−0.06]	[2.14]				1.09* [0.63]	Warracknabeal, Vic., soil; pH 8.0; 0.01 M $CaCl_2$		BE	558
[0.30]	[2.03]				3.20* [1.86]	Warracknabeal, Vic., soil; pH 8.4; 0.01 M $CaCl_2$		BE	558
[0.22]	[1.64]				6.62* [3.84]	Balkuling soil; pH 5.6; 0.01 M $CaCl_2$		BE	558
[0.01]	[1.92]				2.14* [1.24]	Kojonup soil; pH 5.5; 0.01 M $CaCl_2$		BE	558
[−0.01]	[2.08]				1.42* [0.82]	Warranine soil; pH 6.5; 0.01 M $CaCl_2$		BE	558
[0.15]	[1.67]				5.17* [3.00]	Yalanbee soil; pH 6.4; 0.01 M $CaCl_2$		BE	558
[0.17]	[1.95]				2.85* [1.65]	Avondale soil; pH 5.9; 0.01 M $CaCl_2$		BE	558
[0.13]	[2.17]				1.58* [0.92]	Badgingarra soil; pH 6.3; 0.01 M $CaCl_2$		BE	558
[−0.88]	[2.08]				0.19* [0.11]	Badgingarra soil; pH 6.3; 0.01 M $CaCl_2$		BE	558
[0.22]	[1.99]				2.92* [1.69]	Beverley soil; 0.01 M $CaCl_2$		BE	558
[0.38]	[2.04]				3.78* [2.19]	Gabalong soil; pH 5.9; 0.01 M $CaCl_2$		BE	558
[−0.10]	[2.08]				1.13* [0.66]	Perth soil; pH 5.9; 0.01 M $CaCl_2$		BE	558
[0.33]	[2.12]				1.86* [1.08]	Tammin soil; pH 5.9; 0.01 M $CaCl_2$		BE	558
	2.62					Correlation log K_{oc}−log S			564
Cyanazine (**pK_a=5.1**, Ref. 645)									
0.86° (0.51)				100		Almeira montmorillonite (AM)-H+; CE=80 me/100 g; SA(N_2)=734 m^2/g	20	BE	140
0.78° (0.52)						Idem	30		140
0.70° (0.82)				100		AM-Co^{2+}	20	BE	140
0.54° (0.87)						Idem	30		140
1.47° (0.69)				100		AM-Cu^{2+}	20	BE	140
1.20° (0.79)						Idem	30		140
3.17° (0.53)						Padul peat (PP)-H^+; CE=165 me/100 g; SA(N_2)=56 m^2/g	20	BE	140
3.10° (0.55)						Idem	30		140
1.76° (0.90)						PP-K^+	20	BE	140
1.66° (0.91)						Idem	30		140
1.82° (0.84)						PP-Mg^{2+}	20	BE	140
1.71° (0.86)						Idem	30		140
1.93° (0.73)						PP-Ca^{2+}	20	BE	140

TABLE 8. Sorption coefficients for pesticides—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%)				Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
1.73° (0.79)						Idem	30		140
1.88° (0.80)						PP-Co^{2+}	20	BE	140
1.84° (0.78)						Idem	30		140
2.40° (0.85)						PP-Cu^{2+}	20	BE	140
2.31° (0.87)						Idem	30		140
−0.20	[1.78]		20	3	1.8* [1.04]	Calcareous soil; pH 7.4; 0.01 M $CaCl_2$	19	BE	503
0.34° (1.02)	[1.90]		30	27	2.77	Ves soil; pH 5.7; 0.01 M $CaCl_2$	23	BE	643
0.08	[1.86]	30.1	55.2	14.7	1.64	Valois soil; pH 5.9; 0.005 M $CaSO_4$	23–27	BE	527
0.66° (0.96)	[2.57]	10.5	62.5	27	2.15* [1.25]	Monona soil; pH 6.7; CE=20.7 me/100 g	24	BE	644
0.53° (0.86)		90.5	4.5	5	0.75* [0.44]	Valentine soil; pH 6.75;	24	BE	644
0.19° (0.91)	[2.47]	29	55	16	0.53	Conv. tilled soil−ryegrass (0–2 cm); pH 5.87		BE	645
0.25° (0.90)	[2.43]	31	56	13	0.67	No-tilled soil−ryegrass (0–2 cm); pH 5.74		BE	645
0.25° (0.90)	[2.25]	29	58	13	1.01	Conv. tilled soil+ryegrass (0–2 cm); pH 5.83		BE	645
0.41° (0.91)	[2.23]	33	53	14	1.51	No-tilled soil+ryegrass (0–2 cm); pH 5.58		BE	645
1.13° (>0.95)						Ryegrass residue		BE	645
0.78	2.26				3.27	Hickory Hill sediment; coarse si fraction (20–50 μm)	25	BE	130
−1.10	[1.79]	97.1	2.3	0.6	0.13	Tampa aquifer; pH 8 0.01 N $CaCl_2$		BE	521
	2.30					Soil; experimental (literature)			217
	1.85					Correlation $\log K_{oc}-\log K_{ow}$			96
	2.71					Correlation $\log K_{oc}-\log S$			96
	1.75					Correlation $\log K_{oc}-\log S$(mp)			96
	2.42					Correlation $\log K_{oc}-\log S$			564
	2.35					Correlation $\log K_{oc}$–MCI			578
						2,4-D (pK_a=2.80, Ref. 679)			
1.14				100		Illite No. 35 (Fithian, Ill.); SA=50–300 m^2/g	40	BE	146
1.14						Idem	25		146
0.70						Idem	0		146
−0.4				100		Kaolinite (Merck, NFV); SA=4–80 m^2/g	40	BE	146
−0.31						Idem	25		146
−0.41						Idem	0		146
0.88				100		Montmorillonite No. 25 (J.C. Lane Tract, Upton, Wyo.); SA=400–900 m^2/g	40	BE	146
0.95						Idem	25		146
0.96						Idem	0		146
1.54				100		Mississippi bentonite; pH 3.5	0	BE	251
1.56						Idem	50		251
0.23° (0.62)				100	0.2	Montmorillonite (M) SWy-1; CE=76.4 me/100 g; SA(N_2)=60 m^2/g; 0.01 M $CaCl_2$		BE	334
0.30° (0.73)				100	0.1	Santa Olalla vermiculite (V); CE=143.0 me/100 g; SA(N_2)=3 m^2/g; 0.01 M $CaCl_2$		BE	334

TABLE 8. Sorption coefficients for pesticides—Continued

$\log K_\mathrm{d}$ $\log K_\mathrm{f}^0$ $(1/n)$	$\log K_\mathrm{oc}$	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
1.77° (0.91)	[2.75]				10.3	Decylammonium-M (78.9 me/100 g) SA(N_2)=10.0 m²/g; 0.01 M $CaCl_2$		BE	334
2.87° (0.93)	[3.62]				17.5	Decylammonium-V (145 me/100 g) SA(N_2)=3.0 m²/g; 0.01 M $CaCl_2$		BE	334
0.95	[1.29]				77* [44.7]	Houghton muck; pH 5.6	0	BE	251
0.91	[1.26]					Idem	50		251
0.28° (0.90)	[2.04]	12	61	27	3.0* [1.74]	Naff soil; pH 5.9; CE=19 me/100 g; 0.1 N $CaCl_2$		BE	348
−0.68° (0.86)		39	30	31	0.8* [0.46]	Glendale soil; pH 7.7 CE=31.1 me/100 g; 0.1 N $CaCl_2$		BE	348
−0.17	[1.22]	2.9	68.7	28.4	7.1* [4.12]	Lanton soil; pH 6.4; CE=32.8 me/100 g		BE	631
0.11° (1.00)	[1.31]	47.5	33.2	20.3	10.5* [6.09]	Melfort soil; pH 5.9	25	BE	332
0.53	[1.75]					Idem		LE	540
−0.11° (0.98)	[1.04]	45.5	41.0	13.5	12.4* [7.19]	Lacombe soil; pH 7.7	25	BE	332
−0.33° (1.01)	[1.10]	53.3	27.5	19.2	6.46* [3.75]	Weyburn Oxbow soil; pH 6.5	25	BE	332
−0.21	[1.21]					Idem		LE	540
−0.89° (1.00)	[0.73]	5.3	25.3	69.5	4.15* [2.41]	Regina soil; pH 7.7	25	BE	332
−0.51	[1.11]					Idem		LE	540
−0.51° (0.97)	[1.12]	69.3	12.3	18.5	4.07* [2.36]	Indian Head soil; pH 7.8	25	BE	332
−0.36	[1.27]					Idem		LE	540
−0.44° (1.01)	[1.16]	69.0	16.0	15.0	4.28* [2.48]	Weyburn soil; pH 7.8	25	BE	332
−1.05° (0.79)		81.6	10.4	8.0	1.77* [1.03]	Asquith soil; pH 7.5	25	BE	332
−0.85	[1.13]					Idem		LE	540
2.04° (1.64)						Peat, pH 3.4	25	BE	320
0.21° (0.96)	2.09	3.31	21.9	75.0	1.30	Eurosol-1; c; pH 5.1; 0.01 M $CaCl_2$		BE	583
0.34	2.23					Idem; EEC laboratory ringtest			62
−0.39° (1.06)	1.04	3.4	64.1	22.6	3.70	Eurosol-2; sil; pH 7.4; 0.01 M $CaCl_2$		BE	583
−0.12	1.30					Idem; EEC laboratory ringtest			62
−0.06° (0.99)	1.40	46.4	36.8	17.0	3.45	Eurosol-3; 1; pH 5.2; 0.01 M $CaCl_2$		BE	583
0.20	1.66					Idem; EEC laboratory ringtest			62
−1.03	0.78	4.1	75.7	20.3	1.55	Eurosol-4; si; pH 6.5; 0.01 M $CaCl_2$		BE	583
−0.36	1.46					Idem; EEC laboratory ringtest			62
1.68	2.72	81.6	12.6	6.0	9.25	Eurosol-5; EEC laboratory ringtest; pH 3.2; 0.01 M $CaCl_2$			62
−0.80	1.81	1.7	82.4	16.0	0.25	Eurosol-6; EEC laboratory ringtest; pH 7.2; 0.01 M $CaCl_2$			62
0.45° (0.91)	2.30		6	3	1.41	Gribskov soil; A hor.; pH 3.23; CE=4.8 me/100 g; 0.01 M $CaCl_2$	11	BE	131
0.74° (0.91)	2.32		4	7	2.58	Gribskov soil; B hor.; pH 3.59; CE=9.6 me/100 g; 0.01 M $CaCl_2$	21	BE	131
0.43° (0.92)	2.18		3	5	1.82	Gribskov soil; C hor.; pH 4.07; CE=7.0 me/100 g; 0.01 M $CaCl_2$	21	BE	131
0.38° (0.97)	1.70		5	4	5.11	Strodam soil; AB hor.; pH 3.88; CE=13 me/100 g; 0.01 M $CaCl_2$	20	BE	131
−0.80° (0.93)			3	3	0.09	Strodam soil; C hor.; pH 4.95; CE=1.6 me/100 g; 0.01 M $CaCl_2$	6	BE	131
−0.85°			1	2	0.15	Tisvilde soil; C hor.; pH 4.21;	6	BE	131

TABLE 8. Sorption coefficients for pesticides—Continued

log K_d log K_f^0 ($1/n$)	log K_{oc}	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
(0.65)						CE=1.3 me/100 g; 0.01 M $CaCl_2$			
0.39° (0.93)	2.18		18	12	1.64	Roskilde soil; agric.; pH 5.40; CE=14 me/100 g; 0.01 M $CaCl_2$	6	BE	131
−0.64° (1.03)			4	18	0.06	Esrum soil; subsurf.; pH 4.71; CE=9.1 me/100 g; 0.01 M $CaCl_2$	20	BE	131
−0.57° (0.91)			7	3	0.05	Tirstrup soil; subsurf.; pH 6.14; CE=1.4 me/100 g; 0.01 M $CaCl_2$	20	BE	131
−0.89° (0.84)			34	41	0.13	Bjodstrup soil; subsurf.; pH 7.64; CE=40.5 me/100 g; 0.01 M $CaCl_2$	20	BE	131
[−0.38]	[1.46]	74.4	19.5	6.1	2.5* [1.45]	Aguadilla soil; CE=10 me/100 g; pH 7.4; 0.01 M $CaCl_2$		BE	304
[0.31]	[2.43]	27.6	35.6	36.8	1.3* [0.75]	Aguirre soil; CE=14.3 me/100 g; pH 9.0; 0.01 M $CaCl_2$		BE	304
[0.05]	[1.69]	16.6	13.0	70.4	3.9* [2.26]	Aguirre soil; CE=59.0 me/100 g; pH 8.4; 0.01 M $CaCl_2$		BE	304
[0.17]	[1.91]	14.9	39.3	45.8	3.2* [1.86]	Alonso soil; CE=13.8 me/100 g; pH 5.1; 0.01 M $CaCl_2$		BE	304
[−0.28]	[1.39]	49.2	28.8	22.0	3.7* [2.15]	Altura soil; CE=27.6 me/100 g; pH 8.0; 0.01 M $CaCl_2$		BE	304
[−0.06]	[1.95]	68.1	4.4	27.0	1.7* [0.99]	Bayamón; CE=5.0 me/100 g; pH 4.7; 0.01 M $CaCl_2$		BE	304
[0.34]	[2.09]	56.4	8.0	35.9	3.1* [1.80]	Cabo Rojo soil; CE=9.0 me/100 g; pH 4.3; 0.01 M $CaCl_2$		BE	304
[0.69]	[1.37]	36.0	36.0	28.0	36.0* [20.9]	Caño Tiburones soil; pH 5.5; CE=86.0 me/100 g; 0.01 M $CaCl_2$		BE	304
[0.87]	[2.09]	6.6	28.9	64.5	1.9* [1.10]	Catalina soil; CE=11.8 me/100 g; pH 4.7; 0.01 M $CaCl_2$		BE	304
[−0.12]	[1.88]	47.2	17.4	35.4	1.7* [0.99]	Cartagena soil; CE=36.1 me/100 g; pH 7.7; 0.01 M $CaCl_2$		BE	304
[−0.38]	[1.53]	89.0	7.3	3.7	2.1* [1.22]	Cataño soil; CE=6.9 me/100 g; pH 7.9; 0.01 M $CaCl_2$		BE	304
[0.45]	[2.29]	43.4	25.2	31.4	2.5* [1.45]	Cintrona soil; CE=25.0 me/100 g; pH 8.3; 0.01 M $CaCl_2$		BE	304
[0.09]	[2.03]	58.8	23.4	17.8	2.0* [1.16]	Cayaguá soil; CE=7.3 me/100 g; pH 5.2, 0.01 M $CaCl_2$		BE	304
[0.47]	[2.14]	22.7	37.4	39.9	3.7* [2.15]	Coloso soil; CE=23.0 me/100 g; pH 5.7; 0.01 M $CaCl_2$		BE	304
[0.25]	[1.85]	26.0	18.6	55.4	4.3* [2.49]	Corozal soil; CE=17.0 me/100 g; pH 4.6; 0.01 M $CaCl_2$		BE	304
[0.17]	[1.91]	23.4	24.8	51.8	3.2* [1.86]	Coto soil; CE=14.0 me/100 g; pH 7.7; 0.01 M $CaCl_2$		BE	304
[−0.06]	[2.22]	48.0	20.6	31.4	0.9* [0.52]	Estación soil; CE=10.0 me/100 g; pH 5.9; 0.01 M $CaCl_2$		BE	304
[−0.20]	[1.51]	39.1	29.7	32.2	3.4* [1.97]	Fe soil; CE=27.6 me/100 g; pH 7.5; 0.01 M $CaCl_2$		BE	304
[−0.20]	[1.52]	15.0	50.7	34.3	3.3* [1.91]	Fortuna soil; CE=23.3 me/100 g; pH 5.4; 0.01 M $CaCl_2$		BE	304
[−0.12]	[1.79]	15.5	32.5	52.0	2.1* [1.22]	Fraternidad soil; pH 6.3; CE=36.6 me/100 g; 0.01 M $CaCl_2$		BE	304
[0.31]	[1.92]	11.1	23.8	65.1	4.2* [2.44]	Fraternidad soil (Lajas); pH 5.9; CE=58.0 me/100 g; 0.01 M $CaCl_2$		BE	304
[0.00]	[1.55]	6.4	19.6	74.0	4.8* [2.78]	Guánica soil; CE=52.1 me/100 g; pH 8.1; 0.01 M $CaCl_2$		BE	304
[0.05]	[2.24]	84.4	8.4	7.2	1.1* [0.64]	Humacao soil; CE=4.0 me/100 g; pH 6.3; 0.01 M $CaCl_2$		BE	304
[−0.28]	[1.73]	10.1	50.9	39.0	1.7* [0.99]	Humata soil; CE=10.1 me/100 g; pH 4.5; 0.01 M $CaCl_2$		BE	304
[−0.20]	[1.52]	26.6	53.5	20.9	3.3* [1.91]	Josefa soil; CE=16.8 me/100 g; pH 6.0; 0.01 M $CaCl_2$		BE	304
[−0.28]	[1.53]	15.2	41.6	43.2	2.7* [1.57]	Juncos soil; CE=13.4 me/100 g; pH 6.2; 0.01 M $CaCl_2$		BE	304
[−0.12]	[1.52]	19.9	33.4	46.7	3.9* [2.26]	Mabí soil; CE=55.2 me/100 g; pH 7.0; 0.01 M $CaCl_2$		BE	304

TABLE 8. Sorption coefficients for pesticides—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%)				Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
[0.00]	[1.54]	22.7	40.7	36.6	4.9** [2.84]	Mabí soil; CE=31.0 me/100 g; pH 5.7; 0.01 M $CaCl_2$		BE	304
[0.13]	[2.03]	76.0	13.4	10.6	2.2* [1.28]	Machete soil; CE=8.0 me/100 g; pH 6.5; 0.01 M $CaCl_2$		BE	304
[0.09]	[1.95]	14.9	42.8	42.3	2.4* [1.39]	Mercedita soil; CE=19.9 me/100 g; pH 8.1; 0.01 M $CaCl_2$		BE	304
[−0.06]	[1.60]	26.3	27.7	46.0	3.8* [2.20]	Moca soil; CE=31.0 me/100 g; pH 5.8; 0.01 M $CaCl_2$		BE	304
[0.50]	[2.01]	22.0	49.2	28.0	5.3* [3.07]	Nipe soil; CE=11.9 me/100 g; pH 5.7; 0.01 M $CaCl_2$		BE	304
[−0.38]	[1.56]	59.4	28.2	12.4	2.0* [1.16]	Pandura soil; CE=7.7 me/100 g; pH 5.7; 0.01 M $CaCl_2$		BE	304
[0.37]	[2.06]	13.4	43.6	43.0	3.5* [2.03]	Río Piedras soil; pH 4.9; CE=11.5 me/100 g; 0.01 M $CaCl_2$		BE	304
[0.13]	[1.78]	39.0	24.6	36.4	3.9* [2.26]	Sabana Seca soil; pH 7.4; CE=23.0 me/100 g; 0.01 M $CaCl_2$		BE	304
[0.59]	[2.14]	47.0	24.4	28.6	4.9* [2.84]	San Antón soil; pH 7.4; CE=28.0 me/100 g; 0.01 M $CaCl_2$		BE	304
[−0.28]	[1.64]	57.0	18.6	24.4	2.1* [1.22]	Santa Isabel soil; pH 7.4; CE=28.0 me/100 g; 0.01 M $CaCl_2$		BE	304
[0.28]	[1.50]	46.0	20.0	34.0	10.4* [6.03]	Soller soil; CE=53.0 me/100 g; pH 6.9; 0.01 M $CaCl_2$		BE	304
[0.21]	[2.30]	73.4	19.4	7.2	1.4* [0.81]	Talante soil; CE=4.0 me/100 g; pH 5.1; 0.01 M $CaCl_2$		BE	304
[0.17]	[1.70]	35.0	24.6	40.4	5.1* [2.96]	Toa soil; CE=36.0 me/100 g; pH 8.0; 0.01 M $CaCl_2$		BE	304
[−0.12]	[1.81]	41.5	38.3	20.2	2.0* [1.16]	Toa soil; CE=13.0 me/100 g; pH 5.3; 0.01 M $CaCl_2$		BE	304
[−0.28]	[2.18]	60.9	25.1	14.0	0.6* [0.35]	Toa soil; CE=8.0 me/100 g; pH 6.0; 0.01 M $CaCl_2$		BE	304
[−0.28]	[1.41]	73.7	12.6	13.7	3.5* [2.03]	Vega Alta soil; pH 5.0 CE=5.6 me/100 g; 0.01 M $CaCl_2$		BE	304
[0.17]	[2.05]	45.2	36.8	18.0	2.3* [1.33]	Vía soil; CE=39.9 me/100 g; pH 5.1; 0.01 M $CaCl_2$		BE	304
[0.40]	[2.29]	62.4	19.6	18.0	2.2* [1.28]	Viví soil; CE=14.0 me/100 g; pH 4.8; 0.01 M $CaCl_2$		BE	304
[0.89]	[2.48]	15.0	23.4	61.6	4.5* [2.61]	Voladura soil; pH 4.3; CE=17.7 me/100 g; 0.01 M $CaCl_2$		BE	304
−0.51° (0.91)	[1.77]	71.33	18.87	9.80	0.91* [0.53]	Lubheek II surf. soil; pH 6.71; CE=4.5 me/100 g; SA(E)=26 m^2/g; 0.025 M $CaCl_2$	25	BE	333
−1.05° (0.88)		89.02	5.15	5.83	0.12* [0.07]	Lubbeek II subsoil; pH 6.46; CE=2.37 me/100 g; SA(E)=22 m^2/g; 0.025 M $CaCl_2$	25	BE	333
−1.30° (0.88)		91.32	2.12	6.56	0.04* [0.02]	Lubbeek, II subsoil; pH 6.43; CE=2.3 me/100 g; SA(E)=27 m^2/g; 0.025 M $CaCl_2$	25	BE	333
−0.11° (0.92)	[1.83]	14.96	69.92	15.12	1.98* [1.15]	Lubbeek I surf. soil; pH 6.62; CE=9.52 me/100 g; SA(E)=33.5 m^2/g; 0.025 M $CaCl_2$	25	BE	333
−0.37° (0.91)	[1.82]	32.60	55.18	12.22	1.12* [0.65]	Lubbeek III surf. soil; pH 6.91; CE=7.02 me/100 g; SA(E)=38 m^2/g; 0.025 M $CaCl_2$	25	BE	333
0.26° (0.93)	[2.23]	83.95	10.27	5.78	1.85* [1.07]	Stookrooie surf. soil; pH 5.64; CE=2.9 me/100 g; SA(E)=17.5 m^2/g; 0.025 M $CaCl_2$	25	BE	333
0.31° (0.94)	[1.80]	3.05	62.89	34.06	5.59* [3.24]	Fleron surf. soil; pH 3.75; CE=12.29 me/100 g; SA(E)=52 m^2/g; 0.025 M $CaCl_2$	25	BE	333
0.26° (0.91)	[1.77]	23.84	59.84	6.32	5.45* [3.16]	Bullingen surf. soil; pH 3.55; CE=8.23 me/100 g; SA(E)=13 m^2/g; 0.025 M $CaCl_2$	25	BE	333
1.38°		6.58	59.66	33.76	6.70*	Spa surf. soil; pH 3.25;	25	BE	333

TABLE 8. Sorption coefficients for pesticides—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%)				Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
(0.86)					[3.89]	CE=12.1 me/100 g; SA(E)=18.8 m^2/g; 0.025 M $CaCl_2$			
1.12° (0.88)	[2.74]	10.86	61.69	27.45	4.17* [2.42]	Bernard-Fagne surf. soil; pH 3.60; CE=8.75 me/100 g; SA(E)=33.6 m^2/g; 0.025 M $CaCl_2$	25	BE	333
0.88° (0.92)	[2.48]	8.16	69.69	22.15	4.37* [2.53]	Stavelot surf. soil; pH 3.90; CE=5.61 me/100 g; SA(E)=20.4 m^2/g; exch. Al=4.51 me$_q$/100 g; 0.025 M $CaCl_2$	25	BE	333
0.85° (0.88)	[2.30]	18.50	73.00	8.50	6.19* [3.59]	Meerdael surf. soil; pH 4.00; CE=11.74 me/100 g; SA(E)=35 m^2/g; 0.025 M $CaCl_2$	25	BE	333
1.21° (0.76)		31.00	68.50	0.50	8.52* [4.94]	Soignes surf. soil; pH 3.40; CE=16.9 me/100 g; SA(E)=23 m^2/g; 0.025 M $CaCl_2$	25	BE	333
−0.07° (0.92)	[1.77]	76.04	17.06	6.90	2.50* [1.45]	Heverlee surf. soil; pH 5.84; CE=10.7 me/100 g; SA(E)=21 m^2/g; 0.025 M $CaCl_2$	25	BE	333
−0.41° (0.89)	[1.73]	19.30	72.90	7.80	1.25* [0.73]	Nodebais surf. soil; pH 6.20; CE=8.4 me/100 g; SA(E)=40.6 m^2/g; 0.025 M $CaCl_2$	25	BE	333
1.02° (0.86)		94.60	2.11	3.29	3.20* [1.86]	Zolder surf. soil; pH 3.84; CE=1.66 me/100 g; SA(E)=10 m^2/g; 0.025 M $CaCl_2$	25	BE	333
−0.02° (0.88)	[2.71]	96.77	2.59	0.64	0.32* [0.19]	Zolder surf. soil; pH 4.23; CE=0.45 me/100 g; SA(E)=1 m^2/g; 0.025 M $CaCl_2$	25	BE	333
−0.38° (0.93)		96.60	1.30	2.10	0.12* [0.07]	Zolder subsoil; pH 4.73; CE=0.68 me/100 g; SA(E)=6.6 m^2/g; 0.025 M $CaCl_2$	25	BE	333
−0.11	[1.84]			16.2	1.11	Conventional farm soil; pH 5.42; 0.004 M $CaSO_4$		BE	646
−0.22	[1.78]			19.7	1.00	Idem; pH 5.35			646
−0.51	[1.68]			24.7	0.64	Idem; pH 7.12			646
0.10	[1.84]			16.5	1.85	Low-input farm soil; pH 5.53; 0.004 M $CaSO_4$		BE	646
−0.04	[1.86]			16.6	1.26	Idem; pH 5.47			646
−0.27	[1.80]			19.1	0.86	Idem; pH 6.32			646
−0.54° (0.98)	[1.51]				0.90	Glendale c soil; (no addition of sewage sludge); 0.01 N $CaCl_2$		BE	647
−0.58° (0.89)	[1.25]				1.45	Idem; freshly amended (+22.4 metric tons/ha sewage sludge)			647
−0.57° (0.89)	[1.21]				1.66	Idem; freshly amended (+44.9 metric tons/ha sewage sludge)			647
−0.57° (0.77)					0.86	Idem; preconditioned (no addition of sewage sludge)			647
−0.47° (0.81)					1.37	Idem; preconditioned (+44.9 metric tons/ha sewage sludge)			647
−0.42° (0.74)					1.61	Idem; preconditioned (+80.8 metric tons/ha sewage sludge)			647
−0.92° (0.76)					0.60	Harvey fine sl soil; (no addition of sewage sludge); 0.01 N $CaCl_2$		BE	647
−0.77° (0.85)					1.12	Idem; freshly amended (+22.4 metric tons/ha sewage sludge)			647
−0.77° (0.93)	[1.10]				1.36	Idem; freshly amended (+44.9 metric tons/ha sewage sludge)			647
−1.00° (0.75)					0.62	Idem; preconditioned (no addition of sewage sludge)			647
−0.92° (0.72)					0.64	Idem; preconditioned (+44.9 metric tons/ha sewage sludge)			647
−0.72°					0.65	Idem; preconditioned (+89.8			647

TABLE 8. Sorption coefficients for pesticides—Continued

log K_d log K_f^0 (1/*n*)	log K_{oc}	Sorbent composition (%)				Other sorbent and solution data: prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
(0.58)						metric tons/ha sewage sludge)			
−0.80° (0.88)	[1.38]				0.66	Lea sl soil; (no addition of sewage sludge); 0.01 N $CaCl_2$		BE	647
−0.85° (0.91)	[1.06]				1.23	Idem; freshly amended (+22.4 metric tons/ha sewage sludge)			647
−0.80° (0.99)	[1.01]				1.57	Idem; freshly amended (+44.9 metric tons/ha sewage sludge)			647
−0.72° (0.76)					0.74	Idem; preconditioned (no addition of sewage sludge)			647
−0.22° (0.60)					1.31	Idem; preconditioned (+44.9 metric tons/ha sewage sludge)			647
−0.26° (0.57)					1.57	Idem; preconditioned (+89.8 metric tons/ha sewage sludge)			647
	1.76av (three soils)	38	48	14	0.68	Commerce soil; pH 6.7		BE	575
		56	30	14	1.12	Tracy soil; pH 6.2		BE	575
		12	56	32	2.01	Catlin soil; pH 6.2		BE	575
0.46° (0.91)	2.11				2.24	Speyer soil 2.2 (0.15–0.5 mm); pH 5.8	22	BE	181
0.04° (0.69)		12.9	64.3	19.6	0.76	Alfisol soil; pH 7.5	22	BE	181
0.63° (0.70)		81.5	10.0	7.2	3.56	Spodosol soil; pH 3.9	22	BE	181
−0.22° (0.92)						Cellulose	22	BE	181
0.34° (1.04)						Alumina	22	BE	181
−0.66	[1.87]	98.38	1.61	0.74	0.51* [0.30]	Lakeland soil; CE=0.89 me/100 g; 0.01 N $CaSO_4$		BE	648
0.98° (0.89)	2.29	89.2	8.2	2.6	4.85	Podzol soil; pH 2.8; CE=15.1 me/100 g;		BE	163
−0.66° (1.06)	1.23	69.7	14.4	15.9	1.25	Alfisol soil; pH 6.7; CE=12.3 me/100 g;		BE	163
−0.82° (0.94)	1.00	5.5	58.8	35.7	1.58	Lake Constance sedim.; pH 7.1; CE=13.4 me/100 g;		BE	163
	3.38°* (0.75)				56.4	Humic acid from Black Chernozemic soil; pH 3.3–3.6	5	BE	125
	3.21°* (0.79)					Idem	25		125
	3.16° (0.76)				38*	Fulvic acid-montmorillonite complex; pH 3.5	5	BE	649
	3.06° (0.83)					Idem	25		649
	1.30					Soil; experimental (literature)			217
	1.29av					9 soils (literature)			87
	2.59					Cyanopropyl column; pH 3	20–25	RPLC	579
	1.36					C18 column		RPLC	573
	2.00					Correlation log K_{oc}–log S			564
	1.48					Correlation log K_{oc}–MCI			578
						2,4-D amine			
0.66° (0.70)		18.4	45.3	38.3	3.87	Webster soil; pH 7.3; CE=54.7 me/100 g; 0.01 N $CaCl_2$	23	BE	102
−0.19° (0.83)		65.8	19.5	14.7	0.90	Cecil soil; pH 5.6; CE=6.8 me/100 g; 0.01 N $CaCl_2$	23	BE	102
−0.12° (0.73)		93.8	3.0	3.2	0.56	Eustis soil; pH 5.6; CE=5.2 me/100 g; 0.01 N $CaCl_2$		BE	102
	2.04av					3 soils (literature data)			87
						p,p′-DDT			
3.11	5.11			18	0.99	Montcalm soil; sandy loam; CE=5 me/100 g	25	BE	184
4.14	5.55			46	3.86	Sims soil; clay; CE=30 me/100 g;	25	BE	184

TABLE 8. Sorption coefficients for pesticides—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%)				Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
5.03	5.36				46.5	Houghton soil; muck; CE=214 me/100 g;	25	BE	184
	5.18av (three soils)	38	48	14	0.68	Commerce soil; pH 6.7		BE	575
		56	30	14	1.12	Tracy soil; pH 6.2		BE	575
		12	56	32	2.01	Catlin soil; pH 6.2		BE	575
3.94	5.68	25	40	35	1.8	Taichung soil; pH 6.8	25	BE	407
4.89						Sewage effluent; pH 7.6		BE	650
5.32						Idem (after filtration)		BE	650
4.31	5.95				2–4	Boonton Reservoir sed.; pH 8.3		BE	421
	5.61				54.3	Boonton sed. humic acid; pH 8.3; 0.01 M NaCl	25	ED	421, 402
3.66	6.24			6.9	0.45* [0.26]	Mivtahim agricult. surface soil	25	BE	563
3.81	5.95			23.8	1.25* [0.73]	Gilat agricult. surface soil	25	BE	563
3.91	5.69			71.2	2.82* [1.64]	Neve Yaar agricult. surface soil	25	BE	563
3.98	5.45			76.2	5.82* [3.38]	Malkiya agricult. surface soil	25	BE	563
4.54	5.88			60.5	7.85* [4.55]	Kinneret A Lake sediment	25	BE	563
4.18	5.77			63.8	4.39* [2.55]	Kinneret G Lake sediment	25	BE	563
4.68	6.25				2.7	Narragansett Bay (NB) sed.; sea water	25	BE	173
4.82	6.39					Idem	5		173
4.08	6.30				0.6	Idem after treatment with H_2O_2	25		173
5.39	5.63				57	Humic acid from NB sed.; sea water	25	BE	173
5.30	5.54					Idem	5		173
5.48	5.72					Idem; distilled water	25		173
4.48						Montmorillonite clay; sea water	25	BE	173
4.63						Idem	5		173
4.60						Idem; distilled water	25		173
3.78						Kaolinite clay; sea water	25	BE	173
	5.07–5.35				45.8	Pakim Pond humic acid; pH 6.0–9.2; μ=0.01–0.08; 7 values	25	ED	402
	5.61–5.74				54.9	Aldrich humic acid; pH 8.3; 25 μ=0.001–0.08; 3 values		ED	402
	5.61					Boonton Reservoir sediment humic acid; pH 8.3; μ=0.01	25	ED	402
	4.84					Pakim Pond water DOC; pH 8.3; μ=0.001	25	ED	402
	4.83					Boonton water DOC; pH 8.3; μ=0.001	25	ED	402
	5.06				58.0	Sanhedron soil humic acid; pH 6.5	24	SE	220
	4.58				48.7	Sanhedron soil fulvic acid; pH 6.5	24	SE	220
	4.39				54.2	Suwannee River humic acid; pH 6.5	24	SE	220
	4.40				53.8	Suwannee River fulvic acid; pH 6.5	24	SE	220
	5.53					Aldrich humic acid	25	SE	407
	5.56				69.4	Aldrich humic acid Na salt; pH 6.5	24	SE	219
	5.56				65.8	Fluka-Tridom humic acid; pH 6.5	24	SE	219
	4.93				56.7	Calcasieu River Humic extr.; pH 6.5	24	SE	219
	4.39					Suwannee River water; pH 6.5; DOC=37 mg/L	24	SE	219
	4.39					Sopchoppy River water; pH 6.5; DOC=44 mg/L	24	SE	219
	5.11					Aldrich humic acid (DOC=9.4 mg/L); pH 5.8–6.8		RS	414
	5.45					Idem		ED	414

TABLE 8. Sorption coefficients for pesticides—Continued

log K_d log K_f^0 (1/n)	log K_{oc}	Sorbent composition (%)				Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
	5.44					Idem (log K_{doc} is the zero intercept of the regression line of log K_{doc} vs DOC concentration)		RS	414
	4.46					DOC in Lake Erie water (9.6 mg/L)		RS	414
	4.76					Idem		ED	414
	4.23					DOC in Huron River wat. (7.8 mg/L)		RS	414
	5.67					Idem		ED	414
	5.40					Aldrich humic acid	25	RS	409
5.57av	6.36av					Lake suspended matter (three phases distribution)	25	RS	409
	4.26av					Lake dissolved organic matter (same procedure)	25	RS	409
5.46av	6.24av				16	Green Bay suspended matter (same procedure)	25	RS	410
	3.97av					Green Bay DOC (same procedure)	25	RS	410
	5.70					Aldrich humic acid; pH 7.32 (DOC=0–1.7 mg/L)	6.6	RS	546
	4.55					Peat humic acid		ED	423
	3.98					Bermeo soil humic acid		ED	423
	3.09					Bermeo soil fulvic acid		ED	423
	5.63					Cyanopropyl column	20–25	RPLC	579
	[6.23]				58.03	Prediction by limiting vapor sorption on soil humic acid	23	LSC	363
	5.59				50.2	Aldrich and Fluka humic acid		FH	206
	4.64					C18 column		RPLC	573
	5.38					Soil; experimental (literature)			217
	5.39av					2 soils (literature)			87
	5.63av					31 literature data			562
	5.80					Correlation log K_{oc}–log K_{ow}			96
	4.95					Correlation log K_{oc}–log K_{ow}			207
	5.98					Correlation log K_{oc}–log K_{ow}			108
	5.16					Correlation log K_{oc}–log S			564
	5.62					Correlation log K_{oc}–log S			96
	6.81					Correlation log K_{oc}–log S(mp)			96
	5.34					Correlation log K_{oc}–MCI			578
	[5.57]					Correlation log K_{om}–MCI			591
						Diallate			
	3.03°* (0.67)					Peat moss; pH 4.0	25	BE	475
1.56° (0.67)						Silica gel (24–32 mesh/cm); pH 8.2	25	BE	475
2.72° (0.68)						Wheat straw; pH 6.2	25	BE	475
	3.28					Soil; experimental (literature)			217
	3.00					Correlation log K_{oc}–log S			564
	2.77					Correlation log K_{oc}–MCI			578
						Diazinon			
[0.67]	[2.36]				3.53* [2.05]	Batcombe sil soil; pH 6.1; 0.01 M $CaCl_2$	20	BE	120
1.14	2.51	18.9	26.3	54.8	4.24	Tsukuba soil; pH 6.5; 0.01 M $CaCl_2$	25	BE	642
1.07° (0.95)						Idem			642
0.38	2.24	23.1	15.4	61.5	1.35	Kanuma soil; pH 5.7; 0.01 M $CaCl_2$	25	BE	642
0.42° (1.04)						Idem			642
2.51° (1.00)	[2.87]	52	34	14	75.3* [43.7]	Soil; organic; pH 6.1		BE	264
0.85°	[2.64]	71	22	7	2.8*	Big Creek sediment; pH 6.6		BE	264

TABLE 8. Sorption coefficients for pesticides—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
(1.07)					[1.62]				
0.78°	[2.62]	56	30	14	2.5*	Beverly soil; pH 6.8		BE	264
(0.99)					[1.45]				
0.30°	[2.69]	91.5	1.5	7	0.7*	Plainfield soil; pH 7.0		BE	264
(1.08)					[0.41]				
0.56°		35.5	5.3	59.2	0.6*	Soil; pH 6.3	20	BE	651
(0.81)					[0.35]				
1.63°		76.2	12.8	11.0	8.7*	Soil; pH 5.1	20	BE	651
(0.85)					[5.05]				
0.94°	[2.51]	73.9	11.9	14.2	4.7*	Soil; pH 5.1	20	BE	651
(0.88)					[2.73]				
0.28°	[2.61]	66.4	15.6	18.1	0.8*	Soil; pH 7.5	20	BE	651
(0.97)					[0.46]				
1.00°	[3.35]	66.4	15.5	18.1	0.77*	Eutric Cambisol (Ah hor.); pH 7.5;	20	BE	350
(0.91)					[0.45]	CE=9.4 me/100 g;			
1.30°	[3.63]	4.4	53.0	42.6	0.82*	Marismas 1 soil; pH 7.7	20	BE	652
(0.95)					[0.48]				
0.68°	[2.88]	4.2	27.1	68.7	1.10*	Idem 2; pH 7.8			652
(0.98)					[0.64]				
0.85°	[2.90]	11.2	26.7	62.1	1.55*	Idem 3; pH 7.6			652
(0.88)					[0.90]				
0.73°	[3.21]	25.7	32.5	41.8	0.57*	Idem 4; pH 7.7			652
(0.94)					[0.33]				
0.80	[2.70]	26.3	21.9	51.8	2.16*	Idem 5; pH 7.8			652
(0.88)					[1.25]				
0.20°	[2.70]	53.1	11.0	35.9	0.55*	Idem 6; pH 7.9			652
(1.03)					[0.32]				
−0.15°	[2.41]	70.9	5.3	23.8	0.47*	Idem 7; pH 7.9			652
(1.09)					[0.27]				
0.44°	[2.71]	73.0	3.0	24.0	0.93*	Idem 8; pH 7.7			652
(0.97)					[0.54]				
0.16°	[2.65]	53.1	5.9	41.0	0.57*	Idem 9; pH 7.4			652
(1.09)					[0.33]				
0.20°		65.4	5.6	29.0	0.15*	Idem 10; pH 4.6			652
(1.25)					[0.09]				
0.62°	[2.74]	78.2	6.6	15.2	1.30*	Idem 11; pH 5.8			652
(0.91)					[0.75]				
0.41°	[3.31]	75.8	5.7	18.5	0.22*	Idem 12; pH 4.6			652
(1.10)					[0.13]				
0.25°	[2.64]	74.9	8.5	16.6	0.72*	Idem 13; pH 7.9			652
(0.93)					[0.42]				
0.62°	[2.56]	33.1	14.3	52.6	2.01*	Idem 14; pH 7.4			652
(0.93)					[1.17]				
0.71°	[2.53]	13.5	23.9	62.6	2.60*	Idem 15; pH 7.4			652
(0.94)					[1.51]				
0.82°		59.6	12.2	28.2	1.89*	Idem 16; pH 7.9			652
(0.79)					[1.10]				
0.71°	[2.77]	66.6	6.9	26.5	1.52*	Idem 17; pH 7.2			652
(0.90)					[0.88]				
0.39°	[2.91]	65.9	7.5	26.6	0.52*	Idem 18; pH 7.9			652
(1.01)					[0.30]				
0.24°	[2.64]	88.8	2.7	8.5	0.69*	Idem 19; pH 5.2			652
(1.06)					[0.40]				
−0.03°		66.4	15.5	18.1	0.77*	Idem 20; pH 7.5			652
(1.18)					[0.45]				
1.36°	[2.59]	64.3	21.1	14.6	10.2*	Salamanca soil 21; pH 4.7	20	BE	652
(0.93)					[0.93]				
1.41°		67.4	18.7	13.9	8.90*	Idem 22; pH 5.0			652
(0.85)					[5.16]				
1.30°		75.4	13.0	11.6	5.95*	Idem 23; pH 5.3			652
(0.79)					[3.45]				
0.97°		73.9	11.9	14.2	4.66*	Idem 24; pH 5.1			652
(0.85)					[2.70]				

TABLE 8. Sorption coefficients for pesticides—Continued

log K_d log K_f^0 ($1/n$)	log K_{oc}	Sorbent composition (%)				Other sorbent and solution data: prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
0.99° (0.95)	[2.70]	54.2	34.0	11.8	3.44* [2.00]	Idem 25; pH 5.6			652
	5.38					Soil; experimental (literature)			217
	2.76					Correlation log K_{oc}–log S			564
	3.13					Correlation log K_{oc}–MCI			598
						Dicamba (pK_a=1.95, Ref. 680)			
2.82				100		Ca–montmorillonite; pH 6	24	BE	121
NA					94* [54.5]	OM from peaty muck (Histosol) soil; pH 5.5	24	BE	121
−2.0	[−0.46]		59	22	2.8	Waukegan soil; pH 4.1; CE=21 cmol/kg; 0.01 M $CaCl_2$	23	BE	323
−0.66	[0.93]		73	21	2.6	Plano soil; pH 4.7; CE=17 cmol/kg; 0.01 M $CaCl_2$	23	BE	323
−0.89	[0.70]					Idem; pH 5.8			323
−1.05	[0.54]					Idem; pH 6.3			323
−2.0	[−0.04]		62	15	1.1	Walla Walla soil; pH 5.0; CE=20 cmol/kg; 0.01 M $CaCl_2$	23	BE	323
−2.0	[−0.04]					Idem; pH 5.5			323
−2.0	[−0.04]					Idem; pH 6.0			323
0.93° (0.99)						Peat; pH 3.5	25	BE	320
−0.96° (0.72)		47.5	33.2	20.3	10.5* [6.09]	Melfort soil; pH 5.9	25	BE	320
−1.08° (0.74)		25		22	9.0	Elkton soil (Ap horizon); pH 6.1; CE=5.6 me/100 g	25	BE	322
	−0.40					Soil; experimental (literature)			217
	0.34av					5 soils (literature)			87
	1.63					Correlation log K_{oc}–log S			564
	1.46					Correlation log K_{oc}–MCI			598
						Dicrotophos			
−1.15° (0.77)		88	8	4	1.1* [0.64]	Georgia soil; pH 6.7; CE=2.0 me/100 g	25	BE	653
−0.40° (0.96)	[1.73]	60	28	12	1.3* [0.75]	Hanford soil; pH 6.4; CE=7.1 me/100 g	25	BE	653
−0.04° (0.95)	[1.60]	24	52	24	4.0* [2.3]	Catlin soil; pH 5.7; CE=13.0 me/100 g	25	BE	653
0.55° (0.98)	[2.27]	22	34	44	3.3* [1.9]	Soil: clay loam; pH 5.9; CE=23.5 me/100 g	25	BE	653
						Dieldrin			
2.07° (0.79)		77	15	8	3.9* [2.26]	Bondhead soil (2.00E-4 g/mL); pH 6.9	20	BE	486
2.13° (0.78)						Idem (2.00E-3 g/mL)			486
1.59	[3.99]				0.4	Plainfield-Bloomfield s soil; CE=1.7 me/100 g; 0.01 M $CaCl_2$	25	BE	265
2.17	[4.09]				1.2	Gilford-Hoopeston-Ade sl soil; CE=7.5 me/100 g; 0.01 M $CaCl_2$	25	BE	265
2.42	[3.99]				2.7	Bryce-Swygert sic soil; CE=34.4 me/100 g; 0.01 M $CaCl_2$	25	BE	265
2.30	[3.81]				3.1	Drummer sicl soil; CE=24.8 me/100 g; 0.001 M $CaCl_2$	25	BE	265
2.42	[3.87]				3.5	Flanagan sil soil; CE=27.7 me/100 g; 0.01 M $CaCl_2$	25	BE	265
2.47	[3.60]				7.5	Bryce sic soil; CE=55.5 me/100 g; 0.01 M $CaCl_2$	25	BE	265
3.18	[3.95]				16.8	Houghton soil; muck; CE=72.4 me/100 g; 0.01 M $CaCl_2$	25	BE	265
2.29°	4.15				1.42	Soil; cl; (kaolinite);	20	BE	214

TABLE 8. Sorption coefficients for pesticides—Continued

log K_d log K_f^0 $(1/n)$	log K_{oc}	Sorbent composition (%)				Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
(0.954)						pH 5.91; CE=12.4 me$_q$/100 g			
	4.40*av			65-*	85*	Eight sludges from two water treatment plants	22.5	BE	535
[2.42]	[4.11]				3.53* [2.05]	Batcombe sil soil; pH 6.1; 0.01 M $CaCl_2$	20	BE	120
3.63° (1.08)	[3.99]	52	34	14	75.3* [43.7]	Soil; organic; pH 6.1		BE	264
2.65° (0.91)	[4.44]	71	22	7	2.8* [1.62]	Big Creek sediment; pH 6.6		BE	264
2.53° (0.89)	[4.37]	56	30	14	2.5* [1.45]	Beverly soil; pH 6.8		BE	264
2.03° (0.88)	[4.41]	91.5	1.5	7	0.7* [0.41]	Plainfield soil; pH 7.0		BE	264
2.99	4.73	25	40	35	1.8	Taichung soil; pH 6.8	25	BE	407
	4.89					Aldrich humic acid	25	SE	407
	4.55					Correlation log K_{oc}–log S			564
	4.03					Correlation log K_{oc}–MCI			598
						Dimethoate			
[0.73]	[0.96]				3.53* [2.05]	Batcombe silt loam; pH 6.1; 0.01 M $CaCl_2$	20	BE	120
−0.10	1.26	18.9	26.3	54.8	4.24	Tsukuba soil; pH 6.5; 0.01 M $CaCl_2$	25	BE	642
−0.31° (0.85)						Idem	25	BE	642
−0.30	1.56	23.1	15.4	61.5	1.35	Kanuma soil; pH 5.7; 0.01 M $CaCl_2$	25	BE	642
−0.37° (0.95)						Idem	25	BE	642
	1.23					Correlation log K_{oc}–log S			564
	1.39					Correlation log K_{oc}–MCI			598
						Dinoseb			
	2.09					Soil; experimental (literature)			217
	3.82					Cyanopropyl column; pH 3	20–25	RPLC	579
	2.71					Correlation log K_{oc}–log S			564
	2.74					Correlation log K_{oc}–MCI			578
						Diphenamid			
0.41	[1.80]	2.9	68.7	28.4	7.1* [4.1]	Lanton soil; pH 6.4; CE=32.8 me/100 g		BE	631
	2.32					Correlation log K_{oc}–log S			564
						Dipropetryn			
−1.15° (0.97)		100				Quartz sand; pH 5.6; CE=0.4 me/100 g; 0.01 N $CaCl_2$	26	BE	299
0.12° (0.88)	[2.58]	93	4	3	0.6* [0.35]	Cobb soil; pH 7.3; CE=3.8 me/100 g; 0.01 N $CaCl_2$	26	BE	299
1.51° (0.73)		93	4	3	2.1* [1.22]	Cobb soil+2% muck; pH 5.3; CE=9.0 me/100 g; 0.01 N $CaCl_2$	26	BE	299
0.79° (0.86)		58	23	19	1.3* [0.75]	Teller soil; pH 5.7; CE=8.6 me/100 g; 0.01 N $CaCl_2$	26	BE	299
0.95° (0.81)		16	42	42	1.8* [1.04]	Port soil; pH 6.3; CE=17.9 me/100 g; 0.01 N $CaCl_2$	26	BE	299
1.27° (0.89)	[3.06]	27	45	29	2.8* [1.62]	Brewer soil; pH 5.8; CE=13.5 me/100 g; 0.01 N $CaCl_2$	26	BE	299
	3.07					Soil; experimental (literature)			217
	3.07av					5 soils (literature)			87
	3.10					Correlation log K_{oc}–MCI			598
	2.98					Correlation log K_{oc}–log S			564

TABLE 8. Sorption coefficients for pesticides—Continued

log K_d log K_f^0 (1/*n*)	log K_{oc}	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data: prediction procedure	Temp. (°C)	Meth.	Ref.
						Disulfoton			
1.33° (1.00)	[2.90]			18	2.7	Broadbalk FYM plot soil; pH 7.8; CE=19.8 me/100 g; 0.01 M $CaCl_2$	20	BE	262
0.76° (1.01)	[2.81]			18	0.9	Broadbalk nil plot soil; pH 8.1; CE=10.4 me/100 g; 0.01 M $CaCl_2$	20	BE	262
1.30° (1.00)	[3.05]			7	1.8	Woburn plot 2 soil; pH 6.5; CE=10.7 me/100 g; 0.01 M $CaCl_2$	20	BE	262
1.31° (0.85)				6	1.3	Woburn plot 4 soil; pH 6.8; CE=10.6 me/100 g; 0.01 M $CaCl_2$	20	BE	262
1.17° (0.93)	[3.13]			6	1.1	Woburn plot 34 soil; pH 6.8; CE=10.2 me/100 g; 0.01 M $CaCl_2$	20	BE	262
1.17° (0.81)				26	1.4	Stretham soil; pH 7.5; CE=13.0 me/100 g; 0.01 M $CaCl_2$	20	BE	262
1.69° (0.87)				11	7.6	Islcham 1 soil; pH 7.5; CE=44.8 me/100 g; 0.01 M $CaCl_2$	20	BE	262
1.74° (0.88)	[3.30]			2	2.8	Islcham 2 soil; pH 6.3; CE=18.2 me/100 g; 0.01 M $CaCl_2$	20	BE	262
1.77° (0.97)	[2.82]			16	8.8	Bottisham soil; pH 7.7; Ce=48.2 me/100 g; 0.01 M $CaCl_2$	20	BE	262
0.72° (1.09)	[2.88]			8	0.7	Worlington soil; pH 8.1; CE=6.3 me/100 g; 0.01 M $CaCl_2$	20	BE	262
1.98° (0.80)				25	12.0	Spinney soil; pH 7.2; CE=66.4 me/100 g; 0.01 M $CaCl_2$	20	BE	262
1.31° (0.80)				36	1.7	Wicken soil; pH 8.0; CE=21.9 me/100 g; 0.01 M $CaCl_2$	20	BE	262
2.00° (1.00)	[2.83]			62	15.0	Prickwillow soil; pH 5.1; CE=83.4 me/100 g; 0.01 M $CaCl_2$	20	BE	262
1.32° (0.81)				10	1.7	Moulton soil; pH 8.1; CE=10.6 me/100 g; 0.01 M $CaCl_2$	20	BE	262
1.20° (0.92)	[2.95]			21	1.8	Oakington soil; pH 7.2; CE=14.0 me/100 g; 0.01 M $CaCl_2$	20	BE	262
1.85° (0.94)	[2.81]			36	11.0	Peacock soil; pH 7.6; CE=74.0 me/100 g; 0.01 M $CaCl_2$	20	BE	262
2.13° (0.95)	[2.64]				31.0	Adventures peat soil; pH 6.9; CE=118.8 me/100 g; 0.01 M $CaCl_2$	20	BE	262
1.78° (1.18)				75	1.3	Eurosol-1; c; pH 5.1; 0.01 M $CaCl_2$		BE	583
1.71° (1.42)				22.6	3.7	Eurosol-2; sil; pH 7.4; 0.01 M $CaCl_2$		BE	583
1.65° (1.27)				17.0	3.45	Eurosol-3; 1; pH 5.2; 0.01 M $CaCl_2$		BE	583
1.56° (1.34)				20.3	1.55	Eurosol-4; si; pH 6.5; 0.01 M $CaCl_2$		BE	583
3.11° (2.06)				6.0	9.25	Eurosol-5; ls; pH 3.2; 0.01 M $CaCl_2$		BE	583
	3.25					Soil; experimental (literature)			217
	3.20av					20 soils (literature)			87
	2.87					Correlation log K_{oc}–log S			564
	2.91					Correlation log K_{oc}–MCI			598
						Diuron			
1.36° (0.93)				100		Na–montmorillonite (1–0.2 μm); pH 6.80; CE=87.0 me/100 g	25	BE	250
1.85° (1.05)				100		H–montmorillonite (1–0.2 μm); pH 3.35; CE=73.5 me/100 g	25	BE	250
1.64° (0.80)				100		H–montmorillonite; pH 3.6		BE	212
1.38° (0.80)				100		Na–montmorillonite; pH 7.9		BE	212
1.38° (0.80)				100		Ca–montmorillonite; pH 7.9		BE	212
1.36° (0.80)				100		Mg–montmorillonite; pH 8.2		BE	212

TABLE 8. Sorption coefficients for pesticides—Continued

log K_d log K_f^0 ($1/n$)	log K_{oc}	Sorbent composition (%)				Other sorbent and solution data: prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
[0.10]	[2.34]			14.3	0.99* [0.57]	Bosket sil soil; pH 5.8; CE=8.4 me/100 g; 0.01 M $CaCl_2$	26	BE	38
[0.20]	[2.16]			20.1	1.89* [1.10]	Cecil scl soil, pH 5.3; CE=3.6 me/100 g; 0.01 M $CaCl_2$	26	BE	38
[0.35]	[2.36]			29.0	1.67* [0.97]	Dundee sicl soil; pH 5.0; CE=18.1 me/100 g; 0.01 M $CaCl_2$	26	BE	38
[0.22]	[2.07]			22.4	2.42* [1.40]	Beltsville sil soil; pH 4.3; CE=4.2 me/100 g; 0.01 M $CaCl_2$	26	BE	38
[0.45]	[2.22]			23.9	2.90* [1.68]	Chester l soil; pH 4.9; CE=5.2 me/100 g; 0.01 M $CaCl_2$	26	BE	38
[−0.05]	[2.19]			24.4	0.99* [0.57]	Christiana l soil; pH 4.4; CE=5.6 me/100 g; 0.01 M $CaCl_2$	26	BE	38
[0.12]	[2.19]			26.6	1.48* [0.86]	Ascalon scl soil; pH 7.3; CE=12.7 me/100 g; 0.01 M $CaCl_2$	26	BE	38
[−0.26]	[2.34]			13.7	0.44* [0.26]	Truckton sl soil; pH 7.0; CE=4.4 me/100 g; 0.01 M $CaCl_2$	26	BE	38
[0.15]	[2.17]			30.7	1.64* [0.95]	Sterling cl soil; pH 7.7; CE=22.5 me/100 g; 0.01 M $CaCl_2$	26	BE	38
[0.04]	[2.22]			40.6	1.13* [0.66]	Garland c soil; pH 7.7; CE=23.2 me/100 g; 0.01 M $CaCl_2$	26	BE	38
[0.33]	[2.23]			35.7	2.18* [1.26]	Thurlow cl soil; pH 7.7; CE=21.6 me/100 g; 0.01 M $CaCl_2$	26	BE	38
[0.93]	[2.34]			34.4	6.90* [4.00]	Barnes cl soil; pH 7.4; CE=33.8 me/100 g; 0.01 M $CaCl_2$	26	BE	38
[0.63]	[2.35]			18.0	3.30* [1.91]	Crosby sil soil; pH 4.8; CE=11.5 me/100 g; 0.01 M $CaCl_2$	26	BE	38
[0.17]	[2.15]			17.4	1.82* [1.06]	Ruston sl soil; pH 5.1; CE=3.4 me/100 g; 0.01 M $CaCl_2$	26	BE	38
[−0.21]	[2.03]			11.2	0.98* [0.57]	Tifton ls soil; pH 4.9; CE=2.4 me/100 g; 0.01 M $CaCl_2$	26	BE	38
[0.63]	[2.23]			30.0	4.31* [2.50]	Hagerstown sicl soil; pH 5.5; CE=12.5 me/100 g; 0.01 M $CaCl_2$	26	BE	38
[0.33]	[2.21]			32.4	2.26* [1.31]	Hagerstown sicl soil; pH 7.5; CE=8.8 me/100 g; 0.01 M $CaCl_2$	26	BE	38
[0.07]	[2.13]			20.7	1.49* [0.86]	Tripp l soil; pH 7.6; CE=14.7 me/100 g; 0.01 M $CaCl_2$	26	BE	38
[0.75]	[2.30]			52.5	4.85* [2.81]	Toledo sic soil; pH 5.5; CE=29.8 me/100 g; 0.01 M $CaCl_2$	26	BE	38
[0.33]	[2.21]			21.2	2.27* [1.32]	Wooster sil soil; pH 4.7; CE=6.8 me/100 g; 0.01 M $CaCl_2$	26	BE	38
[0.66]	[2.26]			22.1	4.40* [2.55]	Chillum sil soil; pH 4.6; CE=7.6 me/100 g; 0.01 M $CaCl_2$	26	BE	38
[0.04]	[1.76]			10.5	3.26* [1.89]	Lakeland sl soil; pH 6.2; CE=2.9 me/100 g; 0.01 M $CaCl_2$	26	BE	38
[0.84]	[2.35]			23.2	5.27* [3.06]	Iredell sil (topsoil); pH 5.4; CE=17.0 me/100 g; 0.01 M $CaCl_2$	26	BE	38
[−0.02]	[2.19]			44.2	1.07* [0.62]	Iredell c (subsoil); pH 5.6; CE=20.9 me/100 g; 0.01 M $CaCl_2$	26	BE	38
[−0.68]	[1.38]			47.2	1.50* [0.87]	Montalto c (subsoil); pH 5.9; CE=8.4 me/100 g; 0.01 M $CaCl_2$	26	BE	38
[0.80]	[2.45]			67.1	3.90* [2.26]	Sharkey c soil; pH 6.2; CE=40.2 me/100 g; 0.01 M $CaCl_2$	26	BE	38
[0.77]	[2.10]			50.5	8.02* [4.65]	Berkley sic (topsoil); pH 7.1; CE=33.7 me/100 g; 0.01 M $CaCl_2$	26	BE	38
[0.10]	[2.10]			69.2	1.73* [1.00]	Berkley c (subsoil); pH 7.3; CE=34.4 me/100 g; 0.01 M $CaCl_2$	26	BE	38
[0.56]	[2.13]			43.6	4.68* [2.71]	Benevola sic (topsoil); pH 7.7; CE=19.5 me/100 g; 0.01 M $CaCl_2$	26	BE	38
[0.17]	[2.06]			68.0	2.26* [1.31]	Benevola c (subsoil); pH 7.6; CE=20.1 me/100 g; 0.01 M $CaCl_2$	26	BE	38
[0.15]	[2.10]			25.2	1.93* [1.12]	Wehadkee sil soil; pH 5.6; CE=10.2 me/100 g; 0.01 M $CaCl_2$	26	BE	38

TABLE 8. Sorption coefficients for pesticides—Continued

log K_d log K_f^0 (1/n)	log K_{oc}	Sorbent composition (%)				Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
[0.64]	[2.22]				4.54* [2.63]	Warwick, Qld, soil; pH 6.3; 0.01 M $CaCl_2$		BE	558
[0.58]	[2.21]				4.07* [2.36]	Rutherglen, Vic., soil; pH 4.8; 0.01 M $CaCl_2$		BE	558
[0.34]	[2.31]				1.86* [1.08]	Wagga, N.S.W., soil; pH 5.1; 0.01 M $CaCl_2$		BE	558
[0.43]	[2.22]				2.81* [1.63]	Turretfield, S.A., soil; pH 5.2; 0.01 M $CaCl_2$		BE	558
[0.29]	[2.49]				1.09* [0.63]	Warracknabeal, Vic., soil; pH 8.0; 0.01 M $CaCl_2$		BE	558
[0.48]	[2.21]				3.20* [1.86]	Warracknabeal, Vic., soil; pH 8.4; 0.01 M $CaCl_2$		BE	558
[0.42]	[1.84]				6.62* [3.84]	Balkuling soil; pH 5.6; 0.01 M $CaCl_2$		BE	558
[0.39]	[2.30]				2.14* [1.24]	Kojonup soil; pH 5.5; 0.01 M $CaCl_2$		BE	558
[0.22]	[2.31]				1.42* [0.82]	Warranine soil; pH 6.5; 0.01 M $CaCl_2$		BE	558
[0.46]	[1.98]				5.17* [3.00]	Yalanbee soil; pH 6.4; 0.01 M $CaCl_2$		BE	558
[0.40]	[2.18]				2.85* [1.65]	Avondale soil; pH 5.9; 0.01 M $CaCl_2$		BE	558
[0.47]	[2.51]				1.58* [0.92]	Badgingarra soil; pH 6.3; 0.01 M $CaCl_2$		BE	558
[−0.68]	[2.28]				0.19* [0.11]	Badgingarra soil; pH 6.3; 0.01 M $CaCl_2$		BE	558
[0.51]	[2.28]				2.92* [1.69]	Beverley soil; 0.01 M $CaCl_2$		BE	558
[0.70]	[2.36]				3.78* [2.19]	Gabalong soil; pH 5.9; 0.01 M $CaCl_2$		BE	558
[0.14]	[2.32]				1.13* [0.66]	Perth soil; pH 5.9; 0.01 M $CaCl_2$		BE	558
[0.44]	[2.41]				1.86* [1.08]	Tammin soil; pH 5.9; 0.01 M $CaCl_2$		BE	558
1.92° (0.95)	[3.14]	47.5	33.2	20.3	10.5* [6.09]	Melfort soil; pH 5.9	25	BE	260
1.43° (0.55)		53.3	27.5	19.2	6.46* [3.75]	Weybum soil; pH 6.5	25	BE	260
1.13° (0.70)		5.3	25.3	69.5	4.15* [2.41]	Regina soil; pH 7.7	25	BE	260
1.12° (0.78)		69.3	12.3	18.5	4.07* [2.36]	Indian Head soil; pH 7.8	25	BE	260
0.84° (0.63)		81.6	10.4	8.0	1.77* [1.03]	Asquith soil; pH 7.5	25	BE	260
0.45° (0.78)				15.9	0.31	Greenhouse soil; $SA(N_2)=6\ m^2/g$; pH 8.1; CE=3.8 me/100 cm^3; 0.02 M $CaCl_2$	10	BE	245
0.35° (0.76)						Idem	25		245
−0.85° (1.93)						Idem	40		245
0.61° (0.66)						Idem; 0.02 M $CaCl_2$+0.06 M NH_4Cl	25		245
0.86° (0.63)				15.9	0.85	Greenhouse soil; $SA(N_2)=12\ m^2/g$; pH 7.8; CE=13.1 me/100 cm^3; 0.02 M $CaCl_2$	10	BE	245
0.71° (0.81)						Idem	25		245
0.55° (0.84)						Idem	40		245
0.93° (0.71)						Idem; 0.02 M $CaCl_2$+0.06 M NH_4Cl	25		245
0.82°				15.9	0.67	Greenhouse soil; $SA(N_2)=10\ m^2/g$;	10	BE	245

TABLE 8. Sorption coefficients for pesticides—Continued

log K_d log K_f^0 (1/n)	log K_{oc}	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
(0.77)						pH 7.9; CE=9.4 me/100 cm^3; 0.02 M $CaCl_2$			
0.63° (0.77)						Idem	25		245
0.42° (0.68)						Idem	25		245
0.91° (0.67)						Idem 0.02 M $CaCl_2$+0.06 M NH_4Cl			
0.70° (0.61)				15.9	0.45	Greenhouse soil; SA(N_2)=8 m^2/g; pH 8.1; CE=6.3 me/100 cm^3; 0.02 M $CaCl_2$	10	BE	245
0.49° (0.69)						Idem	25		245
0.34° (0.68)						Idem	40		245
0.83° (0.52)						Idem; 0.02 M $CaCl_2$+0.06 M NH_4Cl	25		245
0.43	[2.15]	66.0	18.4	15.6	1.93	Begbroke soil; pH 7.1; 0.1 M $CaCl_2$	22	BE	638
2.43°		7	10	10	36.5	Sunway farm light peat; pH 5.2; CE=60 me/100 g	22	BE	259
1.88°		45.5	15.9	6.6	12.0	Great House E.H.F. soil; pH 6.3; CE=18 me/100 g	22	BE	259
1.72°		23	24.4	28.6	11.7	Toll Farm heavy peat; pH 7.4; CE=41 me/100 g	22	BE	259
1.20°		34.0	33.4	32.6	3.69	Trawscoed E.H.F. soil; pH 6.2; CE=12 me/100 g	22	BE	259
1.13°		66.0	18.4	15.6	1.93	Weed Res. soil; pH 7.1; CE=11 me/100 g	22	BE	259
1.01°		36.0	40.4	23.6	1.76	Rosemaunde E.H.F. soil; pH 6.7; CE=14 me/100 g	22	BE	259
1.40°		44.0	33.4	22.6	3.45	Liscombe E.H.F. soil; pH 6.2; CE=13 me/100 g	22	BE	259
1.08°		40.0	26.4	33.6	3.09	Bridget's E.H.F. soil; pH 8.0; CE=24 me/100 g	22	BE	259
1.18°		40.0	20.4	39.6	2.08	Boxworth E.H.F. soil; pH 7.9; CE=22 me/100 g	22	BE	259
1.15°		42.0	23.4	34.6	1.54	Terrington E.H.F. soil; pH 8.0; CE=15 me/100 g	22	BE	259
1.00°		71.0	13.4	15.6	1.50	Kirton E.H.F. soil; pH 7.6; CE=13 me/100 g	22	BE	259
0.67	[2.51]	74.4	19.5	6.1	2.5* [1.45]	Aguadilla soil; pH 7.4; CE=10 me/100 g; 0.01 M $CaCl_2$		BE	256
0.52	[2.65]	27.6	35.6	36.8	1.3* [0.75]	Aguirre soil; pH 9.0; CE=14.3 me/100 g; 0.01 M $CaCl_2$		BE	256
0.67	[2.40]	14.9	39.3	45.8	3.2* [1.86]	Alonso soil; pH 5.1; CE=13.8 me/100 g; 0.01 M $CaCl_2$		BE	256
0.73	[2.40]	49.2	28.8	22.0	3.7* [2.15]	Altura soil; pH 8.0; CE=27.6 me/100 g; 0.01 M $CaCl_2$		BE	256
0.36	[2.36]	68.1	4.4	27.5	1.7* [0.99]	Bayamòn soil; pH 4.7; CE=5.0 me/100 g; 0.01 M $CaCl_2$		BE	256
2.56	[3.24]	36.0	36.0	28.0	36.0* [20.8]	Cano Tiburones soil; pH 5.5; CE=86.0 me/100 g; 0.01 M $CaCl_2$		BE	256
0.27	[2.23]	6.6	28.9	64.5	1.9* [1.10]	Catalina soil; pH 4.7; CE=11.8 me/100 g; 0.01 M $CaCl_2$		BE	256
0.59	[2.50]	89.0	7.3	2.08	2.1* [1.22]	Catano soil; pH 7.9; CE=6.9 me/100 g; 0.01 M $CaCl_2$		BE	256
0.47	[2.41]	58.8	23.4	17.8	2.0* [1.16]	Cayaguà soil; pH 5.2; CE=7.3 me/100 g; 0.01 M $CaCl_2$		BE	256
1.09	[2.64]	13.3	34.8	51.9	4.9* [2.84]	Cialitos soil; pH 5.4; CE=18.6 me/100 g; 0.01 M $CaCl_2$		BE	256
1.09	[2.75]	22.7	37.4	39.9	3.7*	Coloso soil; pH 5.7;		BE	256

TABLE 8. Sorption coefficients for pesticides—Continued

log K_d log K_f^0 (1/*n*)	log K_{oc}	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data: prediction procedure	Temp. (°C)	Meth.	Ref.
					[2.15]	CE=23.0 me/100 g; 0.01 M $\mathrm{CaCl_2}$			
0.97	[2.70]	23.4	24.8	51.8	3.2* [1.86]	Coto soil; pH 7.7; CE=14.0 me/100 g; 0.01 M $\mathrm{CaCl_2}$		BE	256
0.77	[2.47]	39.1	29.7	32.2	3.4* [1.97]	Fe soil; pH 7.5; CE=27.6 me/100 g; 0.01 M $\mathrm{CaCl_2}$		BE	256
1.13	[2.85]	15.0	50.7	34.3	3.3* [1.91]	Fortuna soil; pH 5.4; CE=23.3 me/100 g; 0.01 M $\mathrm{CaCl_2}$		BE	256
0.84	[2.76]	15.5	32.5	52.0	2.1* [1.22]	Fraternidad soil; pH 6.3; CE=36.0 me/100 g; 0.01 M $\mathrm{CaCl_2}$		BE	256
1.20	[2.81]	11.1	23.8	65.1	4.2* [2.44]	Fraternidad (Lajas) soil; pH 5.9; CE=58.0 me/100 g; 0.01 M $\mathrm{CaCl_2}$		BE	256
0.97	[2.53]	6.4	19.6	74.0	4.8* [2.78]	Guànica soil; pH 8.1; CE=52.1 me/100 g; 0.01 M $\mathrm{CaCl_2}$		BE	256
0.33	[2.33]	10.1	50.9	39.0	1.7* [0.99]	Humata soil; pH 4.5; CE=10.1 me/100 g; 0.01 M $\mathrm{CaCl_2}$		BE	256
1.08	[2.80]	26.6	53.5	20.9	3.3* [1.91]	Josefa soil; pH 6.0; CE=16.8 me/100 g; 0.01 M $\mathrm{CaCl_2}$		BE	256
1.00	[2.81]	15.2	41.6	43.2	2.7* [1.57]	Juncos soil; pH 6.2; CE=13.4 me/100 g; 0.01 M $\mathrm{CaCl_2}$		BE	256
1.16	[2.81]	19.9	33.4	46.7	3.9* [2.26]	Mabi soil; pH 7.0; CE=55.2 me/100 g; 0.01 M $\mathrm{CaCl_2}$		BE	256
1.01	[2.56]	22.7	40.7	36.6	4.9* [2.84]	Mabi soil; pH 5.7; CE=31.0 me/100 g; 0.01 M $\mathrm{CaCl_2}$		BE	256
0.74	[2.59]	14.9	42.8	2.38	2.4* [1.39]	Mercedita soil; pH 8.1; CE=19.9 me/100 g; 0.01 M $\mathrm{CaCl_2}$		BE	256
1.08	[2.74]	26.3	27.7	46.0	3.8* [2.20]	Moca soil; pH 5.8; CE=31.0 me/100 g; 0.01 M $\mathrm{CaCl_2}$		BE	256
0.81	[2.53]	28.0	47.0	25.0	3.3* [1.91]	Mùcara soil; pH 5.8; CE=19.6 me/100 g; 0.01 M $\mathrm{CaCl_2}$		BE	256
1.18	[2.69]	22.8	49.2	28.0	5.3* [3.07]	Nipe soil; pH 5.7; CE=11.9 me/100 g; 0.01 M $\mathrm{CaCl_2}$		BE	256
0.67	[2.61]	59.4	28.2	12.4	2.0* [1.16]	Pandura soil; pH 5.7; CE=7.7 me/100 g; 0.01 M $\mathrm{CaCl_2}$		BE	256
0.56	[2.25]	13.4	43.6	43.0	3.5* [2.03]	Rio Piedras soil; pH 4.9; CE=11.5 me/100 g; 0.01 M $\mathrm{CaCl_2}$		BE	256
1.20	[3.00]	24.3	49.7	26.0	2.7* [1.57]	San Antòn soil; pH 6.7; CE=26.1 me/100 g; 0.01 M $\mathrm{CaCl_2}$		BE	256
0.37	[2.46]	73.4	19.4	7.2	1.4* [0.81]	Talante soil; pH 5.1; CE=4.0 me/100 g; 0.01 M $\mathrm{CaCl_2}$		BE	256
0.55	[2.49]	41.5	38.3	20.2	2.0* [1.16]	Toa soil; pH 5.3; CE=13.0 me/100 g; 0.01 M $\mathrm{CaCl_2}$		BE	256
0.10	[2.56]	60.9	25.1	14.0	0.6* [0.35]	Toa soil; pH 6.0; CE=8.0 me/100 g; 0.01 M $\mathrm{CaCl_2}$		BE	256
0.80	[2.49]	73.7	12.6	13.7	3.5* [2.03]	Vega Alta soil; pH 5.0 CE=5.6 me/100 g; 0.01 M $\mathrm{CaCl_2}$		BE	256
0.71	[2.59]	45.2	36.8	18.0	2.3* [1.33]	Via soil; pH 5.1; CE=39.9 me/100 g; 0.01 M $\mathrm{CaCl_2}$		BE	256
[0.65]	[2.66]	10	33.6	56.4	0.97	Gerif soil; CE=55.4 me/100 g; pH 8.7; SA(W)=150.7 $\mathrm{m^2/g}$;	25	BE	271
[0.24]	[2.64]	22.3	26.1	41.6	0.40	Gash soil; CE=45.6 me/100 g; pH 8.6; SA(W)=105.0 $\mathrm{m^2/g}$	25	BE	271
[0.18]	[2.72]	40.5	22.4	37.1	0.29	Gurier soil; CE=26.0 me/100 g; pH 9.3; SA(W)=104.1 $\mathrm{m^2/g}$;	25	BE	271
[0.32]	[2.66]	40.8	18.6	40.6	0.46	Kassala soil; CE=30.4 me/100 g; pH 9.2; SA(W)=66.1 $\mathrm{m^2/g}$	25	BE	271
1.02	[2.98]			16.2	1.11	Conventional farm soil; pH 5.42; 0.004 M $\mathrm{CaSO_4}$	25	BE	647
0.88	[2.88]			19.7	1.00	Idem; pH 5.35			646
0.48	[2.67]			24.7	0.64	Idem; pH 7.12			646
1.45	[3.18]			16.5	1.85	Low-input farm soil; pH 5.53; 0.004 M $\mathrm{CaSO_4}$		BE	646
1.26	[3.16]			16.6	1.26	Idem; pH 5.47			646

TABLE 8. Sorption coefficients for pesticides—Continued

log K_d log K_f^0 (1/n)	log K_{oc}	Sorbent composition (%)				Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
1.01	[3.08]			19.1	0.86	Idem; pH 6.32			646
1.16° (0.77)		10.5	62.5	27	2.15* [1.25]	Monona soil; pH 6.7; CE=20.7 me/100 g	24	BE	644
0.81° (0.74)		90.5	4.5	5	0.75* [0.44]	Valentine soil; pH 6.75;	24	BE	644
	2.63av	6–94	3–66	3–35	0.8–3.9	5 soils; 0.01 N $CaCl_2$	25	BE	455
	2.62av					5 soils; extrapolated from log K_d–f_c plots (methanol–water)	25	BE	455
	2.55av					5 soils; extrapolated from log K_d–f_c plots (acetone–water)	25	BE	455
1.39° (0.75)		55	20	25	3.34	Webster soil; pH 7.3; CE=22 me/100 g		BE	192
0.16° (0.82)		93.8	3.0	3.2	0.2	Eustis soil; ph 5.7; 0.01 N $CaCl_2$	25	BE	452
0.84° (0.92)	[2.56]	1	48	51	1.9	Mockingbird Can. L. sed.; pH 6.7; CE=39 me/100 g; 0.01 M $CaCl_2$	25	BE	257
0.99° (0.80)		19	27	54	1.8	San Joaquin Marsh sed.; pH 6.7; CE=44 me/100 g; 0.01 M $CaCl_2$	25	BE	257
1.04° (0.89)	[3.08]	4	30	66	0.91	Baldwin Lake sed.; pH 7.6; CE=24 me/100 g; 0.01 M $CaCl_2$	25	BE	257
1.36° (0.76)		4	53	43	2.3	Jenks Lake sed; pH 5.4; CE=33 me/100 g; 0.01 M $CaCl_2$	25	BE	257
1.36° (0.79)		8	38	55	3.6	Hill Slough (Delta) sed.; pH 6.2; CE=39 me/100 g; 0.01 M $CaCl_2$	25	BE	257
1.67° (0.71)		20	29	51	6.2	Big Bear Lake sed.; pH 7.3; CE=57 me/100 g; 0.01 M $CaCl_2$	25	BE	257
1.75° (0.82)		11	36	53	9.3	Clear Lake sed.; pH 6.0; CE=53 me/100 g; 0.01 M $CaCl_2$	25	BE	257
1.99° (0.90)	[2.71]	23	52	25	19	Castle Lake sed.; pH 5.0; CE=48 me/100 g; 0.01 M $CaCl_2$	25	BE	257
0.60° (1.25)					2.1* [1.22]	Keyport soil; silt loam; pH 5.4; aver. particle size=5.6 μm		BE	641
0.38° (0.95)	[2.77]				0.7* [0.41]	Cecil soil; loamy sand; pH 5.8; aver. particle size=10.5		BE	641
	[2.21]av				1.09*–4.25*	4 soils; silt loam; pH 6.1–7.5. 0.01 M $CaCl_2$	20	BE	120
	2.59av (three soils)	38	48	14	0.68	Commerce soil; pH 6.7		BE	575
		56	30	14	1.12	Tracy soil; pH 6.2		BE	575
		12	56	32	2.01	Catlin soil; pH 6.2		BE	575
0.825	2.95				0.74	Eustis soil (<250 μm); K_d extrapolated from log K_d–f_c plots (methanol-water). 0.01 M $CaCl_2$		BE MD	457
	2.48					C18 column		RPLC	573
	2.60					Soil; experimental (literature)			217
	2.58av					84 soils (literature)			87
	2.47av					156 literature data			562
	1.58, 2.42					Correlation log K_{oc}–log K_{ow}			96
	3.06					Correlation log K_{oc}–log S			96
	2.41					Correlation log K_{oc}–log S(mp)			96
	2.75					Correlation log K_{oc}–log S			564
						Endrin			
3.53° (1.08)	[3.89]	52	34	14	75.3* [43.7]	Soil; organic; pH 6.1		BE	264
2.41° (0.99)	[4.20]	71	22	7	2.8* [1.62]	Big Creek sediment; pH 6.6		BE	264
2.05° (1.12)	[3.89]	56	30	14	2.5* [1.45]	Beverly soil; pH 6.8		BE	264
1.76° (1.03)	[4.15]	91.5	1.5	7	0.7* [0.41]	Plainfield soil; pH 7.0		BE	264
	4.41–					DOC in porewater of Lake		RS	547

TABLE 8. Sorption coefficients for pesticides—Continued

log K_d log K_f^0 (1/n)	log K_{oc}	Sorbent composition (%) Sand	 Silt	 Clay	 OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
	5.14					Michigan (LM) sediment after filtration			
	4.44–4.70					DOC in porewater of LM sediment after centrifugation		RS	547
	3.25–4.91					DOC in elutriate of LM sediment after filtration		RS	547
	4.46–4.55					DOC in elutriate of LM sediment after centrifugation		RS	547
	4.53					Correlation log K_{oc}–log S			564
						EPTC			
−0.24	[1.68]			7.0	2.1* [1.22]	Döbrököz soil; SA(N_2)=3.7 m^2/g; SA(Me)=38.2 m^2/g; 0.01 M $CaCl_2$		BE	71
−0.10	[1.96]			10.3	1.5* [0.87]	Jánosháza soil; SA(N_2)=5.8 m^2/g; SA(Me)=40.6 m^2/g; 0.01 M $CaCl_2$		BE	71
0.20	[2.06]			14.0	2.4* [1.39]	Nagybaracska soil; SA(N_2)=9.6 m^2/g; SA(Me)=54.4 m^2/g; 0.01 M $CaCl_2$		BE	71
0.18	[2.13]			16.0	1.9* [1.10]	Simonfa soil; SA(N_2)=10.1 m^2/g; SA(Me)=55.8 m^2/g; 0.01 M $CaCl_2$		BE	71
0.08	[2.11]			26.5	1.6* [0.93]	Aszód soil; SA(N_2)=14.0 m^2/g; SA(Me)=83.9 m^2/g; 0.01 M $CaCl_2$		BE	71
0.54	[2.04]			48.0	5.5* [3.19]	Vizesfás soil; SA(N_2)=18.3 m^2/g; SA(Me)=175 m^2/g; 0.01 M $CaCl_2$		BE	71
−0.14° (0.98)	[2.22]	67.1	25.8	7.1	0.43	Hanford soil; pH 6.05; CE=5.95 cmol/kg; 0.01 M $CaCl_2$	25	BE	528
−0.10° (0.83)		82.0	13.5	4.5	0.33	Tujunga soil; pH 6.30; CE=0.45 cmol/kg; 0.01 M $CaCl_2$	25	BE	528
2.25	[2.60]				76* [44]	OM from peat soil; 0.01 M $BaCl_2$		BE	270
	1.58*					Peat humic acid; 0.01 M $BaCl_2$		BE	270
	2.38					Soil; experimental (literature)			217
	2.23					Correlation log K_{oc}–log S			564
	2.59					Correlation log K_{om}–log S(563)			528
	2.52					Correlation log K_{oc}–log K_{ow}(87)			528
	2.80					Correlation log K_{oc}–log K_{ow}(217)			528
						Fenamiphos			
1.34° (0.80)				75	1.3	Eurosol-1; c; pH 5.1; 0.01 M $CaCl_2$		BE	583
0.82° (0.81)				22.6	3.7	Eurosol-2; sil; pH 7.4; 0.01 M $CaCl_2$		BE	583
0.88° (0.86)				17.0	3.45	Eurosol-3; l; pH 5.2; 0.01 M $CaCl_2$		BE	583
0.51° (0.93)	2.32			20.3	1.55	Eurosol-4; si; pH 6.5; 0.01 M $CaCl_2$		BE	583
1.94° (0.87)				6.0	9.25	Eurosol-5; ls; pH 3.2; 0.01 M $CaCl_2$		BE	583
	[2.52]				3.53* [2.05]	Batcombe si; pH 6.1 0.01 M $CaCl_2$	20	BE	120
	2.08					Correlation log K_{oc}–log S			564
						Fenitrothion			
1.85° (1.16)				100		Na-montmorillonite (<2 μm)	20	BE	246
1.81° (1.95)				100		Ca-montmorillonite (<2 μm)	20	BE	246
2.87° (1.77)				100		Fe-montmorillonite (<2 μm)	20	BE	246
1.40	2.77	18.9	26.3	54.8	4.24	Tsukuba soil; pH 6.5; 0.01 M $CaCl_2$	25	BE	642

TABLE 8. Sorption coefficients for pesticides—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data: prediction procedure	Temp. (°C)	Meth.	Ref.
1.49° (1.07)						Idem	25	BE	642
0.54	2.40	23.1	15.4	61.5	1.35	Kanuma soil; pH 5.7; 0.01 M $CaCl_2$	25	BE	642
0.53° (0.99)						Idem	25	BE	642
	2.83					Correlation $\log K_{oc}-\log S$			564
						Fensulfothion			
1.56° (0.85)				75	1.3	Eurosol-1; c; pH 5.1; 0.01 M $CaCl_2$		BE	583
0.83° (0.93)	2.27			22.6	3.7	Eurosol-2; sil; pH 7.4; 0.01 M $CaCl_2$		BE	583
0.65° (0.93)	2.11			17.0	3.45	Eurosol-3; l; pH 5.2; 0.01 M $CaCl_2$		BE	583
0.45° (0.89)	2.26			20.3	1.55	Eurosol-4; si; pH 6.5; 0.01 M $CaCl_2$		BE	583
1.81° (1.01)	2.85			6.0	9.25	Eurosol-5; ls; pH 3.2; 0.01 M $CaCl_2$		BE	583
0.15° (0.97)	2.54	91.5	1.5	7	0.7* [0.41]	Plainfield soil; pH 6.9	20	BE	261
0.58° (1.08)	2.46	71	22	7	2.3* [1.33]	Big Creek sediment; pH 6.5	20	BE	261
0.83° (0.82)		77	15	8	3.9* [2.26]	Bondhead soil; pH 6.9	20	BE	261
1.71° (0.87)	2.38	52	34	14	36.7* [21.3]	Muck soil; pH 6.3	20	BE	261
						Fenthion			
2.46° (1.12)	4.35			75	1.3	Eurosol-1; c; pH 5.1; 0.01 M $CaCl_2$		BE	583
2.12° (1.15)				22.6	3.7	Eurosol-2; sil; pH 7.4; 0.01 M $CaCl_2$		BE	583
2.00° (1.01)	3.46			17.0	3.45	Eurosol-3; l; pH 5.2; 0.01 M $CaCl_2$		BE	583
1.34° (0.91)	3.15			20.3	1.55	Eurosol-4; si; pH 6.5; 0.01 M $CaCl_2$		BE	583
2.61° (0.82)				6.0	9.25	Eurosol-5; ls; pH 3.2; 0.01 M $CaCl_2$		BE	583
	2.68					Correlation $\log K_{oc}-\log S$			564
						Fenuron			
1.15° (1.00)				100		Na–montmorillonite (1–0.2 μm); pH 6.80; CE=87.0 me/100 g	25	BE	250
2.06° (0.82)				100		H–montmorillonite (1–0.2 μm); pH 3.35; CE=73.5 me/100 g	25	BE	250
0.88				100		Montmorillonite-H(Al) (<0.2 μm;) pH 3.5	3.5	BE	244
1.89				100		Bentonite–H(Al) (<0.2 μm); pH 3.5; CE=0.72 me/g	3.5	BE	244
0.83				100		Bentonite–Na (<0.2 μm); pH 6.7; CE=0.83 me/g; SA(E)=758 m^2/g; Salt conc.=0.1 N	3.5	BE	244
0.94				100		Bentonite-Ca (<0.2 μm); pH 6.7; CE=0.88 me/g; Salt conc.=0.1 N	3.5	BE	244
1.07				100		Bentonite-Mg (<0.2 μm); pH 6.7; CE=0.84 me/g; Salt conc.=0.1 N	3.5	BE	244
0.73av				100		Bentonite-Na (<0.2 μm); pH 6.7; CE=0.83 me/g; SA(E)=758 m^2/g; Salt conc.=0.005–1 N	26.5	BE	244
1.21				100		Idem; Salt conc.=3 N	26.5	BE	244

TABLE 8. Sorption coefficients for pesticides—Continued

log K_d log K_f^0 (1/n)	log K_{oc}	Sorbent composition (%)				Other sorbent and solution data: prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
0.89av				100		Bentonite-Ca (<0.2 μm); pH 6.7 CE=0.88 ne/g; Salt conc.=0.005–1 N	26.5	BE	244
1.49				100		Idem; Salt conc.=3 N	26.5	BE	244
0.94				100		Bentonite-Mg (<0.2 μm); pH 6.7 CE=0.84 me/g; Salt conc.=0.005-1 N	26.5	BE	244
	[1.12]av			1.09*-	4.25*	4 soils; sil; pH 6.1–7.5. 0.01 M $CaCl_2$	20	BE	120
[0.08]	[1.62]				4.54* [2.63]	Warwick, Qld. soil; pH 6.3; 0.01 M $CaCl_2$		BE	558
[−0.39]	[1.24]				4.07* [2.36]	Rutherglen, Vic., soil; pH 4.8; 0.01 M $CaCl_2$		BE	558
[−0.62]	[1.35]				1.86* [1.08]	Wagga, N.S.W., soil; pH 5.1; 0.01 M $CaCl_2$		BE	558
[−0.47]	[1.32]				2.81* [1.63]	Turretfield, S.A., soil; pH 5.2; 0.01 M $CaCl_2$		BE	558
[−1.06]	[1.14]				1.09* [0.63]	Warracknabeal, Vic., soil; pH 8.0; 0.01 M $CaCl_2$		BE	558
[−0.23]	[1.50]				3.20* [1.86]	Warracknabeal, Vic., soil; pH 8.4; 0.01 M $CaCl_2$		BE	558
[−0.07]	[1.35]				6.62* [3.84]	Balkuling soil; pH 5.6; 0.01 M $CaCl_2$		BE	558
[−0.56]	[1.35]				2.14* [1.24]	Kojonup soil; pH 5.5; 0.01 M $CaCl_2$		BE	558
[−0.43]	[1.66]				1.42* [0.82]	Warranine soil; pH 6.5; 0.01 M $CaCl_2$		BE	558
[−0.33]	[1.19]				5.17* [3.00]	Yalanbee soil; pH 6.4; 0.01 M $CaCl_2$		BE	558
[−0.26]	[1.52]				2.85* [1.65]	Avondale soil; pH 5.9; 0.01 M $CaCl_2$		BE	558
[−0.52]	[1.52]				1.58* [0.92]	Badgingarra soil; pH 6.3; 0.01 M $CaCl_2$		BE	558
[−1.54]	[1.42]				0.19* [0.11]	Badgingarra soil; pH 6.3; 0.01 M $CaCl_2$		BE	558
[−0.53]	[1.24]				2.92* [1.69]	Beverley soil; 0.01 M $CaCl_2$		BE	558
[−0.16]	[1.50]				3.78* [2.19]	Gabalong soil; pH 5.9; 0.01 M $CaCl_2$		BE	558
[−0.54]	[1.64]				1.13* [0.66]	Perth soil; pH 5.9; 0.01 M $CaCl_2$		BE	558
[−0.73]	[1.24]				1.86* [1.08]	Tammin soil; pH 5.9; 0.01 M $CaCl_2$		BE	558
0.91° (0.68)		47.5	33.2	20.3	10.5* [6.09]	Melfort soil; pH 5.9	25	BE	260
0.04° (0.92)	[1.47]	53.3	27.5	19.2	6.46* [3.75]	Weyburn soil; pH 6.5	25	BE	260
−0.10° (0.93)	[1.54]	5.3	25.3	69.5	4.15* [2.41]	Regina soil; pH 7.7	25	BE	260
0.20° (0.85)		69.3	12.3	18.5	4.07* [2.36]	Indian Head soil; pH 7.8	25	BE	260
−0.52° (0.97)	[1.52]	81.6	10.4	8.0	1.77* [1.03]	Asquith soil; pH 7.5	25	BE	260
1.08°	[1.52]	7	10	10	36.5	Sunway farm light peat; pH 5.2; CE=60 me/100 g	22	BE	259
0.67°	[1.59]	45.5	15.9	6.6	12.0	Great House E.H.F. soil; pH 6.3; CE=18 me/100 g	22	BE	259
0.46°	[1.39]	23	24.4	28.6	11.7	Toll Farm heavy peat; pH 7.4; CE=41 me/100 g	22	BE	259
−0.14°	[1.30]	34.0	33.4	32.6	3.69	Trawscoed E.H.F. soil; pH 6.2; CE=12 me/100 g	22	BE	259
−0.36°	[1.36]	66.0	18.4	15.6	1.93	Weed Res. soil; pH 7.1; CE=11 me/100 g	22	BE	259

TABLE 8. Sorption coefficients for pesticides—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%)				Other sorbent and solution data: prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
−0.47°	[1.29]	36.0	40.4	23.6	1.76	Rosemaunde E.H.F. soil; pH 6.7; CE=14 me/100 g	22	BE	259
	1.43					Soil; experimental (literature)			217
	1.63av					10 soils (literature)			87
	0.61					Correlation $\log K_{oc}-\log K_{ow}$			96
	1.80, 1.86					Correlation $\log K_{oc}-\log S$			96
	0.72, 0.84					Correlation $\log K_{oc}-\log S(\mathrm{mp})$			96
	1.67					Correlation $\log K_{oc}-\log S$			564
						Fluometuron			
−0.77	[1.62]			5.0	0.70* [0.41]	Eufala 1 fine s soil; pH 6.4; 0.01 N $CaCl_2$	23	BE	300
−0.88	[1.52]				0.70* [0.41]	Idem; 0.5 N $CaCl_2$			300
−0.52	[1.32]			17.5	2.50* [1.45]	Norge 1 soil; pH 6.1; 0.01 N $CaCl_2$	23	BE	300
−0.56	[1.29]				2.50* [1.45]	Idem; pH 5.9; 0.5 N $CaCl_2$			300
−0.51° (0.93)	[1.50]	46	38	16	1.7* [0.99]	Norge soil; pH 6.6; 9.2 me_q /100 g; 0.01 N $CaCl_2$		BE	507
0.34	[1.72]	2.9	68.7	28.4	7.1* [4.12]	Lanton soil; pH 6.4; CE=32.8 me/100 g		BE	631
	[1.82]av				1.09*- 4.25*	4 soils; sil; pH 6.1–7.5; 0.01 M $CaCl_2$	20	BE	120
0.19av (two soils)	[2.43]av	23.4	67.5	9.1	1.1* [0.64]	Taloka soil (10–20 cm); pH 5.2; CE=11 me/100 g; 0.01 N $CaCl_2$	20	BE	285
		22.0	62.2	15.8	0.90* [0.52]	Roxana soil (10–20 cm); pH 6.8; CE=19 me/100 g; 0.01 M $CaCl_2$	20	BE	285
−0.15av (two soils)	[2.30]av	24.2	62.0	13.8	0.70* [0.41]	Taloka soil (40–50 cm); pH 5.5; CE=13 me/100 g; 0.01 M $CaCl_2$	20	BE	285
		30.7	54.7	14.6	0.50* [0.29]	Roxana soil (40–50 cm); pH 7.1; CE=19 me/100 g; 0.01 M $CaCl_2$	20	BE	285
−0.4° (0.98)	[1.61]	46.0	37.6	16.4	1.7* [0.99]	Norge soil; Ca-saturated; pH 6.6; CE=9.2 me/100 g	23	BE	476
0.18° (0.74)		55.4	28.3	16.3	1.6*	Calcic Luvisol; pH 5.5	25	BE	654
0.66° (0.74)		65.4	21.0	13.6	10.2	Humic Cambisol; pH 5.0	25	BE	654
0.35	[2.28]	6	79	15	2.0* [1.16]	Lexington soil (0–4 cm); no-tillage, no cover crop; pH 5.1; CE=8.8 cmol/kg; 0.01 M $CaCl_2$		BE	655
0.22	[2.46]				1.0* [0.58]	Idem (4–8 cm); pH 5.5; CE=7.3 cmol/kg			655
0.14	[2.42]	6	78	16	0.9* [0.52]	Idem (8–15 cm); pH 6.5			655
0.23	[2.36]	7	80	13	1.3* [0.75]	Lexington soil (0–4 cm); convent. tillage, no cover crop; pH 5.5; CE=7.7 cmol/kg; 0.01 M $CaCl_2$		BE	655
0.33	[2.46]	6	80	14		Idem (4–8 cm); pH 5.7; CE=7.5 cmol/kg			655
0.14	[2.33]	7	78	15	1.1* [0.64]	Idem (8–15 cm); pH 6.3			655
0.47	[2.31]	7	78	15	2.5* [1.45]	Lexington soil (0–4 cm); no-tillage, vetch cover crop; pH 4.7; CE=9.6 cmol/kg; 0.01 M $CaCl_2$		BE	655
0.02	[2.21]				1.1* [0.64]	Idem (4–8 cm); pH 4.9; CE=7.2 cmol/kg			655
0.11	[2.39]				0.9* [0.52]	Idem (8–15 cm); pH 5.7			655
0.33	[2.39]	6	80	14	1.5*	Lexington soil (0–4 cm); convent.		BE	655

TABLE 8. Sorption coefficients for pesticides—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
					[0.87]	tillage, vetch cover crop; pH 5.0; CE=7.7 cmol/kg; 0.01 M $CaCl_2$			
0.34	[2.40]	6	79	15		Idem (4–8 cm); CE=7.5 cmol/kg			655
0.21	[2.41]	5	80	15	1.1* [0.64]	Idem (8–15 cm); pH 5.6; CE=7.7 cmol/kg			655
0.098° (0.90)	[2.32]	10.3	54.5	35.2	0.59	Dundee soil (Ap horizon); pH 5.47; 0.01 M $CaCl_2$		BE	149
[0.14]	[1.97]	74.4	19.5	6.1	2.5* [1.45]	Aguadilla soil; CE=10 me/100 g; pH 7.4; 0.01 M $CaCl_2$		BE	304
[0.25]	[2.37]	27.6	35.6	36.8	1.3* [0.75]	Aguirre soil; CE=14.3 me/100 g; pH 9.0; 0.01 M $CaCl_2$		BE	304
[1.00]	[2.64]	16.6	13.0	70.4	3.9* [2.26]	Aguirre soil; CE=59.0 me/100 g; pH 8.4; 0.01 M $CaCl_2$		BE	304
[0.42]	[2.16]	14.9	39.3	45.8	3.2* [1.86]	Alonso soil; CE=13.8 me/100 g; pH 5.1; 0.01 M $CaCl_2$		BE	304
[0.28]	[1.95]	49.2	28.8	22.0	3.7* [2.15]	Altura soil; CE=27.6 me/100 g; pH 8.0; 0.01 M $CaCl_2$		BE	304
[0.05]	[2.05]	68.1	4.4	27.0	1.7* [0.99]	Bayamón soil; CE=5.0 me/100 g; pH 4.7; 0.01 M $CaCl_2$		BE	304
[0.28]	[2.03]	56.4	8.0	35.9	3.1* [1.80]	Cabo Rojo soil; CE=9.0 me/100 g pH 4.3; 0.01 M $CaCl_2$		BE	304
[1.43]	[2.11]	36.0	36.0	28.0	36.0* [20.9]	Caño Tiburones soil; pH 5.5; CE=86.0 me/100 g; 0.01 M $CaCl_2$		BE	304
[0.59]	[2.55]	6.6	28.9	64.5	1.9* [1.10]	Catalina soil; CE=11.8 me/100 g; pH 4.7; 0.01 M $CaCl_2$		BE	304
[0.37]	[2.38]	47.2	17.4	35.4	1.7* [0.99]	Cartagena soil; CE=36.1 me/100 g; pH 7.7; 0.01 M $CaCl_2$		BE	304
[0.52]	[2.44]	89.0	7.3	3.7	2.1* [1.22]	Cataño soil; CE=6.9 me/100 g; pH 7.9; 0.01 M $CaCl_2$		BE	304
[0.59]	[2.43]	43.4	25.2	31.4	2.5* [1.45]	Cintrona soil; CE=25.0 me/100 g; pH 8.3; 0.01 M $CaCl_2$		BE	304
[−0.01]	[1.93]	58.8	23.4	17.8	2.0* [1.16]	Cayaguá soil; CE=7.3 me/100 g; pH 5.2; 0.01 M $CaCl_2$		BE	304
[0.57]	[2.11]	13.3	34.8	51.9	4.9* [2.84]	Cialitos soil; CE=18.6 me/100 g; pH 5.4; 0.01 M $CaCl_2$		BE	304
[0.63]	[2.30]	22.7	37.4	39.9	3.7* [2.15]	Coloso soil; CE=23.0 me/100 g; pH 5.7; 0.01 M $CaCl_2$		BE	304
[0.45]	[2.05]	26.0	18.6	55.4	4.3* [2.49]	Corozal soil; CE=17.0 me/100 g; pH 4.6; 0.01 M $CaCl_2$		BE	304
[0.45]	[2.18]	23.4	24.8	51.8	3.2* [1.86]	Coto soil; CE=14.0 me/100 g; pH 7.7; 0.01 M $CaCl_2$		BE	304
[0.21]	[2.49]	48.0	20.6	31.4	0.9* [0.52]	Estación soil; CE=10.0 me/100 g; pH 5.9; 0.01 M $CaCl_2$		BE	304
[0.69]	[2.40]	39.1	29.7	32.2	3.4* [1.97]	Fe soil; CE=27.6 me/100 g; pH 7.5; 0.01 M $CaCl_2$		BE	304
[0.31]	[2.03]	15.0	50.7	34.3	3.3* [1.91]	Fortuna soil; CE=23.3 me/100 g; pH 5.4; 0.01 M $CaCl_2$		BE	304
[0.28]	[2.19]	15.5	32.5	52.0	2.1* [1.22]	Fraternidad soil; pH 6.3; CE=36.6 me/100 g; 0.01 M $CaCl_2$		BE	304
[0.40]	[2.01]	11.1	23.8	65.1	4.2* [2.43]	Fraternidad soil (Lajas); pH 5.9; CE=58.0 me/100 g; 0.01 M $CaCl_2$		BE	304
[0.63]	[2.19]	6.4	19.6	74.0	4.8* [2.78]	Guánica soil; CE=52.1 me/100 g; pH 8.1; 0.01 M $CaCl_2$		BE	304
[0.17]	[2.37]	84.4	8.4	7.2	1.1* [0.64]	Humacao soil; CE=4.0 me/100 g; pH 6.3; 0.01 M $CaCl_2$		BE	304
[0.37]	[2.38]	10.1	50.9	39.0	1.7* [0.99]	Humata soil; CE=10.1 me/100 g; pH 4.5; 0.01 M $CaCl_2$		BE	304
[0.17]	[1.89]	26.6	53.5	20.9	3.3* [1.91]	Josefa soil; CE=16.8 me/100 g; pH 6.0; 0.01 M $CaCl_2$		BE	304
[0.65]	[2.46]	15.2	41.6	43.2	2.7* [1.57]	Juncos soil; CE=13.4 me/100 g; pH 6.2; 0.01 M $CaCl_2$		BE	304
[0.28]	[1.92]	19.9	33.4	46.7	3.9* [2.26]	Mabí soil; CE=55.2 me/100 g; pH 7.0; 0.01 M $CaCl_2$		BE	304

TABLE 8. Sorption coefficients for pesticides—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
[0.73]	[2.28]	22.7	40.7	36.6	4.9* [2.84]	Mabí soil; CE=31.0 me/100 g; pH 5.7; 0.01 M $CaCl_2$		BE	304
[0.42]	[2.32]	76.0	13.4	10.6	2.2* [1.28]	Machete soil; CE=8.0 me/100 g; pH 6.5; 0.01 M $CaCl_2$		BE	304
[0.05]	[1.90]	14.9	42.8	42.3	2.4* [1.39]	Mercedita soil; CE=19.9 me/100 g; pH 8.1; 0.01 M $CaCl_2$		BE	304
[0.61]	[2.27]	26.3	27.7	46.0	3.8* [2.20]	Moca soil; CE=31.0 me/100 g; pH 5.8; 0.01 M $CaCl_2$		BE	304
[−0.06]	[1.66]	28.0	47.0	25.0	3.3* [1.91]	Múcara soil; CE=19.6 me/100 g; pH 5.8; 0.01 M $CaCl_2$		BE	304
[0.52]	[2.03]	22.0	49.2	28.0	5.3* [3.07]	Nipe soil; CE=11.9 me/100 g; pH 5.7; 0.01 M $CaCl_2$		BE	304
[0.37]	[2.31]	59.4	28.2	12.4	2.0* [1.16]	Pandura soil; CE=7.7 me/100 g; pH 5.7; 0.01 M $CaCl_2$		BE	304
[−0.06]	[1.63]	13.4	43.6	43.0	3.5* [2.03]	Río Piedras soil; pH 4.9; CE=11.5 me/100 g; 0.01 M $CaCl_2$		BE	304
[0.45]	[2.10]	39.0	24.6	36.4	3.9* [2.26]	Sabana Seca soil; pH 7.4; CE=23.0 me/100 g; 0.01 M $CaCl_2$		BE	304
[0.57]	[2.11]	47.0	24.4	28.6	4.9* [2.84]	San Antón soil; pH 7.4; CE=28.0 me/100 g; 0.01 M $CaCl_2$		BE	304
[0.61]	[3.53]	57.0	18.6	24.4	2.1* [1.22]	Santa Isabel soil; pH 7.4; CE=28.0 me/100 g; 0.01 M $CaCl_2$		BE	304
[0.84]	[2.06]	46.0	20.0	34.0	10.4* [6.03]	Soller soil; CE=53.0 me/100 g; pH 6.9; 0.01 M $CaCl_2$		BE	304
[0.13]	[2.23]	73.4	19.4	7.2	1.4* [0.81]	Talante soil; CE=4.0 me/100 g; pH 5.1; 0.01 M $CaCl_2$		BE	304
[0.82]	[2.35]	35.0	24.6	40.4	5.1* [2.96]	Toa soil; CE=36.0 me/100 g; pH 8.0; 0.01 M $CaCl_2$		BE	304
[0.28]	[2.21]	41.5	38.3	20.2	2.0* [1.16]	Toa soil; CE=13.0 me/100 g; pH 5.3; 0.01 M $CaCl_2$		BE	304
[−0.69]	[1.77]	60.9	25.1	14.0	0.6* [0.35]	Toa soil; CE=8.0 me/100 g; pH 6.0; 0.01 M $CaCl_2$		BE	304
[0.65]	[2.34]	73.7	12.6	13.7	3.5* [2.03]	Vega Alta soil; pH 5.0 CE=5.6 me/100 g; 0.01 M $CaCl_2$		BE	304
[0.05]	[1.92]	45.2	36.8	18.0	2.3* [1.33]	Via soil; CE=39.9 me/100 g; pH 5.1; 0.01 M $CaCl_2$		BE	304
[0.40]	[2.29]	62.4	19.6	18.0	2.2* [1.28]	Viví soil; CE=14.0 me/100 g; pH 4.8; 0.01 M $CaCl_2$		BE	304
[0.77]	[2.35]	15.0	23.4	61.6	4.5* [2.61]	Voladura soil; pH 4.3; CE=17.7 me/100 g; 0.01 M $CaCl_2$		BE	304
0.40	[2.28]	4	48	47	2.3* [1.33]	Sharkey soil; pH 6.4; 0.01 M $CaCl_2$		BE	656
−0.20	[1.92]	11	74	15	1.3* [0.75]	Dundee soil; pH 5.9; 0.01 M $CaCl_2$		BE	656
−0.16	[1.87]	2	80	18	1.6* [0.93]	Loring soil; pH 5.2; 0.01 M $CaCl_2$		BE	656
−0.22	2.16	38	50	12	0.72* [0.42]	Beulah soil (0–7.5 cm); pH 6.8; CE=9.9 me/100 g; 0.01 M $CaCl_2$		BE	258
−0.28	2.25	35	52	13	0.50* [0.29]	Idem (7.5–15 cm); pH 6.9; CE=10.3 me/100 g			258
−0.31	2.34	34	51	15	0.38* [0.22]	Idem (15–30 cm); pH 7.0; CE=14.9 me/100 g			258
−0.33	2.33	30	55	15	0.38* [0.22]	Idem (30–45 cm); pH 7.1; CE=16.0 me/100 g			258
−0.35	2.37	35	52	13	0.33* [0.19]	Idem (45–60 cm); pH 7.2; CE=16.6 me/100 g			258
−0.45	2.34	43	46	11	0.28* [0.16]	Idem (60–90 cm); pH 7.3; CE=16.8 me/100 g			258
−0.26	2.48	39	47	14	0.31* [0.18]	Idem (90–120 cm); pH 7.5; CE=16.4 me/100 g			258
2.67	[2.93]				94* [54.5]	OM from peaty muck (Histosol) soil; pH 5.5	24	BE	121
	2.24					Soil; experimental (literature)			217

TABLE 8. Sorption coefficients for pesticides—Continued

log K_d log K_f^0 ($1/n$)	log K_{oc}	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data: prediction procedure	Temp. (°C)	Meth.	Ref.
	0.95					Correlation log K_{oc}–log K_{ow}			96
	2.87					Correlation log K_{oc}–log S			96
	2.02					Correlation log K_{oc}–log S(mp)			96
	2.57					Cor relation log K_{oc}–log S			564
						Heptachlor			
3.16	4.90	25	40	35	1.8	Taichung soil; pH 6.8	25	BE	407
	4.48					Aldrich humic acid	25	SE	407
	4.48					Correlation log K_{oc}–log S			564
						α-Hexachlorocyclohexane			
1.45°		79.6	4.8	15.6	0.75*	Alluvial soil; pH 6.20;	26	BE	185
(1.60)					[0.44]	CE=18.6 me/100 g			
1.72°		69.6	6.8	23.6	2.88*	Lateritic soil; pH 6.30;	26	BE	185
(1.26)					[1.67]	CE=42.8 me/100 g			
1.85°	[3.34]	45.6	7.8	45.6	5.52*	Pokkali soil; pH 5.2;	26	BE	185
(0.94)					[3.20]	CE=19.2 me/100 g			
2.70°		63.6	6.8	29.6	24.6*	Kari soil; pH 3.3;	26	BE	185
(1.16)					[14.3]	CE=28.9 me/100 g			
	4.1				4.1	Lake Ontario sediment trap material		FM	49
	3.42					Correlation log K_{oc}–log K_{ow}			96
	3.5					Correlation log K_{oc}–log K_{ow}(96)			49
	3.90					Correlation log K_{oc}–log S			96
	3.66					Correlation log K_{oc}–log S(mp)			96
	3.53					Correlation log K_{oc}–MCI			598
						β-Hexachlorocyclohexane			
2.66°	[3.55]				22*	Ca-Staten peaty muck	20	BE	390
(0.95)					[12.8]				
2.64°	[3.53]					Idem			390
(0.99)									
1.80°					6*	Ca-Venado clay	20	BE	390
(0.86)					[3.5]	(50% Montmorillonite)			
1.78°						Idem			390
(0.88)									
0.60°						Ca-bentonite (Montmorillonite)	20	BE	390
(0.86)									
0.65°						Idem			390
(0.88)									
0.33°						Silica gel; pH 4.4	20	BE	390
(0.97)									
0.21°						Idem			390
(0.99)									
0.71°		79.6	4.8	15.6	0.75*	Alluvial soil; pH 6.20;	26	BE	185
(0.82)					[0.44]	CE=18.6 me/100 g			
1.60°		69.6	6.8	23.6	2.88*	Lateritic soil; pH 6.30;	26	BE	185
(1.20)					[1.67]	CE=42.8 me/100 g			
1.90°		45.6	7.8	45.6	5.52*	Pokkali soil; pH 5.2;	26	BE	185
(0.80)					[3.20]	CE=19.2 me/100 g			
2.20°		63.6	6.8	29.6	24.6*	Kari soil; pH 3.3;	26	BE	185
(0.80)					[14.3]	CE=28.9 me/100 g			
	3.41					Correlation log K_{oc}–log K_{ow}			96
	3.23					Correlation log K_{oc}–log K_{ow}			207
	3.60					Correlation log K_{oc}–log K_{ow}			108
	4.50					Correlation log K_{oc}–log S			96
	3.17					Correlation log K_{oc}–log S(mp)			96
	3.53					Correlation log K_{oc}–MCI			598
						γ-Hexachlorocyclohexane (Lindane)			
0.47°						Ca-Bentonite (Montmorillonite)	20	BE	390
(0.89)									
0.43°						Idem	30		390

TABLE 8. Sorption coefficients for pesticides—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%)				Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
(0.91)									
0.84° (0.94)						Silica gel; pH 4.4	20	BE	390
0.66° (0.96)						Idem	30		390
0.48				100		Ca-bentonite	20.5	BE	506
[1.36]	[2.86]			19(fine)	3.1	Svea sil soil (A horizon); pH 6.6; CE=26 me/100 g		BE	119
[1.49]	[2.75]			17(fine)	5.4	Bearden sicl soil (A horizon); pH 7.7; CE=31 me/100 g		BE	119
[1.30]	[3.26]			19(fine)	11	Blue earth sil soil (A horizon); pH 7.7; CE=36 me/100 g		BE	119
[2.27]	[3.36]			8(fine)	8.3	Idem (B horizon); pH 7.6; CE=27 me/100 g		BE	119
[1.52]	[3.10]			6(fine)	2.6	Brainerd fsl soil (A horizon); pH 5.4; CE=15 me/100 g		BE	119
[1.68]	[2.82]			19(fine)	7.3	Canisteo 1 (A horizon); pH 7.8; CE=44 me/100 g		BE	119
[1.60]	[2.89]			29(fine)	5.2	Fargo sic soil (A horizon); pH 7.0; CE=45 me/100 g		BE	119
[1.08]	[2.84]			36(fine)	1.7	Fargo sicl soil (B horizon); pH 7.2; CE=38 me/100 g		BE	119
[1.36]	[2.99]			8(fine)	2.3	Fayette sil soil (A horizon); pH 5.4; CE=15 me/100 g		BE	119
[1.52]	[2.88]			24(fine)	4.3	Hegne sic soil (A horizon); pH 8.0; CE=40 me/100 g		BE	119
[0.99]	[2.91]			3(fine)	1.2	Hubbard ls soil (A horizon); pH 5.8; CE=7 me/100 g		BE	119
[1.22]	[2.76]			19(fine)	2.9	Kranzburg sicl soil (A horizon); pH 6.6; CE=28 me/100 g		BE	119
[1.39]	[3.03]			8(fine)	2.3	Lester fsl soil (A horizon); pH 6.3; CE=16 me/100 g		BE	119
[1.15]	[2.92]			2(fine)	1.7	Milaca sl soil (A horizon); pH 5.7; CE=9 me/100 g		BE	119
[1.23]	[2.78]			13(fine)	2.8	Nicollet 1 soil (A horizon); pH 6.0; CE=24 me/100 g		BE	119
[1.35]	[2.80]			18(fine)	3.5	Ontonagon c soil (A horizon); pH 5.2; CE=40 me/100 g		BE	119
[1.43]	[3.17]			1(fine)	1.8	Ulen sl soil (A horizon) pH 8.3; CE=12 me/100 g		BE	119
[1.29]	[3.82]			2(fine)	0.3	Ulen sl soil (B horizon) pH 8.6; CE=2 me/100 g		BE	119
[1.17]	[3.33]			1(fine)	0.7	Zimmerman s soil (A horizon); pH 5.5; CE=4 me/100 g		BE	119
[0.85]	[2.81]	9	68	21	1.9* [1.1]	Woodburn soil	20	BE	198
1.57	3.45	3.31	21.9	75.0	1.30	Eurosol-1; EEC laboratory ringtest; pH 5.1; 0.01 M $CaCl_2$		BE	62
1.61	3.04	3.4	64.1	22.6	3.70	Eurosol-2; EEC laboratory ringtest; pH 7.4; 0.01 M $CaCl_2$		BE	62
1.63	3.09	46.4	36.8	17.0	3.45	Eurosol-3; EEC laboratory ringtest; pH 5.2; 0.01 M $CaCl_2$		BE	62
1.05	2.86	4.1	75.7	20.3	1.55	Eurosol-4; EEC laboratory ringtest; pH 6.5; 0.01 M $CaCl_2$		BE	62
2.36	3.40	81.6	12.6	6.0	9.25	Eurosol-5; EEC laboratory ringtest; pH 3.2; 0.01 M $CaCl_2$		BE	62
−0.41	2.19	1.7	82.4	16.0	0.25	Eurosol-6; EEC laboratory ringtest; pH 7.2; 0.01 M $CaCl_2$		BE	62
0.46	[2.89]			18.4	0.65* [0.38]	Gila soil	21	BE	657
0.74	[3.04]			12.6	0.87* [0.50]	Pachappa soil	21	BE	657

TABLE 8. Sorption coefficients for pesticides—Continued

log K_d log K_f^0 (1/n)	log K_{oc}	Sorbent composition (%)				Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
1.02	[3.06]			10.7	1.60* [0.93]	Kentwood soil	21	BE	657
0.56	[3.12]				0.28	Pachappa sl soil; pH 7.4; 0.005 M $CaCl_2$	20	BE	529
0.36	[2.91]				0.28	Idem	30	BE	529
1.31	[3.00]	51.10	41.42	7.48	3.56* [2.06]	Honeywood soil	20.5	BE	506
1.24	[3.01]	78.21	14.15	7.64	2.90* [1.68]	Fox soil	20.5	BE	506
1.36	[3.09]	62.02	20.45	17.53	3.19* [1.85]	Brookston soil	20.5	BE	506
2.57	[2.98]				66* [38.3]	Muck	20.5	BE	506
1.30	2.60	18.9	26.3	54.8	4.24	Tsukuba soil; pH 6.5; 0.01 M $CaCl_2$	25	BE	642
0.98° (0.86)						Idem			642
0.04	1.93	23.1	15.4	61.5	1.35	Kanuma soil; pH 5.7; 0.01 M $CaCl_2$	25	BE	642
0.36° (1.20)						Idem			642
0.99° (0.79)					1.42	Soil; cl; (kaolinite); pH 5.91; CE=12.4 me/100 g	20	BE	214
1.30° (0.91)	3.11				1.51	Soil; light c; (montmorillonite); pH 5.18; CE=13.2 me/100 g	20	BE	214
1.57° (0.81)					3.23	Soil; light c; (montomorillite) pH 5.26; CE=28.3 me/100 g	20	BE	214
1.88° (1.00)	2.98				7.91	Soil; sl; (allophane); pH 5.41; CE=26.3 me/100 g	20	BE	214
1.90° (0.94)	2.88				10.4	Soil; cl; (allophane); pH 4.89; CE=35.0 me/100 g	20	BE	214
2.58° (0.96)	[3.47]				22* [12.8]	Ca-Staten peaty muck	10	BE	390
2.52° (0.97)	[3.41]					Idem	20		390
2.43° (0.98)	[3.32]					Idem	30		390
2.29° (0.98)	[3.19]					Idem	40		390
2.29° (0.98)	[3.19]					Idem	40		390
1.73° (0.87)					6* [3.5]	Ca-Venado clay (50% Montmorillonite)	10	BE	390
1.66° (0.84)						Idem	20		390
1.62°) (0.85)						Idem	30		390
1.56° (0.85)						Idem	40		390
−1.28° (0.86)					0.10	Portage soil; CE=7.0 me/100 g; 0.01 N Ca^{++}; pH 8		BE	91
−0.44	[2.56]								
−0.32° (0.86)					0.13	Michaywe soil; CE=7.0 me/100 g; 0.01 N Ca^{++}; pH 8		BE	91
0.54	[3.42]								
−0.03° (0.95)					0.12	Delta soil; CE=5.0 me/100 g; 0.01 N Ca^{++}; pH 8		BE	91
0.24	[3.16]								
−0.34° (0.74)					1.14	Ann Arbor soil; CE=6.9 me/100 g; 0.01 N Ca^{++}; pH 8		BE	91
1.18	[3.12]								
2.95° (0.98)	[3.31]	52	34	14	75.3* [43.7]	Soil; organic; pH 6.1		BE	264

TABLE 8. Sorption coefficients for pesticides—Continued

log K_d log K_f^0 $(1/n)$	log K_{oc}	Sorbent composition (%)				Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
1.20^{0} (0.97)	[3.04]	56	30	14	2.5* [1.45]	Beverly soil; pH 6.8		BE	264
0.90^{0} (0.99)	[3.29]	91.5	1.5	7	0.7* [0.41]	Plainfield soil; pH 7.0		BE	264
0.95^{0} (0.90)	[3.31]	79.6	4.8	15.6	0.75** [0.44]	Alluvial soil; pH 6.20; CE=18.6 me/100 g	26	BE	185
1.40^{0} (0.80)		69.6	6.8	23.6	2.88* [1.67]	Lateritic soil; pH 6.30; CE=42.8 me/100 g	26	BE	185
1.50^{0} (0.80)		45.6	7.8	45.6	5.52* [3.20]	Pokkali soil; pH 5.2; CE=19.2 me/100 g	26	BE	185
2.65^{0} (1.10)	[3.50]	63.6	6.8	29.6	24.6* [14.3]	Kari soil; pH 8.3; CE=28.9 me/100 g	26	BE	185
	2.87 av (three soils)	38	48	14	0.68	Commerce soil; pH 6.7		BE	575
		56	30	14	1.12	Tracy soil; pH 6.2		BE	575
		12	56	32	2.01	Catlin soil; pH 6.2		BE	575
0.89^{0} (0.8)		12.9	64.3	19.6	0.76	Alfisol; pH 7.5	22	BE	181
1.23^{0} (1.1)						Cellulose	22	BE	181
2.47^{0} (0.92)	[3.21]	14.4	27.5	26.8	31.1* [18.0]	Lake sediment; pH 5.3 (0.1 μg lindane/mg sedim.)	23	BE	463
2.48^{0} (0.89)	[3.22]					Idem (0.2 μg/mg)			463
2.52^{0} (0.92)	[3.26]					Idem (0.5 μg/mg)			463
2.52^{0} (0.86)						Idem (1.0 μg/mg)			463
2.53^{0} (0.75)						Idem (2.0 μg/mg)			463
2.64^{0} (0.76)						Idem (5.0 μg/mg)			463
1.92	3.27				2-4	Boonton Reservoir sed.; pH 8.3		BE	421
	3.04				54.3	Boonton sed. humic acid		ED	421
1.38^{0} (0.96)	[3.17]	71	22	7	2.8* [1.62]	Big Creek sediment; pH 6.6		BE	264
	3.41* av				65–85*	Eight sludges from two water treatment plants	22.5	BE	535
	2.7				58.03	Sanhedron soil humic acid; pH 6.5	24	BE	220
	1.8				48.71	Sanhedron soil fulvic acid; pH 6.5	24	BE	220
	1.5				54.22	Suwannee River humic acid; pH 6.5	24	BE	220
	1.5				53.78	Suwannee River fulvic acid; pH 6.5	24	BE	220
	2.86					Peat humic acid		ED	423
	2.15					Bermeo soil humic acid		ED	423
	4.3				4.1	Lake Ontario sediment trap material		FM	49
1.90	[2.30]				40.0	Chitin in seawater (2.5 g/L); salinity 36.52‰	22	BE	492
1.83	[2.23]					Idem (4 g/L)			492
1.79	[2.19]					Idem (6.25 g/L)			492
1.78	[2.17]					Idem (7.5 g/L)			492
1.74	[2.14]					Idem (10 g/L)			492
1.68	[2.08]					Idem (12.5 g/L)			492
	4.02					Cyanopropyl column	20–25	RPLC	579
	2.89*				58.03	Prediction by limiting vapor sorption on soil humic acid	23	LSC	363
	2.96					Soil; experimental (literature)			217
	3.03 av					3 soils (literature)			87
	2.98 av					94 literature data			562
	3.33					Correlation log K_{oc}–log K_{ow}			96

TABLE 8. Sorption coefficients for pesticides—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%) Sand	 Silt	 Clay	 OC	Other sorbent and solution data: prediction procedure	Temp. (°C)	Meth.	Ref.
	3.5					Correlation $\log K_{oc}-\log K_{ow}(96)$			49
	3.57					Correlation $\log K_{oc}-\log S$			96
	3.60					Correlation $\log K_{oc}-\log S(\mathrm{mp})$			96
	4.09					Correlation $\log K_{oc}-\log S$			564
	3.54					Correlation $\log K_{oc}-\mathrm{MCI}$			578
	[3.68]					Correlation $\log K_{om}-\mathrm{MCI}$			591
Hexazinone (pK_a=1.09–1.23, Ref. 234)									
0.04	1.41		12	3	4.27	Forest soil (0–5 cm); pH 4.10; CE=12.1 cmol/kg; 0.01 M $CaCl_2$	25	BE	301
−0.70	1.29		10	5	1.02	Idem (5–10 cm); pH 4.22; CE=8.1 cmol/kg			301
−1.2	0.92		8	3	0.76	Idem (15–20 cm); pH 4.64; CE=6.3 cmol/kg			301
−0.10	1.40		8	3	3.19	Forest soil (0–5 cm); pH 4.99; CE=8.9 cmol/kg; 0.01 M $CaCl_2$	25	BE	301
−0.66	1.08		8	3	1.83	Idem (5–10 cm); pH 5.11; CE=5.6 cmol/kg			301
−1.33	0.79		7	4	0.76	Idem (15–20 cm); pH 5.30; CE=4.2 cmol/kg			301
−1.61	1.30		4	3	0.12	Idem (65–70 cm); pH 5.80; CE=1.3 cmol/kg			301
−0.11	0.97		8	4	8.25	Forest soil (0–5 cm); pH 5.45; CE=17.7 cmol/kg; 0.01 M $CaCl_2$	25	BE	301
−0.70	1.09		9	4	1.61	Idem (5–10 cm); pH 5.01; CE=14.4 cmol/kg			301
−1.15	0.91		6	4	0.87	Idem (15–20 cm); pH 5.20; CE=10.2 cmol/kg			301
−0.10	1.18		9	4	5.27	Forest soil (0–5 cm); pH 4.76; CE=10.9 cmol/kg; 0.01 M $CaCl_2$	25	BE	301
−0.90	0.97		9	4	1.34	Idem (5–10 cm); pH 4.79; CE=8.9 cmol/kg			301
−1.08	0.99		9	4	0.86	Idem (15–20 cm); pH 5.02; CE=6.9 cmol/kg			301
−0.16	1.34		3	4	3.18	Forest soil (0–5 cm); pH 5.04; CE=6.9 cmol/kg; 0.01 M $CaCl_2$	25	BE	301
−0.61	1.12		3	4	1.88	Idem (5–10 cm); pH 4.92; CE=5.1 cmol/kg			301
−0.45	1.32		2	5	1.70	Idem (15–20 cm); pH 4.73; CE=5.9 cmol/kg			301
−0.03	1.03		7	4	8.73	Forest soil (0–5 cm); pH 5.06; CE=11.2 cmol/kg; 0.01 M $CaCl_2$	25	BE	301
−0.88	1.17		4	4	0.83	Idem (5–10 cm); pH 4.94; CE=6.3 cmol/kg			301
−1.22	1.01		1	3	0.59	Idem (15–20 cm); pH 4.81; CE=8.1 cmol/kg			301
−1.62	1.30		0	1	0.12	Idem (65–70 cm); pH 5.60; CE=2.1 cmol/kg			301
−0.57° (0.87)		26	63	11	0.63	Taloka soil (Ap horizon); pH 5.6; 0.01 M $CaCl_2$	22	BE	234
0.07° (0.87)		38	50	12	2.41	Mountainburg soil (Oa-A-B hor.); pH 5.5; 0.01 M $CaCl_2$	22	BE	234
0.38° (0.96)	[1.52]	44	47	90	7.31	Idem (Oa-A horizon); pH 6.4; 0.01 M $CaCl_2$	22	BE	234
−0.23° (0.96)	[1.53]	37	45	18	1.73	Idem (B horizon); pH 4.0; 0.01 M $CaCl_2$	22	BE	234
−0.70° (0.95)	[1.15]	56	29	15	1.40* [0.81]	Fallsington soil; pH 5.6; CE=4.8 me/100 g		BE	658
0.00° (1.05)	[1.40]	5	64	31	4.02* [2.33]	Flanagan soil; pH 5.0; CE=23.4 me/100 g		BE BE	658 658

TABLE 8. Sorption coefficients for pesticides—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data: prediction procedure	Temp. (°C)	Meth.	Ref.
						Ipazine (pK_a=1.85, Ref. 247)			
1.42	2.91				3.27	Hickory Hill sediment; coarse si fraction (20–50 μm)	25	BE	130
1.68	[3.39]	66.0	18.4	15.6	1.93	Begbroke soil; pH 7.1; 0.1 M $CaCl_2$	22	BE	638
	3.22					Soil: experimental (literature)			217
	3.55					Correlation $\log K_{oc}-\log K_{ow}$			96
	3.09					Correlation $\log K_{oc}-\log S$			96
	3.10					Correlation $\log K_{oc}-\log S$(mp)			96
	2.76					Correlation $\log K_{oc}-\log S$			564
	2.74					Correlation $\log K_{oc}$–MCI			598
						Isocil (pK_a=9.1, Ref. 679)			
0.31						Silica gel (0.59–0.07 mm)(Grace Div. Chem., Baltimore, Md.): pH 5.2	25	BE	99
0.58						Idem	0		99
0.31						Idem; pH 3.5	25		99
0.97° (0.8)						Idem	0		99
0.3° (0.9)				100		Illite No. 35 (0.83 mm)(Fithian, Ill.); pH 7.4	25	BE	99
0.79° (0.8)						Idem	0		99
0.1° (1.2)				100		Montmorillonite No. 25 (0.83 mm) (J. C. Lane Track, Upton, Wyo.) pH 6.7	25	BE	99 99
0.49° (1.1)						Idem	0		99
−1.07° (1.2)				100		Kaolinite (0.24–1.68 mm) (Merck, NFV); pH 6–7	25	BE	99
−3.6° (1.1)						Idem	0		99
	2.05°* (0.7)					Humic acid (0.59–0.2 mm) extracted from soil; pH 6–7	25	BE	99
	2.19°* (0.7)					Idem	0		99
	2.11					Soil; experimental (literature)			217
	1.81					Correlation $\log K_{oc}-\log S$			564
	2.23					Correlation $\log K_{oc}$–MCI			578
						Leptophos			
3.66	[3.93]				94* [54.5]	OM from peaty much (Histosol) soil; pH 5.5	24	BE	121
	3.97					Soil: experimental (literature)			217
	3.43					Correlation $\log K_{oc}-\log S$			564
						Linuron			
1.45° (0.78)						Bentonite; 0.01 M $CaCl_2$	22	BE	144
	[2.43] av				1.09*- 4.25*	4 soils; silt loam; pH 6.1–7.5. 0.01 M $CaCl_2$	20	BE	120
[0.78]	[2.36]				4.54* [2.63]	Warwick, Qld, soil; pH 6.3; 0.01 M $CaCl_2$		BE	558
[0.74]	[2.37]				4.07* [2.36]	Rutherglen, Vic., soil; pH 4.8; 0.01 M $CaCl_2$		BE	558
[0.43]	[2.40]				1.86* [1.08]	Wagga, N.S.W., soil; pH 5.1; 0.01 M $CaCl_2$		BE	558
[0.47]	[2.26]				2.81* [1.63]	Turretfield, S. A., soil; pH 5.2; 0.01 M $CaCl_2$		BE	558
[0.29]	[2.49]				1.09* [0.63]	Warracknabeal, Vic., soil; pH 8.0; 0.01 M $CaCl_2$		BE	558
[0.65]	[2.38]				3.20*	Warracknabeal, Vic., soil; pH 8.4;		BE	558

TABLE 8. Sorption coefficients for pesticides—Continued

log K_d log K_f^0 ($1/n$)	log K_{oc}	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data: prediction procedure	Temp. (°C)	Meth.	Ref.
					[1.86]	0.01 M $CaCl_2$			
[0.58]	[2.00]				6.62* [3.84]	Balkuling soil; pH 5.6; 0.01 M $CaCl_2$		BE	558
[0.41]	[2.32]				2.14* [1.24]	Kojonup soil; pH 5.5; 0.01 M $CaCl_2$		BE	558
[0.29]	[2.38]				1.42* [0.82]	Warranine soil; pH 6.5; 0.01 M $CaCl_2$		BE	558
[0.58]	[2.10]				5.17* [3.00]	Yalanbee soil; pH 6.4; 0.01 M $CaCl_2$		BE	558
[0.54]	[2.32]				2.85* [1.65]	Avondale soil; pH 5.9; 0.01 M $CaCl_2$		BE	558
[0.51]	[2.55]				1.58* [0.92]	Badgingarra soil; pH 6.3; 0.01 M $CaCl_2$		BE	558
[−0.80]	[2.16]				0.19* [0.11]	Badgingarra soil; pH 6.3; 0.01 M $CaCl_2$		BE	558
[0.61]	[2.38]				2.92* [1.69]	Beverley soil; 0.01 M $CaCl_2$		BE	558
[0.78]	[2.44]				3.78* [2.19]	Gabalong soil; pH 5.9; 0.01 M $CaCl_2$		BE	558
[0.23]	[2.41]				1.13* [0.66]	Perth soil; pH 5.9; 0.01 M $CaCl_2$		BE	558
[0.55]	[2.52]				1.86* [1.08]	Tammin soil; pH 5.9; 0.01 M $CaCl_2$		BE	558
1.99° (0.77)		47.5	33.2	20.3	10.5* [6.09]	Melfort soil; pH 5.9	25	BE	260
1.28° (0.70)		53.3	27.5	19.2	6.46* [3.75]	Weyburn soil; pH 6.5	25	BE	260
1.26° (0.70)		5.3	25.3	69.5	4.15* [2.41]	Regina soil; pH 7.7	25	BE	260
1.25° (0.65)		69.3	12.3	18.5	4.07* [2.36]	Indian Head soil; pH 7.8	25	BE	260
0.84° (0.75)		81.6	10.4	8.0	1.77* [1.03]	Asquith soil; pH 7.5	25	BE	260
1.09° (∼0.9)	[2.80]	66.0	18.4	15.6	1.93	Begbroke soil; pH 7.1; 1:10 soil:water; 0.1 M $CaCl_2$	22	BE	462
1.03	[2.75]					Idem			638
0.64° (∼0.9)	[2.36]	66.0	18.4	15.6	1.93	Begbroke soil; pH 7.1; 1:1 soil:water; 0.01 M $CaCl_2$	22	BE	462
0.43° (∼0.9)	[2.15]	66.0	18.4	15.6	1.93	Begbroke soil; pH 7.1; 4:1 soil;water: 0.1 M $CaCl_2$	22	BE	462
1.39° (0.97)	3.28			75	1.3	Eurosol-1; c soil; pH 5.1; 0.01 M $CaCl_2$		BE	583
0.96° (1.02)	2.39			22.6	3.7	Eurosol-2; sil; pH 7.4; 0.01 M $CaCl_2$		BE	583
1.00° (1.01)	2.46			17.0	3.45	Eurosol-3; l; pH 5.2; 0.01 M $CaCl_2$		BE	583
0.48° (1.09)	2.29			20.3	1.55	Eurosol-4; si; pH 6.5; 0.01 M $CaCl_2$		BE	583
2.09° (0.83)				6.0	9.25	Eurosol-5; ls; pH 3.2; 0.01 M $CaCl_2$		BE	583
2.50°		7	10	10	36.5	Sunway farm light peat; pH 5.2; CE=60 me/100 g	22	BE	259
1.86°		45.5	15.9	6.6	12.0	Grat House E.H.F. soil; pH 6.3; CE=18 me/100 g	22	BE	259
1.80°		23	24.4	28.6	11.7	Toll Farm heavy peat; pH 7.4; CE=41 me/100 g	22	BE	259
1.70°		34.0	33.4	32.6	3.69	Trawscoed E.H.F. soil; pH 6.2; CE=12 me/100 g	22	BE	259
1.67°		66.0	18.4	15.6	1.93	Weed Res. soil; pH 7.1; CE=11 me/100 g	22	BE	259
1.54°		36.0	40.4	23.6	1.76	Rosemaunde E.H.F. soil; pH 6.7; CE=14 me/100 g	22	BE	259
1.83°		45.5	15.9	6.6	12	Great House E.H.F. soil; pH 6.3;	22	BE	144

TABLE 8. Sorption coefficients for pesticides—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%)				Other sorbent and solution data: prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
(0.75)						CE = 18 me/100 g; 0.1 M $CaCl_2$			
1.66° (0.75)		66.0	18.4	15.6	1.93	Weed Res. Orgn. soil; pH 7.1; CE = 11 me/100 g; 0.1 M $CaCl_2$	22	BE	144
0.36° (0.84)				9.8	0.1* [0.06]	Soil; s, mesic; pH 7.0; SA(W) = 14.8 m^2/g		BE	72
0.68° (0.85)				15.0	1.0* [0.58]	Soil; s, mixed, mesic; pH 7.6; SA(W) = 18.1 m^2/g		BE	72
0.69° (0.79)				13.0	1.4* [0.81]	Soil; s, mixed, mesic; pH 7.3; SA(W) = 30.3 m^2/g		BE	72
0.98° (0.73)				6.8	1.5* [0.87]	Soil; s, mixed, mesic; pH 7.1; SA(W) = 15.2 m^2/g		BE	72
0.90° (0.94)	[2.93]			31.5	1.6* [0.93]	Soil; s, clay, mesic; pH 6.6; SA(W) = 72.4 m^2/g		BE	72
1.26° (0.82)				10.6	1.9* [1.10]	Soil; s, mesic; pH 4.2; SA(W) = 38.6 m^2/g		BE	72
1.11° (0.77)				18.3	1.2* [0.70]	Soil, s, mesic; pH 6.9; SA(W) = 55.8 m^2/g		BE	72
1.36° (0.89)	[2.94]			4.5	4.6* [2.67]	Soil, s, mesic; pH 3.7; SA(W) = 22.4 m^2/g		BE	72
0.73° (0.85)			1.5	1.3	1.2* [0.70]	Bassendean soil; pH 5.0; CE = 2.4 cmol/kg; SA(N_2) = 0.4 m^2/g; 0.005 M $CaCl_2$		BE	143
0.56° (0.76)			8.3	15.3	1.7* [0.99]	Gascoyne soil; CE = 24.8 cmol/kg; pH 6.9; SA(N_2) = 22.5 m^2/g; 0.005 M $CaCl_2$		BE	143
0.42 (0.70)			2.5	13.6	0.6* [0.35]	Cobiac soil; CE = 3.5 cmol/kg; pH 5.1; SA(N_2) = 13.4 m^2/g; 0.005 M $CaCl_2$		BE	143
1.43° (0.81)			14.2	63.7	4.6* [2.67]	Wellesley soil; CE = 43.0 cmol/kg; pH 5.9; SA(N_2) = 73.1 m^2/g; 0.005 M $CaCl_2$		BE	143
[1.08]	[3.38]			1	0.5	Lakewood soil (A horizon); pH 8.6; CE = 1.8 me/100 g		BE	242
[0.86]	[3.78]			5	0.12	Idem (B horizon); pH 4.5 CE = 1.4 me/100 g		BE	242
[1.05]	[2.75]			20	2.0	Sassafras soil (A horizon); pH 5.2; CE = 7.7 me/100 g		BE	242
[1.04]	[3.34]			30	0.5	Idem (B horizon); pH 5.1; CE = 7.1 me/100 g		BE	242
[1.16]	[2.75]			17	2.6	Collington soil (A horizon); pH 4.9; CE = 12.8 me/100 g		BE	242
[0.68]	[2.90]			19	0.6	Idem (B horizon); pH 5.7; CE = 11.0 me/100 g		BE	242
[0.83]	[2.75]			11	1.2	Colts Neck soil (A horizon); pH 4.2; CE = 7.7 me/100 g		BE	242
[0.55]	[2.65]			15	0.8	Idem (B horizon); pH 4.6; CE = 8.4 me/100 g		BE	242
[1.07]	[2.84]			21	1.7	Annandale soil (A horizon); pH 5.9; CE = 11.3 me/100 g		BE	242
[0.80]	[2.68]			24	1.3	Idem (B horizon); pH 6.8; CE = 12.0 me/100 g		BE	242
[1.14]	[2.94]			31	1.6	Bermudian soil (A horizon); pH 6.0; CE = 13.2 me/100 g		BE	242
[0.89]	[2.99]			35	0.8	Idem (B horizon); pH 6.0; CE = 12.6 me/100 g		BE	242
[0.94]	[2.66]			20	1.9	Whippany soil (A horizon); pH 5.6; CE = 9.4 me/100 g		BE	242
[0.54]	[2.77]			21	0.6	Idem (B horizon); pH 6.2; CE = 16.9 me/100 g		BE	242
[1.13]	[2.67]			24	2.9	Dutchess soil (A horizon); pH 5.4; CE = 12.7 me/100 g		BE	242
[1.13]	[3.01]			22	1.3	Idem (B horizon); pH 5.8; CE = 5.8 me/100 g		BE	242

TABLE 8. Sorption coefficients for pesticides—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data: prediction procedure	Temp. (°C)	Meth.	Ref.
[1.02]	[2.79]			17	1.7	Squires soil (A horizon); pH 6.6; CE=7.0 me/100 g		BE	242
[0.70]	[2.70]			16	1.0	Idem (B horizon): pH 6.9; CE=7.5 me/100 g		BE	242
[1.13]	[2.75]			20	2.4	Washington soil (A horizon); pH 6.1; CE=11.2 me/100 g		BE	242
[0.70]	[2.55]			21	1.4	Idem (B horizon); pH 6.5; CE=9.2 me/100 g		BE	242
[2.20]	[2.64]				63* [36.5]	Mesic peat (acid treated); 0.01 M $CaCl_2$		BE	477
2.59° (0.95)	[2.94]				76* [44]	OM from peat soil; 0.1 M $CaCl_2$	22	BE	144
2.65	[3.00]				76* [44]	OM from peat soil; 0.1 M $BaCl_2$		BE	270
	2.37*					Peat humic acid; 0.1 M $BaCl_2$		BE	270
0.98	2.94		27.4	72.1	1.1	Bear Creek 5290 sedim.; pH 5.7	25	BE	478
1.26	2.66		21.5	77.2	3.9	Bear Creek 5356 sedim.; pH 4.4	25	BE	478
0.67	2.56		37.6	59.7	1.3	Lake Chicot 5636 sedim.; pH 6.3	25	BE	478
0.48	2.74		48.1	30.9	0.55	Lake Chicot 5643 sedim.; pH 7.3	25	BE	478
0.80	2.65		14.2	85.3	1.4	Lake Chicot 5700 sedim.; pH 6.2	25	BE	478
0.93	2.82		18.6	80.9	1.3	Wolf Lake 6262 sedim.; pH 4.5	25	BE	478
0.77	2.93		54.4	25.6	0.69	Wolf Lake 6268 sedim.; pH 7.7	25	BE	478
0.95	2.81		45.0	49.6	1.4	Wolf Lake 6272 sedim.; pH 5.7	25	BE	478
0.85	2.94		47.8	51.8	0.81	McWilliams Pond 1 sedim.; pH 5.8	25	BE	478
0.65	2.81		67.3	30.8	0.69	McWilliams Pond 2 sedim.; pH 6.8	25	BE	478
1.20	2.82		42.6	57.2	2.9	Beaver Pond sedim.; pH 5.2	25	BE	478
0.34	2.65		88.6	9.9	0.51	Lake Washington sedim.; pH 7.7	25	BE	478
	[3.02]				52.54	Humic acid from peat; pH 5.0		BE	242
	[3.03]					Idem; pH 5.3			242
	[3.29]					Idem; pH 4.4			242
	[3.48]					Idem; pH 4.2			242
	2.84°* (0.78)					Humic acid from a black chernozemic Ah hor. (56.4% C); saturated with Al^{3+}	5	BE	396
	2.80°* (0.79)					Idem; saturated with Al^{3+}	25		396
	2.96°* (0.68)					Idem; saturated with Fe^{3+}	5		396
	2.86°* (0.79)					Idem; saturated with Fe^{3+}	25		396
	2.79°* (0.71)					Idem; saturated with Cu^{2+}	2		396
	2.72°* (0.72)					Idem; saturated with Cu^{2+}	25		396
	2.74°* (0.74)					Idem; saturated with Zn^{2+}	5		396
	2.70°* (0.74)					Idem; saturated with Zn^{2+}	25		396
	2.72°* (0.81)					Idem; saturated with Ni^{2+}	5		396
	2.68°* (0.85)					Idem; saturated with Ni^{2+}	25		396
	2.76°* (0.72)					Idem; saturated with Ca^{2+}	5		396
	2.71°* (0.73)					Idem; saturated with Ca^{2+}	25		396
	2.97°* (0.73)					Idem; saturated with H^+	5		396
	2.92°* (0.80)					Idem; saturated with H^+	25		396
	3.83					Patuxent River colloidal fraction; TOC=49.0 mg/L. Salinity=13.5‰	20	BE	406

TABLE 8. Sorption coefficients for pesticides—Continued

log K_d log K_f^0 (1/n)	log K_{oc}	Sorbent composition (%) Sand	 Silt	 Clay	 OC	Other sorbent and solution data: prediction procedure	Temp. (°C)	Meth.	Ref.
	3.79					Idem; TOC=52.5 mg/L; salinity=14.5/mL			406
	2.67					Cyanopropyl column; ring test		RPLC	581
	2.91					Soil; experimental (literature)			217
	2.94av					33 soils (literature)			87
	1.80					Correlation log K_{oc}–log K_{ow}			96
	2.93					Correlation log K_{oc}–log S			96
	2.80					Correlation log K_{oc}–log S(mp)			96
	2.61					Correlation log K_{oc}–log S			564
						Malathion			
[0.63]	[2.93]			1	0.5	Lakewood soil (A horizon); pH 4.6; CE=1.8 me/100 g		BE	242
[0.39]	[3.31]			5	0.12	Idem (B horizon); pH 4.8 CE=1.4 me/100 g		BE	242
[1.41]	[3.11]			20	2.0	Sassafras soil (A horizon); pH 5.2; CE=7.7 me/100 g		BE	242
[0.62]	[2.92]			30	0.5	Idem (B horizon); pH 5.3; CE=7.1 me/100 g		BE	242
[1.67]	[3.25]			17	2.6	Collington soil (A horizon); pH 5.7; CE=12.8 me/100 g		BE	242
[1.00]	[3.22]			19	0.6	Idem (B horizon); pH 5.7; CE=11.0 me/100 g		BE	242
[0.90]	[2.82]			11	1.2	Colts Neck soil (A horizon); pH 5.7; CE=7.7 me/100 g		BE	242
[0.53]	[2.63]			15	0.8	Idem (B horizon); pH 4.7; CE=8.4 me/100 g		BE	242
[1.74]	[3.51]			21	1.7	Annandale soil (A horizon); pH 6.2; CE=11.3 me/100 g		BE	242
[1.24]	[3.12]			24	1.3	Idem (B horizon); pH 6.5; CE=12.0 me/100 g		BE	242
[1.73]	[3.53]			31	1.6	Bermudian soil (A horizon); pH 6.4; CE=13.2 me/100 g		BE	242
[1.19]	[3.29]			35	0.8	Idem (B horizon); pH 5.2; CE=12.6 me/100 g		BE	242
[1.18]	[2.90]			20	1.9	Whippany soil (A horizon); pH 5.7; CE=9.4 me/100 g		BE	242
[0.46]	[2.68]			21	0.6	Idem (B horizon); pH 5.7; CE=16.9 me/100 g		BE	242
[1.76]	[3.29]			24	2.9	Dutchess soil (A horizon); pH 5.8; CE=12.7 me/100 g		BE	242
[1.17]	[3.06]			22	1.3	Idem (B horizon); pH 5.6; CE=5.8 me/100 g		BE	242
[1.70]	[3.47]			17	1.7	Squires soil (A horizon); pH 6.5; CE=7.0 me/100 g		BE	242
[0.80]	[2.81]			16	1.0	Idem (B horizon); pH 6.7; CE=7.5 me/100 g		BE	242
[1.41]	[3.03]			20	2.4	Washington soil (A horizon); pH 6.1; CE=11.2 me/100 g		BE	242
[0.77]	[2.62]			21	1.4	Idem (B horizon); pH 5.8; CE=9.2 me/100 g		BE	242
	[2.82]av				52.54	4 humic acid samples from peat; pH 5.1–5.3		BE	242
	3.26av					20 soils (literature)			87
	2.50					Correlation log K_{oc}–log K_{ow}			96
	2.83					Correlation log K_{oc}–log S			96
	3.29					Correlation log K_{oc}–log S (mp)			96
	2.45					Correlation log K_{oc}–log S			564
						Methazole			
2.71				100		Ca–montmorillonite; pH 6	24	BE	121
3.16	[3.42]				94* [54.5]	OM from peaty muck (Histosol) soil; pH 6.5	24	BE	121

TABLE 8. Sorption coefficients for pesticides—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
	3.42					Soil; experimental (literature)			217
	3.54					Correlation $\log K_{oc}-\log S$			564
Methiocarb									
1.23° (0.83)				75	1.3	Eurosol-1; c; pH 5.1; 0.01 M $CaCl_2$		BE	583
1.02° (0.89)	2.45			22.6	3.7	Eurosol-2; sil; pH 7.4; 0.01 M $CaCl_2$		BE	583
0.92° (0.91)	2.38			17.0	3.45	Eurosol-3; l; pH 5.2; 0.01 M $CaCl_2$		BE	583
0.58° (0.92)	2.38			20.3	1.55	Eurosol-4; si; pH 6.5; 0.01 M $CaCl_2$		BE	583
1.76° (0.79)				6.0	9.25	Eurosol-5; ls; pH 3.2; 0.01 M $CaCl_2$		BE	583
	[2.32]av				1.09* 2.51*	2 Batcombe sil soils; pH 7.5; 6.7. 0.01 M $CaCl_2$	20	BE	120
Methoxychlor									
1.72	4.61				0.13	Hickory Hill sedim.; s (>50 μm)	25	BE	108
3.42	4.90				3.27	Idem; coarse si (50–20 μm)			108
3.26	4.96				1.98	Idem; medium si (20–5 μm)			108
3.15	5.00				1.34	Idem; fine si (5–2 μm)			108
3.04	4.96				1.20	Idem; c (>2 μm)			108
0.92	3.99				0.09	Doe Run sedim.: s	25	BE	108
3.34	4.90				2.78	Idem; coarse si			108
3.23	4.86				2.34	Idem; medium si			108
3.36	4.90				2.89	Idem; fine si			108
3.38	4.86				3.29	Idem; c			108
1.98	4.23				0.57	Oconee River sedim.; s	25	BE	108
3.40	4.93				2.92	Idem; coarse si			108
3.30	5.00				1.99	Idem; medium si			108
3.32	4.97				2.26	Idem; fine si			108
	4.99					Cyanopropyl column	20–25	RPLC	579
	4.90					Soil; experimental (literature)			217
	4.69					Correlation $\log K_{oc}-\log K_{ow}$			96
	5.54					Correlation $\log K_{oc}-\log S$(mp)			96
	5.03					Correlation $\log K_{oc}-\log S$			564
	4.63					Correlation $\log K_{oc}-$MCI			598
Methyl parathion									
1.82° (1.03)				100		Na–montmorillonite (<2 μm)	20	BE	246
1.75° (1.66)				100		Ca–montmorillonite (<2 μm)	20	BE	246
2.17° (1.46)				100		Fe–montmorillonite (<2 μm)	20	BE	246
1.13° (0.75)		18.4	45.3	38.3	3.87	Webster soil; pH 7.3; CE=54.7 me/100 g; 0.01 N $CaCl_2$	23	BE	102
0.60° (0.85)		65.8	19.5	14.7	0.90	Cecil soil; pH 5.6; CE=6.8 me/100 g; 0.01 N $CaCl_2$	23	BE	102
0.43° (0.86)		93.8	3.0	3.2	0.56	Eustis soil; pH 5.6; CE=5.2 me/100 g; 0.01 N $CaCl_2$	23	BE	102
1.24	[2.87]			37.7	4.03* [2.34]	Mollic-Solonetz soil	20	BE	659
0.96	[3.12]			46.4	1.19* [0.69]	Idem			659
1.08	[2.59]			9.5	5.30* [3.08]	Humic Cambisol	20	BE	659
1.21	[2.59]			15.9	7.13* [4.15]	Idem			659
0.56	[2.91]			62.0	0.77* [0.45]	Pellic Vertisol	20	BE	659
0.51	[3.18]			48.5	0.36*	Chromic Luvisol	20	BE	659

TABLE 8. Sorption coefficients for pesticides—Continued

log K_d log K_f^0 $(1/n)$	log K_{oc}	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data: prediction procedure	Temp. (°C)	Meth.	Ref.
					[0.21]				
0.74	[2.59]			10.7	2.40* [1.40]	Humic Cambisol	20	BE	659
1.44	[2.67]			13.6	10.2* [5.93]	Idem			659
	3.99					Soil; experimental (literature)			217
	3.71av					7 soils (literature)			87
	2.93					Correlation log K_{oc}−log K_{ow}			96
	3.02					Correlation log K_{oc}−log S			96
	3.47					Correlation log K_{oc}−log S(mp)			96
	2.67					Correlation log K_{oc}−log S			564
						Metobromuron			
[0.54]	[2.12]				4.54* [2.63]	Warwick, Qld, soil; pH 6.3; 0.01 M $CaCl_2$		BE	558
[0.30]	[1.93]				4.07* [2.36]	Rutherglen, Vic., soil; pH 4.8; 0.01 M $CaCl_2$		BE	558
[−0.01]	[1.96]				1.86* [1.08]	Wagga, N.S.W., soil; pH 5.1; 0.01 M $CaCl_2$		BE	558
[0.02]	[1.81]				2.81* [1.63]	Turretfield, S. A., soil; pH 5.2; 0.01 M $CaCl_2$		BE	558
[−0.18]	[2.02]				1.09* [0.63]	Warracknabeal, Vic., soil; pH 8.0; 0.01 M $CaCl_2$		BE	558
[0.27]	[2.00]				3.20* [1.86]	Warracknabeal, Vic., soil; pH 8.4; 0.01 M $CaCl_2$		BE	558
[0.25]	[1.67]				6.62* [3.84]	Balkuling soil; pH 5.6; 0.01 M $CaCl_2$		BE	558
[0.10]	[2.01]				2.14* [1.24]	Kojonup soil; pH 5.5; 0.01 M $CaCl_2$		BE	558
[−0.02]	[2.07]				1.42* [0.82]	Warranine soil; pH 6.5; 0.01 M $CaCl_2$		BE	558
[0.24]	[1.76]				5.17* [3.00]	Yalanbee soil; pH 6.4; 0.01 M $CaCl_2$		BE	558
[0.15]	[1.93]				2.85* [1.65]	Avondale soil; pH 5.9; 0.01 M $CaCl_2$		BE	558
[0.08]	[2.12]				1.58* [0.92]	Badgingarra soil; pH 6.3; 0.01 M $CaCl_2$		BE	558
[−0.81]	[2.15]				0.19* [0.11]	Badgingarra soil; pH 6.3; 0.01 M $CaCl_2$		BE	558
[0.22]	[1.99]				2.92* [1.69]	Beverley soil; 0.01 M $CaCl_2$		BE	558
[0.47]	[2.02]				3.78* [2.19]	Gabalong soil; pH 5.9; 0.01 M $CaCl_2$		BE	558
[−0.08]	[2.10]				1.13* [0.66]	Perth soil; pH 5.9; 0.01 M $CaCl_2$		BE	558
[0.12]	[2.09]				1.86* [1.08]	Tammin soil; pH 5.9; 0.01 M $CaCl_2$		BE	558
1.79° (0.49)		47.5	33.2	20.3	10.5* [6.09]	Melfort soil; pH 5.9	25	BE	260
1.05° (0.64)		53.3	27.5	19.2	6.46* [3.75]	Weyburn soil; pH 6.5	25	BE	260
0.63° (0.83)		5.3	25.3	69.5	4.15* [2.41]	Regina soil; pH 7.7	25	BE	260
0.97° (0.68)		69.3	12.3	18.5	4.07* [2.36]	Indian Head soil; pH 7.8	25	BE	260
0.32° (0.89)	[2.31]	81.6	10.4	8.0	1.77* [1.03]	Asquith soil; pH 7.5	25	BE	260
0.40° (0.58)				9.8	0.1* [0.06]	Soil; s, mesic; pH 7.0; SA(W)=14.8 m^2/g		BE	72
0.32° (0.78)				15.0	1.0* [0.58]	Soil; s, mixed, mesic; pH 7.6; SA(W)=18.1 m^2/g		BE	72
0.34° (0.82)				13.0	1.4* [0.81]	Soil; s, mixed, mesic; pH 7.3; SA(W)=30.3 m^2/g		BE	72

TABLE 8. Sorption coefficients for pesticides—Continued

log K_d log K_f^0 ($1/n$)	log K_{oc}	Sorbent composition (%)				Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
0.29° (0.82)				6.8	1.5* [0.87]	Soil; s, mixed, mesic; pH 7.1; SA(W) = 15.2 m^2/g		BE	72
0.66° (0.85)				31.5	1.6* [0.93]	Soil; s, c, mesic; pH 6.6; SA(W) = 72.4 m^2/g		BE	72
0.79° (0.80)				10.6	1.9* [1.10]	Soil; s, mesic; pH 4.2; SA(W) = 38.6 m^2/g		BE	72
0.79° (0.82)				18.3	1.2* [0.70]	Soil; s, mesic; pH 6.9; SA(W) = 55.8 m^2/g		BE	72
1.01° (0.81)				4.5	4.6* [2.67]	Soil; s, mesic; pH 3.7; SA(W) = 22.4 m^2/g		BE	72
	1.78					Soil; experimental (literature)			217
	2.43av					4 soils (literature)			87
	2.26					Correlation log K_{oc} – log S			564
						Metolachlor			
2.10° (1.01)						Ca–montmorillonite; pH 7; 0.01 M $CaCl_2$	25	BE	660
0.17av (two soils)	[2.41]av	23.4	67.5	9.1	1.1* [0.64]	Taloka soil (10–20 cm); pH 5.2; CE = 11 me/100 g; 0.01 M $CaCl_2$	20	BE	285
		22.0	62.2	15.8	0.90* [0.52]	Roxana soil (10–20 cm); pH 6.8; CE = 19 me/100 g; 0.01 M $CaCl_2$	20	BE	285
−0.04av (two soils)	[2.42]av	24.2	62.0	13.8	0.70* [0.41]	Taloka soil (40–50 cm); pH 5.5; CE = 13 me/100 g; 0.01 M $CaCl_2$	20	BE	285
		30.7	54.7	14.6	0.50* [0.29]	Roxana soil (40–50 cm); pH 7.1; CE = 19 me/100 g; 0.01 M $CaCl_2$	20	BE	285
0.64° (~0.90)	2.06	15	71	14	3.8	Tanana Alaskan agric soil (0–15 cm); pH 6.5; 0.01 M $CaCl_2$	5	BE	398
0.67° (~0.90)	2.09					Idem	28		398
0.85° (~0.90)	2.04	42	50	8	6.4	Beales Alaskan agric. soil (0–15 cm); pH 6.4; 0.01 M $CaCl_2$	5	BE	398
0.96° (~0.90)	2.16					Idem	28		398
0.11° (~0.95)	2.27	26	63	11	0.69	Tanana Alaskan agric. soil (30–45 cm); pH 7.4; 0.01 M $CaCl_2$	5	BE	398
0.08° (~0.95)	2.23					Idem	28		398
−0.23° (~0.95)	2.01	67	25	8	0.74	Beales Alaskan agric. soil (30–45 cm); pH 5.1; 0.01 M $CaCl_2$	5	BE	398
−0.09° (~0.95)	2.14					Idem	28		398
0.93	[2.20]		28	11	9.2* [5.34]	Cape Fear soil; pH 6.0; CE = 10.3 me/100 g; SA = 77.2 m^2/g		BE	279
0.51	[2.35]		41	7	2.5* [1.45]	Rains soil; pH 6.0; CE = 7.1 me/100 g; SA = 18.2 m^2/g		BE	279
0.34	[2.35]		11	2	1.7* [0.99]	Norfolk soil; pH 6.0; CE = 2.3 me/100 g; SA = 4.4 m^2/g		BE	279
0.74	3.03	43	24	33	0.51	Pullman soil; pH 7.9; CE = 29.2 me/100 g	24	BE	281
0.68	3.14	70	14	16	0.35	Amarillo soil; pH 8.2; CE = 15.6 me/100 g	24	BE	281
0.58	3.14	74	10	16	0.27	Patricia soil; pH 8.2; CE = 14.9 me/100 g	24	BE	281
0.47	[2.10]		32.8	13.7	2.37	CVa, Merrimac f_{sl} soil (0–15 cm); 0.01 M $CaCl_2$	21	BE	481
0.16	[1.95]		42.7	8.7	1.65	CVb, Merrimac f_{sl} soil (5–30 cm); 0.01 M $CaCl_2$	21	BE	481
0.11	[2.15]				0.91	W1, Merrimac sl soil (0–15 cm); 0.01 M $CaCl_2$	21	BE	481
−0.11	[2.11]		10.3	8.0	0.60	W2, Merrmac sl soil (0–15 cm); 0.01 M $CaCl_2$	21	BE	481
−0.32	[2.22]	80	15	5	0.5*	Augusta soil; pH 5.7;	28	BE	280

TABLE 8. Sorption coefficients for pesticides—Continued

log K_d log K_f^0 (1/n)	log K_{oc}	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data: prediction procedure	Temp. (°C)	Meth.	Ref.
					[0.29]	CE=3.2 me/100 g; SA(E)=3.3 m^2/g			
−0.28	[2.26]	89	9	2	0.5* [0.29]	Norfolk soil; pH 5.4; CE=2.3 me/100 g; SA(E)=4.4 m^2/g	28	BE	280
0.15	[2.30]	72	23	5	1.2* [0.70]	Goldsboro soil; pH 5.3; CE=3.3 me/100 g; SA(E)=7.0 m^2/g	28	BE	280
0.03	[2.12]	82	10	8	1.4* [0.81]	Appling soil; pH 6.8; CE=6.9 me/100 g; SA(E)=12.8 m^2/g	28	BE	280
0.39	[2.23]	70	22	8	2.5* [1.45]	Lynchburg soil; pH 5.5; CE=6.6 me/100 g; SA(E)=13.6 m^2/g	28	BE	280
0.00	[2.00]	76	16	8	1.7* [0.99]	Cecil soil; pH 5.4; CE=3.1 me/100 g; SA(E)=16.3 m^2/g	28	BE	280
0.37	[2.38]	26	64	10	1.7* [0.99]	Rains soil; pH 6.0; CE=7.1 me/100 g; SA(E)=18.8 m^2/g	28	BE	280
0.52	[2.11]	61	26	12	4.4* [2.55]	Portsmouth soil; pH 5.4; CE=10.6 me/100 g; SA(E)=20.6 m^2/g	28	BE	280
1.04	[2.32]	52	36	13	8.7* [5.05]	Cape Fear soil; pH 5.1; CE=10.3 me/100 g; SA(E)=77.2 m^2/g	28	BE	280
0.86° (0.84)		53	26	21	5.7	Cape Fear soil; pH 4.7; CE=12.7 me/100 g; 0.01 M CaCl$_2$	25	BE	660
0.81° (0.84)		28	45	27	4.9	Webster soil; pH 7.4; CE=20.2 me/100 g; 0.01 M CaCl$_2$	25	BE	660
−0.36° (0.74)		74	20	6	1.1	Norfolk soil; pH 5.9; CE=2.7 me/100 g; 0.01 M CaCl$_2$	25	BE	660
−0.44° (0.92)	[1.60]	60	24	16	0.9	Rion soil; pH 5.7; CE=3.8 me/100 g; 0.01 M CaCl$_2$	25	BE	660
	2.36°* (0.94) [2.59]				0.58	Ca–OM from a muck (Histosol); pH 4; 0.01 M CaCl$_2$	25	BE	660
0.24av	2.32av	30.6av	56.9av	12.6av	1.4*av [0.81]	Captina-Johnsburg; Ap horizons association from 135 sampling locations; pH 5.8av	25	BE	661
−0.12av	2.50av	23.1av	53.7av	23.2av	0.44*av [0.26]	Idem; Bt horizons; pH 5.6av			661
−0.12av	2.67av	22.3av	51.6av	26.1av	0.33*av [0.19]	Idem; Btx horizons; pH 5.1av			661
	2.33av					45 literature data			562
	2.15					Correlation log K_{oc}−log S			564
	2.46					Correlation log K_{oc}−MCI			598
						Metoxuron			
[0.30]	[1.88]				4.54* [2.63]	Warwick, Qld, soil; pH 6.3; 0.01 M CaCl$_2$		BE	558
[−0.01]	[1.62]				4.07* [2.36]	Rutherglen, Vic., soil; pH 4.8; 0.01 M CaCl$_2$		BE	558
[−0.01]	[1.96]				1.86* [1.08]	Wagga, N.S.W., soil; pH 5.1; 0.01 M CaCl$_2$		BE	558
[0.08]	[1.87]				2.81* [1.63]	Turretfield, S.A., soil; pH 5.2; 0.01 M CaCl$_2$		BE	558
[−0.02]	[2.18]				1.09* [0.63]	Warracknabeal, Vic., soil; pH 8.0; 0.01 M CaCl$_2$		BE	558
[0.12]	[1.85]				3.20* [1.86]	Warracknabeal, Vic., soil; pH 8.4; 0.01 M CaCl$_2$		BE	558
[0.16]	[1.58]				6.62* [3.84]	Balkuling soil; pH 5.6; 0.01 M CaCl$_2$		BE	558

TABLE 8. Sorption coefficients for pesticides—Continued

log K_d log K_f^0 ($1/n$)	log K_{oc}	Sorbent composition (%)				Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
[−0.09]	[1.82]				2.14* [1.24]	Kojonup soil; pH 5.5; 0.01 M $CaCl_2$		BE	558
[−0.14]	[1.95]				1.42* [0.82]	Warranine soil; pH 6.5; 0.01 M $CaCl_2$		BE	558
[−0.05]	[1.47]				5.17* [3.00]	Yalanbee soil; pH 6.4; 0.01 M $CaCl_2$		BE	558
[−0.20]	[1.58]				2.85* [1.65]	Avondale soil; pH 5.9; 0.01 M $CaCl_2$		BE	558
[−0.18]	[1.86]				1.58* [0.92]	Badgingarra soil; pH 6.3; 0.01 M $CaCl_2$		BE	558
[−1.23]	[1.73]				0.19* [0.11]	Badgingarra soil; pH 6.3; 0.01 M $CaCl_2$		BE	558
[−0.02]	[1.75]				2.92* [1.69]	Beverley soil; 0.01 M $CaCl_2$		BE	558
[0.16]	[1.82]				3.78* [2.19]	Gabalong soil; pH 5.9; 0.01 M $CaCl_2$		BE	558
[−0.25]	[1.93]				1.13* [0.66]	Perth soil; pH 5.9; 0.01 M $CaCl_2$		BE	558
[−0.07]	[1.90]				1.86* [1.08]	Tammin soil; pH 5.9; 0.01 M $CaCl_2$		BE	558
	2.08					Correlation log K_{oc}–log S			564
Metribuzin (pK_a=0.99, Ref. 289)									
−0.24av (two soils)	[1.99]av	23.4	67.5	9.1	1.1* [0.64]	Taloka soil (10–20 cm); pH 5.2; CE=11 me/100 g; 0.01 M $CaCl_2$	20	BE	285
		22.0	62.2	15.8	0.90* [0.52]	Roxana soil (10–20 cm); pH 6.8; CE=19 me/100 g; 0.01 M $CaCl_2$	20	BE	285
−0.49av (two soils)	[1.96]av	24.2	62.0	13.8	0.70* [0.41]	Taloka soil (40–50 cm); pH 5.5; CE=13 me/100 g; 0.01 M $CaCl_2$	20	BE	285
		30.7	54.7	14.6	0.50* [0.29]	Roxana soil (40–50 cm); pH 7.1; CE=19 me/100 g; 0.01 M $CaCl_2$	20	BE	285
0.18° (~0.92)	1.59	15	71	14	3.8	Tanana Alaskan agric. soil (0–15 cm); pH 6.5; 0.01 M $CaCl_2$	5	BE	398
0.11° (~0.92)	1.53					Idem	28		398
0.51° (~0.92)	1.70	42	50	8	6.4	Beales Alaskan agric. soil (0–15 cm); pH 6.4; 0.01 M $CaCl_2$	5	BE	398
0.38° (~0.92)	1.58					Idem	28		398
−0.41° (~0.96)	1.75	26	63	11	0.69	Tanana Alaskan agric. soil (30–45 cm); pH 7.4; 0.01 M $CaCl_2$	5	BE	398
−0.44° (~0.96)	1.71					Idem	28		398
−0.48° (~0.96)	1.67	67	25	8	0.74	Beales Alaskan agric. soil (30–45 cm); pH 5.1; 0.01 M $CaCl_2$	5	BE	398
−0.52° (~0.96)	1.71					Idem	28		398
−0.04° (~0.92)	[2.06]	10.4	58.5	31.2	1.4* [0.81]	Dundee soil (0–10 cm); pH 6.65; CE=23.5 cmol/kg; 0.01 M $CaCl_2$	25	BE	288
−0.11° (~0.92)	[2.25]	10.5	59.6	29.8	0.75* [0.44]	Idem (10–35 cm); pH 6.50; CE=22.1 cmol/kg			288
−0.02° (~0.92)	[2.37]	10.5	59.6	29.8	0.70* [0.41]	Idem (35–80 cm); pH 6.45; CE=22.6 cmol/kg			288
0.01° (~0.92)	[2.37]	7.3	57.5	35.2	0.75* [0.44]	Idem (80–125 cm); pH 6.55; CE=25.3 cmol/kg			288
0.13° (~0.92)	[2.49]	2.2	51.6	46.3	0.75* [0.44]	Idem (125–150 cm); pH 6.95; CE=31.8 cmol/kg			288
−0.03° (~0.92)	[2.36]	5.6	55.2	39.3	0.70* [0.41]	Idem (150–175 cm); pH 7.20; CE=26.7 cmol/kg			288
−0.52° (0.90)	[1.71]	31	49	20	0.58	Dundee soil; pH 6.53; 0.01 M $CaCl_2$		BE	662
[0.40]	[2.24]	74.4	19.5	6.1	2.5* [1.45]	Aguadilla soil; CE=10 me/100 g; pH 7.4; 0.01 M $CaCl_2$		BE	304

TABLE 8. Sorption coefficients for pesticides—Continued

log K_d log K_f^0 (1/*n*)	log K_{oc}	Sorbent composition (%)				Other sorbent and solution data: prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
[0.57]	[2.69]	27.6	35.6	36.8	1.3* [0.75]	Aguirre soil; CE=14.3 me/100 g; pH 9.0; 0.01 M $\mathrm{CaCl_2}$		BE	304
[0.42]	[2.07]	16.6	13.0	70.4	3.9* [2.26]	Aguirre soil; CE=59.0 me/100 g; pH 8.4; 0.01 M $\mathrm{CaCl_2}$		BE	304
[0.50]	[2.23]	14.9	39.3	45.8	3.2* [1.86]	Alonso soil; CE=13.8 me/100 g; pH 5.1; 0.01 M $\mathrm{CaCl_2}$		BE	304
[−0.06]	[1.61]	49.2	28.8	22.0	3.7* [2.15]	Altura soil; CE=27.6 me/100 g; pH 8.0; 0.01 M $\mathrm{CaCl_2}$		BE	304
[0.87]	[2.14]	68.1	4.4	27.0	1.7* [0.99]	Bayamón soil; CE=5.0 me/100 g; pH 4.7; 0.01 M $\mathrm{CaCl_2}$		BE	304
[0.73]	[2.48]	56.4	8.0	35.9	3.1* [1.80]	Cabo Rojo soil; CE=9.0 me/100 g pH 4.3; 0.01 M $\mathrm{CaCl_2}$		BE	304
[1.16]	[1.84]	36.0	36.0	28.0	36.0* [20.9]	Caño Tiburones soil; pH 5.5; CE=86.0 me/100 g; 0.01 M $\mathrm{CaCl_2}$		BE	304
[0.93]	[2.89]	6.6	28.9	64.5	1.9* [1.10]	Catalina soil; CE=11.8 me/100 g; pH 4.7; 0.01 M $\mathrm{CaCl_2}$		BE	304
[0.52]	[2.53]	47.2	17.4	35.4	1.7* [0.99]	Cartagena soil; CE=36.1 me/100 g; pH 7.7; 0.01 M $\mathrm{CaCl_2}$		BE	304
[−0.06]	[1.85]	89.0	7.3	3.7	2.1* [1.22]	Cataño soil; CE=6.9 me/100 g; pH 7.9; 0.01 M $\mathrm{CaCl_2}$		BE	304
[0.50]	[2.34]	43.4	25.2	31.4	2.5* [1.45]	Cintrona soil; CE=25.0 me/100 g; pH 8.3; 0.01 M $\mathrm{CaCl_2}$		BE	304
[−0.01]	[1.93]	58.8	23.4	17.8	2.0* [1.16]	Cayaguá soil; CE=7.3 me/100 g; pH 5.2; 0.01 M $\mathrm{CaCl_2}$		BE	304
[0.45]	[2.00]	13.3	34.8	51.9	4.9* [2.84]	Cialitos soil; CE=18.6 me/100 g; pH 5.4; 0.01 M $\mathrm{CaCl_2}$		BE	304
[0.28]	[1.95]	22.7	37.4	39.9	3.7* [2.15]	Coloso soil; CE=23.0 me/100 g; pH 5.7; 0.01 M $\mathrm{CaCl_2}$		BE	304
[0.61]	[2.21]	26.0	18.6	55.4	4.3* [2.49]	Corozal soil; CE=17.0 me/100 g; pH 4.6; 0.01 M $\mathrm{CaCl_2}$		BE	304
[0.52]	[2.26]	23.4	24.8	51.8	3.2* [1.86]	Coto soil; CE=14.0 me/100 g; pH 7.7; 0.01 M $\mathrm{CaCl_2}$		BE	304
[0.13]	[2.42]	48.0	20.6	31.4	0.9* [0.52]	Estación soil; CE=10.0 me/100 g; pH 5.9; 0.01 M $\mathrm{CaCl_2}$		BE	304
[0.48]	[2.18]	39.1	29.7	32.2	3.4* [1.97]	Fe soil; CE=27.6 me/100 g; pH 7.5; 0.01 M $\mathrm{CaCl_2}$		BE	304
[0.40]	[2.12]	15.0	50.7	34.3	3.3* [1.91]	Fortuna soil; CE=23.3 me/100 g; pH 5.4; 0.01 M $\mathrm{CaCl_2}$		BE	304
[0.25]	[2.16]	15.5	32.5	52.0	2.1* [1.22]	Fraternidad soil; pH 6.3 CE=36.6 me/100 g; 0.01 M $\mathrm{CaCl_2}$		BE	304
[0.59]	[2.20]	11.1	23.8	65.1	4.2* [2.44]	Fraternidad soil (Lajas); pH 5.9; CE=58.0 me/100 g; 0.01 M $\mathrm{CaCl_2}$		BE	304
[0.63]	[2.19]	6.4	19.6	74.0	4.8* [2.78]	Guánica soil; CE=52.1 me/100 g; pH 8.1; 0.01 M $\mathrm{CaCl_2}$		BE	304
[0.13]	[2.33]	84.4	8.4	7.2	1.1* [0.64]	Humacao soil; CE=4.0 me/100 g; pH 6.3; 0.01 M $\mathrm{CaCl_2}$		BE	304
[0.21]	[2.22]	10.1	50.9	39.0	1.7* [0.99]	Humata soil; CE=10.1 me/100 g; pH 4.5; 0.01 M $\mathrm{CaCl_2}$		BE	304
[0.13]	[1.85]	26.6	53.5	20.9	3.3* [1.91]	Josefa soil; CE=16.8 me/100 g; pH 6.0; 0.01 M $\mathrm{CaCl_2}$		BE	304
[0.34]	[2.15]	15.2	41.6	43.2	2.7* [1.57]	Juncos soil; CE=13.4 me/100 g; pH 6.2; 0.01 M $\mathrm{CaCl_2}$		BE	304
[0.67]	[2.32]	19.9	33.4	46.7	3.9* [2.26]	Mabí soil; CE=55.2 me/100 g; pH 7.0; 0.01 M $\mathrm{CaCl_2}$		BE	304
[1.19]	[2.74]	22.7	40.7	36.6	4.9* [2.84]	Mabí soil; CE=31.0 me/100 g; pH 5.7; 0.01 M $\mathrm{CaCl_2}$		BE	304
[0.50]	[2.39]	76.0	13.4	10.6	2.2* [1.28]	Machete soil; CE=8.0 me/100 g; pH 6.5; 0.01 M $\mathrm{CaCl_2}$		BE	304
[0.73]	[2.59]	14.9	42.8	42.3	2.4* [1.39]	Mercedita soil; CE=19.9 me/100 g; pH 8.1; 0.01 M $\mathrm{CaCl_2}$		BE	304
[0.61]	[2.27]	26.3	27.7	46.0	3.8* [2.20]	Moca soil; CE=31.0 me/100 g; pH 5.8; 0.01 M $\mathrm{CaCl_2}$		BE	304
[−0.28]	[1.44]	28.0	47.0	25.0	3.3*	Múcara soil; CE=19.6 me/100 g;		BE	304

TABLE 8. Sorption coefficients for pesticides—Continued

log K_d log K_f^0 (1/n)	log K_{oc}	Sorbent composition (%)				Other sorbent and solution data: prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
					[1.91]	pH 5.8; 0.01 M $CaCl_2$			
[0.48]	[1.99]	22.0	49.2	28.0	5.3* [3.07]	Nipe soil; CE=11.9 me/100 g; pH 5.7; 0.01 M $CaCl_2$		BE	304
[0.09]	[2.03]	59.4	28.2	12.4	2.0* [1.16]	Pandura soil; CE=7.7 me/100 g; pH 5.7; 0.01 M $CaCl_2$		BE	304
[0.55]	[2.24]	13.4	43.6	43.0	3.5* [2.03]	Río Piedras soil; pH 4.9 CE=11.5 me/100 g; 0.01 M $CaCl_2$		BE	304
[0.52]	[2.17]	39.0	24.6	36.4	3.9* [2.26]	Sabana Seca soil; pH 7.4; CE=23.0 me/100 g; 0.01 M $CaCl_2$		BE	304
[0.82]	[2.37]	47.0	24.4	28.6	4.9* [2.84]	San Antón soil; pH 7.4; CE=28.0 me/100 g; 0.01 M $CaCl_2$		BE	304
[0.55]	[2.46]	57.0	18.6	24.4	2.1* [1.22]	Santa Isabel soil; pH 7.4; CE=28.0 me/100 g; 0.01 M $CaCl_2$		BE	304
[0.67]	[1.89]	46.0	20.0	34.0	10.4* [6.03]	Soller soil; CE=53.0 me/100 g; pH 6.9; 0.01 M $CaCl_2$		BE	304
[0.48]	[2.57]	73.4	19.4	7.2	1.4* [0.81]	Talante soil; CE=4.0 me/100 g; pH 5.1; 0.01 M $CaCl_2$		BE	304
[0.90]	[2.42]	35.0	24.6	40.4	5.1* [2.96]	Toa soil; CE=36.0 me/100 g; pH 8.0; 0.01 M $CaCl_2$		BE	304
[−0.20]	[1.74]	41.5	38.3	20.2	2.0* [1.16]	Toa soil; CE=13.0 me/100 g; pH 5.3; 0.01 M $CaCl_2$		BE	304
[−1.00]	[1.46]	60.9	25.1	14.0	0.6* [0.35]	Toa soil; CE=8.0 me/100 g; pH 6.0; 0.01 M $CaCl_2$		BE	304
[0.45]	[2.14]	73.7	12.6	13.7	3.5* [2.03]	Vega Alta soil; pH 5.0; CE=5.6 me/100 g; 0.01 M $CaCl_2$		BE	304
[−0.20]	[1.68]	45.2	36.8	18.0	2.3* [1.33]	Vía soil; CE=39.9 me/100 g; pH 5.1; 0.01 M $CaCl_2$		BE	304
[0.31]	[2.21]	62.4	19.6	18.0	2.2* [1.28]	Viví soil; CE=14.0 me/100 g; pH 4.8;0.01 M $CaCl_2$		BE	304
[0.45]	[2.03]	15.0	23.4	61.6	4.5* [2.61]	Voladura soil; pH 4.3; CE=17.7 me/100 g; 0.01 M $CaCl_2$		BE	304
−0.21	[1.74]			16.2	1.11	Conventional farm soil; pH 5.42; 0.004 M$CaSO_4$		BE	646
−0.25	[1.75]			19.7	1.00	Idem; pH 5.35; 0.004 M $CaSO_4$			646
−0.51	[1.68]			24.7	0.64	Idem; pH 7.12; 0.004 M $CaSO_4$			646
0.11	[1.84]			16.5	1.85	Low-input farm soil; pH 5.53; 0.004 M$CaSO_4$		BE	646
−0.03	[1.87]			16.6	1.26	Idem; pH 5.47; 0.004 M $CaSO_4$			646
−0.18	[1.88]			19.1	0.86	Idem; pH 6.32; 0.004 M $CaSO_4$			646
−0.49	[1.49]		20	3	1.8* [1.04]	Calcareous soil; pH 7.4; 0.01 M $CaCl_2$	19	BE	503
0.85	[2.70]	16		32	2.4* [1.39]	Woodburn soil; pH 4.6; CE=13.2 cmol/kg		BE	290
0.38	[2.24]	57		19	2.4* [1.39]	Chealis soil; pH 6.0; CE=19.5 cmol/kg		BE	290
0.53	[2.02]	30		19	5.5* [3.19]	Ontko soil; pH 6.2; CE=44.2 cmol/kg		BE	290
0.33	[2.56]	40		38	1.0* [0.58]	Barshaw soil; pH 6.2; CE=35.1 cmol/kg		BE	290
0.05	[2.24]	70		17	1.1* [0.64]	Crooked soil; pH 8.2; CE=13.7 cmol/kg		BE	290
−0.68	[1.86]	80	15	5	0.5* [0.29]	Augusta soil; SA(E)=3.3 m^2/g; pH 5.7; CE=3.2 me/100 g	28	BE	291
−1.19	[1.35]	89	9	2	0.5* [0.29]	Norfolk soil; SA(E)=4.4 m^2/g; pH 5.4; CE=2.3 me/100 g	28	BE	291
−0.13	[2.02]	72	23	5	1.2* [0.70]	Goldsboro soil; SA(E)=7.0 m^2/g; pH 5.3; CE=3.3 me/100 g	28	BE	291
−0.55	[1.54]	82	10	8	1.4* [0.81]	Appling soil; SA(E)=12.8 m^2/g; pH 6.8; CE=6.9 me/100 g	28	BE	291
−0.12	[1.72]	70	22	8	2.5* [1.45]	Lynchburg soil; SA(E)=13.6 m^2/g; pH 5.5; CE=6.6 me/100 g	28	BE	291
−0.66	[1.34]	76	16	8	1.7* [0.99]	Cecil soil; SA(E)=16.3 m^2/g; pH 5.4; CE=3.1 me/100 g	28	BE	291

TABLE 8. Sorption coefficients for pesticides—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%)				Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
−0.14	[1.87]	26	64	10	1.7* [0.99]	Rains soil; SA(E)=18.8 m^2/g; pH 6.0; CE=7.1 me/100 g	28	BE	291
0.15	[1.74]	61	26	12	4.4* [2.55]	Portsmouth soil; SA(E)=20.6 m^2/g; pH 5.4; CE=10.6 me/100 g	28	BE	291
0.61	[1.91]	52	36	13	8.7* [5.05]	Cape Fear soil; SA(E)=77.2 m^2/g; pH 5.1; CE=10.3 me/100 g	28	BE	291
0.09	[2.03]	6	36	58	1.98* [1.15]	Alligator soil; pH 4.8	27	BE	117
−0.57	[1.79]	69	20	11	0.75* [0.44]	Bosket soil; pH 6.7	27	BE	117
−0.30	[1.82]	25	43	36	1.30* [0.75]	Bosket soil; pH 6.8	27	BE	117
−0.49		59	32	9	0.10* [0.06]	Bosket soil; pH 7.7	27	BE	117
−0.43	[1.90]	22	61	17	0.81* [0.47]	Brittain soil; pH 4.8	27	BE	117
0.08	[2.14]	19	50	30	1.52* [0.88]	Dundee soil; pH 6.1	27	BE	117
−0.06	[1.87]	44	36	20	2.02* [1.17]	Dundee soil; pH 7.1	27	BE	117
0.00	[2.02]	26	55	29	1.65* [0.96]	Dundee soil; pH 7.2	27	BE	117
0.12	[2.00]	6	40	54	2.26* [1.31]	Dowling soil; pH 6.7	27	BE	117
−0.11	[2.24]	5	49	46	0.78* [0.45]	Forestdale soil; pH 5.6	27	BE	117
−0.04	[1.90]	6	63	31	2.01* [1.17]	Forestdale soil; pH 5.8	27	BE	117
−0.16	[1.61]	29	36	35	2.93* [1.70]	Forestdale soil; pH 6.2	27	BE	117
−0.16	[1.94]	34	48	18	1.38* [0.80]	Pearson soil; pH 5.5	27	BE	117
−0.28	[2.05]	25	45	30	0.81* [0.47]	Pearson soil; pH 6.8	27	BE	117
0.53	[2.15]	4	25	71	4.20* [2.44]	Sharkey soil; pH 5.5	27	BE	117
−0.15	[1.89]	22	46	32	1.55* [0.90]	Tunica soil; pH 6.4	27	BE	117
	1.98					Soil; experimental (literature)			217
	1.94					Correlation $\log K_{oc}-\log S$			564
	1.79					Correlation $\log K_{oc}$−MCI			578
						Mirex			
	6.45					Aldrich humic acid (1.1 mg/L DOC); pH 6.7		GP	417
[4.71]	6.1				4.1	Lake Ontario sediment trap material		FM	49
	3.76					Soil; experimental (literature)			217
	5.9					Correlation $\log K_{oc}-\log K_{ow}$(96)			49
	3.08					Correlation $\log K_{oc}-\log S$			564
	5.67					Correlation $\log K_{oc}$−MCI			598
						Molinate			
0.57	1.95	18.9	26.3	54.8	4.24	Tsukuba soil; pH 6.5; 0.01 M $CaCl_2$	25	BE	642
0.33° (0.85)						Idem	25	BE	642
0.04	1.90	23.1	15.4	61.5	1.35	Kanuma soil; pH 5.7; 0.01 M $CaCl_2$	25	BE	642
−0.002° (0.99)						Idem	25	BE	642

TABLE 8. Sorption coefficients for pesticides—Continued

log K_d log K_f^0 (1/n)	log K_{oc}	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
	2.04					Correlation log K_{oc}−log S			564
	2.46					Correlation log K_{oc}−MCI			598
						Monolinuron			
[0.39]	[1.97]				4.54* [2.63]	Warwick, Qld, soil; pH 6.3; 0.01 M $CaCl_2$		BE	558
[0.10]	[1.73]				4.07* [2.36]	Rutherglen, Vic., soil; pH 4.8; 0.01 M $CaCl_2$		BE	558
[−0.19]	[1.78]				1.86* [1.08]	Wagga, N.S.W., soil; pH 5.1; 0.01 M $CaCl_2$		BE	558
[−0.12]	[1.67]				2.81* [1.63]	Turretfield, S.A., soil; pH 5.2; 0.01 M $CaCl_2$		BE	558
[−0.23]	[1.97]				1.09* [0.63]	Warracknabeal, Vic., soil; pH 8.0; 0.01 M $CaCl_2$		BE	558
[0.03]	[1.76]				3.20* [1.86]	Warracknabeal, Vic., soil; pH 8.4; 0.01 M $CaCl_2$		BE	558
[0.00]	[1.42]				6.62* [3.84]	Balkuling soil; pH 5.6; 0.01 M $CaCl_2$		BE	558
[−0.18]	[1.73]				2.14* [1.24]	Kojonup soil; pH 5.5; 0.01 M $CaCl_2$		BE	558
[−0.16]	[1.93]				1.42* [0.82]	Warranine soil; pH 6.5; 0.01 M $CaCl_2$		BE	558
[−0.02]	[1.50]				5.17* [3.00]	Yalanbee soil; pH 6.4; 0.01 M $CaCl_2$		BE	558
[−0.06]	[1.72]				2.85* [1.65]	Avondale soil; pH 5.9; 0.01 M $CaCl_2$		BE	558
[−0.06]	[1.98]				1.58* [0.92]	Badgingarra soil; pH 6.3; 0.01 M $CaCl_2$		BE	558
[−1.34]	[1.87]				0.19* [0.11]	Badgingarra soil; pH 6.3; 0.01 M $CaCl_2$		BE	558
[0.03]	[1.80]				2.92* [1.69]	Beverley soil; 0.01 M $CaCl_2$		BE	558
[0.16]	[1.82]				3.78* [2.19]	Gabalong soil; pH 5.9; 0.01 M $CaCl_2$		BE	558
[−0.26]	[1.92]				1.13* [0.66]	Perth soil; pH 5.9; 0.01 M $CaCl_2$		BE	558
[0.03]	[2.00]				1.86* [1.08]	Tammin soil; pH 5.9; 0.01 M $CaCl_2$		BE	558
1.51° (0.69)		47.5	33.2	20.3	10.5* [6.09]	Melfort soil; pH 5.9	25	BE	260
0.74° (0.80)		53.3	27.5	19.2	6.46* [3.75]	Weyburn soil; pH 6.5	25	BE	260
0.56° (0.80)		5.3	25.3	69.5	4.15* [2.41]	Regina soil; pH 7.7	25	BE	260
0.76° (0.69)		69.3	12.3	18.5	4.07* [2.36]	Indian Head soil; pH 7.8	25	BE	260
0.08° (0.84)		81.6	10.4	8.0	1.77* [1.03]	Asquith soil; pH 7.5	25	BE	260
0.55° (0.79)				75	1.3	Eurosol-1; c; pH 5.1; 0.01 M $CaCl_2$		BE	583
0.07° (1.37)				22.6	3.7	Eurosol-2; sil; pH 7.4; 0.01 M $CaCl_2$		BE	583
0.25° (1.09)	1.71			17.0	3.45	Eurosol-3; l; pH 5.2; 0.01 M $CaCl_2$		BE	583
−0.06° (0.82)				20.3	1.55	Eurosol-4; si; pH 6.5; 0.01 M $CaCl_2$		BE	583
1.41° (0.83)				6.0	9.25	Eurosol-5; ls; pH 3.2; 0.01 M $CaCl_2$		BE	583
1.91°		7	10	10	36.5	Sunway farm light peat; pH 5.2; CE=60 me/100 g	22	BE	259
1.40°		45.5	15.9	6.6	12.0	Grat House E.H.F. soil; pH 6.3; CE=18 me/100 g	22	BE	259

TABLE 8. Sorption coefficients for pesticides—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%)				Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
1.32°		23	24.4	28.6	11.7	Toll Farm heavy peat; pH 7.4; CE=41 me/100 g	22	BE	259
1.04°		34.0	33.4	32.6	3.69	Trawscoed E.H.F. soil; pH 6.2; CE=12 me/100 g	22	BE	259
0.98°		66.0	18.4	15.6	1.93	Weed Res. soil; pH 7.1; CE=11 me/100 g	22	BE	259
0.91°		36.0	40.4	23.6	1.76	Rosemaunde E.H.F. soil; pH 6.7; CE=14 me/100 g	22	BE	259
0.39° (0.50)				9.8	0.1* [0.06]	Soil; s, mesic; pH 7.0; SA(W)=14.8 m^2/g		BE	72
0.52° (0.86)				15.0	1.0* [0.58]	Soil; s, mixed mesic; pH 7.6; SA(W)=18.1 m^2/g		BE	72
0.51° (0.60)				13.0	1.4* [0.81]	Soil; s, mixed, mesic; pH 7.3; SA(W)=30.3 m^2/g		BE	72
0.69° (0.81)				6.8	1.5* [0.87]	Soil; s, mixed, mesic; pH 7.1; SA(W)=15.2 m^2/g		BE	72
0.53° (0.91)	[2.56]			31.5	1.6* [0.93]	Soil; s, c, mesic; pH 6.6; SA(W)=72.4 m^2/g		BE	72
0.62° (0.82)				10.6	1.9* [1.10]	Soil; s, mesic; pH 4.2; SA(W)=38.6 m^2/g		BE	72
0.80° (0.87)				18.3	1.2* [0.70]	Soil; s, mesic; pH 6.9; SA(W)=55.8 m^2/g		BE	72
1.10° (0.90)	[2.68]			4.5	4.6* [2.67]	Soil; s, mesic; pH 3.7; SA(W)=22.4 m^2/g		BE	72
	2.30					Soil; experimental (literature)			217
	2.45av					10 soils (literature)			87
	1.21					Correlation $\log K_{oc}-\log K_{ow}$			96
	2.36					Correlation $\log K_{oc}-\log S$			96
	2.08					Correlation $\log K_{oc}-\log S$(mp)			96
	2.11					Correlation $\log K_{oc}-\log S$			564
						Monuron			
1.38° (0.48)				100		Na–montmorillonite (1–0.2 μm); pH 6.80; CE=87.0 me/100 g	25	BE	250
2.00° (0.98)				100		H–montmorillonite (1–0.2 μm); pH 3.35; CE=73.5 me/100 g	25	BE	250
1.51° (0.80)				100		H–montmorillonite; pH 3.6		BE	212
1.38° (0.80)				100		Na–montmorillonite; pH 7.9		BE	212
1.38° (0.80)				100		Ca–montmorillonite; pH 7.9		BE	212
1.36° (0.80)				100		Mg–montmorillonite; pH 8.2		BE	212
0.88				100		Montmorillonite-H(Al) (<0.2 μm); pH 3.5	3.5	BE	244
1.46				100		Bentonite–H(Al) (<0.2 μm): pH 3.5; CE=0.72 me/g	3.5	BE	244
1.36				100		Bentonite–Al(H) (<0.2 μm)	3.5	BE	244
1.00				100		Bentonite–Na (<0.2 μm); pH 6.7; CE=0.83 me/g; SA(E)=758 m^2/g Salt conc.=0.1 N	3.5	BE	244
1.11				100		Bentonite–Ca (<0.2 μm); pH 6.7; CE=0.88 me/g; Salt conc.=0.1 N	3.5	BE	244
1.31				100		Bentonite–Mg (<0.2 μm); pH 6.7; CE=0.84 me/g; Salt conc.=0.1 N	3.5	BE	244
1.01av				100		Bentonite–Na (<0.2 μm); pH 6.7; CE=0.83 me/g; Salt conc.=0.005–1 N	26.5	BE	244
1.45				100		Idem; Salt conc.=3 N	26.5	BE	244
1.12av				100		Bentonite–Ca (<0.2 μm); pH 6.7; CE=0.88 me/g; Salt conc.=0.005–1 N	26.5	BE	244

TABLE 8. Sorption coefficients for pesticides—Continued

log K_d log K_f^0 $(1/n)$	log K_{oc}	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data: prediction procedure	Temp. (°C)	Meth.	Ref.
1.65				100		Idem; Salt conc. = 3 N	26.5	BE	244
1.17				100		Bentonite–Mg (<0.2 μm); pH 6.7; CE = 0.84 me/g; Salt conc. = 0.1 N	26.5	BE	244
1.21° (0.80)						Bentonite; 0.1 MCaCl$_2$	22	BE	144
1.65				100		Mississippi bentonite; pH 8.5	0	BE	251
0.64						Idem	50		251
1.61	[1.96]				77* [44.7]	Houghton muck; pH 5.6	0	BE	251
1.66	[2.01]					Idem	50		251
	[1.70]av			1.09-*	4.25*	4 soils; slit loam; pH 6.1–7.5 0.01 M CaCl$_2$	20	BE	120
[0.42]	[2.00]				4.54* [2.63]	Warwick, Qld, soil; pH 6.3; 0.01 M CaCl$_2$		BE	558
[0.01]	[1.64]				4.07* [2.36]	Rutherglen, Vic., soil; pH 4.8; 0.01 M CaCl$_2$		BE	558
[−0.20]	[1.77]				1.86* [1.08]	Wagga, N.S.W., soil; pH 5.1; 0.01 M CaCl$_2$		BE	558
[−0.13]	[1.66]				2.81* [1.63]	Turretfield, S.A., soil; pH 5.2; 0.01 M CaCl$_2$		BE	558
[−0.35]	[1.85]				1.09* [0.63]	Warracknabeal, Vic., soil; pH 8.0; 0.01 M CaCl$_2$		BE	558
[0.05]	[1.78]				3.20* [1.86]	Warracknabeal, Vic., soil; pH 8.4; 0.01 M CaCl$_2$		BE	558
[−0.03]	[1.39]				6.62* [3.84]	Balkuling soil; pH 5.6; 0.01 M CaCl$_2$		BE	558
[−0.24]	[1.67]				2.14* [1.24]	Kojonup soil; pH 5.5; 0.01 M CaCl$_2$		BE	558
[−0.19]	[1.90]				1.42* [0.82]	Warranine soil; pH 6.5; 0.01 M CaCl$_2$		BE	558
[−0.08]	[1.44]				5.17* [3.00]	Yalanbee soil; pH 6.4; 0.01 M CaCl$_2$		BE	558
[−0.20]	[1.58]				2.85* [1.65]	Avondale soil; pH 5.9; 0.01 M CaCl$_2$		BE	558
[−0.18]	[1.86]				1.58* [0.92]	Badgingarra soil; pH 6.3; 0.01 M CaCl$_2$		BE	558
[−1.11]	[1.85]				0.19* [0.11]	Badgingarra soil; pH 6.3; 0.01 M CaCl$_2$		BE	558
[0.00]	[1.77]				2.92* [1.69]	Beverly soil; 0.01 M CaCl$_2$		BE	558
[0.07]	[1.73]				3.78* [2.19]	Gabalong soil; pH 5.9; 0.01 M CaCl$_2$		BE	558
[−0.29]	[1.89]				1.13* [0.66]	Perth soil; pH 5.9; 0.01 M CaCl$_2$		BE	558
[−0.15]	[1.82]				1.86* [1.08]	Tammin soil; pH 5.9; 0.01 M CaCl$_2$		BE	558
1.52° (0.67)		47.5	33.2	20.3	10.5* [6.09]	Melfort soil; pH 5.9	25	BE	260
0.76° (0.80)		53.3	27.5	19.2	6.46* [3.75]	Weybum soil; pH 6.5	25	BE	260
0.51° (0.84)		5.3	25.3	69.5	4.15* [2.41]	Regina soil; pH 7.7	25	BE	260
0.71° (0.72)		69.3	12.3	18.5	4.07* [2.36]	Indian Head soil; pH 7.8	25	BE	260
0.00° (1.04)	[1.97]	81.6	10.4	8.0	1.77* [1.03]	Asquith soil; pH 7.5	25	BE	260
0.69° (0.90)	2.58			75	1.3	Eurosol-1; c; pH 5.1; 0.01 M CaCl$_2$		BE	583
0.33° (0.86)				22.6	3.7	Eurosol-2; sil; pH 7.4; 0.01 M CaCl$_2$		BE	583
0.39° (0.81)				17.0	3.45	Eurosol-3; l; pH 5.2; 0.01 M CaCl$_2$		BE	583

TABLE 8. Sorption coefficients for pesticides—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%) Sand	 Silt	 Clay	 OC	Other sorbent and solution data: prediction procedure	Temp. (°C)	Meth.	Ref.
−0.04° (0.80)				20.3	1.55	Eurosol-4; si; pH 6.5; 0.01 M $CaCl_2$		BE	583
1.34° (0.85)				6.0	9.25	Eurosol-5; ls; pH 3.2; 0.01 M $CaCl_2$		BE	583
[1.31]	[1.75]				63* [36.5]	Mesic peat (acid treated); 0.01 M $CaCl_2$		BE	477
1.88°		7	10	10	36.5	Sunway farm light peat; pH 5.2; CE=60 me/100 g	22	BE	259
1.42°		45.5	15.9	6.6	12.0	Great House E.H.F. soil; pH 6.3; CE=18 me/100 g	22	BE	259
1.34°		23	24.4	28.6	11.7	Toll Farm heavy peat; pH 7.4; CE=41 me/100 g	22	BE	259
0.86°		34.0	33.4	32.6	3.69	Trawscoed E.H.F. soil; pH 6.2; CE=12 me/100g	22	BE	259
0.74°		66.6	18.4	15.6	1.93	Weed Res. soil; pH 7.1; pH 6.7; CE=11 me/100 g	22	BE	259
0.68°		36.0	40.4	23.6	1.76	Rosemaunde E.H.F. soil; pH 6.7; CE=14 me/100 g	22	BE	259
1.37° (0.83)		45.5	15.9	6.6	12	Great House E.H.F. soil; pH 6.3; CE=18 me/100 g; 0.1 M $CaCl_2$	22	BE	144
0.78° (0.74)		66.0	18.4	15.6	1.93	Weed Res. Orgn. soil; pH 7.1; CE=11 me/100 g; 0.1 M $CaCl_2$	22	BE	144
1.96	[2.32]				76* [44]	OM from peat soil; 0.1 M $CaCl_2$	22	BE	144
0.04° (0.70)				18	3.3* [1.91]	Lakeland sl soil; pH 6.2; CE=2.9 me/100 g; 0.01 M $CaCl_2$	26	BE	633
0.28° (0.71)				43	1.1.9* [1.10]	Wehadkee sil soil; pH 5.6; CE=10.2 me/100 g; 0.01 M $CaCl_2$	26	BE	633
0.52° (0.84)				38	4.4* [2.55]	Chillum sil soil; pH 4.6; CE=7.6 me/100 g; 0.01 M $CaCl_2$	26	BE	633
0.60° (0.76)				48	4.3* [2.49]	Hagerstown sicl soil; pH 5.5; CE=12.5 me/100 g; 0.01 M $CaCl_2$	26	BE	633
0.42° (0.68)					2.1* [1.22]	Keyport sil soil; pH 5.4; average particle size=5.6 μm		BE	641
−0.40° (1.2)					0.7* [0.41]	Cecil ls soil; pH 5.8; average particle size=10.5 μm		BE	641
	2.00					Cyanopropyl column; ring test		RPLC	581
	2.00					Soil; experimental (literature)			217
	2.26av					18 soils (literature)			87
	1.07, 1.73					Correlation $\log K_{oc}$–$\log K_{ow}$			96
	2.58					Correlation $\log K_{oc}$–log S			96
	1.52					Correlation $\log K_{oc}$–log S(mp)			96
	2.34					Correlation $\log K_{oc}$–log S			564
						Napropamide			
0.30av	2.56av				0.55av	Tujunga agricul. ls soil; 36 samples; 0.01 N $CaCl_2$	20	BE	276
0.28av	2.52av				0.57av	Idem; 36 soil columns; 8 me/L $CaSO_4$ irrigation solut.		MD	276
−0.57				7.5	0.06	Mivtachim agric. surface soil; pH 8.5; 3.5% $CaCO_3$		BE	277
0.15	2.54			13.7	0.40	Bet Degan I agric. surface soil; pH 7.9; 2.3% $CaCO_3$		BE	277
0.28	2.54			23.1	0.55	Gilat agric. surface soil; pH 7.8; 12.9% $CaCO_3$		BE	277
0.47	2.47			42.5	1.01	Bet Degan II agric. surface soil; pH 7.8; 2.6% $CaCO_3$		BE	277
0.37	2.51			70.0	0.72	Shefer agric. surface soil; pH 7.2; 0.2% $CaCO_3$		BE	277
0.47	2.40			70.0	1.18	Neve Yaar agric. surface soil; pH 7.7; 8.9%$CaCO_3$		BE	277

TABLE 8. Sorption coefficients for pesticides—Continued

log K_d log K_f^0 (1/*n*)	log K_{oc}	Sorbent composition (%)				Other sorbent and solution data: prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
0.07	[2.62]				0.28	Pachappa s1 soil; pH 7.4; 0.005 M $CaCl_2$	20	BE	529
0.03	[2.59]					Idem	30		529
1.41° (1.04)	[3.32]	93	4	3	2.1* [1.22]	Cobb s+2% muck; pH 5.3; CE=9.0 me/100 g;		BE	278
0.94° (1.0)	[2.92]	96	3	1	1.8* [1.04]	Cobb s+1% muck; pH 5.6; CE=7.8 me/100 g		BE	278
0.95° (0.83)		26	28	46	1.6* [0.93]	Port soil; pH 6.4; CE=14.6 me/100 g;		BE	278
0.55° (0.84)		60	20	20	1.2* [0.70]	Teller soil; pH 6.6; CE=7.3 me/100 g;		BE	278
0.30° (0.84)		87	4	9	0.6* [0.35]	Cobb soil; pH 6.0; CE=3.0 me/100 g		BE	278
1.36	2.40			35	9.1	Eversham c soil; (0–0.02 m depth); pH 7.8. 0.005 M $CaCl_2$		BE	137
1.25	2.38			>35	7.3	Idem (0.02–0.22 m depth)			137
[0.06]	2.66		14.2	4.5	0.25	Tujunga soil; pH 6.7		BE	423
[1.73]	2.88		33.4	50.4	7.10	Bermeo soil; pH 5.3		BE	423
−0.05	2.95			11.2	0.17* [0.10]	Netanya agricult. surface soil	25	BE	641
−0.33	2.26			6.9	0.45* [0.26]	Mivtahim agricult. surface soil	25	BE	563
0.50	2.67			63.1	1.18* [0.68]	Golan agricult. surface soil 25	25	BE	563
0.27	2.40			23.8	1.25* [0.73]	Gilat agricult. surface soil	25	BE	563
0.46	2.54			72.5	1.42* [0.82]	Shefer agricult. surface soil	25	BE	563
0.35	2.42			10.6	1.45* [0.84]	Bet Degan agricult. surface soil	25	BE	563
0.64	2.43			71.2	2.82* [1.64]	Neve Yaar agricult. surface soil	25	BE	563
0.89	2.36			76.2	5.82* [3.38]	Malkiya agricult. surface soil	25	BE	563
0.88	2.63				3.08* [1.79]	Kinneret Lake sediment	25	BE	563
1.49	2.83			60.5	7.85* [4.55]	Kinneret A Lake sediment	25	BE	563
1.44	2.81			63.2	7.43* [4.31]	Kinneret F Lake sediment	25	BE	563
1.33	2.92			63.8	4.39* [2.55]	Kinneret G Lake sediment	25	BE	563
	3.21					Peat humic acid		ED	423
	2.98av					Soil humic acid		ED	423
	1.69av					Soil fulvic acid		ED	423
	2.83					Soil; experimental (literature)			217
	2.94av					33 soils (literature)			87
	2.62av					36 literature data			562
	2.61					Correlation log K_{oc}−log S			564
						Neburon			
2.82°		7	10	10	36.5	Sunway farm light peat; pH 5.2; CE=60 me/100 g	22	BE	259
2.51°		45.5	15.9	6.6	12.0	Grat House E.H.F. soil; pH 6.3; CE=18 me/100 g	22	BE	259
2.38°		23	24.4	28.6	11.7	Toll Farm heavy peat; pH 7.4; CE=41 me/100 g	22	BE	259
2.14°		34.0	33.4	32.6	3.69	Trawscoed E.H.F. soil; pH 6.2; CE=12 me/100 g	22	BE	259
1.86°		66.0	18.4	15.6	1.93	Weed Res. soil; pH 7.1; CE=11 me/100 g	22	BE	259
1.76°		36.0	40.4	23.6	1.76	Rosemaunde E.H.F. soil; pH 6.7; CE=14 me/100 g	22	BE	259

TABLE 8. Sorption coefficients for pesticides—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
	3.36					Soil; experimental (literature)			217
	3.49av					5 soils (literature)			87
	3.26					Correlation $\log K_{oc}-\log S$			564
	2.95					Correlation $\log K_{oc}$–MCI			598
						Nitralin			
1.70	[3.33]	6	71	23	4.0* [2.32]	Plano soil (soil/solut.=1 g/100 mL) pH 6.3; CE=20 me/100 g	25	BE	351
1.58	[3.22]	6	71	23	4.0* [2.32]	Idem (soil/solut.=2 g/100 mL)	25	BE	351
1.63	[3.27]	6	71	23	4.0* [2.32]	Idem (soil/solut.=4 g/100 mL)	25	BE	351
2.33	[3.97]	6	71	23	4.0* [2.32]	Idem (soil/solut.=2 g/100 mL)	5	BE	351
	2.98					Soil; experimental (literature)			217
	3.76					Correlation $\log K_{oc}-\log S$			564
						Nitrapyrin			
	[2.24]av				1.35*, 5.92*	2 Cottenham sl soils; ph 7.2; 6.8, 0.01 M $CaCl_2$	20	BE	120
	2.66av	38	48	14	0.68	Commerce soil; pH 6.7		BE	575
	(three	56	30	14	1.12	Tracy soil; pH 6.2		BE	575
	soils)	12	56	32	2.01	Catlin soil; pH 6.2		BE	575
	2.62					Soil; experimental (literature)			217
	2.87					C18 column		RPLC	573
	2.76					Correlation $\log K_{oc}-\log S$			564
						Oxadiazon			
3.24	[3.51]				94* [54.5]	OM from peaty muck (Histosol) soil; pH 5.5	24	BE	121
	3.51					Soil; experimental (literature)			217
	3.72					Correlation $\log K_{oc}-\log S$			564
						Oxamyl			
−1.30	1.90			7.5	0.11* [0.06]	Mivtahim agricult. surface soil	25	BE	563
−0.64	1.53			63.1	1.18* [0.68]	Golan agricult. surface soil	25	BE	563
−0.82	1.44			23.1	0.95* [0.55]	Gilat agricult. surface soil	25	BE	563
−0.58	1.56			70.0	1.23* [0.71]	Shefer agricult. surface soil	25	BE	563
−1.10	1.31			13.7	0.68* [0.39]	Bet Degan agricult. surface soil	25	BE	563
−0.51	1.42			70.0	2.03* [1.18]	Neve Yaar agricult. surface soil	25	BE	563
−0.62	0.85			76.2	5.82* [3.38]	Malkiya agricult. surface soil	25	BE	563
−0.39	0.95			60.5	7.85* [4.55]	Kinneret A sediment	25	BE	563
−0.39	0.98			63.2	7.43* [4.31]	Kinneret F sediment	25	BE	563
−0.29	1.30			63.8	4.39* [2.55]	Kinneret G sediment	25	BE	563
	[0.71]av				1.35*, 5.92*	2 Cottenham sl soils; pH 7.2; 6.8; 0.01 M $CaCl_2$	20	BE	120
	0.60					Correlation $\log K_{oc}-\log S$			564
						Paraoxon			
1.73° (1.16)				100		Na–montmorillonite (<2 μm)	20	BE	246
1.63° (1.45)				100		Ca–montmorillonite (<2 μm)	20	BE	246

TABLE 8. Sorption coefficients for pesticides—Continued

log K_d log K_f^0 (1/n)	log K_{oc}	Sorbent composition (%) Sand	 Silt	 Clay	 OC	Other sorbent and solution data: prediction procedure	Temp. (°C)	Meth.	Ref.
1.91° (1.38)				100		Fe–montmorillonite (< 2μm)	20	BE	246
						Paraquat			
4.86						Li–montmorillonite (<0:15 μm)		BE	650
3.85°					45.2	Acid light peat; pH 5.3	22	BE	306
3.70°					33.1	Alkaline light peat; pH 7.2	22	BE	306
3.70°					44.0	Lightpeat; pH 6.8	22	BE	306
3.97°					53.3	Fine sphagnum peat; pH 3.3	22	BE	306
3.49°					44.0	Top 2.5 cm below turf layer; pH 5.7	22	BE	306
3.52°					27.2	2.5–5 cm below turf layer; pH 4.4	22	BE	306
3.57°						Grass	22	BE	306
	4.62°*					Humic acid from peat soil		ED	306
	3.42°*					Lignin	22	BE	306
	1.81°*					Whatman cellulose powder	22	BE	306
3.00°		67	18	15	2.5* [1.45]	Begbroke soil; pH 7.3; CE=11.8 me/100 g	22	BE	306
4.78*						Fuller's earth (Ca–montmorillonite) CE=84–88 me/100 g	22	BE	306
	4.19					Soil; experimental (literature)			217
	0.30					Correlation log K_{oc}–log S			564
						Parathion			
2.10* (1.04)				100		Na–montmorillonite (<2 μm)	20	BE	246
2.36° (1.51)				100		Ca–montmorollonite (<2 μm)	20	BE	246
2.89° (1.19)				100		Fe–montmorillonite (<2 μm)	20	BE	246
1.94° (1.04)				100		Ca–illite (<2 mm) (3.33E-3 g/mL)	20	BE	486
1.90° (0.98)						Idem (3.33E-2 g/mL)			486
1.89° (0.97)						Idem (1.00E-1 g/mL)			486
1.55° (0.90)	[3.19]				3.9° [2.26]	Bondhead sl soil (6.67E-3 g/mL)	20	BE	486
1.52° (0.88)	[3.15]					Idem (1.67E-2 g/mL)			486
1.53° (0.83)						Idem (3.33E-2 g/mL)			486
1.51° (0.84)						Idem (6.67E-2 g/mL)			486
1.49° (0.82)						Idem (1.67E-1 g/mL)			486
1.43° (0.82)						Idem (3.33E-1 g/mL)			486
1.56° (0.89)	[3.17]					Idem (variable sorbent conc.)			486
1.46° (0.98)	[3.11]	77	15	8	3.9* [2.26]	Bondhead soil; pH 6.9		BE	536
[1.33]	[3.02]				3.53* [2.05]	Batcombe sil soil; pH 6.1; 0.01 M $CaCl_2$	20	BE	120
[0.65]	[2.93]		23	42	0.9* [0.52]	Panoche soil; CE=15.4 me/100 g; pH 7.5; SA=100 m^2/g		BE	269
[1.47]	[3.23]		61	27	3.0* [1.74]	Palouse soil; CE=10.0 me/100 g; pH 5.9; SA=42 m^2/g		BE	269
[1.15]	[3.11]	9	68	21	1.9* [1.1]	Woodburn soil	20	BE	198
0.66° (0.83)		77	15	8	0.51	Sarpy soil; pH 7.3; CE=5.7 me/100 g; 0.01 M $CaCl_2$	24	BE	122
0.95° (0.83)		83	9	8	1.07	Thurman soil; pH 6.83; CE=6.1 me/100 g; 0.01 M $CaCl_2$	24	BE	122

TABLE 8. Sorption coefficients for pesticides—Continued

log K_d log K_f^0 (1/*n*)	log K_{oc}	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
1.47° (0.88)	[3.05]	37	42	21	2.64	Clarion agric. soil; pH 5.00; CE=21.0 me/100 g; 0.01 M $CaCl_2$	24	BE	122
1.50° (0.80)		21	55	24	3.80	Harps agric. soil; pH 7.30; CE=37.8 me/100 g; 0.01 M $CaCl_2$	24	BE	122
2.31° (0.81)		42	39	19	18.36	Peat; pH 6.98; CE=77.3 me/100 g; 0.01 M $CaCl_2$	24	BE	122
2.69° (0.95)	[3.05]	52	34	14	75.3* [43.7]	Soil; organic; pH 6.1		BE	264
1.30° (0.99)	[3.09]	71	22	7	2.8* [1.62]	Big Creek sediment; pH 6.6		BE	264
1.19° (1.01)	[3.03]	56	30	14	2.5* [1.45]	Beverly soil; pH 6.8		BE	264
0.78° (0.98)	[3.17]	91.5	1.5	7	0.7* [0.41]	Plainfield soil; pH 7.0		BE	264
1.59	[3.22]			63	3.72* [2.16]	Meron soil; pH 6.6		BE	267
1.88	[2.89]			64	4.88* [2.83]	Golan soil; pH 7.1		BE	267
2.21	[3.89]			72	4.55* [2.64]	Bet Guvrin soil; pH 7.1		BE	267
2.94	[3.18]				95* [55.1]	Peat soil		BE	267
1.08	[3.20]			33	1.3* [0.75]	Hoban sicl soil; pH 7.7; CE=22 me/100 g		BE	268
1.12				72		Harlingen c soil; pH 8.2		BE	268
1.00						Idem		LE	268
0.64	[2.44]			44	0.4* [0.23]	Nacogdoches c soil; pH 5.0; CE=14 me/100 g		BE	268
0.35	[2.99]					Idem		LE	268
0.37				17		Norwood sil soil; pH 8.2		LE	268
0.71	[2.39]			8	0.5* [0.29]	Amarillo fine sl soil; pH 7.7; CE=8 me/100 g		LE	268
0.78	[2.13]			6	1.0* [0.58]	Katy sil soil; pH 5.1		LE	268
0.88° (1.04)	[3.24]	79.6	4.8	15.6	0.75* [0.44]	Alluvial soil; pH 6.20; CE=18.6 me/100 g;		BE	129
1.09° (1.05)	[3.12]	75.9	3.4	20.7	1.62* [0.94]	Lateritic soil; pH 6.25; CE=26.6 me/100 g		BE	129
0.50° (1.33)						Idem; oxidized with H_2O_2			129
1.58° (1.11)	[3.36]	69.6	6.8	23.6	2.88* [1.67]	Lateritic soil; pH 6.30; CE=42.8 me/100 g		BE	129
1.03° (1.33)						Idem; oxidized with H_2O_2			129
2.10° (1.05)	[3.60]	45.6	7.8	45.6	5.52* [3.20]	Pokkali soil; pH 5.2; CE=19.2 me/100 g		BE	129
2.33° (1.03)	[3.65]	53.6	12.8	33.6	8.21* [4.76]	Kari soil; pH 3.5; CE=21.2 me/100 g;		BE	129
2.66° (1.02)	[3.51]	63.6	6.8	29.6	24.6* [14.3]	Kari soil; pH 3.3; CE=28.9 me/100 g;		BE	129
[0.80]	[3.56]			6	0.3* [0.17]	Mivtahim s regosol; pH 8; CE=4 me/100 g; SA=39 m^2/g	10	BE	139
[0.75]	[3.51]					Idem	30		139
[0.54]	[3.31]					Idem	50		139
[1.25]	[3.20]			56	1.9* [1.1]	Har-Bargan calcareous reddish-brown alluv. grumsol; pH 7.7; CE=63 me/100 g; SA=410 m^2/g	10	BE	139
[1.01]	[2.97]					Idem	30		139
[0.96]	[2.92]					Idem	50		139
[1.02]	[3.41]			14	0.7* [0.41]	Netanya scl; pH 6.3; CE=8 me/100 g; SA=90 m^2/g	10	BE	139
[0.86]	[3.25]					Idem	30		139
[0.73]	[3.11]					Idem	50		139

TABLE 8. Sorption coefficients for pesticides—Continued

log K_d log K_f^0 $(1/n)$	log K_{oc}	Sorbent composition (%)				Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
−0.11	2.89			11.2	0.17* [0.10]	Netanya agricult. surface soil	25	BE	563
0.14	2.72			6.9	0.45* [0.26]	Mivtahim agricult. surface soil	25	BE	563
0.56	2.73			63.1	1.18* [0.68]	Golan agricult. surface soil	25	BE	563
0.73	2.87			23.8	1.25* [0.73]	Gilat agricult. surface soil	25	BE	563
0.70	2.78			72.5	1.42* [0.82]	Shefer agricult. surface soil	25	BE	563
0.72	2.79			10.6	1.45* [0.84]	Bet Degan agricult. surface soil	25	BE	563
1.09	2.88			71.2	2.82* [1.64]	Neve Yaar agricult. surface soil	25	BE	563
1.45	2.92			76.2	5.82* [3.38]	Malkiya agricult. surface soil	25	BE	563
1.48	3.22				3.08* [1.79]	Kinneret Lake sediment	25	BE	563
1.80	3.15			60.5	7.85* [4.55]	Kinneret A Lake sediment	25	BE	563
1.81	3.18			63.2	7.43* [4.31]	Kinneret F Lake sediment	25	BE	563
1.60	3.20			63.8	4.39* [2.55]	Kinneret G Lake sediment	25	BE	563
	2.95*av [3.18]av					94 soils (literature)			663
	3.68					Soil: experimental (literature)			217
	3.17av					89 literature data			562
	3.42					Correlation log K_{oc}−log K_{ow}			96
	3.23					Correlation log K_{oc}−log K_{ow}			207
	3.60					Correlation log K_{oc}−log K_{ow}			108
	3.25					Correlation log K_{oc}−log S			96
	3.95					Correlation log K_{oc}−log S(mp)			96
	2.88					Correlation log K_{oc}−log S			564
						Permethrin			
[2.60]	[4.80]				1.09* [0.63]	Warracknabeal, Vic., soil; pH 8.0; 0.01 M $CaCl_2$		BE	558
[2.64]	[4.37]				3.20* [1.86]	Warracknabeal, Vic., soil; pH 8.4; 0.01 M $CaCl_2$		BE	558
[1.83]	[3.92]				1.42* [0.82]	Warranine soil; pH 6.5; 0.01 M $CaCl_2$		BE	558
[2.34]	[4.38]				1.58* [0.92]	Badgingarra soil; pH 6.3; 0.01 M $CaCl_2$		BE	558
[1.85]	[4.81]				0.19* [0.11]	Badgingarra soil; pH 6.3; 0.01 M $CaCl_2$		BE	558
[2.60]	[4.26]				3.78* [2.19]	Gabalong soil; pH 5.9; 0.01 M $CaCl_2$		BE	558
2.59	[3.19]	18	34	48	43* [24.9]	Sediment (Lake St. George, Can.)	21	BE	126
	5.25					Correlation log K_{oc}−MCI			598
	4.03					Correlation log K_{oc}−log S			564
						Phorate			
0.34° (0.94)	[2.63]	77	15	8	0.51	Sarpy soil; pH 7.3; CE=5.7 me/100 g; 0.01 M $CaCl_2$	24	BE	122
0.69° (0.91)	[2.66]	83	9	8	1.07	Thurman soil; pH 6.83; CE=6.1 me/100 g; 0.01 M $CaCl_2$	24	BE	122
0.93° (0.92)	[2.51]	37	42	21	2.64	Clarion agricultural soil; pH 5.00; CE=21.0 me/100 g; 0.01 M $CaCl_2$	24	BE	122
1.14° (0.88)	[2.56]	21	55	24	3.80	Harps agricultural soil; pH 7.30; CE=37.8 me/100 g; 0.01 M $CaCl_2$	24	BE	122
1.88°	[2.62]	42	39	19	18.36	Peat; pH 6.98;	24	BE	122

TABLE 8. Sorption coefficients for pesticides—Continued

log K_d log K_f^0 (1/n)	log K_{oc}	Sorbent composition (%) Sand	 Silt	 Clay	 OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
(1.01)						CE=77.3 me/100 g; 0.01 M $CaCl_2$			
	[2.82]				3.53* [2.05]	Batcombe sil soil; pH 6.1; 0.01 M $CaCl_2$	20	BE	120
	3.51					Soil; experimental (literature)			217
	2.71					Correlation log K_{oc}–log S			564
Picloram (pK_a=3.6, Ref. 674)									
1.57° (0.78)				100		H-montmorillonite (1–0.2 μm); pH=3.35; CE=73.5 me/100 g;	25	BE	250
1.34° (0.82)		45	44	11	6.80* [3.94]	Aiken soil; pH 6.0; pH (corrected, HNO_3) 3.63; CE=8.4 me/100 g;		BE	319
1.25° (0.83)						Idem; pH (corrected, HNO_3)3.80			319
1.06° (0.76)						Idem; pH (corrected, HNO_3)4.22			319
0.74° (0.92)	[2.14]					Idem; pH (corrected, HNO_3)4.83			319
−0.22° (0.89)	[1.18]					Idem; pH 6.03			319
−0.55° (1.08)	[0.85]					Idem; pH(corrected, NaOH)9.06			319
−0.27° (0.97)	[1.14]					Idem; pH(corrected, NaOH)10.4			319
NA			23	42	0.9* [0.52]	Panoche soil (<1 mm); pH 7.5; CE=15.4 me/100 g; SA=100 m^2/g	25	BE	315
−0.46° (0.86)						Idem; pH(corrected, HCl)4.2	15		315
−0.68° (0.92)	[1.61]					Idem; pH(corrected, HCl)4.2	25		315
−0.84° (0.98)	[1.45]					Idem; pH(corrected, HCl)4.2	35		315
1.11° (0.90)	[3.39]					Idem; pH(corrected, HCl)1.2	10		315
0.55° (0.89)	[2.84]					Idem; pH (corrected, HCl)1.2	20		315
0.18° (0.97)	[2.46]					Idem; pH(corrected, HCl)1.2	30		315
−0.55° (1.00)	[1.85]		32	8	0.7* [0.41]	Ephrata soil (<1 mm); pH 7.2; CE=8.2 me/100 g; SA=28 m^2/g	15	BE	315
−0.76° (0.99)	[1.63]					Idem	25		315
−1.04° (0.99)	[1.36]					Idem	35		315
0.30° (0.90)	[2.06]		61	27	3.0* [1.74]	Palouse soil (<1 mm); pH 5.9; CE=19 me/100 g; SA=42 m^2/g	15	BE	315
0.24° (1.09)	[2.00]					Idem	25		315
0.14° (1.09)	[1.90]					Idem	35		315
−0.74° (0.97)	[1.27]	46	38	16	1.7* [0.99]	Norge soil; pH 6.6; CE=9.2 me/100 g; 0.01 N $CaCl_2$		BE	508
[0.81]	[3.75]	21	45	34	0.2* [0.12]	Soil 4; pH 2	25	BE	314
[−0.81]	[2.12]					Idem; pH 9			314
[1.23]	[3.86]	48	36	16	0.3* [0.17]	Soil 3; pH 2	25	BE	314
[−0.59]	[2.17]					Idem; pH 9			314
[−0.36]	[2.28]	87	10	3	0.4* [0.23]	Soil 7; pH 2	25	BE	314
[−0.85]	[1.79]					Idem; pH 9			314
[0.58]	[2.82]	42	46	12	1.0* [0.58]	Soil D1; pH 2	25	BE	314

TABLE 8. Sorption coefficients for pesticides—Continued

log K_d log K_f^0 (1/*n*)	log K_{oc}	Sorbent composition (%) Sand	 Silt	 Clay	 OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
[1.13]	[2.93]	13	39	48	2.7* [1.57]	Soil N1; pH 2	25	BE	314
[−1.32]	[0.49]					Idem; pH 9			314
[1.51]	[3.13]	58	35	7	4.1* [2.38]	Soil B2; pH 2	25	BE	314
[−0.30]	[1.32]					Idem; pH 9			314
[1.81]	[3.02]	26	52	22	10.7* [6.21]	Soil B1; pH 2	25	BE	314
[−0.01]	[1.20]					Idem; pH 9			314
[2.29]	[3.02]	39	38	23	32.2* [18.7]	Soil Q1; pH 2	25	BE	314
[0.29]	[1.02]					Idem; pH 9			314
[0.41]	[1.03]	68	26	6	44.3* [25.7]	Soil Q3; pH 9	25	BE	314
−1.12° (0.94)	[0.74]				1.4	Wyoming Borollic Haplargids soil (A horizon); pH 6.0–7.8		BE	321
−0.59° (1.02)	[1.16]				1.8	Idem (Bt horizon)			321
−4.0° (1.02)	[1.92]				0.85	Idem (2Btk1 horizon)			321
−0.74° (0.97)	[1.26]	46	38	16	1.7* [0.99]	Norge soil; pH 6.6; CE=9.2 me_q/100 g; 0.01 N $CaCl_2$		BE	507
−0.01° (0.85)				18	4.2* [2.44]	Fiddletown sil soil; pH 5.60; CE=20 me/100 g	20	BE	316
−0.26° (0.82)				27	3.6* [2.09]	Palouse sil soil; pH 5.68; CE=19 me/100 g;	20	BE	316
−0.51° (0.83)				83	2.4* [1.39]	Molokai c soil; pH 6.97; CE=14 me/100 g	20	BE	316
−0.39° (0.74)				33	2.4* [1.39]	Linne cl soil; pH 7.40; CE=41 me/100 g	20	BE	316
−0.93° (0.84)				9	1.6* [0.93]	Kentwood sl soil; pH 6.40; CE=12 me/100 g	20	BE	316
−0.15° (0.60)				8	0.94* [0.55]	Ephrata sl soil; pH 7.14; CE=8 me/100 g;	20	BE	316
−0.12	[1.02]			13.5	12.4* [7.19]	Lacombe l soil; pH 7.9	25	BE	317
−0.31	[0.91]			20.3	10.5* [6.09]	Melfort l soil; pH 6.5	25	BE	317
−0.31	[0.91]					Idem		LE	540
−0.51	[0.92]			19.2	6.5* [3.77]	Weyburn Oxbow 1 soil; pH 7.9	25	BE	317
−0.62	[0.81]					Idem		LE	540
−0.64	[0.93]			57.3	4.7* [2.73]	Indian Head c soil; pH 8.1	25	BE	317
−1.00	[0.63]					Idem		LE	540
−0.62	[0.99]			15.0	4.3* [2.49]	Weyburn light l soil; pH 8.2	25	BE	317
N.A.				69.5	4.2* [2.44]	Regina heavy c soil; pH 8.0	25	BE	317
−1.00	[0.62]					Idem		LE	540
−0.62	[1.01]			18.5	4.1* [2.38]	Indian Head cl soil; pH 8.1	25	BE	317
−1.05	[0.94]			8.0	1.8* [1.04]	Asquith sl soil; pH 6.9	25	BE	317
−1.52	[0.46]					Idem		LE	540
−0.72° (0.88)	[1.28]	14.5	52.5	33.0	1.7* [0.99]	Amsterdam soil; pH 7.8	20	BE	664
−0.22° (0.83)				24	6.6*	Minam loam soil (0–23 cm); pH 7.0; Al=0.3 me/100 g; CE=28.3 me/100 g	25	BE	313
−0.52° (0.76)				26	3.8*	Idem (23–33 cm); pH 7.3; Al=0.3 me/100 g; CE=24.4 me/100 g			313

TABLE 8. Sorption coefficients for pesticides—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%)				Other sorbent and solution data: prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
−0.52° (0.85)				17	7.7*	Woodcock 1 soil (0–10 cm); Al=9.9 me/100 g; CE=12.9 me/100 g;	25	BE	313
−0.22° (0.99)	[1.38]			13	4.3* [2.49]	Idem (36–51 cm); pH 5.8; Al=26.8 me/100 g; CE=3.6 me/100 g			313
−0.40° (1.02)	[1.63]			8	1.6* [0.93]	Idem (69–111 cm); pH 5.6; Al=34.6 me/100 g; CE=3.2 me/100 g			313
0.66° (0.84)				36	7.4*	Kinney clay loam soil (23–38 cm); pH; 5.2; Al=58.0 me/100 g; CE=6.5 me/100 g	25	BE	313
0.36° (0.93)	[2.20]			42	2.5* [1.45]	Idem (23–46 cm); pH 5.2; Al=53.2 me/100 g; CE=8.9 me/100 g			313
0.20° (1.00)	[2.54]			31	0.8* [0.46]	Idem (46–69 cm); pH 5.0; Al=41.6 me/100 g; CE=16.1 me/100 g			313
−1.10	1.05	34	46	20	0.74	Commerce soil; pH 7.3		BE	135
−0.19	1.34	12	28	60	2.92	Fargo soil; pH 6.1		BE	135
−0.92	1.05	18	62	20	1.03	Walla-Walla soil; pH 6.3		BE	135
−0.77	1.10	78	14	8	1.36	Kawkawlin soil; pH 6.8		BE	135
−1.10	1.26	82	10	8	0.45	Norfolk soil; pH 5.9		BE	135
−0.41	1.31	14	54	32	1.89	Catlin soil; pH 6.1		BE	135
−0.92	1.00	38	42	20	1.17	Holdredge soil; pH 5.4		BE	135
−0.74° (0.94)	[1.27]	46	38	16	1.7* [0.99]	Norge soil; pH 6.6; CE=9.2 me/100 g. 0.01 N $CaCl_2$		BE	485
	3.52°* (0.75)				56.4	Humic acid from Black Chernozemic soil; pH 3.3–3.6	5	BE	125
	3.43°* (0.79)					Idem	25	BE	125
	1.23					Soil; experimental (literature)			217
	1.49av					59 literature data			562
	1.41av					26 soils (literature)			87
	2.20					Correlation $\log K_{oc}$–$\log S$			564
	1.47					Correlation $\log K_{oc}$–MCI			578
Profluralin									
2.74				100		Ca–montmorillonite; pH 6	24	BE	121
3.26	[3.52]				94* [54.5]	OM from peaty muck soil; pH 6.5	24	BE	121
	3.93					Soil; experimental (literature)			217
	4.19					Correlation $\log K_{oc}$–$\log S$			564
Prometone (pK_a=**4.28**, Ref. 247)									
TA				100		H–montmorillonite (1–0.2 μm); pH 3.35; CE=73.5 me/100 g	25	BE	250
2.18° (0.64)				100		Na–montmorillonite (1–0.2 μm); pH 6.80; CEC=87.0 me_g/100 g	25	BE	250
0.35	[1.74]	2.9	68.7	28.4	7.1* [4.12]	Lanton soil; pH 6.4; CE=32.8 me/100 g		BE	631
0.00° (0.79)				18	3.3* [1.91]	Lakeland sl soil; pH 6.2; CE=2.9 me/100 g; 0.01 M $CaCl_2$	26	BE	633
0.59° (0.77)				43	1.9* [1.10]	Wehadkee sil soil; ph 5.6; CE=10.2 me/100 g; 0.01 M $CaCl_2$	26	BE	633
0.73° (0.84)				38	4.4* [2.55]	Chillum sil soil; pH 4.6; CE=7.6 me/100 g; 0.01 M $CaCl_2$	26	BE	633
0.63° (0.84)				48	4.3* [2.49]	Hagertown sicl soil; pH 5.5; CE=12.5 me/100 g; 0.01 M $CaCl_2$	26	BE	633
0.45	[2.41]	6	74	20	1.9* [1.1]	Putnam soil; pH 5.3; CE=12.3 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.94	[2.56]	4	66	30	4.2* [2.4]	Marshall soil; pH 5.4; CE=21.3 me/100 g; 0.01 M $CaCl_2$	20	BE	145

TABLE 8. Sorption coefficients for pesticides—Continued

log K_d log K_f^0 (1/n)	log K_{oc}	Sorbent composition (%)				Other sorbent and solution data: prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
0.80	[2.48]	3	67	30	3.6* [2.1]	Grundy soil; pH 5.6; CE=13.5 me/100 g; 0.01 M $CaCl_2$	20	BE	145
1.17	[3.26]	9	74	17	1.4* [0.81]	Marian soil; pH 4.6; CE=9.9 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.81	[2.58]	4	72	24	2.9* [1.7]	Knox soil; pH 5.4; CE=18.8 me/100 g; 0.01 M $CaCl_2$	20	BE	145
1.35	[3.03]	26	43	31	3.6* [2.1]	Shelby soil; pH 4.3; CE=20.1 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.67	[2.73]	30	44	26	1.5* [0.87]	Lindley soil; pH 4.7; CE=6.9 me/100 g; 0.01 M $CaCl_2$	20	BE	145
1.23	[3.12]	1	36	63	2.2* [1.3]	Wabash soil; pH 5.7; CE=40.3 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.66	[2.58]	32	50	18	2.1* [1.2]	Salix soil; pH 6.3; CE=17.9 me/100 g 0.01 M $CaCl_2$	20	BE	145
0.18	[2.30]	40	41	19	1.3* [0.75]	Sarpy soil; pH 7.1; CE=14.3 me/100 g 0.01 M $CaCl_2$	20	BE	145
1.06	[2.61]	5	48	47	4.9* [2.8]	Summit soil; pH 4.8; CE=35.1 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.53	[2.31]	5	67	28	2.9* [1.7]	Oswego soil; pH 6.4; CE=21.0 me/100 g; 0.01 M $CaCl_2$	20	BE	145
−0.22	[1.87]	1	76	23	1.4* [0.81]	Bates soil; pH 6.5; CE=9.3 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.78	[2.58]	1	76	23	2.7* [1.6]	Gerald soil; pH 4.7; CE=11.0 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.38	[2.41]	11	75	14	1.6* [0.93]	Newtonia soil; pH 5.2; CE=8.8 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.11	[1.87]	8	72	20	3.0* [1.7]	Eldon soil; pH 5.9; CE=12.9 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.23	[2.14]	9	72	19	2.1* [1.2]	Baxter soil; pH 6.0; CE=11.2 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.08	[1.93]	4	85	11	2.4* [1.4]	Menfro soil; pH 5.3; CE=9.1 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.79	[2.77]	2	79	19	1.8* [1.04]	Union soil; pH 5.4; CE=6.8 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.89	[2.88]	13	70	17	1.8* [1.04]	Lebanon soil; pH 4.9; CE=7.7 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.34	[2.43]	20	67	13	1.4* [0.81]	Clarksville soil; pH 5.7; CE=5.7 me/100 g; 0.01 M $CaCl_2$	20	BE	145
−0.30	[1.85]	20	63	17	1.2* [0.70]	Cumberland soil; pH 6.4; CE=6.5 me/100 g; 0.01 M $CaCl_2$	20	BE	145
1.74	[3.58]	25	30	45	2.5* [1.5]	Sharkey soil; pH 5.0; CE=28.2 me/100 g; 0.01 M $CaCl_2$	20	BE	145
−0.15	[2.30]	84	11	5	0.6* [0.35]	Lintonia soil; pH 5.3; CE=3.2 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.58	[2.51]	14	66	20	2.0* [1.2]	Waverley soil; pH 6.4; CE=12.8 me/100 g; 0.01 M $CaCl_2$	20	BE	145
−0.44° (0.87)		67.1	25.8	7.1	0.43	Hanford soil; pH 6.05; CE=5.95 cmol/kg; 0.01 M $CaCl_2$	25	BE	528
0.66° (0.96)	[1.82]	82.0	13.5	4.5	0.33	Tuiunga soil; pH 6.30; CE=0.45 cmol/kg; 0.01 M $CaCl_2$	25	BE	528
	2.54					Soil; experimental (literature)			217
	2.72av					29 soils (literature)			87
	2.42					Correlation log K_{om}−log S(563)			528
	2.30					Correlation log K_{oc}−log K_{ow}(87)			528
	2.69					Correlation log K_{oc}−log K_{ow}(217)			528
	2.04					Correlation log K_{oc}−log S			564
	2.20					Correlation log K_{oc}−MCI			598
						Prometryne (pK_a=4.05, Ref. 247)			
T.A.				100		H−montmorillonite; pH 3.6		BE	212
1.45				100		Na−montmorillonite; pH 7.9		BE	212
1.26				100		Ca−montmorillonite; pH 7.9		BE	212

TABLE 8. Sorption coefficients for pesticides—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%)				Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
1.26				100		Mg–montmorillonite; pH 8.2		BE	212
3.27				100		Ca–montmorillonite; pH 6.0	24	BE	121
4.09	[4.35]				94* [54.5]	OM from peaty muck soil; pH 5.5	24	BE	121
−0.44	[1.95]			5.0	0.70* [0.41]	Eufala loamy fine s soil; pH 6.4; 0.01 N $CaCl_2$	23	BE	300
−0.33	[2.06]					Idem; 0.5 N $CaCl_2$			300
−0.15	[1.69]			17.5	2.50* [1.45]	Norge 1 soil; pH 6.1 0.01 N $CaCl_2$	23	BE	300
−0.02	[1.82]					Idem; pH 5.9; 0.5 N $CaCl_2$			300
0.17° (0.86)		46	38	16	1.7* [0.99]	Norge soil; pH 6.6; 9.2 me_q/100 g; 0.01 N $CaCl_2$		BE	507
1.65° (0.67)				75	1.3	Eurosol-1; c soil; pH 5.1; 0.01 M $CaCl_2$		BE	583
0.16° (0.90)	1.60			22.6	3.7	Eurosol-2 sil; pH 7.4; 0.01 M $CaCl_2$		BE	583
0.51° (0.80)				17.0	3.45	Eurosol-3; 1; pH 5.2; 0.01 M $CaCl_2$		BE	583
−0.04° (0.65)				20.3	1.55	Eurosol-4; si; pH 6.5; 0.01 M $CaCl_2$		BE	583
1.64° (0.72)				6.0	9.25	Eurosol-5; 1s; pH 3.2; 0.01 M $CaCl_2$		BE	583
[0.59]	[2.43]	74.4	19.5	6.1	2.5* [1.45]	Aguadilla soil; CE=10 me/100 g; pH 7.4; 0.01 M $CaCl_2$		BE	304
[0.31]	[2.43]	27.6	35.6	36.8	1.3* [0.75]	Aguirre soil; CE=14.3 me/100 g; pH 9.0; 0.01 M $CaCl_2$		BE	304
[0.63]	[2.28]	16.6	13.0	70.4	3.9* [2.26]	Aguirre soil; CE=59.0 me/100 g; pH 8.4; 0.01 M $CaCl_2$		BE	304
[0.86]	[2.59]	14.9	39.3	45.8	3.2* [1.86]	Alonso soil; CE=13.8 me/100 g; pH 5.1; 0.01 M $CaCl_2$		BE	304
[0.57]	[2.24]	49.2	28.8	22.0	3.7* [2.15]	Altura soil; CE=27.6 me/100 g; pH 8.0; 0.01 M $CaCl_2$		BE	304
[0.52]	[2.53]	68.1	4.4	27.0	1.7* [0.99]	Bayamón soil; CE=5.0 me/100 g; pH 4.7; 0.01 M $CaCl_2$		BE	304
[1.00]	[2.76]	56.4	8.0	35.9	3.1* [1.80]	Cabo Rojo soil; CE=9.0 me/100 g; pH 4.3; 0.01 M $CaCl_2$		BE	304
[3.00]	[3.67]	36.0	36.0	28.0	36.0* [20.9]	Caño Tiburones soil; pH 5.5; CE=86.0 me/100 g; 0.01 M $CaCl_2$		BE	304
[0.77]	[2.73]	6.6	28.9	64.5	1.9* [1.10]	Catalina soil; CE=11.8 me/100 g; pH 4.7; 0.01 M $CaCl_2$		BE	304
[0.45]	[2.46]	47.2	17.4	35.4	1.7* [0.99]	Cartagena soil; CE=36.1 me/100 g; pH 7.7; 0.01 M $CaCl_2$		BE	304
[−0.12]	[1.79]	89.0	7.3	3.7	2.1* [1.22]	Cataño soil; CE=6.9 me/100 g; pH 7.9; 0.01 M $CaCl_2$		BE	304
[0.71]	[2.55]	43.4	25.2	31.4	2.5* [1.45]	Cintrona soil; CE=25.0 me/100 g; pH 8.3; 0.01 M $CaCl_2$		BE	304
[0.59]	[2.53]	58.8	23.4	17.8	2.0* [1.16]	Cayaguá soil; CE=7.3 me/100 g; pH 5.2; 0.01 M $CaCl_2$		BE	304
[0.82]	[2.52]	13.3	34.8	51.9	4.9* [2.84]	Cialitos soil; CE=18.6 me/100 g; pH 5.4; 0.01 M $CaCl_2$		BE	304
[0.91]	[2.58]	22.7	37.4	39.9	3.7* [2.15]	Coloso soil; CE=23.0 me/100 g; pH 5.7; 0.01 M $CaCl_2$		BE	304
[0.91]	[2.52]	26.0	18.6	55.4	4.3* [2.49]	Corozal soil; CE=17.0 me/100 g; pH 4.6; 0.01 M $CaCl_2$		BE	304
[0.59]	[2.32]	23.4	24.8	51.8	3.2* [1.86]	Coto soil; CE=14.0 me/100 g; pH 7.7; 0.01 M $CaCl_2$		BE	304
[0.48]	[2.76]	48.0	20.6	31.4	0.9* [0.52]	Estación soil; CE=10.0 me/100 g; pH 5.9; 0.01 M $CaCl_2$		BE	304
[0.98]	[2.69]	39.1	29.7	32.2	3.4* [1.97]	Fe soil; CE=27.6 me/100 g; pH 7.5; 0.01 M $CaCl_2$		BE	304
[1.19]	[2.91]	15.0	50.7	34.3	3.3* [1.91]	Fortuna soil; CE=23.3 me/100 g; pH 5.4; 0.01 M $CaCl_2$		BE	304
[0.52]	[2.44]	15.5	32.5	52.0	2.1*	Fraternidad soil; pH 6.3;		BE	304

TABLE 8. Sorption coefficients for pesticides—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
					[1.22]	CE=36.6 me/100 g; 0.01 M $CaCl_2$			
[0.73]	[2.34]	11.1	23.8	65.1	4.2* [2.44]	Fraternidad soil (Lajas); pH 5.9; CE=58.0 me/100 g; 0.01 M $CaCl_2$		BE	304
[0.71]	[2.27]	6.4	19.6	74.0	4.8* [2.78]	Guánica soil; CE=52.1 me/100 g; pH 8.1; 0.01 M $CaCl_2$		BE	304
[0.59]	[2.79]	84.4	8.4	7.2	1.1* [0.64]	Humacao soil; CE=4.0 me/100 g; pH 6.3; 0.01 M $CaCl_2$		BE	304
[0.97]	[2.97]	10.1	50.9	39.0	1.7* [0.99]	Humata soil; CE=10.1 me/100 g; pH 4.5; 0.01 M $CaCl_2$		BE	304
[0.95]	[2.67]	26.6	53.5	20.9	3.3* [1.91]	Josefa soil; CE=16.8 me/100 g; pH 6.0; 0.01 M $CaCl_2$		BE	304
[0.61]	[2.42]	15.2	41.6	43.2	2.7* [1.57]	Juncos soil; CE=13.4 me/100 g; pH 6.2; 0.01 M $CaCl_2$		BE	304
[0.31]	[1.96]	19.9	33.4	46.7	3.9* [2.26]	Mabí soil; CE=55.2 me/100 g; pH 7.0; 0.01 M $CaCl_2$		BE	304
[0.81]	[2.35]	22.7	40.7	36.6	4.9* [2.84]	Mabí soil; CE=31.0 me/100 g; pH 5.7; 0.01 M $CaCl_2$		BE	304
[0.67]	[2.57]	76.0	13.4	10.6	2.2* [1.28]	Machete soil; CE=8.0 me/100 g; pH 6.5; 0.01 M $CaCl_2$		BE	304
[0.59]	[2.45]	14.9	42.8	42.3	2.4* [1.39]	Mercedita soil; CE=19.9 me/100 g; pH 8.1; 0.01 M $CaCl_2$		BE	304
[1.02]	[2.67]	26.3	27.7	46.0	3.8* [2.20]	Moca soil; CE=31.0 me/100 g; pH 5.8; 0.01 M $CaCl_2$		BE	304
[0.93]	[2.65]	28.0	47.0	25.0	3.3* [1.91]	Múcara soil; CE=19.6 me/100 g; pH 5.8; 0.01 M $CaCl_2$		BE	304
[1.09]	[2.60]	22.0	49.2	28.0	5.3* [3.07]	Nipe soil; CE=11.9 me/100 g; pH 5.7; 0.01 M $CaCl_2$		BE	304
[−0.12]	[1.81]	59.4	28.2	12.4	2.0* [1.16]	Pandura soil; CE=7.7 me/100 g; pH 5.7; 0.01 M $CaCl_2$		BE	304
[0.91]	[2.61]	13.4	43.6	43.0	3.5* [2.03]	Río Piedras soil; pH 4.9; CE=11.5 me/100 g; 0.01 M $CaCl_2$		BE	304
[0.48]	[2.12]	39.0	24.6	36.4	3.9* [2.26]	Sabana Seca soil; pH 7.4; CE=23.0 me/100 g; 0.01 M $CaCl_2$		BE	304
[0.42]	[1.97]	47.0	24.4	28.6	4.9* [2.84]	San Antón soil; pH 7.4; CE=28.0 me/100 g; 0.01 M $CaCl_2$		BE	304
[0.95]	[2.86]	57.0	18.6	24.4	2.1* [1.22]	Santa Isabel soil; pH 7.4; CE=28.0 me/100 g; 0.01 M $CaCl_2$		BE	304
[2.51]	[3.73]	46.0	20.0	34.0	10.4* [6.03]	Soller soil; CE=53.0 me/100 g; pH 6.9; 0.01 M $CaCl_2$		BE	304
[0.45]	[2.54]	73.4	19.4	7.2	1.4* [0.81]	Talante soil; CE=4.0 me/100 g; pH 5.1; 0.01 M $CaCl_2$		BE	304
[1.12]	[2.65]	35.0	24.6	40.4	5.1* [2.96]	Toa soil; CE=36.0 me/100 g; pH 8.0; 0.01 M $CaCl_2$		BE	304
[0.73]	[2.67]	41.5	38.3	20.2	2.0* [1.16]	Toa soil; CE=13.0 me/100 g; pH 5.3; 0.01 M $CaCl_2$		BE	304
[0.13]	[2.59]	60.9	25.1	14.0	0.6* [0.35]	Toa soil; CE=8.0 me/100 g; pH 6.0; 0.01 M $CaCl_2$		BE	304
[0.61]	[2.30]	73.7	12.6	13.7	3.5* [2.03]	Vega Alta soil; pH 5.0; CE=5.6 me/100 g; 0.01 M $CaCl_2$		BE	304
[0.67]	[2.55]	45.2	36.8	18.0	2.3* [1.33]	Vía soil; CE=39.9 me/100 g; pH 5.1; 0.01 M $CaCl_2$		BE	304
[0.75]	[2.64]	62.4	19.6	18.0	2.2* [1.28]	Viví soil; CE=14.0 me/100 g; pH 4.8; 0.01 M $CaCl_2$		BE	304
[1.19]	[2.78]	15.0	23.4	61.6	4.5* [2.61]	Voladura soil; pH 4.3; CE=17.7 me/100 g; 0.01 M $CaCl_2$		BE	304
[0.45]	[1.84]	2.9	68.7	28.4	7.1* [4.12]	Lanton soil; pH 6.4; CE=32.8 me/100 g;		BE	631
−1.15° (−0.54)		100				Quartz s; pH 5.6; CE=0.4 me/100 g; 0.01 N $CaCl_2$	26	BE	299
−0.18° (0.77)		93	4	3	0.6* [0.35]	Cobb soil; pH 7.3; CE=3.8 me/100 g; 0.01 N $CaCl_2$	26	BE	299
1.46°		93	4	3	2.1*	Cobb soil+2% muck; pH 5.3;	26	BE	299

TABLE 8. Sorption coefficients for pesticides—Continued

log K_d log K_f^0 ($1/n$)	log K_{oc}	Sorbent composition (%)				Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
(0.79)					[1.22]	CE=9.0 me/100 g; 0.01 N $CaCl_2$			
0.54°		58	23	19	1.3*	Teller soil; pH 5.7;	26	BE	299
(0.80)					[0.75]	CE=8.6 me/100 g; 0.01 N $CaCl_2$			
0.69°		16	42	42	1.8*	Port soil; pH 6.3;	26	BE	299
(0.76)					[1.04]	CE=17.9 me/100 g; 0.01 N $CaCl_2$			
1.0°		27	45	29	2.8*	Brewer soil; pH 5.8;	26	BE	299
(0.83)					[1.62]	CE=13.5 me/100 g; 0.01 N $CaCl_2$			
0.28°				18	3.3*	Lakeland sl soil; pH 6.2;	26	BE	633
(0.88)					[1.91]	CE=2.9 me/100 g; 0.01 M $CaCl_2$			
0.79°				43	1.9*	Wehadkee sil soil; pH 5.6;	26	BE	633
(0.84)					[1.10]	CE=10.2 me/100 g; 0.01 M $CaCl_2$			
1.11°				38	4.4*	Chillum sil soil; pH 4.6;	26	BE	633
(0.86)					[2.55]	CE=7.6 me/100 g; 0.01 M $CaCl_2$			
1.01°				48	4.3*	Hagerstown sicl soil; pH 5.5;	26	BE	633
(0.84)					[2.49]	CE=12.5 me/100 g; 0.01 M $CaCl_2$			
0.04	[2.03]				1.77*	Cecil soil; pH 6.3		BE	665
					[1.03]				
0.58	[2.54]	6	74	20	1.9*	Putnam soil; pH 5.3;	20	BE	145
					[1.1]	CE=12.3 me/100 g; 0.01 M $CaCl_2$			
1.09	[2.71]	4	66	30	4.2*	Marshall soil; pH 5.4;	20	BE	145
					[2.4]	CE=21.3 me/100 g; 0.01 M $CaCl_2$			
0.96	[2.64]	3	67	30	3.6*	Grundy soil; pH 5.6;	20	BE	145
					[2.1]	CE=13.5 me/100 g; 0.01 M $CaCl_2$			
1.15	[3.24]	9	74	17	1.4*	Marian soil; pH 4.6;	20	BE	145
					[0.81]	CE=9.9 me/100 g; 0.01 M $CaCl_2$			
0.92	[2.70]	4	72	24	2.9*	Knox soil; pH 5.4;	20	BE	145
					[1.7]	CE=18.8 me/100 g; 0.01 M $CaCl_2$			
1.34	[3.02]	26	43	31	3.6*	Shelby soil; pH 4.3;	20	BE	145
					[2.1]	CE=20.1 me/100 g; 0.01 M $CaCl_2$			
0.90	[2.96]	30	44	26	1.5*	Lindley soil; pH 4.7;	20	BE	145
					[0.87]	CE=6.9 me/100 g; 0.01 M $CaCl_2$			
1.24	[3.13]	1	36	63	2.2*	Wabash soil; pH 5.7;	20	BE	145
					[1.3]	CE=40.3 me/100 g; 0.01 M $CaCl_2$			
0.81	[2.72]	32	50	18	2.1*	Salix soil; pH 6.3;	20	BE	145
					[1.2]	CE=17.9 me/100 g; 0.01 M $CaCl_2$			
0.46	[2.59]	40	41	19	1.3*	Sarpy soil; pH 7.1;	20	BE	145
					[0.75]	CE=14.3 me/100 g; 0.01 M $CaCl_2$			
1.25	[2.79]	5	48	47	4.9*	Summit soil; pH 4.8;	20	BE	145
					[2.8]	CE=35.1 me/100 g; 0.01 M $CaCl_2$			
0.70	[2.47]	5	67	28	2.9*	Oswego soil; pH 6.4;	20	BE	145
					[1.7]	CE=21.0 me/100 g; 0.01 M $CaCl_2$			
0.20	[2.30]	1	76	23	1.4*	Bates soil; pH 6.5;	20	BE	145
					[0.81]	CE=9.3 me/100 g; 0.01 M $CaCl_2$			
0.97	[2.78]	1	76	23	2.7*	Gerald soil; pH 4.7;	20	BE	145
					[1.6]	CE=11.0 me/100 g; 0.01 M $CaCl_2$			
0.54	[2.58]	11	75	14	1.6*	Newtonia soil; pH 5.2;	20	BE	145
					[0.93]	CE=8.8 me/100 g; 0.01 M $CaCl_2$			
0.56	[2.32]	8	72	20	3.0*	Eldon soil; pH 5.9;	20	BE	145
					[1.7]	CE=12.9 me/100 g; 0.01 M $CaCl_2$			
0.63	[2.55]	9	72	19	2.1*	Baxter soil; pH 6.0;	20	BE	145
					[1.2]	CE=11.2 me/100 g; 0.01 M $CaCl_2$			
0.52	[2.37]	4	85	11	2.4*	Menfro soil; pH 5.3;	20	BE	145
					[1.4]	CE=9.1 me/100 g; 0.01 M $CaCl_2$			
0.93	[2.92]	2	79	19	1.8*	Union soil; pH 5.4;	20	BE	145
					[1.04]	CE=6.8 me/100 g; 0.01 M $CaCl_2$			
0.95	[2.94]	13	70	17	1.8*	Lebanon soil; pH 4.9;	20	BE	145
					[1.04]	CE=7.7 me/100 g; 0.01 M $CaCl_2$			
0.71	[2.80]	20	67	13	1.4*	Clarksville soil; pH 5.7;	20	BE	145
					[0.81]	CE=5.7 me/100 g; 0.01 M $CaCl_2$			
0.15	[2.30]	20	63	17	1.2*	Cumberland soil; pH 6.4;	20	BE	145
					[0.70]	CE=6.5 me/100 g; 0.01 M $CaCl_2$			
1.64	[3.48]	25	30	45	2.5*	Sharkey soil; pH 5.0;	20	BE	145

TABLE 8. Sorption coefficients for pesticides—Continued

log K_d log K_f^0 (1/n)	log K_{oc}	Sorbent composition (%) Sand	 Silt	 Clay	 OC	Other sorbent and solution data: prediction procedure	Temp. (°C)	Meth.	Ref.
					[1.5]	CE=28.2 me/100 g; 0.01 M $CaCl_2$			
−0.05	[2.41]	84	11	5	0.6* [0.35]	Lintonia soil; pH 5.3; CE=3.2 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.76	[2.70]	14	66	20	2.0* [1.2]	Waverley soil; pH 6.4; CE=12.8 me/100 g; 0.01 M $CaCl_2$	20	BE	145
2.93	[4.20]		28	11	9.2* [5.34]	Cape Fear soil; CE=10.3 me/100 g; pH 6; SA=77.2 m^2/g		BE	279
2.14	[3.99]		41	7	2.5* [1.45]	Rains soil; CE=7.1 me/100 g; pH 6; SA=18.2 m^2/g		BE	279
1.94	[3.95]		11	2	1.7* [0.99]	Norfolk soil; CE=2.3 me/100 g; pH 6; SA=4.4 m^2/g		BE	279
	[2.30]				63* [36.5]	Mesic peat (acid treated); 0.01 M $CaCl_2$		BE	477
	2.30					Peat humic acid		ED	423
	2.91					Soil; experimental (literature)			217
	2.79av					38 soils (literature)			87
	2.72					Correlation log K_{oc}−log S			564
Propazine (**pK_a=1.85**, Ref. 247)									
TA				100		H−montmorillonite (1−0.2 μm); pH 3.35; CE=73.5 me/100 g;	25	BE	250
1.26° (1.12)				100		Na−montmorillonite (1−0.2 μm); pH 6.80; CE=87.0 me/100 g	25	BE	250
0.67° (0.98)	2.16	57.8	19.6	22.6	5.6* [3.25]	Vetroz soil; pH 6.7;	20	BE	630
0.36° (1.15)		38.4	49.4	12.2	3.6* [2.09]	Evouettes soil; pH 6.1	20	BE	630
0.70	2.59			75	1.3	Eurosol-1; c soil; pH 5.1; 0.01 M $CaCl_2$		BE	583
0.49	1.93			22.6	3.7	Eurosol-2; sil; pH 7.4; 0.01 M $CaCl_2$		BE	583
0.61	2.08			17.0	3.45	Eurosol-3; l; pH 5.2; 0.01 M $CaCl_2$		BE	583
0.14	1.95			20.3	1.55	Eurosol-4; si; pH 6.5; 0.01 M $CaCl_2$		BE	583
1.66	2.70			6.0	9.25	Eurosol-5; ls; pH 3.2; 0.01 M $CaCl_2$		BE	583
−0.10° (0.91)	[1.62]			18	3.3* [1.91]	Lakeland sl soil; pH 6.2; CE=2.9 me/100 g; 0.01 M $CaCl_2$	26	BE	633
0.20° (0.99)	[2.16]			43	1.9* [1.10]	Wehadkee sil soil; pH 5.6; CE=10.2 me/100 g; 0.01 M $CaCl_2$	26	BE	633
0.66° (0.96)	[2.26]			38	4.4* [2.55]	Chillum sil soil; pH 4.6; CE=7.6 me/100 g; 0.01 M $CaCl_2$	26	BE	633
0.57° (0.94)	[2.17]			48	4.3* [2.49]	Hagerstown sicl soil; pH 5.5; CE=12.5 me/100 g; 0.01 M $CaCl_2$	26	BE	633
0.04	[2.00]	6	74	20	1.9* [1.1]	Putnam soil; pH 5.3; CE=12.3 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.48	[2.10]	4	66	30	4.2* [2.4]	Marshall soil; pH 5.4; CE=21.3 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.45	[2.12]	3	67	30	3.6* [2.1]	Grundy soil; pH 5.6; CE=13.5 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.32	[2.41]	9	74	17	1.4* [0.81]	Marian soil; pH 4.6; CE=9.9 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.43	[2.21]	4	72	24	2.9* [1.7]	Knox soil; pH 5.4; CE=18.8 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.45	[2.12]	26	43	31	3.6* [2.1]	Shelby soil; pH 4.3; CE=20.1 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.34	[2.40]	30	44	26	1.5* [0.87]	Lindley soil; pH 4.7; CE=6.9 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.49	[2.38]	1	36	63	2.2* [1.3]	Wabash soil; pH 5.7; CE=40.3 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.28	[2.19]	32	50	18	2.1*	Salix soil; pH 6.3;	20	BE	145

TABLE 8. Sorption coefficients for pesticides—Continued

log K_d log K_f^0 (1/n)	log K_{oc}	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
					[1.2]	CE=17.9 me/100 g; 0.01 M $CaCl_2$			
0.08	[2.20]	40	41	19	1.3* [0.75]	Sarpy soil; pH 7.1; CE=14.3 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.53	[2.08]	5	48	47	4.9* [2.8]	Summit soil; pH 4.8; CE=35.1 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.28	[1.92]	5	67	28	2.9* [1.7]	Oswego soil; pH 6.4; CE=21.0 me/100 g; 0.01 M $CaCl_2$	20	BE	145
−0.15	[1.93]	1	76	23	1.4* [0.81]	Bates soil; pH 6.5; CE=9.3 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.26	[2.06]	1	76	23	2.7* [1.6]	Gerald soil; pH 4.7; CE=11.0 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.15	[2.18]	11	75	14	1.6* [0.93]	Newtonia soil; pH 5.2; CE=8.8 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.26	[2.01]	8	72	20	3.0* [1.7]	Eldon soil; pH 5.9; CE=12.9 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.28	[2.19]	9	72	19	2.1* [1.2]	Baxter soil; pH 6.0; CE=11.2 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.26	[2.11]	4	85	11	2.4* [1.4]	Menfro soil; pH 5.3; CE=9.1 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.38	[2.36]	2	79	19	1.8* [1.04]	Union soil; pH 5.4; CE=6.8 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.30	[2.28]	13	70	17	1.8* [1.04]	Lebanon soil; pH 4.9; CE=7.7 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.32	[2.41]	20	67	13	1.4* [0.81]	Clarksville soil; pH 5.7; CE=5.7 me/100 g; 0.01 M $CaCl_2$	20	BE	145
−0.15	[2.00]	20	63	17	1.2* [0.70]	Cumberland soil; pH 6.4; CE=6.5 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.48	[2.32]	25	30	45	2.5* [1.5]	Sharkey soil; pH 5.0; CE=28.2 me/100 g; 0.01 M $CaCl_2$	20	BE	145
−1.00	[1.46]	84	11	5	0.6* [0.35]	Lintonia soil; pH 5.3; CE=3.2 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.30	[2.24]	14	66	20	2.0* [1.2]	Waverley soil; pH 6.4; CE=12.8 me/100 g; 0.01 M $CaCl_2$	20	BE	145
1.08	2.56				3.27	Hickory Hill sediment; coarse silt fraction (20–50 μm)	25	BE	130
	2.20					Soil; experimental (literature)			217
	2.19av					36 soils (literature)			87
	2.55					Correlation log K_{oc}–log K_{ow}			96
	3.47					Correlation log K_{oc}–log S			96
	2.49					Correlation log K_{oc}–log S(mp)			96
	3.11					Correlation log K_{oc}–log S			564
						Simazine (**pK_a=1.65**, Ref. 679)			
2.82				100		Mississippi bentonite; pH 8.5	0	BE	251
1.45						Idem	50		251
1.23° (0.95)						Ca-Wyoming smectite; pH 7.9; SA(N_2)=23 m^2/g; 0.01 M $CaCl_2$	20	BE	640
3.60° (0.88)						Fe-Wyoming smectite; pH 2.9; SA(N_2)=36 m^2/g; 0.01 M $CaCl_2$	20	BE	640
0.93°						Illite; pH 7; CE=24 me/100 g; 0.01 M $CaCl_2$	20	BE	145
1.05						Idem; pH 5			145
0.43						Putnam clay; pH 7; CE=42 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.78						Idem; pH 5			145
1.09						Montmorillonite; pH 7; CE=105 me/100 g; 0.01 M $CaCl_2$	20	BE	145
1.09						Idem; pH 5			145
1.59	[1.94]				77* [44.7]	Houghton muck; pH 5.6	0	BE	251
1.58	[1.93]					Idem	50		251
[0.82]	[2.83]			29.0	1.67*	Dundee sicl soil; pH 5.0;	26	BE	38

TABLE 8. Sorption coefficients for pesticides—Continued

$\log K_d$ $\log K_f^0$ ($1/n$)	$\log K_{oc}$	Sorbent composition (%) Sand	 Silt	 Clay	 OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
					[0.97]	CE=18.1 me/100 g; 0.01 M $CaCl_2$			
[0.56]	[1.96]			34.4	6.90* [4.00]	Barnes cl soil; pH 7.4; CE=33.8 me/100 g; 0.01 M $CaCl_2$	26	BE	38
[0.54]	[2.06]			23.2	5.27* [3.06]	Iredell sil (topsoil); pH 5.4; CE=17.0 me/100 g; 0.01 M $CaCl_2$	26	BE	38
[0.77]	[2.41]			67.1	3.90* [2.26]	Sharkey c soil; pH 6.2; CE=40.2 me/100 g; 0.01 M $CaCl_2$	26	BE	38
−0.26	[2.63]	97.1	2.3	0.6	0.13	Tampa aquifer; pH 8; 0.01 N $CaCl_2$		BE	521
0.46° (0.84)		57.8	19.6	22.6	5.6* [3.25]	Vetroz soil; pH 6.7	20	BE	630
0.25° (0.78)		38.4	49.4	12.2	3.6* [2.09]	Evouettes soil; pH 6.1	20	BE	630
−0.19° (0.83)		87.0	10.2	2.8	2.2* [1.28]	Collombey soil; pH 7.8	20	BE	630
0.29	[2.08]	30.1	55.2	14.7	1.64	Valois soil; pH 5.9; 0.005 M $CaSO_4$	23–27	BE	527
1.18	3.07			75	1.3	Eurosol-1; c; pH 5.1; 0.01 M $CaCl_2$		BE	583
0.21	1.64			22.6	3.7	Eurosol-2; sil; pH 7.4; 0.01 M $CaCl_2$		BE	583
0.22	1.68			17.0	3.45	Eurosol-3; l; pH 5.2; 0.01 M $CaCl_2$		BE	583
−0.20	1.61			20.3	1.55	Eurosol-4; si; pH 6.5; 0.01 M $CaCl_2$		BE	583
1.45	2.48			6.0	9.25	Eurosol-5; ls; pH 3.2; 0.01 M $CaCl_2$		BE	583
0.40	[1.79]	2.9	68.7	28.4	7.1* [4.12]	Lanton soil; pH 6.4; CE=32.8 me/100 g;		BE	631
−0.05° (0.75)				18	3.3* [1.91]	Lakeland sl soil; pH 6.2; CE=2.9 me/100 g; 0.01 M $CaCl_2$	26	BE	633
0.43° (0.76)				43	1.9* [1.10]	Wehadkee sil soil; pH 5.6; CE=10.2 me/100 g; 0.01 M $CaCl_2$	26	BE	633
0.52° (0.84)				38	4.4* [2.55]	Chillum sil soil; pH 4.6; CE=7.6 me/100 g; 0.01 M $CaCl_2$	26	BE	633
0.52° (0.78)				48	4.3* [2.49]	Hagerstown sicl soil; pH 5.5; CE=12.5 me/100 g; 0.01 M $CaCl_2$	26	BE	633
−0.82	1.88	61	25	14	0.20	Hanford sl soil; CE=6.25 me/100 g	20	BE, MD	422
[−0.01]	[1.68]				3.53* [2.05]	Batcombe sil soil; pH 6.1; 0.01 M $CaCl_2$	20	BE	120
0.02° (0.90)	[2.18]		1.5	1.3	1.2* [0.70]	Bassendean soil; CE=2.4 cmol/kg; pH 5.0; SA(N_2)=0.4 m^2/g; 0.005 M $CaCl_2$		BE	143
−0.05° (0.97)	[1.95]		8.3	15.3	1.7* [0.99]	Gascoyne soil; CE=24.8 cmol/kg; pH 6.9; SA(N_2)=22.5 m^2/g; 0.005 M $CaCl_2$		BE	143
−0.28	[2.18]		2.5	13.6	0.6* [0.35]	Cobiac soil; CE=3.5 cmol/kg; pH 5.1; SA(N_2)=13.4 m^2/g; 0.005 M $CaCl_2$		BE	143
0.93° (0.70)			14.2	63.7	4.6* [2.67]	Wellesley soil; CE=43.0 cmol/kg; pH 5.9; SA(N_2)=73.1 m^2/g; 0.005 M $CaCl_2$		BE	143
0.34	[2.30]	6	74	20	1.9* [1.1]	Putnam soil; pH 5.3; CE=12.3 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.86	[2.48]	4	66	30	4.2* [2.4]	Marshall soil; pH 5.4; CE=21.3 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.81	[2.49]	3	67	30	3.6* [2.1]	Grundy soil; pH 5.6; CE=13.5 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.54	[2.64]	9	74	17	1.4* [0.81]	Marian soil; pH 4.6 CE=9.9 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.71	[2.48]	4	72	24	2.9*	Knox soil; pH 5.4	20	BE	145

TABLE 8. Sorption coefficients for pesticides—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%)				Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
					[1.7]	CE=18.8 me/100 g; 0.01 M $CaCl_2$			
0.71	[2.39]	26	43	31	3.6* [2.1]	Shelby soil; pH 4.3; CE=20.1 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.42	[2.48]	30	44	26	1.5* [0.87]	Lindley soil; pH 4.7; CE=6.9 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.78	[2.67]	1	36	63	2.2* [1.3]	Wabash soil; pH 5.7; CE=40.3 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.54	[2.46]	32	50	18	2.1* [1.2]	Salix soil; pH 6.3; CE=17.9 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.30	[2.43]	40	41	19	1.3* [0.75]	Sarpy soil; pH 7.1; CE=14.3 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.90	[2.44]	5	48	47	4.9* [2.8]	Summit soil; pH 4.8; CE=35.1 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.59	[2.37]	5	67	28	2.9* [1.7]	Oswego soil; pH 6.4; CE=21.0 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.00	[2.09]	1	76	23	1.4* [0.81]	Bates soil; pH 6.5; CE=9.3 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.62	[2.43]	1	76	23	2.7* [1.6]	Gerald soil; pH 4.7; CE=11.0 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.48	[2.51]	11	75	14	1.6* [0.93]	Newtonia soil; pH 5.2; CE=8.8 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.46	[2.22]	8	72	20	3.0* [1.7]	Eldon soil; pH 5.9; CE=12.9 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.36	[2.28]	9	72	19	2.1* [1.2]	Baxter soil; pH 6.0; CE=11.2 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.40	[2.26]	4	85	11	2.4* [1.4]	Menfro soil; pH 5.3; CE=9.1 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.58	[2.56]	2	79	19	1.8* [1.04]	Union soil; pH 5.4; CE=6.8 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.45	[2.43]	13	70	17	1.8* [1.04]	Lebanon soil; pH 4.9; CE=7.7 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.15	[2.24]	20	67	13	1.4* [0.81]	Clarksville soil; pH 5.7; CE=5.7 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.08	[2.23]	20	63	17	1.2* [0.70]	Cumberland soil; pH 6.4; CE=6.5 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.85	[2.68]	25	30	45	2.5* [1.5]	Sharkey soil; pH 5.0; CE=28.2 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.00	[2.46]	84	11	5	0.6* [0.35]	Lintonia soil; pH 5.3; CE=3.2 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.49	[2.43]	14	66	20	2.0* [1.2]	Waverley soil; pH 6.4; CE=12.8 me/100 g; 0.01 M $CaCl_2$	20	BE	145
1.33						Wisconsin peat; pH 7; CE=118 me/100 g; 0.01 M $CaCl_2$	20	BE	145
1.36						Idem; pH 5	20	BE	145
1.92						Peal moss; pH 7; CE=106 me/100 g; 0.01 M $CaCl_2$	20	BE	145
0.85	2.33				3.27	Hickory Hill sediment; coarse si fraction (20–50 μm)	25	BE	130
1.84° (0.91)	[2.41]				50.16	Soil humic acid; pH 2.9; 0.01 M $CaCl_2$	20	BE	640
2.11° (0.91)	[2.41]				49.83	Fluka humic acid; pH 4.6; 0.01 M $CaCl_2$	20	BE	640
	2.13					Soil; experimental (literature)			217
	2.14av					147 soils (literature)			87
	1.77					Correlation $\log K_{oc}-\log K_{ow}$			96
	3.66					Correlation $\log K_{oc}-\log S$			96
	2.53					Correlation $\log K_{oc}-\log S$(mp)			96
	3.34					Correlation $\log K_{oc}-\log S$			564
						Simetone ($\mathbf{pK_a=4.15}$, Ref. 247)			
TA				100		H–montmorillonite (1–0.2 μm); pH 3.35; CE=73.5 me/100 g	25	BE	250

TABLE 8. Sorption coefficients for pesticides—Continued

log K_d log K_f^0 $(1/n)$	log K_{oc}	Sorbent composition (%)				Other sorbent and solution data: prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
3.34° (0.31)				100		Na–montmorillonite (1–0.2 μm); pH=6.80; CEC=87.0 me$_q$/100 g	25	BE	250
						Simetryne			
TA				100		H–montmorillonite; pH 3.6		BE	212
1.30				100		Na–montmorillonite; pH 7.9		BE	212
1.59				100		Ca–montmorillonite; pH 7.9		BE	212
1.65				100		Mg–montmorillonite; pH 8.2		BE	21″
	2.18					Correlation log K_{oc}–log S			564
						Sulfometuron methyl (pK$_a$=5.3, Ref. 674)			
−0.25	1.12		12	3	4.27	Forest soil (0–5 cm); pH 4.10; CE=12.1 cmol/kg; 0.01 M CaCl$_2$	25	BE	301
−0.89	1.10		10	5	1.02	Idem (5–10 cm); pH 4.22; CE=8.1 cmol/kg			301
−1.35	0.77		8	3	0.76	Idem (15–20 cm); pH 4.64; CE=6.3 cmol/kg			301
−0.95	0.55		8	3	3.19	Forest soil (0–5 cm); pH 4.99; CE=8.9 cmol/kg; 0.01 M CaCl$_2$	25	BE	301
−1.23	0.51		8	3	1.83	Idem (5–10 cm); pH 5.11; CE=5.6 cmol/kg			301
−1.35	0.77		7	4	0.76	Idem (15–20 cm); pH 5.30; CE=4.2 cmol/kg			301
−1.38	1.54		4	3	0.12	Idem (65–70 cm); pH 5.80; CE=1.3 cmol/kg			301
−0.99	0.10		8	4	8.25	Forest soil (0–5 cm); pH 5.45; CE=17.7 cmol/kg; 0.01 M CaCl$_2$	25	BE	301
−1.15	0.64		9	4	1.61	Idem (5–10 cm); pH 5.01; CE=14.4 cmol/kg			301
−1.39	0.67		6	4	0.87	Idem (15–20 cm); pH 5.20; CE=10.2 cmol/kg			301
−0.92	0.36		9	4	5.27	Forest soil (0–5 cm); pH 4.76; CE=10.9 cmol/kg; 0.01 M CaCl$_2$	25	BE	301
−0.28	0.59		9	4	1.34	Idem (5–10 cm); pH 4.79; CE=8.9 cmol/kg			301
−1.42	0.65		9	4	0.86	Idem (15–20 cm); pH 5.02; CE=6.9 cmol/kg			301
−1.06	0.44		3	4	3.18	Forest soil (0–5 cm); pH 5.04; CE=6.9 cmol/kg; 0.01 M CaCl$_2$	25	BE	301
−1.13	0.60		3	4	1.88	Idem (5–10 cm); pH 4.92; CE=5.1 cmol/kg			301
−0.86	0.91		2	5	1.70	Idem (15–20 cm); pH 4.73; CE=5.9 cmol/kg			301
−0.85	0.21		7	4	8.73	Forest soil (0–5 cm); pH 5.06; CE=11.2 cmol/kg; 0.01 M CaCl$_2$	25	BE	301
−1.19	0.86		4	4	0.83	Idem (5–10 cm); pH 4.94; CE=6.3 cmol/kg			301
−1.32	0.91		1	3	0.59	Idem (15–20 cm); pH 4.81; CE=8.1 cmol/kg			301
−1.72	1.19		0	1	0.12	Idem (65–70 cm); pH 5.60; CE=2.1 cmol/kg			301
−0.92-−0.17	0.85-2.08			10-48	0.6-3.0	5 soils; pH 5.4–7.7		BE	666
						2,4,5-T (pK$_a$=2.84, Ref. 679)			
2.02° (0.42)				100		H–montmorillonite (1–0.2 μm); pH 3.35; CE=73.5 me/100 g	25	BE	250
0.81° (0.81)			61	27	3* [1.7]	Palouse soil; pH 5.9	23	BE	667
−0.04° (0.85)			30	31	0.8* [0.46]	Glendale soil; pH 7.7	23	BE	667
0.50°	[2.26]		61	27	3.0*	Palouse soil; pH 5.9;	25	BE	668

TABLE 8. Sorption coefficients for pesticides—Continued

log K_d log K_f^0 (1/*n*)	log K_{oc}	Sorbent composition (%)				Other sorbent and solution data: prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
(0.90)					[1.74]	soil:solut.=1:1			
0.85° (0.91)	[2.60]					Idem; pH 5.80; 0.01 N $CaCl_2$ soil:solut.=1:1			668
1.08° (0.89)	[2.84]					Idem; pH 5.15; 0.1 N $CaCl_2$ soil:solut=1:1			668
0.77° (0.84)						Idem; pH 5.85; 0.01 N $CaSO_4$ soil:solut=1:1			668
0.91° (0.84)						Idem; pH 5.85; 0.01 N $CaSO_4$; soil:solut.=1:3.3			668
0.92° (0.80)						Idem; pH 5.85; 0.01 N $CaSO_4$: soil:solut.=1:10			668
0.93° (0.86)						Idem; pH 5.85; 0.01 N $CaSO_4$; solut.=1:33			668
0.86° (0.92)	[2.62]					Idem; pH 5.85; 0.01 N $CaSO_4$; soil:solut.=1:1	5		668
0.79° (0.91)	[2.55]					Idem; pH 5.85; 0.01 N $CaSO_4$; soil:solut.=1:1	15		668
0.72° (0.90)	[2.48]					Idem; pH 5.85; 0.01 N $CaSO_4$; soil:solut.=1:1	35		668
0.79° (0.78)		55	20	25	3.34	Webster soil; pH 7.3; CE=22 me/100 g		BE	192
−0.31° (0.94)	[1.97]				0.53	Glendale soil; pH 8.5		BE	669
0.48° (0.86)					2.43	Palouse soil; pH 6.5		BE	669
−0.51° (1.50)					0.80	Ephrata soil; pH 7.5		BE	669
0.38° (0.95)	[1.82]				3.66	Ordnance soil; pH 6.6		BE	669
−0.37° (0.85)				31.4	0.47	Glendale cl soil; pH 7.9. 0.01 N $CaSO_4$		BE	484
0.04° (0.87)					0.90	Glendale c soil: (no addition of sewage sludge); 0.01 N $CaCl_2$		BE	647
0.03° (0.93)	[1.87]				1.45	Idem; freshly amended (+22.4 metric tons/ha sewage sludge)			647
0.03° (0.94)	[1.81]				1.66	Idem; freshly amended (+44.9 metric tons/ha sewage sludge)			647
0.06° (0.87)					0.86	Idem; preconditioned (no addition of sewage sludge)			647
0.12° (0.90)	[1.98]				1.37	Idem; preconditioned (+44.9 metric tons/ha sewage sludge)			647
0.15° (0.91)	[1.94]				1.61	Idem; preconditioned (+80.8 metric tons/ha sewage sludge)			647
−0.37° (0.90)	[1.86]				0.60	Harvey fine sl soil; (no addition of sewage sludge); 0.01 N $CaCl_2$		BE	647
−0.36° (0.96)	[1.59]				1.12	Idem; freshly amended (+22.4 metric tons/ha sewage sludge)			647
−0.26° (0.98)	[1.61]				1.36	Idem; freshly amended (+44.9 metric tons/ha sewage sludge)			647
−0.43° (0.91)	[1.78]				0.62	Idem; preconditioned (no addition of sewage sludge)			647
−0.39° (0.90)	[1.83]				0.64	Idem; preconditioned (+44.9 metric tons/ha sewage sludge)			647
−0.28° (0.92)	[1.91]				0.65	Idem; preconditioned (+89.8 metric tons/ha sewage sludge)			647
−0.15° (0.89)					0.66	Lea sl soil; (no addition of sewage sludge); 0.01 N $CaCl_2$		BE	647
−0.21° (0.93)	[1.70]				1.23	Idem; freshly amended (+22.4 metric tons/ha sewage sludge)			647
−0.17° (0.95)	[1.64]				1.57	Idem: freshly amended (+44.9 metric tons/ha sewage sludge)			647
−0.18° (0.86)					0.74	Idem; preconditioned (no addition of sewage sludge)			647

TABLE 8. Sorption coefficients for pesticides—Continued

log K_d log K_f^0 (1/n)	log K_{oc}	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
−0.04° (0.91)	[1.85]				1.31	Idem; preconditioned (+44.9 metric tons/ha sewage sludge)			647
0.06° (0.95)	[1.86]				1.57	Idem; preconditioned (+89.8 metric tons/ha sewage sludge)			647
− 0.21° (0.79)		38.8	29.8	31.4	0.8* [0.46]	Glendale soil; pH 7.7; CE=31.1 me/100 g; 0.01 N $CaCl_2$		BE	509
1.32° (0.97)	2.63	89.2	8.2	2.6	4.85	Podzol soil; pH 2.8; CE=15.1 me/100 g		BE	163
−0.13° (1.14)		69.7	14.4	15.9	1.25	Alfisol soil; pH 6.7; CE=12.3 me/100 g		BE	163
0.14° (0.84)		5.5	58.8	35.7	1.58	Lake Constance sedim.; pH 7.1; CE=13.4 me/100 g		BE	163
	1.72					Soil; experimental (literature)			217
	1.90av					4 soils (literature)			87
	2.34					Correlation log K_{oc}−log S			564
	1.70					Correlation log K_{oc}−MCI			578
					Tebuthiuron (pK_a=1.2, Ref. 287)				
0.56	1.92		12	3	4.27	Forest soil (0–5 cm); pH 4.10; CE=12.1 cmol/kg; 0.01 M $CaCl_2$	25	BE	301
−0.26	1.74		10	5	1.02	Idem (5–10 cm); pH 4.22; CE=8.1 cmol/kg			301
−0.81	1.31		8	3	0.76	Idem (15–20 cm); pH 4.64; CE=6.3 cmol/kg			301
0.20	1.69		8	3	3.19	Forest soil (0–5 cm); pH 4.99; CE=8.9 cmol/kg; 0.01 M $CaCl_2$	25	BE	301
−0.24	1.50		8	3	1.83	Idem (5–10 cm); pH 5.11; CE=5.6 cmol/kg			301
−1.02	1.10		7	4	0.76	Idem (15–20 cm); pH 5.30; CE=4.2 cmol/kg			301
−1.56	1.36		4	3	0.12	Idem (65–70 cm); pH 5.80; CE=1.3 cmol/kg			301
0.31	1.39		8	4	8.25	Forest soil (0–5 cm); pH 5.45; CE=17.7 cmol/kg; 0.01 M $CaCl_2$	25	BE	301
−0.28	1.51		9	4	1.61	Idem (5–10 cm); pH 5.01; CE=14.4 cmol/kg			301
−0.64	1.42		6	4	0.87	Idem (15–20 cm); pH 5.20; CE=10.2 cmol/kg			301
0.26	1.54		9	4	5.27	Forest soil (0–5 cm); pH 4.76; CE=10.9 cmol/kg; 0.01 M $CaCl_2$	25	BE	301
−0.55	1.32		9	4	1.34	Idem (5–10 cm); pH 4.79; CE=8.9 cmol/kg			301
−0.75	1.31		9	4	0.86	Idem (15–20 cm); pH 5.02; CE=6.9 cmol/kg			301
0.15	1.64		3	4	3.18	Forest soil (0–5 cm); pH 5.04; CE=6.9 cmol/kg; 0.01 M $CaCl_2$	25	BE	301
−0.07	1.65		3	4	1.88	Idem (5–10 cm); pH 4.92; CE=5.1 cmol/kg			301
0.05	1.82		2	5	1.70	Idem (15–20 cm); pH 4.73; CE=5.9 cmol/kg			301
0.39	1.45		7	4	8.73	Forest soil (0–5 cm); pH 5.06; CE=11.2 cmol/kg; 0.01 M $CaCl_2$	25	BE	301
−0.42	1.63		4	4	0.83	Idem (5–10 cm); pH 4.94; CE=6.3 cmol/kg			301
−0.92	1.31		1	3	0.59	Idem (15–20 cm); pH 4.81; CE=8.1 cmol/kg			301
−1.41	1.51		0	1	0.12	Idem (65–70 cm); pH 5.60; CE=2.1 cmol/kg			301
−1.0–0.40	1.59				0.17–2.78	4 soils (0–20 cm)		BE	670
	2.79					Soil; experimental (literature)			217
	1.79					Correlation log K_{oc}−log S			564

TABLE 8. Sorption coefficients for pesticides—Continued

log K_d log K_f^0 (1/n)	log K_{oc}	Sorbent composition (%)				Other sorbent and solution data: prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
Terbacil (pK_a~9, Ref. 679)									
0.39° (0.88)	1.80	18.4	45.3	38.3	3.87	Webster soil; pH 7.3; CE=54.7 me/100 g; 0.01 N $CaCl_2$	23	BE	102
−0.42° (0.99)	1.63	65.8	19.5	14.7	0.90	Cecil soil; pH 5.6; CE=6.8 me/100 g; 0.01 N $CaCl_2$	23	BE	102
−0.92° (0.88)	1.33	93.8	3.0	3.2	0.56	Eustis soil; pH 5.6; CE=5.2 me/100 g; 0.01 N $CaCl_2$	23	BE	102
0.23° (0.50)					2.1* [1.2]	Keyport sil soil; pH 5.4; average particle size=5.6 μm		BE	641
−0.82° (0.96)	[1.56]				0.7* [0.41]	Cecil ls soil; pH 5.8; aver. particle size=10.5		BE	641
	1.71					Soil; experimental (literature)			217
	1.61av					4 soils (literature)			87
	1.50					Correlation log K_{oc}−log K_{ow}			96
	2.32					Correlation log K_{oc}−log S			96
	1.05					Correlation log K_{oc}−log S(mp)			96
	2.08					Correlation log K_{oc}−log S			564
Terbufos									
0.49° (0.95)	[2.78]	77	15	8	0.51	Sarpy soil; pH 7.3; CE=5.7 me/100 g; 0.01 M $CaCl_2$	24	BE	122
1.03° (0.94)	[3.00]	83	9	8	1.07	Thurman soil; pH 6.83; CE=6.1 me/100 g; 0.01 M $CaCl_2$	24	BE	122
0.90° (0.96)	[2.48]	37	42	21	2.64	Clarion agricultural soil; pH 5.00; CE=21.0 me/100 g; 0.01 M $CaCl_2$	24	BE	122
1.31° (0.97)	[2.73]	21	55	24	3.80	Harps agricultural soil; pH 7.30; CE=37.8 me/100 g; 0.01 M $CaCl_2$	24	BE	122
1.70° (0.97)	[2.44]	42	39	19	18.36	Peat; pH 6.98; CE=77.34 me/100 g	24	BE	122
0.94° (0.83)		15.2	63.8	20.5	1.94* [1.13]	Soil (Versailles); pH 6.4; CE=10 me/100 g		BE	671
[1.08]	[3.03]					Idem (linear isotherm)			671
1.08° (0.87)		2.0	14.9	8.7	2.82* [1.64]	Soil (Chalons/Marne); pH 8.1; CE=7.9 me/100 g		BE	671
[1.21]	[3.00]					Idem (linear isotherm)			671
1.21° (0.85)		30.3	52.6	16.9	7.18* [4.16]	Soil, l; pH 6.5; CE=16.7 me/100 g		BE	671
	[2.75]					Idem (linear isotherm)			671
	3.04					Correlation log K_{oc}−log S			564
Terbutryn									
2.73	4.62			75	1.3	Eurosol-1; c soil; pH 5.1; 0.01 M $CaCl_2$		BE	583
2.08	3.51			22.6	3.7	Eurosol-2; sil; pH 7.4; 0.01 M $CaCl_2$		BE	583
1.99	3.45			17.0	3.45	Eurosol-3; l; pH 5.2; 0.01 M $CaCl_2$		BE	583
1.63	3.44			20.3	1.55	Eurosol-4; si; pH 6.5; 0.01 M $CaCl_2$		BE	583
2.91	3.94			6.0	9.25	Eurosol-5; ls; pH 3.2; 0.01 M $CaCl_2$		BE	583
	2.85					Soil; experimental (literature)			217
	2.87					Correlation log K_{oc}−log S			564
Tetrachlorvinphos									
1.30	[3.05]		5.2	3.6	3.1* [1.80]	Surface soil (Naaldwijk); pH 6.9; 0.007 M $CaCl_2$		BE	663
1.29	[2.98]		18.8	9.2	3.6* [2.09]	Surface soil (Honselersdijk II); pH 7.0; 0.007 M $CaCl_2$		BE	663
2.06	[3.32]		37.0	19.8	9.7* [5.63]	Surface soil (Aalsmeer); pH 7.1; 0.007 M $CaCl_2$		BE	663
	3.07					Correlation log K_{oc}−log S			564

TABLE 8. Sorption coefficients for pesticides—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data: prediction procedure	Temp. (°C)	Meth.	Ref.
						Triallate			
1.20° (0.97)				100		Georgia kaolinite No. 4; pH 7.1	25	BE	475
1.00° (0.99)				100		Wyoming montmorillonite No. 25; pH 9.9	25	BE	475
2.85° (0.94)						Peat moss; pH 3.8	25	BE	475
1.66° (0.97)						Silica gel (24–32 mesh/cm); pH 7.0	25	BE	475
2.56° (1.04)						Wheat straw; pH 6.0	25	BE	475
−0.28	[1.68]			16.2	1.11	Conventional farm soil; pH 5.42; 0.004 M $CaSO_4$		BE	646
−0.28	[1.72]			19.7	1.00	Idem; pH 5.35			646
−0.54	[1.66]			24.7	0.64	Idem; pH 7.12			646
−0.08	[1.65]			16.5	1.85	Low-input farm soil; pH 5.53; 0.004 M $CaSO_4$		BE	646
−0.14	[1.76]			16.6	1.26	Idem; pH 5.47			646
−0.29	[1.77]			19.1	0.86	Idem; pH 6.32			646
1.51	[3.65]	48.2	42.1	9.7	1.24* [0.72]	San Joaquin soil; pH 7.2	25	BE	672
1.91	[3.44]	5.8	69.0	25.2	5.1* [2.96]	Flanagan soil; pH 5.5	25	BE	672
1.08° (0.94)	[3.45]	67.1	25.8	7.1	0.43	Hanford soil; pH 6.05; CE=5.95 cmol/kg; 0.01 M $CaCl_2$	25	BE	528
0.97° (0.77)		82.0	13.5	4.5	0.33	Tuiunga soil; pH 6.30; CE=0.45 cmol/kg; 0.01 M $CaCl_2$	25	BE	528
[2.38]	[3.52]	45.5	41.0	13.5	12.4* [7.19]	Lacombe soil; pH 7.7; 0.1 M $CaCl_2$		BE	33
[2.12]	[3.55]	53.5	27.5	19.2	6.5* [3.77]	Weyburn soil; pH 6.5; 0.1 M $CaCl_2$		BE	33
[2.06]	[3.67]	5.3	25.3	69.5	4.2* [2.44]	Regina soil; pH 7.8; 0.1 M $CaCl_2$		BE	33
[1.58]	[3.56]	81.6	10.4	8	1.8* [1.04]	Asquith soil; pH 7.5; 0.1 M $CaCl_2$		BE	33
	3.35					Soil; experimental (literature)			217
	3.70					Correlation $\log K_{om}-\log S$(563)			528
	3.94					Correlation $\log K_{oc}-\log K_{ow}$(87)			528
	3.55					Correlation $\log K_{oc}-\log K_{ow}$(217)			528
	3.30					Correlation $\log K_{oc}-\log S$			564
	3.22					Correlation $\log K_{oc}$−MCI			598
						Triazophos			
1.26	[3.01]		5.2	3.6	3.1* [1.80]	Surface soil (Naaldwijk); pH 6.9; 0.007 M $CaCl_2$		BE	663
1.08	[2.76]		18.8	9.2	3.6* [2.09]	Surface soil (Honselersdijk II); pH 7.0; 0.007 M $CaCl_2$		BE	663
1.68	[2.93]		37.0	19.8	9.7* [5.63]	Surface soil (Aalsmeer); pH 7.1; 0.007 M $CaCl_2$		BE	663
	2.76					Correlation $\log K_{oc}-\log S$			564
						Trietazine (**pK_a=1.88**, Ref. 231)			
TA				100		H-montmorillonite (1–0.2 μm); pH 3.35; CE=73.5 me/100 g	25	BE	250
1.76				100		Na-montmorillonite (1–0.2 μm); pH 6.8; CE=87.0 me/100 g	25	BE	250
1.25	2.74				3.27	Hickory Hill sediment; coarse si fraction (20–50 μm)	25	BE	130
−0.31	[2.58]	97.1	2.3	0.6	0.13	Tampa aquifer; pH 8; 0.01 N $CaCl_2$		MD	521
	2.78					Soil; experimental (literature)			217
	2.96					Correlation $\log K_{oc}-\log K_{ow}$			96

TABLE 8. Sorption coefficients for pesticides—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%)				Other sorbent and solution data: prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
	3.25					Correlation $\log K_{oc}-\log S$			96
	2.36					Correlation $\log K_{oc}-\log S$(mp)			96
	2.92					Correlation $\log K_{oc}-\log S$			564
	2.60					Correlation $\log K_{oc}$ −MCI			578
						Trifluralin			
1.81° (0.96)				100		Georgia kaolinite No. 4; pH 6.7	25	BE	475
1.54				100		Wyoming montmorillonite No. 25; pH 9.5	25	BE	475
4.13° (1.41)						Peat moss; pH 3.6	25	BE	475
1.72° (0.88)						Silica gel (24–32 mesh/cm); pH 6.7	25	BE	475
2.92° (1.04)						Wheat straw; pH 5.8	25	BE	475
2.48	[4.12]	6	71	23	4.0* [2.32]	Plano soil (soil/solut. = 1 g/100 mL) pH 6.3; CE = 20 me/100 g	25	BE	351
2.39	[4.03]					Idem (soil/solut. = 2 g/100 mL)	25		351
2.27	[3.90]					Idem (soil/solut. = 4 g/100 mL)	25		351
2.76	[4.40]					Idem (soil/solut. = 2 g/100 mL)	5		351
1.53	[2.95]	17	64	19	6.5* [3.77]	Adolph soil; pH 6.2; CE = 22.5 me/100 g	22	BE	345
0.92	[2.81]	9	78	13	2.2* [1.28]	Fayette soil; pH 6.5; CE = 7.7 me/100 g	22	BE	345
1.04	[2.98]	23	42	35	2.0* [1.16]	Kewaunee soil; pH 7.8; CE = 19.2 me/100 g	22	BE	345
1.26	[2.93]	12	61	27	3.7* [2.15]	Ontonagon soil; pH 6.6; CE = 13.8 me/100 g	22	BE	345
1.13	[3.07]	27	12	61	2.0* [1.16]	Peebles soil; pH 7.4; CE = 23.4 me/100 g	22	BE	345
0.57	[2.91]	89	6	5	0.8* [0.46]	Plainfield soil; pH 6.6; CE = 3.7 me/100 g	22	BE	345
1.06	[2.62]	17	66	17	4.8* [2.78]	Plano soil; pH 6.7; CE = 17.4 me/100 g	22	BE	345
1.46	[2.72]	23	62	15	9.5* [5.51]	Poigan soil; pH 7.0; CE = 33.6 me/100 g	22	BE	345
1.58	[2.75]	59	30	11	11.7* [6.79]	Sebewa soil; pH 6.8; CE = 28.4 me/100 g	22	BE	345
1.39	[3.02]	17	73	10	4.1* [2.38]	Withee soil; pH 6.5; CE = 10.9 me/100 g	22	BE	345
1.44	[2.83]	2.9	68.7	28.4	7.1* [4.12]	Lanton soil; pH 6.4; CE = 32.8 me/100 g		BE	631
1.75	3.13	18.9	26.3	54.8	4.24	Tsukuba soil; pH 6.5; 0.01 M $CaCl_2$	25	BE	642
3.36° (1.64)						Idem			642
0.72	2.60	23.1	15.4	61.5	1.35	Kanuma soil; pH 5.7; 0.01 M $CaCl_2$	25	BE	642
0.56° (0.94)						Idem			642
2.61	4.71			26	0.8	Agricultural soil; pH 7.4; CE = 31 cmol/kg; 0.01 M $CaCl_2$	20	BE	297
2.79	4.71			54	1.2	Idem; pH 7.8; CE = 24 cmol/kg			297
2.04	4.44			11	0.4	Idem; pH 8.0; CE = 11 cmol/kg			297
3.48	4.59			6	7.6	Idem; pH 4.4; CE = 27 cmol/kg			297
	3.64av	38	48	14	0.68	Commerce soil; pH 6.7		BE	575
	(three	56	30	14	1.12	Tracy soil; pH 6.2		BE	575
	soils)	12	56	32	2.01	Catlin soil; pH 6.2		BE	575
3.00	4.49				3.27	Hickory Hill sediment; coarse si fraction (20–50 μm)	25	BE	130

TABLE 8. Sorption coefficients for pesticides—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
2.08	[4.22]		31.2	68.6	0.72	Missouri Riv. sed. (Big Ben Lake, SD)(18 g/L); pH 7.83; equilibr. time=10 d		GP	156
1.36	[4.32]		75.6	17.4	0.11	Loess soil (Turin, IA) (10 g/L); pH 8.34; equilibr. time=10 d		GP	156
2.98	[4.50]		27.1	52.6	3.04	Ohio Riv. sed. (Ceredo, WV) (2.5 g/L); pH 6.90; equilibr. time=21 d		GP	156
1.59	4.18			6.9	0.45* [0.26]	Mivtahim agricult. surface soil	25	BE	563
1.77	3.91			23.8	1.25* [0.73]	Gilat agricult. surface soil	25	BE	563
2.14	3.93			71.2	2.82* [1.64]	Neve Yaar agricult. surface soil	25	BE	563
2.63	4.10			76.2	5.82* [3.38]	Malkiya agricult. surface soil	25	BE	563
3.13	4.47			60.5	7.85* [4.55]	Kinneret A Lake sediment	25	BE	563
2.84	4.44			63.8	4.39* [2.55]	Kinneret G Lake sediment	25	BE	563
	3.95av					22 literature data			562
	5.13					Cyanopropyl column	20–25	RPLC	579
	3.98					C18 column		RPLC	573
	4.14					Soil; experimental (literature)			217
	3.76					Correlation $\log K_{oc}-\log S$			564

NA Not adsorbed.

TA Totally adsorbed.

Values in square parentheses have been calculated by the author.

*log K_{om} in column 2 and % OM content in column 6.

**log nonlinear K_{om} with the respective value of $(1/n)$ in below, when available.

av average value.

Idem refers to the sorbent reported just above; only the data (texture, OC, temperature, method) which were changed are specified.

TABLE 9. Sorption coefficients for miscellaneous compounds

log K_d log K_f^0 (1/n)	log K_{oc}	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
						Acetophenone			
[0.20]	2.26	4	10	86	0.11	Apison soil; pH 4.5; CE=76 me/100 g		BE	570
[0.16]		11	21	68	0.06	Fullerton soil; pH 4.4; CE=64 me/100 g		BE	570
[1.26]	2.02	2	38	60	1.2	Dormont soil; pH 4.2; CE=129 me/100 g		BE	570
−0.85	2.15			11.2	0.17* [0.10]	Netanya agricult. surface soil	25	BE	563
−1.30	1.29			6.9	0.45* [0.26]	Mivtahim agricult. surface soil	25	BE	563
−0.43	1.74			63.1	1.18* [0.68]	Golan agricult. surface soil	25	BE	563
−0.82	1.31			23.8	1.25* [0.73]	Gilat agricult. surface soil	25	BE	563
−0.52	1.56			72.5	1.42* [0.82]	Shefer agricult. surface soil	25	BE	563
−0.66	1.42			10.6	1.45* [0.84]	Bet Degan agricult. surface soil	25	BE	563
−0.41	1.38			71.2	2.82* [1.64]	Neve Yaar agricult. surface soil	25	BE	563
−0.28	1.19			76.2	5.82* [3.38]	Malkiya agricult. surface soil	25	BE	563
−0.37	1.38				3.08* [1.79]	Kinneret Lake sediment	25	BE	563
0.04	1.38			60.5	7.85* [4.55]	Kinneret A Lake sediment	25	BE	563
0.04	1.41			63.2	7.43* [4.31]	Kinneret F Lake sediment	25	BE	563
0.02	1.61			63.8	4.39* [2.55]	Kinneret G Lake sediment	25	BE	563
−0.05	1.63	3.0	41.8	55.2	2.07	River sediment; pH 7.79; CE=23.7 me/100 g	25	BE	210
−0.25	1.38	33.6	35.4	31.0	2.28	River sediment; pH 7.44; CE=19 me/100 g	25	BE	210
−0.17	1.98	0.2	31.2	68.6	0.72	River sediment; pH 7.83; CE=33 me/100 g	25	BE	210
−1.15	1.68	82.4	10.7	6.8	0.15	River sediment; pH 8.32; CE=3.7 me/100 g	25	BE	210
−1.05	1.91	7.1	75.6	17.4	0.11	Loess; pH 8.34; CE=12.4 me/100 g	25	BE	210
−0.92	1.40	2.1	34.4	63.6	0.48	Soil; pH 4.45; CE=18.9 me/100 g	25	BE	210
−0.57	1.45	15.6	48.7	35.7	0.95	River sediment; pH 7.79; CE=11.3 me/100 g	25	BE	210
−0.52	1.66	34.6	25.8	39.5	0.66	River sediment; pH 7.76; CE=15.4 me/100 g	25	BE	210
−0.54	1.34	0.0	71.4	28.6	1.30	Soil, pH 5.50; CE=8.5 me/100 g	25	BE	210
−0.07	1.65	50.2	42.7	7.1	1.88	River sediment; pH 7.60; CE=8.33 me/100 g	25	BE	210
−0.28	1.49	26.2	52.7	21.2	1.67	River sediment; pH 7.55; CE=8.53 me/100 g	25	BE	210
−0.17	1.46	17.3	13.6	69.1	2.38	River sediment; pH 6.70; CE=31.2 me/100 g	25	BE	210
−0.18	1.65	1.6	55.4	42.9	1.48	River sediment; pH 7.75; CE=20.9 me/100 g	25	BE	210
−0.36	1.56	67.6	13.9	18.6	1.21	Stream sediment; pH 6.35; CE=3.72 me/100 g	25	BE	210
0.03	[1.71]		48	35	2.08	Sangamon sediment	25	BE	673
−0.05	[1.45]		12	69	3.16	Crane Island sediment	25	BE	673
	1.73					Cyanopropyl column	20–25	RPLC	579
	1.79					C18 column; correlation log K_{oc}–(log k' + $\Delta^0\chi$)		RPLC	577

TABLE 9. Sorption coefficients for miscellaneous compounds—Continued

log K_d log K_f^0 (1/n)	log K_{oc}	Sorbent composition (%)				Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
	1.63					C18 column; correlation log K_{oc}-(log k' + hydrogen bonding index)		RPLC	577
	1.57av					30 literature data			562
	1.20					Correlation log K_{oc} – log K_{ow}			96
	1.63					Correlation log K_{oc} – log K_{ow}			207
	1.42					Correlation log K_{oc} – log K_{ow}			108
	1.64					Correlation log K_{oc} – log S			96
	1.40					Correlation log K_{oc} – log S(mp)			96
Anthraquinone									
2.35	4.24			75	1.3	Eurosol-1; c; pH 5.1; 0.01 M $CaCl_2$		BE	583
2.08	3.51			22.6	3.7	Eurosol-2; sil; pH 7.4; 0.01 M $CaCl_2$		BE	583
1.99	3.45			17.0	3.45	Eurosol-3; l; pH 5.2; 0.01 M $CaCl_2$		BE	583
1.63	3.44			20.3	1.55	Eurosol-4; si; pH 6.5; 0.01 M $CaCl_2$		BE	583
2.91	3.94			6.0	9.25	Eurosol-5; ls; pH 3.2; 0.01 M $CaCl_2$		BE	583
Benzidine (pK_{a_1}=4.66, pK_{a_2}=3.57, Ref. 681)									
2.28° (0.42)				18.6	1.21	Stream sed.; CE=3.7 me/100 g; pH 6.35; SA(E)=49.2 m^2/g	25	BE	302
2.40° (0.51)				55.2	2.07	River sed.; CE=23.7 me/100 g; pH 7.79; SA(E)=187.1 m^2/g	25	BE	302
2.38° (0.47)				31.0	2.28	River sed.; CE=19.0 me/100 g; pH 7.74; SA(E)=130.7 m^2/g	25	BE	302
2.90° (0.57)				68.6	0.72	River sed.; CE=33.0 me/100 g; pH 7.83; SA(E)=268.5 m^2/g	25	BE	302
1.57° (0.50)				6.8	0.15	River sed.; CE=3.7 me/100 g; pH 8.32; SA(E)=51.9 m^2/g	25	BE	302
2.28° (0.37)				17.4	0.11	Loess; CE=12.4 me/100 g; pH 8.37; SA(E)=109.0 m^2/g	25	BE	302
3.35° (0.66)				63.6	0.48	Soil; CE=18.9 me/100 g; pH 4.54; SA(E)=145.0 m^2/g	25	BE	302
2.69° (0.27)				35.7	0.95	River sed.; CE=11.3 me/100 g; pH 7.79; SA(E)=96.2 m^2/g	25	BE	302
2.32° (0.41)				39.5	0.66	River sed.; CE=15.4 me/100 g; pH 7.76; SA(E)=135.8 m^2/g	25	BE	302
2.95° (0.43)				28.6	1.30	Soil; CE=8.5 me/100 g; pH 5.50; SA(E)=77.6 m^2/g	25	BE	302
1.47° (0.69)				7.1	1.88	River sed.; CE=8.3 me/100 g; pH 7.60; SA(E)=72.8 m^2/g	25	BE	302
1.60° (0.64)				21.2	1.67	River sed.; CEC=8.5 me_q/100 g; pH 7.55; SA(E)=64.0 m^2/g	25	BE	302
2.71° (0.57)				69.1	2.38	River sed.; CEC=31.2 me_q/100 g; pH 6.7; SA(E)=233.2 m^2/g	25	BE	302
1.78° (0.66)				42.9	1.48	River sed.; CEC=20.9 me_q/100 g; pH 7.75; SA(E)=164.8 m^2/g	25	BE	302
	3.44					Correlation log K_{oc} – MCI			598
Dibenzothiophene									
2.07	3.99	67.6	13.9	18.6	1.21	Stream sed.; CE=3.72 me/100 g pH 6.35; SA(E)=49.18 m^2/g	25	BE	179
2.26	3.94	3.0	41.8	55.2	2.07	River sed.; CE=23.72 me/100 g pH 7.79; SA(E)=187.05 m^2/g	25	BE	179
2.22	3.87	33.6	35.4	31.0	2.28	River sed.; CE=19.00 me/100 g pH 7.44; SA(E)=130.76 m^2/g	25	BE	179
1.78	3.93	0.2	31.2	68.6	0.72	River sed.; CE=33.01 me/100 g pH 7.83; SA(E)=268.54 m^2/g	25	BE	179
0.97	3.80	82.4	10.7	6.8	0.15	River sed.; CE=3.72 me/100 g pH 8.32; SA(E)=51.94 m^2/g	25	BE	179

TABLE 9. Sorption coefficients for miscellaneous compounds—Continued

log K_d log K_f^0 (1/n)	log K_{oc}	Sorbent composition (%)				Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
		Sand	Silt	Clay	OC				
0.76	3.72	7.1	75.6	17.4	0.11	Loess; CE=12.4 me/100 g pH 8.34; SA(E)=108.96 m^2/g	25	BE	179
1.70	4.01	2.1	34.4	63.6	0.48	Soil; CE=18.86 me/100 g pH 4.54; SA(E)=145.04 m^2/g	25	BE	179
2.26	4.28	15.6	48.7	35.7	0.95	River sed.; CE=11.30 me/100 g pH 7.79; SA(E)=96.20 m^2/g	25	BE	179
1.81	3.99	34.6	25.8	39.5	0.66	River sed.; CE=15.43 me/100 g pH 7.76; SA(E)=135.76 m^2/g	25	BE	179
2.01	3.89	0.0	71.4	28.6	1.30	Soil; CE=8.50 me/100 g pH 5.50; SA(E)=77.58 m^2/g	25	BE	179
2.44	4.17	50.2	42.7	7.1	1.88	River sed.; CE=8.33 me/100 g pH 7.60; SA(E)=72.83 m^2/g	25	BE	179
2.25	4.02	26.2	52.7	21.2	1.67	River sed.; CE=8.53 me/100 g pH 7.55; SA(E)=64.04 m^2/g	25	BE	179
2.59	4.21	17.3	13.6	69.1	2.38	River sed.; CE=31.15 me/100 g pH 6.70; SA(E)=233.19 m^2/g	25	BE	179
2.13	3.96	1.6	55.4	42.9	1.48	River sed.; CE=20.86 me/100 g pH 7.75; SA(E)=164.83 m^2/g	25	BE	179
1.06° (0.85)					0.25	Kaolinite coated with Pohokee peat humic acid. 0.1 M $NaClO_4$	25	BE	228
0.48° (0.91)					0.02	Idem			228
1.69° (0.97)	[4.24]				0.28	Hematite coated with Pohokee peat humic acid. 0.1 M $NaClO_4$	25	BE	228
1.26° (0.79)					0.47	Idem			228
−0.41° (0.65)					0.02	Idem			228
	4.05					Sediments (experimental)			211
	3.99					Correlation log K_{oc}−log K_{ow}			96
	4.17					Correlation log K_{oc}−log K_{ow}(108)			228
	3.87					Correlation log K_{oc}−log S			96
	4.20					Correlation log K_{oc}−log S(mp)			96
	4.18					Correlation log K_{oc}−log S(mp)(52)			228
	4.00					Correlation log K_{oc}−MCI			597
	4.06					Correlation log K_{oc}−MCI			578
Dimethylphthalate									
−1.82	0.88	97.3	2.2	0.5	0.2	Forest soil; ph 5.6; CE=0.48 me/100 g		LE	344
−0.03	1.63	65.2	25.6	9.2	2.2	Agricultural soil; pH 7.4; CE=9.0 me/100 g		LE	344
0.41	1.84	69.5	20.5	10.1	3.7	Forest soil; pH 4.2; CE=2.9 me/100 g		LE	344
	1.64					Correlation log K_{oc}−log S			564
α-Naphthol (pK_a=9.34, Ref. 681)									
0.87	[2.58]				1.94	Hagerstown soil; silt loam; 0.01 N $CaCl_2$	23	BE	454
1.20° (0.44)				55.2	2.07	River sed.; CE=23.7 me/100 g; pH 7.79; SA(E)=187.1 m^2/g	25	BE	97
0.91° (0.55)				31.0	2.28	River sed.; CE=19.0 me/100 g; pH 7.74; SA(E)=130.7 m^2/g	25	BE	97
1.48° (0.31)				68.6	0.72	River sed.; CE=33.0 me/100 g; pH 7.83; SA(E)=268.5 m^2/g	25	BE	97
0.42° (0.61)				6.8	0.15	River sed.; CE=3.7 me/100 g; pH 8.32; SA(E)=51.9 m^2/g	25	BE	97
1.24° (0.22)				17.4	0.11	Loess sed.; CE=12.4 me/100 g; pH 8.34; SA(E)=109.0 m^2/g	25	BE	97
1.00° (.36)				52.6	3.04	River sed.; CE=12 me/100 g; pH 6.90	25	BE	97
0.45°				63.6	0.48	Soil; CE=18.9 me/100 g;	25	BE	97

TABLE 9. Sorption coefficients for miscellaneous compounds—Continued

$\log K_d$ $\log K_f^0$ $(1/n)$	$\log K_{oc}$	Sorbent composition (%) Sand	Silt	Clay	OC	Other sorbent and solution data; prediction procedure	Temp. (°C)	Meth.	Ref.
(0.56)						pH 4.54; SA(E)=145.0 m^2/g			
1.41° (0.32)				35.7	0.95	River sed.; CE=11.3 me/100 g; pH 7.79; SA(E)=96.2 m^2/g	25	BE	97
1.14° (0.28)				39.5	0.66	River sed.; CE=15.4 me/100 g; pH 7.76; SA(E)=135.8 m^2/g	25	BE	97
1.33° (0.31)				28.6	1.30	Soil; CE=8.5 me/100 g; pH 5.50; SA(E)=77.6 m^2/g	25	BE	97
0.92° (0.50)				7.1	1.88	River sed.; CE=8.3 me/100 g; pH 7.60; SA(E)=72.8 m^2/g	25	BE	97
0.94° (0.64)				21.2	1.67	River sed.; CE=8.5 me/100 g; pH 7.55; SA(E)=64.0 m^2/g	25	BE	97
1.15° (0.39)				69.1	2.38	River sed.; CE=31.2 me/100 g; pH 6.7; SA(E)=233.2 m^2/g	25	BE	97
1.01° (0.44)				42.9	1.48	River sed.; CE=20.9 me/100 g; pH 7.75; SA(E)=164.8 m^2/g	25	BE	97
0.91° (0.55)				22.5	0.90	Soil; CE=3 me/100 g; pH 6.40	25	BE	97
1.00° (0.36)				18.6	1.21	Stream sed.; CE=3.7 me/100 g; pH 6.35; SA(E)=49.2 m^2/g	25	BE	97
	5.57	4	10	86	0.11	Apison soil; pH 4.5; CE=76 me/100 g		BE	570
	>5.78	11	21	68	0.06	Fullerton soil; pH 4.4; CE=64 me/100 g		BE	570
	3.11	2	38	60	1.2	Dormont soil; pH 4.2; CE=129 me/100 g		BE	570
2.46	2.64				65.8	Lignin (organisolv); pH 6.5; 0.03 M $CaCl_2$	25	BE	346
2.15	2.40				57.1	Lignin (alkali); pH 6.5; 0.03 M $CaCl_2$	25	BE	346
1.93	2.19				56.0	Collagen; pH 6.5; 0.03 M $CaCl_2$	25	BE	346
1.64	1.92				52.8	Collagen/(annic acid=1/5); pH 6.5; 0.03 M $CaCl_2$	25	BE	346
1.08	1.43				44.6	Chitin; pH 6.5; 0.03 M $CaCl_2$	25	BE	346
0.04	0.39				44.4	Cellulose; pH 6.5; 0.03 M $CaCl_2$	25	BE	346
	3.31					Humic acid-silica column	20–23	RPLC	587
	2.91					Salicylic acid-silica column	20–23	RPLC	587
	2.61					8-Hydroxyquinoline-silica column	20–23	RPLC	587
	2.89					Correlation $\log K_{oc}$–MCI			578
	3.41					Correlation $\log K_{oc}$–MCI			597
	2.72					Correlation $\log K_{oc}$–LSER			602

Values in square parentheses have been calculated by the author.
*% OM in column 6.
Idem refers to the sorbent reported just above; only the data (texture, OC, temperature, method) which were changed are specified.

TABLE 10. Comparison of sorption data on soils obtained by batch equilibration and miscible displacement technique

	BE		MD		
Compound	N	K_{oc} (aver±SD)	N	K_{oc} (aver±SD)	Deviation factor[a]
Benzene	11	38±17	6	31±18	1.23
Toluene	4	100±65	7	90±80	1.11
Nitrobenzene	6	217±187	3	74±3	2.93
Naphthalene	13	2930±7250	6	906±1150	3.23
TCE	4	70±31	6	71±46	−1.01
TeCE	6	249±143	6	196±113	1.27
Chlorobenzene	3	182±120	5	118±98	1.54
1,2,4-Trichlorobenzene	8	2600±3210	5	1150±970	2.26

[a] Deviation factor is calculated as the ratio of the average K_{oc} values obtained by BE to average values obtained by MD. When this ratio is less than 1 the negative reciprocal is reported.

well below the solubility limit (<0.5 S), where sorption isotherm could be considered linear.[562] Sorption data were derived from graphical isotherms, when only those were available.

Sorption data (K_{oc}) obtained with different methods were examined at first with the aim to detect any significant difference among them. Tables 1–9 show that batch equilibration (BE) is the method most frequently used, especially with pesticides. Miscible displacement (MD) was often experimented in support to studies of migration of organic compounds through soil columns. Finally, only few data were obtained by head space (HS) and gas purge (GP); anyway, average values obtained using HS for toluene and TCE and GP for TCE are higher than those obtained with BE for the same compounds. However, due of the scarcity of data, the only significant comparison seems to be that between the average of the data obtained by BE and those obtained by MD. Table 10 shows this comparison, using soil samples with OC⩾0.1 and excluding any other sorbent. Although the values of deviation factors indicate a general tendency of BE to give sorption coefficients greater than those obtained by MD, the variability of the data is such to raise some doubts on the certainty of this result.

The possibility of measurement errors and errors due to the solids effect using the BE method were then taken into consideration.

The first point was discussed at the end of Sec. 11.1, where it was specified that the measurement errors can be reduced if the percent solute removed from the solution is in between 20% and 80%. Some indicative values of sorbent concentration necessary to stay in this range were given in that section as a function of K_d. Sorbent concentrations, used in the literature, were then collected when possible, for the systems listed in Tables 1–9 having K_d values ranging from less than 0.1 to about 10^5 (data not reported). The result of this investigation was that almost 30% of those sorbent concentrations was out of the previous recommended range, but most of the corresponding values of K_d were in the range of variability of all other results, so making difficult any attempt to quantify the error involved.

The second cause of error in measuring K_d is connected to the solids effect due, for instance, to the possibility of interference of nonsettling particles released by the sorbent during BE measurements. This possibility seems strongly reduced when the sorbent concentration is ⩽1 g/dm^3, as demonstrated with chlorobenzenes and PCBs.[495] By examining the literature listed in Tables 1–9, it is possible to observe that such values of concentration (data not reported) were used with compounds having K_ds greater than 100, like asulam, butralin, dicamba, fluometuron, leptophos, DDT, PCBs etc. For compounds having smaller K_ds, the data available for the systems listed in Tables 1–9 do not allow any conclusion and other studies would be necessary to estimate the entity of this effect in each specific case. However, a reduced solids effect is expected for these compounds (Sec. 8).

At the end of this first series of examinations of the sorption data, the effect of type of sorbent has been investigated. Preliminary results indicated without any doubt that soil, sediment, and possibly dissolved organic matter give different values of sorption coefficients and, therefore, have to be treated separately. Other variables, like those discussed so far (effect of the experimental method, measurement error and solids effect), do not allow to discard any of the sorption coefficients listed in Tables 1–9.

13.2. Effect of Sorbent Properties on Sorption Coefficients

Table 11 shows the correlation coefficients between K_d and four sorbent properties, OC, pH, CE, and clay. Correlations between K_d and SA were not taken into consideration due to lack of SA data obtained with a single method. For two cases, concerning TeCM and 1,2-DCBz, for which several values of SA(N_2) were available, K_d did not appear to correlate with SA.

The data of Table 11 indicate that OC content in soil/sediment (⩾0.1%) is the property most highly correlated with adsorption. CE and pH are the next in importance, while clay content does not correlate with K_d, except for few cases. However, correlation coefficients with CE, although significant for many compounds, do not allow any comment, because CE generally correlates with OC.

Although correlation coefficients between K_d values and the respective OC content in sorbent are high for most compounds listed in Table 11, some anomalous results can be evidenced. Among nonpolar compounds, naphthalene gives an r value lower than expected due to the negative contribution of one K_d value exceptionally high, for which the authors[181] did not find any explanation. If this value is subtracted from the correlation, r increases from 0.451 to 0.808. Also for acetophenone a single point changes the r value from 0.457 to 0.848. Situations of this type also concern TeCE, 1,2,4-TCBz, 1,2,3,4-TeCBz, atrazine, benefin, monolinuron, and napropamide. Finally, the low correlation coefficients found for prometone and sulfometuron methyl were expected looking to the results by Talbert and Fletchall[145] and by Koskinen *et al.*,[301] respectively. However, for these two compounds the $\log K_{oc}$ values have also been calculated and then correlated with pH, as shown in the next tables. The results seem to indicate that a real dependence might exist.

Table 11 also shows that for several compounds, among those indicated with an asterisk, the K_d–OC correlation coefficients increase considerably when the K_d data obtained with high organic sorbents, peats, or mucks are included in the correlation. This effect appears more relevant for 2,2′,4,4′,5,5′-HCB, some triazines, carbaryl, 2,4-D(d), diazinon, dieldrin, diuron, fluometuron, metribuzin monuron, and picloram. For these compounds, the K_d–OC plots show that at low OC content ($\leqslant$5%–7%) the slope of the regression is lower than that obtained when results with high organic sorbents are included; furthermore, the slope shows a positive intercept, indicating a possible contribution of the mineral components to sorption. These results seem to indicate that there may be a change in sorption mechanism or in the nature of the organic matter when OC content increases in the range of the high-organic soils (typically from 10% to 60% OC). This effect is much less pronounced in other cases, expecially those concerning hydrophobic compounds, like benzene, TeCM, TCE, MCBz, 1,2-DCBz, DDT, and lindane, and some pesticides of different chemical composition.

The K_d-pH correlation coefficients are also generally low for the most polar and for ionic compounds. However, if the sorption data of some acidic and basic compounds are expressed as $\log K_{oc}$, the effect of pH appears more evident. Table 12 shows the correlation coefficients between $\log K_{oc}$ and pH for some acidic and basic compound, for which the pK_as are known. Two correlation coefficients are reported for each pH range, calculated for sorbents having OC $\geqslant$0.1% and OC$\geqslant$0.5%, respectively. This choice is justified taking into consideration the observations by Hassett *et al.*[211] and by Gerstl and Mingelgrin,[563] who suggested the possibility that, at low OC content in sorbent, the K_{oc} values could be inflated due to the contribution of sorption by the inorganic components of the sorbent. For acidic compounds the pH range of the available experimental data is chosen to account for the particular form of the molecule: undissociated ($pH<pK_a-2$), dissociated ($pH>pK_a+2$), or partially dissociated in the intermediate range between these two pH limits. Phenol, as an example of the unionized forms, behaves like a hydrophobic compound and its $\log K_{oc}$ values do not correlate with pH. Similarly, for the totally dissociated forms of 2,4-D and picloram, $\log K_{oc}$ does not correlate with pH, although for 2,4-D some uncertainty may exist in the definition of the corresponding pH range. Also for basic compounds, except hexazinone and metribuzin, $\log K_{oc}$ correlates with pH, but correlation coefficients are generally lower, between 0.33 and 0.63. For all compounds, acidic and basic, the respective regression equations have been obtained taking only the data concerning soil OC$\geqslant$0.5% and assuming linear behavior in the pH range taken into consideration. These equations have negative values of the slope at both limits of the confidence intervals, at 95% probability. As a matter of fact, it has been demonstrated that basic compounds, like triazine herbicides, show a decrease of the sorption coefficients by increasing pH.[145,284] This effect was explained with the gradual loss of a H^+ ion from the protonated molecule starting from $pH=pK_a$. It is interesting to note that from the regression equations (Table 12) for ametryne and atrazine, K_{oc} values at pH 4 are about three times larger than at pH 8; a similar difference was observed in the same range of pH for K_d of atrazine on a soil.[286] However, the K_d of ametryne on a soil decreased from 28 to about 3 when pH increased from 4 to 8.[256]

It appears interesting to note that $\log K_{oc}$ values of napropamide also correlate very well with pH at both OC $\geqslant$0.1% and OC$\geqslant$0.5%. Regressing $\log K_{oc}$ as a function of pH, the following equation is obtained:

$$\log K_{oc} = -0.252\,\mathrm{pH} + 4.397$$

with eight data and OC$\geqslant$0.5% ($r=-0.912$). A similar equation is obtained with 11 data and OC$\geqslant$0.1% ($r=-0.899$). More studies are necessary to ascertain if this behavior is true.

Table 13 shows the average $\log K_{oc}$ values with the respective 68% confidence limits between brackets for a large number of compounds of different nature. Two averages are reported, calculated for soils or sediments having OC$\geqslant$0.1% and OC$\geqslant$0.5%, respectively. When possible, the averages for sorbents with OC contents between 0.1% and 0.5% have been calculated. The results do not seem conclusive to evidence differences which can be connected to different OC content, but this seems to be due to the fact that the number of data might not be enough for this purpose. However, in the case of atrazine, for which the number of data available are of several tens, the average $\log K_{oc}$ for 0.1%$\leqslant$OC <0.5% is sensibly greater than the average $\log K_{oc}$ for OC $\geqslant$0.5%.

From Table 13 it appears that about 40% of the $\log K_{oc}$ values obtained with sorbents having OC$\geqslant$0.1% vary within 1 log unit, about 50% vary within 1 or 2 log units and the rest show variations larger than 2 log units. The second and third groups of data also include many hydrophobic compounds, perhaps because of the presence of some outliers in

TABLE 11. Correlation coefficients (r) between average K_d values and four soil or sediment properties

Compound		Soil or sedim. (So,Se)	OC(number of data)	pH (number of data)	CE (number of data)	Clay (number of data)
Benzene		So	0.865(18)	−0.013 (10)	0.011 (9)	0.347 (15)
			0.923(23)*			
Toluene		So	0.905 (14)	−0.551 (8)	−0.375 (5)	0.134 (10)
			0.791 (16)*			
Ethylbenzene		So	0.906 (10)	−0.17 (6)	0.047 (7)	0.278 (9)
Naphthalene		So	0.451 (25)			−0.027 (12)
			0.808 (24)			
Pyrene		Se	0.894 (28)	−0.430 (14)	0.376(12)	0.323 (14)
TeCM		So	0.954 (34)			
			0.952 (37)*			
		Se	0.951 (33)			
TCE		So	0.824 (19)			0.268 (18)
			0.907 (23)*			0.538 (17)
TeCE		So	0.744 (16)			0.149 (13)
			0.984 (15)			
MCBz		So	0.941 (9)			
			0.968 (10)*			
1,2-DCBz		So	0.843 (36)			
			0.962 (37)*			
		Se	0.984 (36)			
1,2,4-TCBz		So	0.649 (15)			
			0.867 (14)			
1,2,3,4-TeCBz		So	0.705 (11)	−0.542 (8)		
			0.931 (10)			
Phenol	(u) (pH 3.2–7.4)	So	0.972 (12)	−0.293 (10)		−0.081 (10)
			0.538 (13)*			
2,4-DCP	(pH 2.0–7.4)	So	0.934 (12)	−0.410 (12)		
2,3,4,6-TeCP	(pH 2.0–7.5)	So	0.698 (11)	−0.460 (11)		
PCP	(pH 2.0–10)	So	0.589 (26)	−0.322 (26)		0.023 (16)
	(pH 3.4–6.9)	So	0.810 (14)	−0.426 (14)		0.421 (8)
	(d) (pH 7.0–10.0)	So	0.747 (9)	−0.343 (9)		
2,2′,4,4′,5,5′-(153)		Se	0.311 (18)			
			0.855 (19)*			
Aroclor-1242		So	0.772 (12)			
Alachlor		So	0.926 (21)	−0.467 (13)	0.672 (7)	0.456 (12)
Ametrine		So	0.412 (33)	−0.143 (34)	0.634(34)	−0.013 (34)
			0.982 (34)*			
			0.971(130)*			0.197 (33)
Atrazine		So	0.656 (128)	−0.182(122)	0.469(46)	0.194 (108)
			0.971 (130)*			0.690 (104)
		Se	0.512 (13)	−0.806 (12)		0.525 (12)
			0.798 (12)			
Benefin		So	0.082 (12)	−0.358 (12)	0.208(12)	0.033 (12)
			0.903 (10)			
Bromacil		So	0.825 (18)	−0.788 (11)		0.108 (15)
			0.972 (19)*			0.762 (13)
Carbaryl		So	0.251 (11)	0.031 (11)		
			0.998 (12)*	−0.083 (12)		
Carbofuran		So	0.859 (12)	−0.230 (6)	0.811(10)	−0.224 (7)
			0.989 (15)*	−0.504 (8)	0.823(12)	
Chlorbromuron		So	0.647 (17)	−0.222 (16)		
Chlorpropham		So	0.933 (15)	0.074 (15)	0.137(14)	0.001 (14)
			0.995 (16)*		−0.045(15)	−0.467 (15)
Chlortoluron		So	0.666 (17)	−0.072 (16)		
Cyanazine		So	0.686 (10)	−0.396 (9)		0.826 (9)
2,4-D	(pH 2.8–9.0)	So	0.554 (94)	−0.391 (92)	−0.123(67)	−0.104 (92)
			0.381 (95)*	−0.392 (93)	−0.029(68)	−0.103 (93)
	(pH 2.8–5.0)	So	0.827 (21)	−0.484 (21)	0.247(20)	−0.203 (21)
	(d) (pH 5.1–9.0)	So	0.164 (71)	−0.160 (71)	0.087(46)	0.229 (70)
			0.498 (72)*	−0.298 (72)	0.341(47)	0.198 (71)
p,p′-DDT		So	0.835 (7)			0.600 (7)
			0.998 (8)*			
Diazinon		So	0.367 (28)	−0.268 (28)		0.027 (27)

TABLE 11. Correlation coefficients (r) between average K_d values and four soil or sediment properties—Continued

Compound		Soil or sedim. (So.Se)	OC(number of data)	pH (number of data)	CE (number of data)	Clay (number of data)
			0.993 (29)*	−0.155(29)		−0.162(28)
Dieldrin		So	0.122 (11)		0.875 (7)	
			0.972 (13)*		0.808 (8)	
Disulfoton		So	0.888 (9)	−0.205 (9)	0.864 (9)	0.372 (9)
			0.946 (11)*	−0.489(11)	0.962(11)	0.725(10)
Diuron		So	0.593 (95)	−0.064(93)	0.467(68)	−0.022(76)
			0.932 (96)*	−0.076(94)	0.541(69)	−0.027(77)
Fenuron		So	0.951 (25)	0.110(24)		−0.258 (8)
			0.992 (26)*	−0.192(25)		−0.340 (9)
Fluometuron		So	0.661 (77)	0.152(77)	0.522(68)	0.571(71)
			0.915 (78)*	0.022(78)	0.668(69)	0.299(72)
Lindane		So	0.832 (45)	−0.230(38)		−0.102(37)
			0.911 (49)*	−0.276(40)		
Hexazinone		So	0.744 (24)	0.252(24)	0.663(22)	0.792(24)
Linuron		So	0.290 (44)	−0.351(43)	−0.046(20)	0.343(26)
			0.970 (45)*			
Malathion		So	0.751 (20)	0.311(20)	0.384(20)	0.314(20)
Metobromuron		So	0.668 (18)	0.008(17)		
Metolachlor		So	0.826 (24)	0.135(20)	0.514(16)	0.348(23)
Metoxuron		So	0.698 (17)	0.044(16)		
Metribuzin		So	0.451 (94)	−0.015(95)	0.474(68)	0.355(95)
			0.618 (95)*			
Monolinuron		So	0.296 (20)	−0.498(19)		
			0.674 (18)	−0.019(18)		
Monuron		So	0.210 (19)	−0.210(18)		
			0.962 (21)*	−0.152(19)		
Napropamide		So	0.641 (20)	−0.376(11)		−0.124(19)
			0.876 (19)			
Parathion		So	0.805 (33)	−0.405(23)	0.059(15)	0.287(30)
			0.940 (36)*	−0.465(25)	0.154(16)	−0.005(32)
Picloram	(pH 2.0–10.4)	So	0.245 (50)	−0.517(50)		−0.024(48)
			0.448 (53)*	−0.411(53)		0.000(51)
	(pH 2.0–6.0)	So	0.737 (16)	−0.538(16)		−0.035(16)
			0.968 (17)*	−0.421(17)		0.013(17)
	(d) (pH 6.1–10.4)	So	0.773 (33)	0.086(33)		−0.057(31)
			0.963 (35)*	0.290(35)		−0.136(33)
Prometone		So	0.141 (27)	−0.426(27)	0.465(27)	0.574(27)
Prometryne		So	0.550 (80)	0.004(80)	0.016(76)	−0.121(79)
			0.819 (81)*	−0.036(81)	0.367(77)	−0.088(80)
Propazine		So	0.892 (35)	−0.507(35)	0.496(29)	−0.134(35)
Simazine		So	0.704 (42)	−0.542(41)	0.634(34)	0.322(41)
			0.835 (43)*	−0.369(42)		
Sulfometuron methyl		So	0.225 (20)	−0.547(20)	0.319(20)	
2,4,5-T		So	0.722 (21)			
Tebuthiuron		So	0.812 (20)	−0.387(20)	0.583(20)	
Triallate		So	0.941 (13)	0.554(13)		0.202(12)
Trifluralin		So	0.532 (23)	−0.566(19)	0.253(16)	−0.117(23)
Acetophenone		So	0.457 (13)			0.404(13)
			0.848 (12)			
		Se	0.802 (17)	−0.222(11)	0.540(11)	0.560(16)
Dibenzothiophene		Se	0.817 (11)	−0.510(11)	0.291(11)	0.248(11)

(d) dissociated.

(u) undissociated.

*correlation coefficients calculated including K_d data obtained with high organic soils or sediments.

TABLE 12. Correlation coefficients (r) between log K_{oc} values and pH for some acidic and basic compounds

Compound	pK$_a$	pH range	Soil OC content (%)	Number of data points	r
Acidic					
Bromacil	9.3	6.3–7.9	⩾0.1	11	−0.695
		6.3–7.8	⩾0.5	9	−0.904
		log K_{oc} = −0.295 pH+3.737			
Phenol	9.8	3.2–7.4 (u)	⩾0.1	10	0.218
		3.2–7.4	⩾0.5	9	0.302
2,3,4,6-TeCP	5.22	3.4–7.5	⩾0.1	10	−0.945
		3.4–7.5	⩾0.5	8	−0.957
		log K_{oc} = −0.443 pH+5.575			
PCP	4.74	3.4–6.9	⩾0.1	14	−0.747
		3.4–6.9	⩾0.5	11	−0.644
		log K_{oc} = −0.284 pH+4.921			
2,4-D	2.80	2.8–5.0	⩾0.1	21	−0.414
		2.8–5.0	⩾0.5	20	−0.464
		2.8–5.5	⩾0.5	35	−0.533
		log K_{oc} = −0.260 pH+3.187 (pH 2.8–5.0)			
		5.1–9.0 (d)	⩾0.1	72	−0.310
		5.1–9.0	⩾0.5	71	−0.310
		5.5–9.0	⩾0.5	56	−0.157
Picloram	3.4	2.0–6.0	⩾0.1	17	−0.828
		2.0–6.0	⩾0.5	12	−0.881
		log K_{oc} = −0.371 pH+3.692			
		6.1–10.4 (d)	⩾0.1	35	0.134
		6.1–10.4	⩾0.5	31	−0.205
Sulfometuron methyl	5.2	4.1–5.8	⩾0.1	20	−0.017
		4.1–5.5	⩾0.5	18	−0.708
		log K_{oc} = −0.581 pH+3.497			
Basic					
Ametryne	4.0	4.5–9.0	⩾0.1	34	−0.533
		4.5–9.0	⩾0.5	33	−0.538
		log K_{oc} = −0.111 pH+3.198			
Atrazine	1.68	3.2–8.2	⩾0.1	122	−0.157
		3.2–8.15	⩾0.5	77	−0.476
		log K_{oc} = −0.114 pH+2.846			
Hexazinone	1.09	4.0–6.4	⩾0.1	24	−0.065
		4.0–6.4	⩾0.5	22	−0.156
Metribuzin	0.99	4.3–9.0	⩾0.1	95	0.108
		4.3–9.0	⩾0.5	83	0.065
Prometone	4.28	4.3–7.1	⩾0.1	27	−0.627
		4.3–7.1	⩾0.5	25	−0.618
		log K_{oc} = −0.391 pH+4.682			
Prometryne	4.05	4.3–9.0	⩾0.1	81	−0.325
		4.3–9.0	⩾0.5	78	−0.328
		log K_{oc} = −0.138 pH+3.453			
Propazine	1.85	3.2–7.4	⩾0.1	35	−0.452
		3.2–7.4	⩾0.5	34	−0.556
		log K_{oc} = −0.133 pH+2.909			
Simazine	1.65	3.2–8.0	⩾0.1	42	−0.382
		3.2–7.4	⩾0.5	39	−0.497
		log K_{oc} = −0.188 pH+3.354			
Tebuthiuron	1.2	4.1–5.8	⩾0.1	20	−0.535
		4.1–5.45	⩾0.5	18	−0.584
		log K_{oc} = −0.366 pH+3.303			

(d) dissociated.
(u) undissociated.

TABLE 13. Average log K_{oc} data as a function of sorbent type and organic carbon content

Compound	Soil or sedim. (So, Se)	OC (%)	Number of data points	Range	Average log K_{oc}
Benzene	So	⩾0.1	23	1.90	1.64 (1.24–2.04)[a]
	So	⩾0.5	16	0.73	1.58 (1.37–1.79)
	So	0.1⩽OC<0.5	7	1.90	1.78 (1.11–2.45)
Toluene	So	⩾0.1	17	1.65	1.89 (1.49–2.29)
	So	⩾0.5	8	0.57	2.00 (1.78–2.22)
	So	0.1⩽OC<0.5	9	1.65	1.79 (1.29–2.29)
m-Xylene	So	⩾0.1	5	1.23	2.06 (1.58–2.54)
	So	⩾0.5	3	0.26	2.33 (2.20–2.46)
p-Xylene	So	⩾0.1	8	0.85	2.27 (1.99–2.55)
	So	⩾0.5	5	0.85	2.31 (2.00–2.62)
	So	0.1⩽OC<0.5	3	0.49	2.21 (1.94–2.48)
Ethylbenzene	So	⩾0.1	10	1.24	2.04 (1.66–2.42)
	So	⩾0.5	5	0.30	2.18 (2.05–2.31)
	So	0.1⩽OC<0.5	5	1.19	1.90 (1.40–2.40)
Nitrobenzene		⩾0.1	9	1.28	2.09 (1.75–2.43)
	So	⩾0.5	6	0.82	2.16 (1.84–2.48)
	So	0.1⩽OC<0.5	3	0.71	1.95 (1.55–2.35)
Naphthalene	So	⩾0.1	25	3.20	2.91 (2.31–3.51)
	So	⩾0.5	16	1.95	3.02 (2.52–3.52)
	So	0.1⩽OC<0.5	9	2.64	2.71 (1.98–3.44)
	Se	⩾0.5	7	0.83	3.06 (2.77–3.35)
Phenanthrene	So	⩾0.1	6	0.66	4.03 (3.72–4.34)
	So	⩾0.5	4	0.66	4.08 (3.72–4.44)
	Se	⩾0.5	5	0.28	4.34 (4.21–4.48)
Fluoranthene	So	⩾0.5	5	0.66	4.65 (4.37–4.93)
	Se	⩾0.5	9	0.93	4.86 (4.48–5.24)
Pyrene	So	⩾0.1	5	0.63	4.66 (4.39–4.93)
	So	⩾0.5	3	0.03	4.78 (4.76–4.80)
	Se	⩾0.1	28	1.05	4.88 (4.65–5.11)
	Se	⩾0.5	26	1.05	4.90 (4.68–5.12)
Benzo(a)pyrene	Se	⩾0.5	4	1.47	6.23 (5.61–6.85)
TeCM	So	⩾0.1	37	0.51	1.80 (1.71–1.89)
	So	⩾0.5	33	0.51	1.80 (1.70–1.90)
	So	0.1⩽OC<0.5	4	0.10	1.78 (1.74–1.82)
	Se	⩾0.1	36	0.26	2.01 (1.96–2.06)
	Se	⩾0.5	28	0.26	2.00 (1.95–2.05)
	Se	0.1⩽OC<0.5	8	0.12	2.02 (1.98–2.06)
1,2-ED	So	⩾0.5	9	1.11	1.64 (1.20–2.08)
1,1,1-TCA	So	⩾0.1	6	1.16	2.16 (1.75–2.57)
1,1,2-TCA	So	⩾0.1	4	0.25	1.88 (1.77–1.99)
TCE	So	⩾0.1	23	2.05	1.92 (1.53–2.31)
	So	⩾0.5	16	1.10	2.00 (1.73–2.27)
	So	0.1⩽OC<0.5	7	1.79	1.75 (1.20–2.30)
TeCE	So	⩾0.1	16	1.91	2.32 (1.91–2.73)
	So	⩾0.5	7	1.17	2.45 (2.09–2.81)
	So	0.1⩽OC<0.5	9	1.36	2.22 (1.78–2.66)
MCBz	So	⩾0.1	11	1.82	1.97 (1.49–2.36)
	So	⩾0.5	6	0.59	2.14 (1.49–2.36)
	So	0.1⩽OC<0.5	5	1.74	1.77 (1.12–2.42)
1,2-DCBz	So	⩾0.1	40	0.75	2.50 (2.35–2.65)
	So	⩾0.5	34	0.75	2.50 (2.35–2.65)
	So	0.1⩽OC<0.5	6	0.09	2.47 (2.43–2.51)
	Se	⩾0.1	36	0.30	2.70 (2.64–2.76)
	Se	⩾0.5	28	0.30	2.69 (2.62–2.76)

TABLE 13. Average $\log K_{oc}$ data as a function of sorbent type and organic carbon content—Continued

Compound		Soil or sedim. (So, Se)	OC (%)	Number of data points	Range	Average $\log K_{oc}$
		Se	$0.1 \leq OC < 0.5$	8	0.10	2.71 (2.67–2.75)
1,3-DCBz		So	≥ 0.1	5	0.30	2.49 (2.38–2.60)
		So	≥ 0.5	3	0.24	2.53 (2.40–2.66)
1,4-DCBz		So	≥ 0.1	9	0.43	2.66 (2.50–2.82)
		So	≥ 0.5	5	0.34	2.57 (2.43–2.71)
		So	$0.1 \leq OC < 0.5$	4	0.27	2.77 (2.65–2.89)
1,2,3-TCBz		So	≥ 0.1	9	1.22	3.48 (3.08–3.88)
		So	≥ 0.5	7	0.77	3.37 (3.11–3.63)
1,2,4-TCBz		So	≥ 0.1	15	2.23	3.15 (2.62–3.68)
		So	≥ 0.5	8	1.29	3.19 (2.81–3.57)
		So	$0.1 \leq OC < 0.5$	7	2.23	3.10 (2.42–3.78)
1,3,5-TCBz		So	≥ 0.1	4	1.66	3.69 (2.92–4.46)
1,2,3,4-TeCBz		So	≥ 0.1	11	1.38	3.70 (3.27–4.13)
		So	≥ 0.5	8	1.09	3.64 (3.31–3.97)
		So	$0.1 \leq OC < 0.5$	3	1.38	3.84 (3.15–4.53)
		Se	≥ 0.5	4	0.34	4.14 (3.98–4.30)
1,2,4,5-TeCBz		So	≥ 0.1	3	1.14	3.48 (2.87–4.09)
PCBz		Se	≥ 0.5	6	1.04	4.91 (4.46–5.36)
HCBz		So	≥ 0.1	5	3.30	4.23 (2.93–5.53)
		So	≥ 0.5	4	2.03	3.79 (2.81–4.77)
		Se	≥ 0.1	8	1.04	5.53 (5.16–5.90)
		Se	≥ 0.5	7	1.04	5.48 (5.11–5.85)
Phenol	(u) (pH 3.2–7.4)	So	≥ 0.1	13	1.18	1.37 (0.99–1.75)
		So	≥ 0.5	12	1.18	1.34 (0.97–1.71)
4MCP	(u) (pH 2.0–7.4)	So	≥ 0.1	7	1.00	2.15 (1.79–2.51)
		So	≥ 05	5	0.66	2.33 (1.09–2.57)
2,4-DCP	(pH 2.0–7.4)	So	≥ 0.1	12	1.06	2.49 (2.16–2.82)
	(u) (pH $\leq$5.8)	So	≥ 0.1	9	1.06	2.57 (2.21–2.93)
		So	≥ 0.5	5	0.50	2.77 (2.57–2.97)
		So	$0.1 \leq OC < 0.5$	4	0.95	2.33 (1.93–2.73)
3,4-DCP	(u) (pH $\leq$6.0)	So	≥ 0.5	4	0.20	3.03 (2.93–3.13)
2.4.6-TCP	(pH >4.2)	So	≥ 0.1	5	1.33	2.52 (1.97–3.07)
	(u) (pH $\leq$4.2)	So	≥ 0.1	3	1.02	2.86 (2.33–3.39)
2,4,5-TCP	(pH 3.4–6.0)	So	≥ 0.1	6	0.72	3.11 (2.81–3.41)
	(u) (pH $\leq$4.9)	So	≥ 0.5	4	0.10	3.35 (3.30–3.40)
2.3,4.6-TeCP	(pH 3.4–7.5)	So	≥ 0.1	10	1.71	3.02 (2.35–3.69)
		So	≥ 0.5	8	1.71	3.06 (2.31–3.81)
	(u) (pH $\leq$3.4)	So	≥ 0.5	2	0.09	3.75 (3.69–3.81)
	(d) (pH $\geq$7.4)	So	≥ 0.5	4	0.26	2.28 (2.16–2.40)
PCP	(pH 2.0–>10)	So	≥ 0.1	26	2.08	3.28 (2.69–3.77)
		So	≥ 0.5	17	1.70	3.28 (2.79–3.77)
		So	$0.1 \leq OC < 0.5$	9	2.08	3.15 (2.52–3.78)
	(pH 3.4–6.9)	So	≥ 0.1	14	1.60	3.38 (2.93–3.83)
		So	≥ 0.5	11	1.60	3.51 (3.09–3.93)
		So	$0.1 \leq OC < 0.5$	3	0.17	2.92 (2.83–3.01)
	(u) (pH $\leq$3)	So	≥ 0.1	10	2.26	4.48 (3.60–5.36)
		So	≥ 0.5	6	2.09	4.54 (3.63–5.45)
		So	$0.1 \leq OC < 0.5$	4	2.26	4.38 (3.41–5.35)
	(d) (pH $\geq$7.1)	So	≥ 0.1	12	0.94	2.82 (2.50–3.14)
		So	≥ 0.5	9	0.86	2.89 (2.59–3.19)
		So	$0.1 \leq OC < 0.5$	3	0.74	2.63 (1.89–3.37)
4-NP	(u) (pH $\leq$5.4)	So	≥ 0.1	6	0.70	2.03 (1.78–2.28)

TABLE 13. Average log K_{oc} data as a function of sorbent type and organic carbon content—Continued

Compound		Soil or sedim. (So, Se)	OC (%)	Number of data points	Range	Average log K_{oc}
		So	≥0.5	5	0.36	1.94 (1.79–2.09)
Biphenyl		So	≥0.1	7	1.46	3.03 (2.56–3.50)
		So	≥0.5	5	0.38	3.12 (2.96–3.28)
2,2′,5-(18)		Se	≥0.5	4	0.90	4.85 (4.41–5.29)
2,2′,5,5′-(52)		So	≥0.1	5	2.72	5.02 (4.01–6.03)
		So	≥0.5	3	1.98	4.55 (3.59–5.56)
		Se	≥0.5	5	1.02	5.58 (5.17–5.99)
2,2′,6,6′-(54)		Se	≥0.1	4	0.39	4.91 (4.75–5.07)
		Se	≥0.5	3	0.19	4.84 (4.74–4.94)
2,3′,4′,5-(70)		Se	≥0.1	4	0.33	4.86 (4.72–5.00)
		Se	≥0.5	3	0.17	4.80 (4.70–4.90)
2,2′,4,5,5′-(101)		Se	≥0.5	5	0.23	5.73 (5.63–5.83)
2,2′,3,3′,6,6′-(136)		Se	≥0.5	5	0.85	6.04 (5.73–6.35)
2,2′,3,5,5′,6-(151)		Se	≥0.5	5	1.23	5.75 (4.96–6.18)
2,2′,4,4′,5,5′-(153)		Se	≥0.1	19	1.55	5.86 (5.45–6.27)
		Se	≥0.5	18	1.34	5.81 (5.46–6.16)
Aroclor-1016		Se	≥0.1	4	0.50	5.03 (4.80–5.26)
		Se	≥0.5	3	0.50	4.97 (4.72–5.22)
Aroclor-1242		So	≥0.1	12	1.37	4.30 (3.94–4.66)
		So	≥0.5	8	0.85	4.12 (3.85–4.39)
		So	0.1≤OC<0.5	4	0.57	4.64 (4.37–4.91)
		Se	≥0.1	5	1.01	4.82 (4.41–5.23)
		Se	≥0.5	4	1.01	4.74 (4.31–5.17)
Aroclor-1254		Se	≥0.5	8	0.90	6.02 (5.73–6.31)
Alachlor		So	≥0.1	21	1.09	2.22 (1.97–2.47)
		So	≥0.5	18	1.09	2.22 (1.96–2.48)
		So	0.1≤OC<0.5	3	0.28	2.20 (2.05–2.35)
Aldicarb		So	≥0.5	5	0.85	1.30 (0.97–1.63)
Ametryne	(pH 4.5–9.0)	So	≥0.5	33	0.90	2.52 (2.27–2.77)
	(pH 4.5–5.4)	So	≥0.5	12	0.78	2.63 (2.39–2.87)
	(pH 5.5–6.0)	So	≥0.5	9	0.62	2.60 (2.41–2.79)
	(pH ≥6.1)	So	≥0.5	12	0.76	2.35 (2.13–2.57)
Atrazine	(pH 3.2–8.2)	So	≥0.1	130	2.34	2.31 (1.80–2.82)
		So	≥0.5	84	1.32	2.17 (1.92–2.42)
		So	0.1≤OC<0.5	46	2.25	2.56 (1.84–3.28)
	(pH 3.2–5.0)	So	≥0.5	14	0.53	2.34 (2.18–2.50)
	(pH 5.1–5.9)	So	≥0.5	22	1.08	2.24 (2.00–2.48)
	(pH ≥6.0)	So	≥0.5	41	1.05	2.06 (1.83–2.29)
	(pH 4.4–7.7)	Se	≥0.5	13	1.65	2.59 (2.21–2.97)
Benefin		So	≥0.5	12	1.38	2.96 (2.59–3.33)
Bromacil	(pH 6.3–7.9)	So	≥0.1	19	1.04	1.48 (1.23–1.73)
		So	≥0.5	15	0.70	1.46 (1.26–1.66)
		So	0.1≤OC<0.5	4	1.04	1.53 (1.10–1.96)
	(u) (pH ≤7.3)	So	≥0.1	5	0.58	1.80 (1.59–2.01)
		So	≥0.5	4	0.30	1.72 (1.58–1.86)
		Se	≥0.5	4	0.13	1.43 (1.38–1.48)
Carbaryl		So	≥0.5	12	0.81	2.20 (1.92–2.48)
Carbofuran		So	≥0.1	15	0.68	1.63 (1.45–1.81)
		So	≥0.5	13	0.68	1.64 (1.46–1.82)
		Se	≥0.5	3	0.88	1.55 (1.07–2.03)

TABLE 13. Average log K_{oc} data as a function of sorbent type and organic carbon content—Continued

Compound		Soil or sedim. (So, Se)	OC (%)	Number of data points	Range	Average log K_{oc}
Chlorbromuron		So	≥0.1	17	0.59	2.54 (2.38–2.70)
		So	≥0.5	16	0.59	2.55 (2.39–2.71)
Chlorpropham		So	≥0.5	16	0.86	2.62 (2.37–2.87)
Chlorpyrifos		So	≥0.1	7	1.01	3.63 (3.30–3.96)
		So	≥0.5	6	1.01	3.62 (3.25–3.99)
Chlortoluron		So	≥0.1	17	0.53	2.00 (1.85–2.15)
		So	≥0.5	16	0.53	2.00 (1.85–2.15)
Cyanazine	(pH 5.6–8.0)	So	≥0.1	9	0.79	2.14 (1.83–2.45)
		So	≥0.5	8	0.79	2.19 (1.89–2.49)
2,4-D	(pH 2.8–9.0)	So	≥0.1	95	2.01	1.79 (1.36–2.22)
		So	≥0.5	91	2.01	1.77 (1.35–2.19)
	(pH 2.8–5.0)	So	≥0.1	23	1.33	2.16 (1.80–2.52)
		So	≥0.5	20	1.33	2.13 (1.78–2.48)
	(d) (pH >5)	So	≥0.1	72	1.70	1.68 (1.30–2.06)
		So	≥0.5	71	1.70	1.68 (1.29–2.07)
p,p′-DDT		So	≥0.1	8	1.13	5.63 (5.28–5.68)
		So	≥0.5	7	0.84	5.54 (5.27–5.81)
		Se	≥0.5	6	0.59	6.08 (5.84–6.32)
Diazinon		So	≥0.1	29	1.39	2.74 (2.44–3.14)
		So	≥0.5	17	0.66	2.64 (2.46–2.82)
		So	0.1≤OC<0.5	12	1.22	2.90 (2.52–3.28)
Dieldrin		So	≥0.1	13	1.13	4.08 (3.79–4.37)
		So	≥0.5	11	1.13	4.06 (3.76–4.36)
Disulfoton		So	≥0.5	11	0.66	2.92 (2.74–3.10)
Diuron		So	≥0.1	96	1.86	2.44 (2.12–2.76)
		So	≥0.5	89	1.86	2.43 (2.10–2.76)
		So	0.1≤OC<0.5	7	0.49	2.57 (2.38–2.76)
		Se	≥0.5	3	0.52	2.78 (2.51–3.05)
EPTC		So	≥0.1	7	0.54	2.03 (1.86–2.20)
		So	≥0.5	6	0.45	2.00 (1.83–2.17)
Fensulfothion		So	≥0.1	6	0.74	2.40 (2.14–2.66)
		So	≥0.5	5	0.74	2.37 (2.09–2.65)
Fenuron		So	≥0.1	26	0.52	1.42 (1.27–1.57)
		So	≥0.5	25	0.52	1.41 (1.26–1.56)
Fluometuron		So	≥0.1	78	2.24	2.17 (1.84–2.50)
		So	≥0.5	68	2.24	2.18 (1.85–2.51)
		So	0.1≤OC<0.5	10	0.96	2.12 (1.77–2.47)
Lindane		So	≥0.1	49	1.89	3.02 (2.70–3.34)
		So	≥0.5	40	1.57	3.00 (2.72–3.28)
		So	0.1≤OC<0.5	9	1.63	3.08 (2.60–3.56)
		Se	≥0.5	4	1.13	3.49 (2.95–4.03)
Hexazinone		So	≥0.1	24	0.74	1.18 (0.97–1.39)
		So	≥0.5	22	0.74	1.16 (0.95–1.37)
Linuron		So	≥0.1	45	1.78	2.65 (2.29–3.01)
		So	≥0.5	43	1.38	2.64 (2.33–2.95)
		Se	≥0.5	12	0.38	2.78 (2.65–2.91)
Malathion		So	≥0.1	20	0.91	3.08 (2.80–3.36)
		So	≥0.5	19	0.91	3.06 (2.77–3.35)
Methylparathion		So	≥0.1	8	0.59	2.82 (2.58–3.06)
		So	≥0.5	6	0.53	2.74 (2.52–2.96)
Metobromuron		So	≥0.1	18	0.64	2.00 (1.85–2.15)
		So	≥0.5	17	0.64	2.00 (1.85–2.15)

TABLE 13. Average log K_{oc} data as a function of sorbent type and organic carbon content—Continued

Compound		Soil or sedim. (So, Se)	OC (%)	Number of data points	Range	Average log K_{oc}
Metolachlor		So	≥0.1	23	1.54	2.28 (1.91–2.65)
		So	≥0.5	19	1.43	2.19 (1.92–2.46)
		So	0.1≤OC<0.5	4	0.92	2.69 (2.17–3.21)
Metoxuron		So	≥0.1	17	0.71	1.81 (1.64–1.98)
		So	≥0.5	16	0.71	1.81 (1.63–1.99)
Metribuzin		So	≥0.1	95	1.55	2.05 (1.72–2.38)
		So	≥0.5	83	1.55	2.06 (1.74–2.38)
		So	0.1≤OC<0.5	12	1.14	2.04 (1.67–2.41)
Monolinuron		So	≥0.1	20	1.26	1.88 (1.58–2.18)
		So	≥0.5	19	1.26	1.88 (1.57–2.19)
Monuron		So	≥0.1	21	1.19	1.80 (1.56–2.04)
		So	≥0.5	20	1.19	1.80 (1.55–2.05)
Napropamide		So	≥0.1	20	1.06	2.58 (2.32–2.84)
		So	≥0.5	15	0.96	2.58 (2.31–2.85)
		So	0.1≤OC<0.5	5	0.69	2.61 (2.36–2.86)
		Se	≥0.5	4	0.29	2.80 (2.68–2.92)
Oxamil		So	≥0.1	7	1.05	1.43 (1.11–1.75)
		So	≥0.5	5	0.71	1.36 (1.07–1.65)
		Se	≥0.5	3	0.35	1.08 (0.89–1.27)
Parathion		So	≥0.1	36	1.76	3.05 (2.70–3.40)
		So	≥0.5	27	1.76	3.09 (2.75–3.43)
		So	0.1≤OC<0.5	9	1.11	2.94 (2.57–3.31)
		Se	≥0.5	5	0.13	3.17 (3.12–3.22)
Permethrin		So	≥0.1	6	0.89	4.42 (4.08–4.76)
		So	≥0.5	5	0.88	4.35 (4.03–4.67)
Phorate		So	≥0.5	6	0.31	2.63 (2.52–2.74)
Picloram	(pH 2.0–10.4)	So	≥0.1	53	3.40	1.55 (0.71–2.39)
		So	≥0.5	44	2.67	1.39 (0.66–2.12)
		So	0.1≤OC<0.5	9	2.60	2.38 (1.49–3.27)
	(u) (pH ≤2.0)	So	≥0.1	9	1.58	3.07 (2.59–3.55)
		So	≥0.5	6	0.31	2.96 (2.84–3.08)
		So	0.1≤OC<0.5	3	1.58	3.30 (2.42–4.18)
	(pH 4.2–5.9)	So	≥0.1	8	1.54	1.80 (1.28–2.32)
		So	≥0.5	6	1.20	1.76 (1.31–2.21)
	(d) (pH ≥6.0)	So	≥0.1	36	1.71	1.12 (0.74–1.50)
		So	≥0.5	32	0.92	1.02 (0.77–1.27)
		So	0.1≤OC<0.5	4	0.54	1.93 (1.67–2.19)
Prometone	(pH 4.3–7.1)	So	≥0.1	27	1.84	2.47 (2.01–2.93)
		So	≥0.5	25	1.84	2.50 (2.04–2.96)
	(pH 4.3–4.9)	So	≥0.5	6	0.68	2.85 (2.59–3.11)
	(pH 5.0–5.9)	So	≥0.1	12	1.71	2.54 (2.07–3.01)
		So	≥0.5	11	1.71	2.56 (2.08–3.04)
	(pH ≥6.0)	So	≥0.1	9	0.84	2.12 (1.80–2.44)
		So	≥0.5	8	0.84	2.16 (1.84–2.48)
Prometryne	(pH 4.3–9.0)	So	≥0.1	81	2.60	2.61 (2.14–3.08)
		So	≥0.5	78	2.60	2.62 (2.14–3.10)
		So	0.1≤OC<0.5	3	0.64	2.32 (1.99–2.65)
	(pH 4.3–4.9)	So	≥0.5	14	0.72	2.81 (2.61–3.01)
	(pH 5.0–5.9)	So	≥0.5	28	1.86	2.65 (2.29–3.01)
	(pH ≥6.0)	So	≥0.5	36	2.60	2.53 (1.93–3.13)
Propazine	(pH 3.2–7.4)	So	≥0.1	35	1.24	2.15 (1.91–2.39)
		So	≥0.5	34	1.08	2.17 (1.96–2.38)

TABLE 13. Average log K_{oc} data as a function of sorbent type and organic carbon content—Continued

Compound		Soil or sedim. (So, Se)	OC (%)	Number of data points	Range	Average log K_{oc}
	(pH 3.2–5.0)	So	⩾0.5	9	0.64	2.29 (2.09–2.49)
	(pH 5.1–5.9)	So	⩾0.5	14	0.59	2.21 (2.02–2.38)
	(pH ⩾6.0)	So	⩾0.5	11	0.62	2.03 (1.85–2.21)
Simazine	(pH 3.2–8.0)	So	⩾0.1	43	1.46	2.29 (1.96–2.62)
		So	⩾0.5	39	1.46	2.29 (1.96–2.62)
		So	0.1⩽OC<0.5	4	0.75	2.29 (1.96–2.62)
	(pH 3.2–5.0)	So	⩾0.5	10	0.65	2.50 (2.32–2.68)
	(pH 5.1–5.9)	So	⩾0.5	15	1.39	2.34 (2.01–2.67)
	(pH ⩾6.0)	So	⩾0.5	14	0.85	2.10 (1.78–2.42)
Sulfometuron m.	(pH 4.1–5.8)	So	⩾0.1	20	1.44	0.73 (0.38–1.08)
		So	⩾0.5	18	1.02	0.65 (0.37–0.93)
2,4,5-T		So	⩾0.5	21	1.25	1.99 (1.63–2.35)
Tebuthiuron	(pH 4.1–5.8)	So	⩾0.1	20	0.82	1.51 (1.31–1.71)
		So	⩾0.5	18	0.82	1.51 (1.30–1.70)
Terbacil		So	⩾0.5	4	0.47	1.58 (1.38–1.78)
Terbufos		So	⩾0.5	8	0.59	2.78 (2.55–3.01)
Terbutryn		So	⩾0.5	5	1.18	3.79 (3.28–4.30)
Triallate		So	⩾0.1	13	2.02	2.70 (1.74–3.66)
		So	⩾0.5	12	2.02	2.64 (1.67–3.61)
Trifluralin		So	⩾0.1	23	2.11	3.53 (2.76–4.39)
		So	⩾0.5	20	2.11	3.45 (2.68–4.22)
		So	0.1⩽OC<0.5	4	1.53	3.96 (3.25–4.67)
		Se	⩾0.5	5	0.28	4.42 (4.30–4.54)
Acetophenone		So	⩾0.1	13	1.07	1.61 (1.25–1.97)
		So	⩾0.5	8	0.83	1.50 (1.23–1.77)
		So	0.1⩽OC<0.5	5	0.97	1.80 (1.36–2.24)
		Se	⩾0.1	17	0.60	1.56 (1.40–1.72)
		Se	⩾0.5	16	0.60	1.55 (1.39–1.71)
Anthraquinone		So	⩾0.5	5	0.80	3.72 (3.36–4.08)
Dibenzothiophene		So	⩾0.1	3	0.29	3.87 (3.72–4.02)
		Se	⩾0.1	11	0.48	4.02 (3.87–4.17)
		Se	⩾0.5	10	0.41	4.04 (3.90–4.18)

[a] 68% confidence limits between brackets.

(u) undissociated.

(d) dissociated.

TABLE 14. Comparison between average $\log K_{oc}$ values for soils and sediments (OC$\geq$0.5%)

Compound	$\log K_{oc}$ (av.) (sediments) (A)	$\log K_{oc}$ (av.) (soils) (B)	A−B	$\log S$	Ref.
Naphthalene	3.06	3.02	0.04	2.38	12
Phenanthrene	4.34	4.08	0.26	0.85	12
Fluoranthene	4.91	4.65	0.26	0.08	12
Pyrene	4.90	4.78	0.12	−0.13	12
TeCM	2.00	1.80	0.20	3.72	12
1,2-DCBz	2.69	2.50	0.19	2.96	12
1,2,3,4-TeCBz	4.14	3.64	0.50	1.30	12
HCBz	5.48	3.79	1.69	−1.76	12
2,4-DCP (u)	2.62	2.77	−0.15	1.45	335
2,2′,5,5′-(52)	5.58	5.02	0.56	−0.89	16
Atrazine	2.59	2.16	0.43	2.19	564
Bromacil	1.43	1.72	−0.29	3.61	563
Carbofuran	1.55	1.64	−0.09	3.50	15
p,p′-DDT	6.08	5.54	0.54	−1.90	563
Lindane	3.49	3.00	0.49	1.42	15
Linuron	2.78	2.64	0.14	2.48	15
Napropamide	2.80	2.58	0.22	2.40	563
Oxamil	1.08	1.36	−0.28	6.11	674
Parathion	3.17	3.09	0.08	1.68	563
Trifluralin	4.42	3.45	0.97	0.35	563
Acetophenone	1.55	1.50	0.05	1.66	570

(u) undissociated.
S water solubility (μmol dm^{-3}).

the respective $\log K_{oc}$ values. The same consideration can be done by looking to the confidence limits. However, the largest dispersion of the data is concentrated on polar and ionizable compounds.

Looking to the ionizable compounds, acidic or basic, the dependence on pH is quantified as average $\log K_{oc}$ in selected pH ranges. The average $\log K_{oc}$ values for acidic compounds, like phenols, bromacil, picloram, and 2,4-D, were fractionated choosing, when possible, suitable pH ranges to discriminate the sorption of undissociated (neutral) form ($\mathrm{pH}<\mathrm{p}K_a-2$) from that of dissociated (ionic) form ($\mathrm{pH}>\mathrm{p}K_a+2$), and selecting an intermediate range where $\log K_{oc}$ varies with pH. Different sorption coefficients were found for undissociated and dissociated forms, for which $\log K_{oc}$ is expected to remain constant with pH. In the intermediate range of pH, K_{oc} values for single pH values can be calculated using Eq. (13), knowing both the average values of K_{oc} for ionic and neutral forms, and the pK_a. The average $\log K_{oc}$ for dissociated and undissociated 2,3,4,6-tetrachlorophenol and pentachlorophenol are in satisfactory agreement with the results of the literature.[111,337,339]

Table 13 also shows that the average $\log K_{oc}$ values for sediments are different from those for soils. This result, already obtained by Gerstl and Mingelgrin[563] with seven compounds included in this study, was interpreted as being due to the difference in chemical nature or lipophilicity of the organic matter in sediments and soils, with sediment organic matter being less polar and, thus, adsorbing nonpolar compounds preferentially to soil organic matter.[230,563] The difference between $\log K_{oc}$ (sediments) and $\log K_{oc}$ (soils) for 21 compounds are shown in Table 14 together with the respective $\log S$ (μmol dm^{-3}), with S spanning 8 orders of magnitude. Linear regression of the data gives the following equation:

$$[\log K_{oc}(\text{sediment}) - \log K_{oc}(\text{soil})] = -0.161 \log S + 0.538 \quad r = -0.700.$$

For the less soluble hydrophobic organic compounds, the sorption on sediments is greater than that on soils and the difference between the two decreases by decreasing the hydrophobic character of the compounds. The regression shows that, for very soluble polar compounds ($S > \sim 3000\,\mu$mol dm^{-3}) sorption on soils becomes greater than that on sediments. This behavior appears to be due again to the more polar character of soil organic matter than that of sediments.

Table 15 shows a comparison of the average K_{oc} values derived from Table 13 with other averages available in the literature. Except for very high deviation factors, concerning however values measured in the field,[544] all other data give low deviation factors, between 1 and 3.7. Only in one case (methylparathion) was the factor as large as 8. In particular, when the values presented by Gerstl[562] and Karickhoff[96] obtained by collecting data obtained with soils and sediments, are compared to the average values reported separately for soils and sediments, are two values of deviation factors indicated for each compound. For these cases, it has to be taken into consideration that the values of deviation factors are affected by the relative different contributions in the literature averages of K_{oc}s obtained with soils or sediments, which are unknown. However, it seems interesting to notice that, when comparison is done with a very large number of these

TABLE 15. Comparison between average K_{oc} values for soils or sediments and other literature averages

Compound	Sorbent type	Number of data points	K_{oc}[a] (average)	Deviation factor[b]	Ref.
Nitrobenzene	So	9	1.23E2		T.W.
	So	4	8.70E1	1.41	120
Naphthalene	So	25	8.13E2		T.W.
	So	5	4.17E2	1.95	120
	Se	7	1.15E3		T.W.
	Se	23	1.00E5	−87	544
	Se	2	1.29E3	−1.12	108
	So+Se	17	8.70E2	1.32 (Se) −1.07 (So)	96
Phenanthrene	So	6	1.07E4		T.W.
	Se	5	2.19E4		T.W.
	Se	23	1.32E6	−60	544
	Se	2	2.29E4	−1.04	108
	Se	8	3.89E4	−1.78	612
	So+Se	17	1.20E4	1.83 (Se) −1.12 (So)	96
Fluoranthene	Se	9	8.13E4		T.W.
	Se	23	2.40E6	−30	544
	Se	6	6.17E4	1.32	612
Pyrene	So	5	4.61E4		T.W.
	Se	28	7.59E4		T.W.
	Se	23	3.24E6	−43	544
	Se	8	4.68E4	1.62	612
	So+Se	17	6.76E4	1.12 (Se) −1.47 (So)	96
	So+Se	33	7.08E4	1.07 (Se) −1.54 (So)	562
Benzo(a)pyrene	Se	4	1.70E6		T.W.
	Se	23	1.82E6	−1.07	544
	Se	8	6.46E5	2.63	612
1,1,1-TCA	So	6	1.45E2		T.W.
	So	17	1.07E2	1.36	472
TCE	So	23	8.32E1		T.W.
	So	18	1.02E2	−1.23	472
TeCE	So	16	2.09E2		T.W.
	So	18	2.40E2	−1.15	472
Ametryne	So	33	3.31E2		T.W.
	So	33	3.90E2	−1.18	87
Atrazine	So	134	2.00E2		T.W.
	So	5	9.60E2	−4.80	455
	So	6	1.26E2	1.59	634
	So	6	1.62E2	1.23	634
	So	56	1.48E2	1.35	87
	So	109	2.14E2	−1.07	227
	Se	13	3.89E2		T.W.
	So+Se	217	1.55E2	2.51 (Se) 1.29 (So)	562
Carbaryl	So	12	1.59E2		T.W.
	So	5	1.29E2	1.23	590
Carbofuran	So	15	4.27E1		T.W.
	So	5	3.00E1	1.42	87
	So+Se	52	4.30E1	−1.01	562
Chlorbromuron	So	17	3.47E2		T.W.
	So	5	1.00E3	−2.88	87
Chlorpropham	So	16	4.17E2		T.W.
	So+Se	57	3.47E2	1.20	562

TABLE 15. Comparison between average K_{oc} values for soils or sediments and other literature averages—Continued

Compound	Sorbent type	Number of data points	$K_{oc}{}^{a}$ (average)	Deviation factor[b]	Ref.
p,p′-DDT	So	8	4.27E5		T.W.
	So	3	1.51E5	2.83	575
	So	2	2.46E5	1.74	87
	Se	8	1.20E6		T.W.
	So+Se	31	4.27E5	2.81 (Se) 1.00 (So)	562
Disulfoton	So	11	8.32E2		T.W.
	So	20	1.59E3	−1.91	87
Diuron	So	96	2.75E2		T.W.
	So	3	3.90E2	−1.42	575
	So	84	3.80E2	−1.38	87
	So	5	4.27E2	−1.55	455
	Se	3	6.03E2		T.W.
	So+Se	156	2.95E2	−2.19 (Se) −1.07 (So)	562
Fenuron	So	26	2.63E1		T.W.
	So	10	4.30E1	−1.63	87
	So	4	1.30E1	2.02	120
Fluometuron	So	78	1.48E2		T.W.
	So	4	6.60E1	2.24	120
Lindane	So	49	1.05E3		T.W.
	So	3	1.07E3	−1.02	87
	Se	4	3.09E3		T.W.
	So+Se	94	9.55E2	3.24 (Se) 1.10 (So)	562
Linuron	So	45	4.47E2		T.W.
	So	33	8.71E2	−1.95	87
	So	4	2.70E2	1.65	120
Malathion	So	20	1.20E3		T.W.
	So	20	1.82E3	−1.52	87
Methyl parathion	So	8	6.61E2		T.W.
	So	7	5.10E3	−7.72	87
Metobromuron	So	18	1.00E2		T.W.
	So	4	2.70E2	−2.70	87
Metolachlor	So	23	1.91E2		T.W.
	So+Se	45	2.14E2	−1.12	562
Monolinuron	So	20	7.59E1		T.W.
	So	10	2.80E2	−3.69	87
Monuron	So	21	6.31E1		T.W.
	So	18	1.82E2	−2.88	87
Napropamide	So	20	3.80E2		T.W.
	So	33	8.71E2	−2.29	87
	Se	4	6.31E2		T.W.
	So+Se	36	4.17E2	1.51 (Se) −1.10 (So)	562
Parathion	So	36	1.12E3		T.W.
	So	94	1.52E3	−1.36	663
	Se	5	1.48E3		T.W.
	So+Se	89	1.48E3	1.00 (Se) −1.32 (So)	562
Prometone	So	27	2.95E2		T.W.
	So	29	5.25E2	−1.78	87
Prometryne	So	81	4.07E2		T.W.
	So	38	6.17E2	−1.52	87
Propazine	So	35	1.41E2		T.W.

TABLE 15. Comparison between average K_{oc} values for soils or sediments and other literature averages—Continued

Compound	Sorbent type	Number of data points	K_{oc}[a] (average)	Deviation factor[b]	Ref.
	So	36	1.55E2	−1.10	87
Simazine	So	43	1.95E2		T.W.
	So	147	1.38E2	1.41	87
Terbacil	So	4	3.80E1		T.W.
	So	4	4.10E1	−1.08	87
Trifluralin	So	24	3.39E3		T.W.
	Se	5	2.63E4		T.W.
	So+Se	22	8.90E3	2.95(Se) −2.63(So)	562
Acetophenone	So	14	4.07E1		T.W.
	Se	17	3.63E1		T.W.
	So+Se	30	3.70E1	−1.02(Se) 1.10(So)	562

[a] Average K_{oc} values are taken as the antilog of the average $\log K_{oc}$ values (Tables 1–9 and Table 13).

[b] Deviation factor is calculated as the ratio of the average K_{oc} values for soils (So) or sediments (Se) derived from Table 13 to average K_{oc} values derived from other pools of data (Tables 1–9). When this ratio is less than 1 the negative reciprocal is reported.

T.W. This work.

TABLE 16. Comparison between average K_{oc} values for soils and sediments (OC≥0.5%) and prediction data

		Deviation factor[b]			
Compound	K_{oc}[a] (average)	Soil	Sediment	Method	Ref.
Benzene	3.82E1 (So)				T.W.
	7.41E1	−1.94		RPLC (humic acid)	585
	6.61E1	−1.73		RPLC (humic acid)	584
	3.72E1	1.02		RPLC (humic acid)	587
	4.17E1	−1.09		RPLC (salicylic acid)	587
	5.50E1	−1.44		RPLC (8-hydroxyquin.)	587
	6.61E1	−1.74		RPLC (C18)	577
	6.92E1	−1.81		RPLC (C18)	577
	5.25E1	−1.37		$\log K_{oc}-\log K_{ow}$	96
	7.94E1	−2.08		$\log K_{oc}-\log K_{ow}$	108
	1.02E2	−2.67		$\log K_{oc}-\log K_{ow}$	207
	7.08E1	−1.85		$\log K_{oc}-\log S$	564
	6.61E1	−1.73		$\log K_{oc}-\log S$	96
	5.25E1	−1.37		$\log K_{oc}-\log S$(mp)	96
	2.14E2	−5.60		$\log K_{oc}$−MCI	591
	5.13E1	−1.34		$\log K_{oc}$−CRI	601
	3.98E1	−1.04		$\log K_{oc}$−LSER	602
Nitrobenzene	1.45E2 (So)				T.W.
	1.12E2	1.29		RPLC (humic acid)	587
	6.92E1	2.10		RPLC (C18)	577
	9.77E1	1.48		RPLC (C18)	577
	1.45E2	1.00		RPLC (salicylic acid)	587
	1.41E2	1.03		RPLC (8-hydroxyquin.)	587
	7.08E1	2.05		$\log K_{oc}-\log S$	564
	1.48E2	−1.02		$\log K_{oc}$−MCI	578
	7.08E1	2.05		$\log K_{oc}$−LSER	602
Naphthalene	1.05E3 (So)				T.W.
	1.15E3 (Se)				T.W.
	1.43E3	−1.36	−1.24	RPLC (humic acid)	585
	1.12E3	−1.07	1.03	RPLC (salicylic acid)	587
	1.15E3	−1.09	1.00	RPLC (8-hydroxyquin.)	587
	9.33E2	1.13	1.23	$\log K_{oc}-\log K_{ow}$	96
	1.41E3	−1.34	−1.23	$\log K_{oc}-\log K_{ow}$	108
	8.13E2	1.29	1.41	$\log K_{oc}-\log K_{ow}$	207
	6.46E2	1.63	1.78	$\log K_{oc}-\log S$	564
	9.55E2	1.10	1.20	$\log K_{oc}-\log S$	96
	1.00E3	1.05	1.15	$\log K_{oc}-\log S$(mp)	96
	1.86E3	−1.77	−1.62	$\log K_{oc}$−MCI	578
	2.63E3	−2.50	−2.29	$\log K_{oc}$−MCI	591
	1.29E3	−1.23	−1.12	$\log K_{oc}$−LSER	602
Phenanthrene	1.20E4 (So)				T.W.
	2.19E4 (Se)				T.W.
	1.66E4	−1.38	1.32	RPLC (humic acid)	585
	1.91E4	−1.59	1.15	RPLC (humic acid)	587
	1.32E4	−1.10	1.66	RPLC (salicylic acid)	587
	1.70E4	−1.42	1.29	RPLC (8-hydroxyquin.)	587
	1.51E4	−1.26	1.45	$\log K_{oc}-\log K_{ow}$	96
	3.80E3	3.16	5.76	$\log K_{oc}-\log S$	564
	7.94E3	1.51	2.76	$\log K_{oc}-\log S$	96
	1.66E4	−1.38	1.32	$\log K_{oc}-\log S$(mp)	96
	2.09E4	−1.74	1.05	$\log K_{oc}$−MCI	578
	3.24E4	−2.70	−1.48	$\log K_{oc}$−MCI	591
	8.32E3	1.44	2.63	$\log K_{oc}$−LSER	602
	1.26E4	−1.05	1.74	Ring fragments	96
Fluoranthene	4.47E4 (So)				T.W.
	8.13E4 (Se)				T.W.
	4.17E4	1.07	1.94	RPLC (humic acid)	585
	5.50E4	−1.23	1.48	RPLC (humic acid)	585
	6.46E4	−1.45	1.26	$\log K_{oc}-\log K_{ow}$(180)	388
	1.23E5	−2.75	−1.51	$\log K_{oc}-\log K_{ow}$(96)	613

TABLE 16. Comparison between average K_{oc} values for soils and sediments (OC≥0.5%) and prediction data—Continued

Compound	K_{oc}^{a} (average)	Deviation factor^{b}		Method	Ref.
		Soil	Sediment		
	5.37E4	−1.20	1.51	log K_{oc}−log S(180)	388
	7.08E4	−1.58	1.15	log K_{oc}−MCI	598
Pyrene	6.03E4 (So)				T.W.
	7.94E4 (Se)				T.W.
	5.89E4	1.02	1.35	RPLC (humic acid)	585
	6.61E4	−1.10	1.20	RPLC (humic acid)	585
	6.31E4	−1.05	1.26	RPLC (humic acid)	587
	6.46E4	−1.07	1.23	RPLC (salicylic acid)	587
	5.25E4	1.15	1.51	RPLC (8-hydroxyquin.)	587
	6.17E4	−1.02	1.29	log K_{oc}−log K_{ow}	96
	9.33E4	−1.55	−1.18	log K_{oc}−log K_{ow}	108
	1.66E4	3.63	4.78	log K_{oc}−log K_{ow}	207
	1.29E4	4.67	6.16	log K_{oc}−log S	564
	3.24E4	1.86	2.45	log K_{oc}−log S	96
	4.37E4	1.38	1.82	log K_{oc}−log S(mp)	96
	6.92E4	−1.15	1.15	log K_{oc}−MCI	578
	1.12E5	−1.86	−1.41	log K_{oc}−MCI	591
	3.16E4	1.91	2.51	log K_{oc}−LSER	602
1,1,1-TCA (OC≥0.1)	1.45E2 (So)				T.W.
	1.29E2	1.12		RPLC (cyanopropyl)	579
	1.20E2	1.21		log K_{oc}−log K_{ow}	96
	1.05E2	1.38		log K_{oc}−log S	96
	1.10E2	1.32		log K_{oc}−log S(mp)	96
	5.01E1	2.89		log K_{oc}−MCI	578
	6.17E1	2.35		log K_{oc}−MCI	591
	1.20E2	1.21		log K_{oc}−LSER	602
TCE	1.00E2 (So)				T.W.
	1.29E2	−1.29		RPLC (cyanopropyl)	579
	1.38E2	−1.38		log K_{oc}−log K_{ow}(207)	193
	1.23E2	−1.23		log K_{oc}−log K_{ow}(108)	193
	4.57E1	2.19		log K_{oc}−log S(180)	193
	6.92E1	1.45		log K_{oc}−MCI	578
	5.01E1	2.00		log K_{oc}−MCI	597
TeCE	2.82E2 (So)				T.W.
	2.46E2	1.15		log K_{oc}−log K_{ow}	108
	1.38E2	2.04		log K_{oc}−log K_{ow}	96
	6.03E2	−2.14		log K_{oc}−log K_{ow}	217
	1.91E2	1.48		log K_{oc}−log K_{ow}(180)	88
	3.16E2	−1.12		log K_{oc}−log K_{ow}(87)	88
	1.82E2	1.55		log K_{oc}−log K_{ow}(120)	88
	2.75E2	1.03		log K_{oc}−log K_{ow}(130)	88
	6.46E2	−2.29		log K_{oc}−log K_{ow}(55)	88
	2.29E2	1.23		log K_{oc}−log K_{ow}	207
	2.40E2	1.18		log K_{oc}−log S	564
	2.24E2	1.26		log K_{oc}−log S	96
	3.72E2	−1.32		log K_{oc}−log S	96
	3.47E2	−1.23		log K_{oc}−log S(mp)	96
	7.76E2	−2.75		log K_{oc}−log S(mp)	96
	1.38E2	2.04		log K_{oc}−MCI	591
	3.31E2	−1.17		log K_{oc}−LSER	602
Phenol (u)	2.91E1 (So)				T.W.
	2.24E1	−1.02		RPLC (cyanopropyl)	579
	2.63E1	−1.20		RPLC (humic acid)	587
	1.00E1	2.19		RPLC (salycilic acid)	587
	1.74E1	1.26		RPLC (8-hydroxyqin.)	587
	3.89E1	−1.78		RPLC (C18)	577
	4.68E1	−2.14		RPLC (C18)	577
	1.48E2	−6.76		log K_{oc}−log K_{ow}	618
	7.24E0	3.02		log K_{oc}−log S(180)	335

TABLE 16. Comparison between average K_{oc} values for soils and sediments (OC≥0.5%) and prediction data—Continued

Compound	K_{oc}[a] (average)	Deviation factor[b]		Method	Ref.
		Soil	Sediment		
	8.91E0	2.46		$\log K_{oc}-\log S$	564
	7.24E1	−3.31		$\log K_{oc}$–MCI	578
	2.69E2	−12.3		$\log K_{oc}$–MCI	598
	7.08E1	−3.23		$\log K_{oc}$–CRI	601
	3.16E1	−1.44		$\log K_{oc}$–LSER	602
4-MCP (u)	2.14E2 (So)				T.W.
	1.70E1	12.6		$\log K_{oc}-\log S(180)$	335
	2.24E2	−1.05		$\log K_{oc}$–CRI	601
2,4-DCP (u)	5.89E2 (So)				T.W.
	2.95E2	2.00		RPLC (C18)	577
	3.39E2	1.74		RPLC (C18)	577
	5.75E1	10.2		$\log K_{oc}-\log S(180)$	335
	1.95E2	3.02		$\log K_{oc}$–MCI	578
	5.75E2	1.02		$\log K_{oc}$–MCI	597
	7.76E2	−1.32		$\log K_{oc}$–CRI	601
3,4-DCP (u)	1.07E3 (So)				T.W.
	7.24E2	1.48		$\log K_{oc}$–MCI	598
	7.59E2	1.41		$\log K_{oc}$–CRI	601
2,4,6-TCP (u)	7.24E2 (So)				T.W.
	3.16E2	2.29		$\log K_{oc}$–MCI	578
	9.77E2	−1.35		$\log K_{oc}$–MCI	597
	2.46E3	−3.40		$\log K_{oc}$–CRI	601
2,4,5-TCP (u)	2.24E3 (So)				T.W.
	1.02E2	22.0		$\log K_{oc}-\log S(180)$	335
	9.77E2	2.29		$\log K_{oc}$–MCI	597
	2.34E3	−1.04		$\log K_{oc}$–CRI	601
2,3,4,6-TeCP (u)	5.62E3 (So)				T.W.
	7.94E3	−1.41		$\log K_{oc}-\log K_{ow}$	111
	5.25E2	10.7		$\log K_{oc}$–MCI	578
	2.09E3	2.69		$\log K_{oc}$–MCI	597
	1.62E4	−2.88		$\log K_{oc}-\log K_{ow}(108)$	597
	5.89E3	−1.05		$\log K_{oc}-\log K_{ow}(217)$	597
	8.72E2	6.44		$\log K_{oc}-\log K_{ow}(120)$	597
	1.29E4	−2.30		$\log K_{oc}-\log K_{ow}(180)$	597
	1.59E3	3.53		$\log K_{oc}-\log K_{ow}(55)$	597
	6.76E3	−1.20		$\log K_{oc}$–CRI	601
PCP (u)	3.47E4 (So)				T.W.
	1.10E4	3.15		RPLC (cyanopropyl)	579
	2.51E4	1.38		$\log K_{oc}-\log K_{ow}$	111
	1.00E3	34.7		$\log K_{oc}-\log S$	564
	8.91E2	38.9		$\log K_{oc}$–MCI	578
	2.88E3	12.0		$\log K_{oc}$–MCI	597
	1.86E4	1.87		$\log K_{oc}$–CRI	601
4-NP (u)	8.71E1 (So)				T.W.
	1.51E2	−1.73		RPLC (cyanopropyl)	579
	1.45E2	−1.66		RPLC (C18)	577
	1.18E2	−1.35		RPLC (C18)	577
	2.34E1	3.72		$\log K_{oc}-\log S(180)$	335
	3.09E2	−3.35		$\log K_{oc}$–MCI	598
Atrazine	1.45E2 (So)				T.W.
	3.89E2 (Se)				T.W.
	8.71E1	1.66	4.47	$\log K_{oc}-\log K_{ow}$	96
	2.63E2	−1.81	1.48	$\log K_{oc}-\log K_{ow}$	96
	1.91E3	−13.2	−4.91	$\log K_{oc}-\log K_{ow}(87)$	528
	1.59E3	−11.0	−4.09	$\log K_{oc}-\log K_{ow}(217)$	528
	1.51E3	−10.4	−3.83	$\log K_{oc}-\log S(180)$	528

TABLE 16. Comparison between average K_{oc} values for soils and sediments (OC⩾0.5%) and prediction data—Continued

Compound	K_{oc}[a] (average)	Deviation factor[b]		Method	Ref.
		Soil	Sediment		
	6.46E2	−4.46	−1.66	$\log K_{oc}-\log S$	564
	1.29E3	−8.90	−3.32	$\log K_{oc}-\log S$	96
	2.04E2	−1.41	1.91	$\log K_{oc}-\log S$(mp)	96
	2.19E2	−1.51	1.78	$\log K_{oc}-$MCI	578
Bromacil	2.88E1 (So)				T.W.
	2.69E1 (Se)				T.W.
	4.27E1	−1.48	−1.59	$\log K_{oc}-\log K_{ow}$	96
	1.35E3	−46.9	−50.2	$\log K_{oc}-\log S$	564
	2.14E2	−7.43	−7.96	$\log K_{oc}-\log S$	96
	2.19E1	1.32	1.23	$\log K_{oc}-\log S$(mp)	96
	3.63E2	−12.6	−13.5	$\log K_{oc}-$MCI	578
Carbaryl	1.59E2 (So)				T.W.
	2.00E2	−1.26		RPLC (cyanopropyl)	579
	3.72E2	−2.34		RPLC (C18)	573
	2.63E2	−1.65		$\log K_{oc}-\log K_{ow}$	96
	5.75E2	−3.62		$\log K_{oc}-\log S$	564
	1.10E3	−6.92		$\log K_{oc}-\log S$	96
	3.16E2	−1.99		$\log K_{oc}-\log S$(mp)	96
	1.70E2	−1.07		$\log K_{oc}-$MCI	578
Carbofuran	4.37E1 (So)				T.W.
	1.29E2	−2.95		RPLC (C18)	573
	4.79E1	−1.10		$\log K_{oc}-\log K_{ow}$	96
	1.59E2	−3.64		$\log K_{oc}-\log S$	564
	2.88E1	1.52		$\log K_{oc}-\log S$	96
	3.24E1	1.35		$\log K_{oc}-\log S$(mp)	96
Chlorpropham	4.17E2 (So)				T.W.
	4.68E2	−1.12		$\log K_{oc}-\log K_{ow}$	96
	3.72E2	1.12		$\log K_{oc}-\log S$	564
	7.08E2	−1.70		$\log K_{oc}-\log S$	96
	6.31E2	−1.51		$\log K_{oc}-\log S$	96
	1.48E3	−3.55		$\log K_{oc}-\log S$(mp)	96
	1.20E3	−2.88		$\log K_{oc}-\log S$(mp)	96
p,p′-DDT	3.47E5 (So)				T.W.
	1.20E6 (Se)				T.W.
	6.31E5	−1.82	1.90	$\log K_{oc}-\log K_{ow}$	96
	8.91E4	3.89	13.5	$\log K_{oc}-\log K_{ow}$	207
	9.55E5	−2.75	1.26	$\log K_{oc}-\log K_{ow}$	108
	1.45E5	2.39	8.28	$\log K_{oc}-\log S$	564
	4.17E5	−1.20	2.88	$\log K_{oc}-\log S$	96
	6.46E6	−18.6	−5.38	$\log K_{oc}-\log S$(mp)	96
	2.19E5	1.58	5.48	$\log K_{oc}-$MCI	578
	3.72E5	−1.07	3.23	$\log K_{oc}-$MCI	591
Diuron	2.69E2 (So)				T.W.
	3.02E2	−1.12		RPLC (C18)	573
	3.80E1	7.08		$\log K_{oc}-\log K_{ow}$	96
	2.63E2	1.02		$\log K_{oc}-\log K_{ow}$	96
	5.62E2	−2.09		$\log K_{oc}-\log S$	564
	1.15E3	−4.28		$\log K_{oc}-\log S$	96
	2.57E2	1.05		$\log K_{oc}-\log S$(mp)	96
Fenuron	2.57E1 (So)				T.W.
	4.07E0	6.31		$\log K_{oc}-\log K_{ow}$	96
	4.68E1	−1.82		$\log K_{oc}-\log S$	564
	6.31E1	−2.46		$\log K_{oc}-\log S$	96
	7.24E1	−2.82		$\log K_{oc}-\log S$	96
	5.25E0	4.90		$\log K_{oc}-\log S$(mp)	96
	6.92E0	3.71		$\log K_{oc}-\log S$(mp)	96
Lindane	1.00E3 (So)				T.W.

TABLE 16. Comparison between average K_{oc} values for soils and sediments (OC≥0.5%) and prediction data—Continued

Compound	K_{oc}[a] (average)	Deviation factor[b]		Method	Ref.
		Soil	Sediment		
	3.09E3 (Se)				T.W.
	2.14E3	−2.14	1.44	log K_{oc}−log K_{ow}	96
	3.16E3	−3.16	−1.02	log K_{oc}−log K_{ow}(96)	49
	1.23E4	−12.3	−3.98	log K_{oc}−log S	564
	3.72E3	−3.72	−1.20	log K_{oc}−log S	96
	3.98E3	−3.98	−1.29	log K_{oc}−log S(mp)	96
	3.47E3	−3.47	−1.12	log K_{oc}−MCI	578
	4.79E3	−4.79	−1.55	log K_{oc}−MCI	591
Linuron	4.37E2 (So)				T.W.
	6.03E2 (Se)				T.W.
	4.68E2	−1.07	1.29	RPLC (cyanopropyl)	581
	6.31E1	6.93	9.56	log K_{oc}−log K_{ow}	96
	4.07E2	1.07	1.48	log K_{oc}−log S	564
	8.51E2	−1.95	−1.41	log K_{oc}−log S	96
	6.31E2	−1.44	−1.05	log K_{oc}−log S(mp)	96
Malathion	1.15E3 (So)				T.W.
	3.16E2	3.64		log K_{oc}−log K_{ow}	96
	2.82E2	4.08		log K_{oc}−log S	564
	6.76E2	1.70		log K_{oc}−log S	96
	1.95E3	−1.70		log K_{oc}−log S(mp)	96
Metolachlor	1.55E2 (So)				T.W.
	1.41E2	1.10		log K_{oc}−log S	564
	2.88E2	−1.86		log K_{oc}−MCI	598
Napropamide	3.80E2 (So)				T.W.
	6.31E2 (Se)				T.W.
	4.07E2	−1.07	1.55	log K_{oc}−log S	564
Parathion	1.23E3 (So)				T.W.
	1.48E3 (Se)				T.W.
	2.63E3	−2.14	−1.78	log K_{oc}−log K_{ow}	96
	1.70E3	−1.38	−1.15	log K_{oc}−log K_{ow}	207
	3.98E3	−3.24	−2.69	log K_{oc}−log K_{ow}	108
	7.59E2	1.62	1.95	log K_{oc}−log S	564
	1.78E3	−1.45	−1.20	log K_{oc}−log S	96
	8.91E3	−7.24	−6.02	log K_{oc}−log S(mp)	96
Prometone	3.16E2 (So)				T.W.
	2.00E2	1.58		log K_{oc}−log K_{ow}(87)	528
	4.90E2	−1.55		log K_{oc}−log K_{ow}(217)	528
	2.63E2	1.20		log K_{oc}−log S(180)	528
	1.10E2	2.87		log K_{oc}−log S	564
	1.59E2	1.99		log K_{oc}−MCI	598
Prometryne	4.17E2 (So)				T.W.
	5.25E2	−1.26		log K_{oc}−log S	564
Propazine	1.48E2 (So)				T.W.
	3.55E2	−2.40		log K_{oc}−log K_{ow}	96
	1.29E3	−8.72		log K_{oc}−log S	564
	2.95E3	−19.9		log K_{oc}−log S	96
	3.09E2	−2.09		log K_{oc}−log S(mp)	96
Simazine	1.95E2 (So)				T.W.
	5.89E1	3.31		log K_{oc}−log K_{ow}	96
	2.19E3	−11.2		log K_{oc}−log S	564
	4.57E3	−23.4		log K_{oc}−log S	96
	3.39E2	−1.74		log K_{oc}−log S(mp)	96
Terbacil	3.80E1 (So)				T.W.
	3.16E1	1.20		log K_{oc}−log K_{ow}	96
	1.20E2	−3.16		log K_{oc}−log S	564

TABLE 16. Comparison between average K_{oc} values for soils and sediments (OC≥0.5%) and prediction data—Continued

Compound	K_{oc}[a] (average)	Deviation factor[b] Soil	Deviation factor[b] Sediment	Method	Ref.
	2.09E2	−5.50		$\log K_{oc}-\log S$	96
	1.12E1	3.39		$\log K_{oc}-\log S$(mp)	96
Trifluralin	2.82E3 (So)				T.W.
	2.63E4 (Se)				T.W.
	1.35E5	−47.9	−5.13	RPLC (cyanopropyl)	579
	9.55E3	−3.39	2.75	RPLC (C18)	573
	5.75E3	−2.04	4.57	$\log K_{oc}-\log S$	564
Acetophenone	3.16E1 (So)				T.W.
	3.55E1 (Se)				
	1.59E1	1.99	2.23	$\log K_{oc}-\log K_{ow}$	96
	4.27E1	−1.35	−1.20	$\log K_{oc}-\log K_{ow}$	207
	2.63E1	1.20	1.35	$\log K_{oc}-\log K_{ow}$	108
	4.37E1	−1.38	1.23	$\log K_{oc}-\log S$	96
	2.51E1	1.26	1.41	$\log K_{oc}-\log S$(mp)	96

[a] Average K_{oc} values are taken as the antilog of the average $\log K_{oc}$ values (Tables 1–9 and Table 13).

[b] Deviation factor is calculated as the ratio of the average K_{oc} values for soils (So) or sediments (Se) derived from Table 13 to predicted values derived from Tables 1–9. When this ratio is less than 1 the negative reciprocal is reported.

T.W. This work.

literature data, a maximum factor of about 3 is obtained, which is indicative of a satisfactory accuracy at least for the nonionizable compounds listed in Table 15.

13.3. Comments on Prediction Methods

Finally, to evaluate the reliability of the prediction methods the estimated K_{oc} data were compared with the averages derived in Table 13 for soils and sediments. The results in Table 16 show that for hydrophobic compounds deviation factors are mostly within a value of 2 in the absolute value, while for polar and ionizable compounds factors often reach values higher than 1 order of magnitude. In particular:

(i) RPLC with C18 and other types of stationary phases gives estimates (47 values) of K_{oc} with deviation factors equal to or lower than 5 with both hydrophobic and polar compounds. One exception seems to be the value of -48 found for trifluralin with cyanopropyl as stationary phase;

(ii) About one half of the 61 data concerning K_{oc}–K_{ow} relationships give deviation factors within 2, which regard especially nonpolar compounds. The remaining data give factors within 13.5, with only 3 being greater than 10. This second group of data concern phenols, triazines, and other pesticides;

(iii) K_{oc}–S relationships (87 data) give the worst results with factors >5 and >10 for 28% and 14% of the data, respectively. The greatest values are concentrated on phenols, triazines, and bromacil. Introducing the correction for the melting point, generally an improvement is obtained: in 22 cases only five give factors lower than expected. However, as pointed out by Gerstl,[562] the crystal energy term was derived for rigid molecules and therefore it may not give the same result for all compounds;

(iv) Finally, 26 of the total 54 data concerning prediction of K_{oc} based on correlations with parameters connected to molecular structure give deviation factors within 2, while 20 data give factors between 2 and 5, and the rest between 5 and about 40, with only 6 data >10. These concern especially phenols and bromacil.

In conclusion, predictions of sorption coefficients for nonpolar compounds are generally satisfactory with all methods, while K_{oc} predicted for polar or ionizable compounds may show large differences from average experimental K_{oc} values. For these compounds, predictions may be complicated due to the great uncertainty of the log–log plots using the experimental values of K_{oc} to calibrate the systems. This uncertainty may depend on possible contribution of several sorption mechanisms for compounds belonging to different classes. Therefore, for these compounds, a specific correlation equation for each class may be better than a single equation for the total data base, as suggested by some authors.[120,561,562]

14. Acknowledgment

The author wishes to thank Dr. L. Monte for valuable comments.

15. Nomenclature

AG	adsorption to glass container walls
BDHA	benzyldimethylhexadecylammonium ion
BE	batch equilibration
BU	batch equilibration and ultrafiltration
CE	cation exchange capacity [m equivalent $(100\ g)^{-1}$ or cmol kg^{-1}]
CRI	characteristic root index
DDPA	dodecyldimethyl(2-phenoxyethyl)ammonium ion
DDTMA	dodecyltrimethylammonium ion
DF	diffusion
DHS	dissolved humic substances
DOC	dissolved organic carbon
DOM	dissolved organic matter
DTMA	decyltrimethylammonium ion (Ref. 93)
DTMA	dodecyltrimethylammonium ion (Ref. 93)
DTMDA	decyltrimethyldiammonium ion
ED	equilibrium dialysis
FE	flow equilibration
FH	Flory–Huggins model
FM	field measurement
f_c	volume fraction of cosolvent
f_{oc}	fraction of sorbent organic carbon
f_{om}	fraction of sorbent organic matter
FQ	fluorescence quenching
ΔG	Gibbs energy (J mol^{-1})
GP	gas purge
H	Henry's Law constant
ΔH	enthalpy (J mol^{-1})
ΔH_f	enthalpy of fusion (J mol^{-1})
HDTMA	hexadecyltrimethylammonium ion
HS	head space
HT	humic acid titration
HTMA	hexadecyltrimethylammonium ion (Ref. 93)
k'	chromatographic capacity factor
K_a	acid dissociation constant
K_d	linear sorption coefficient ($cm^3\ g^{-1}$ or $dm^3\ kg^{-1}$)
K_{doc}	dissolved organic carbon–water partition coefficient ($cm^3\ g^{-1}$)
K_{dom}	dissolved organic matter–water partition coefficient ($cm^3\ g^{-1}$)
K_f	Frendlich sorption coefficient ($\mu g l^{-1/n}\ cm^{3/n}\ g^{-1}$)
K_{oc}	organic carbon-normalized partition coefficient ($cm^3\ g^{-1}$ of organic carbon)
K_{ow}	octanol/water partition coefficient
K_{sg}	solid–gas sorption coefficient ($cm^3\ g^{-1}$)
LE	leaching equilibration
LSER	linear solvation energy relationship

LSC	limiting sorption capacity
μ	ionic strength
MCI	molecular connectivity index
MD	miscible displacement
mp	melting point (K or °C)
$1/n$	Freundlich exponent
NTMA	nonyltrimethylammonium ion
OC	soil or sediment organic carbon (%)
OM	soil or sediment organic matter (%)
R	gas constant (8.314510 J $\mathrm{mol^{-1}\ K^{-1}}$)
RPLC	reversed-phase high pressure liquid chromatography
RS	reversed-phase separation by C18 column
R_t	retardation factor
r_t	chromatographic retention time
ΔS	entropy (J $\mathrm{mol^{-1}\ K^{-1}}$)
ΔS_f	entropy of fusion (J $\mathrm{mol^{-1}\ K^{-1}}$)
S	water solubility (g $\mathrm{m^{-3}}$ or mol $\mathrm{m^{-3}}$)
SA	surface area ($\mathrm{m^2\ g^{-1}}$); method not specified
SA(CO_2)	surface area measured by carbon dioxide sorption
SA(E)	surface area measured by ethylene glycol monoethyl ether (EGME) sorption
SA(M)	surface area measured by methylene blue sorption
S(mp)	water solubility for subcooled liquids
SA(N_2)	surface area measured by nitrogen (BET) sorption
SA(W)	surface area measured by water vapor sorption
SE	solubility enhancement
Soil texture:	
c	clay
cl	clay loam
l	loam
ls	loamy sand
s	sand
sc	sandy clay
scl	sandy clay loam
sl	sandy loam
si	silt
sic	silty clay
sicl	silty clay loam
sil	silt loam
T	temperature (K)
T_m	melting point (K)
TOC	total organic carbon
TTMA	tetradecyltrimethylammonium ion

16. References

[1] Environmental Protection Agency, Guidelines for Registering Pesticides in United States, Federal Register 40 (123), 26802–26928 (1975).

[2] OECD Chemical Testing Program-Expert Group Physical Chemistry, Final Report, Berlin (December 1979).

[3] M. F. Kovacs, Jr., Residue Review **85**, 4 (1983).

[4] P. J. Mc Call, R. L. Swann, and D. A. Laskowski, in *Fate of Chemicals in the Environment*, edited by R. L. Swann and A. Eschenroeder, N. 225 (ACS, Washington, D.C., 1983).

[5] Environmental Protection Agency, Exposure Analysis Modeling System (EXAMS): User Manual and System Documentation, EPA Publication, EPA-600-3-82-023 (1981).

[6] K. Yoshida, T. Shigeoka, and F. Yamauchi, Ecotoxicol. Environ. Safety **7**, 179 (1983).

[7] D. Mackay, Environ. Sci. Technol. **13**, 1218 (1979).

[8] D. Mackay and S. Paterson, Environ. Sci. Technol. **15**, 1006 (1981).

[9] D. Mackay and S. Paterson, Environ. Sci. Technol. **16**, 654A (1982).

[10] P. Y. Lu and R. Metcalf, Environ. Health Perspect. **10**, 269 (1975).

[11] W. J. Lyman, W. F. Reehl, and D. H. Rosenblatt, editors, *Handbook of Chemical Property Estimation Methods* (McGraw-Hill, New York, 1982).

[12] D. Mackay and W. Y. Shiu, J. Phys. Chem. Ref. Data **10**, 1175 (1981).

[13] D. Mackay, W. Y. Shiu, and K. C. Ma, *Illustrated Handbook of Physical-Chemical Properties and Environmental Fate of Organic Chemicals* (Lewis, Boca Raton, 1992).

[14] R.-M. Dannenfelser, M. Paric, M. White, and S. H. Yalkowsky, Chemosphere **23**, 141 (1991).

[15] L. R. Suntio, W. Y. Shiu, D. Mackay, J. N. Seiber, and D. Glotfelty, Rev. Environ. Contam. Toxicol. **103**, 1 (1988).

[16] W. Y. Shiu and D. Mackay, J. Phys. Chem. Ref. Data **15**, 911 (1986).

[17] A. Delle Site, J. Phys Chem. Ref. Data **26**, 157 (1997).

[18] C. A. Edwards, Soils Fertilizers **27**, 451 (1964).

[19] T. J. Sheets, J. Agric. Food Chem. **12**, 30 (1964).

[20] D. F. Goerlitz, D. E. Troutman, E. M. Godsy, and B. J. Franks, Environ. Sci. Technol. **19**, 955 (1985).

[21] J. F. Mc Carthy and J. M. Zachara, Environ. Sci. Technol. **23**, 496 (1989).

[22] R. P. Schwarzenbach, W. Giger, E. Hoehn, and J. K. Schneider, Environ. Sci Technol. **17**, 472 (1983).

[23] L. B. Barber, II, E. M. Thurman, M. P. Schroeder, and D. R. Le Blanc, Environ. Sci. Technol. **22**, 205 (1988).

[24] D. Mackay, D. L. Freyberg, P. V. Roberts, and J. A. Cherry, Water Resour. Res. **22**, 2017 (1986).

[25] G. W. Page, Environ. Sci. Technol. **15**, 1475 (1981).

[26] S. M. Lambert, P. E. Porter, and H. Schieferstein, Weeds **13**, 185 (1965).

[27] R. P. Upchurch and W. C. Pierce, Weeds **6**, 24 (1958).

[28] W. J. Weber, P. M. Mc Ginley, and L. E. Katz, Water Res. **25**, 499 (1991).

[29] W. A. Jury, D. Russo, G. Streile, and H. Elabd, Water Resour. Res. **26**, 13 (1990).

[30] R. Haque, D. W. Schmedding, and V. H. Freed, Environ. Sci. Technol. **8**, 139 (1974).

[31] W. F. Spencer and M. M. Cliath, Environ. Sci. Technol. **3**, 670 (1969).

[32] W. F. Spencer, T. D. Shoup, M. M. Cliath, W. J. Farmer, and R. Haque, J. Agric. Food Chem. **27**, 273 (1979).

[33] A. E. Smith, Weed Res. **10**, 331 (1970).

[34] R. G. Thomas, in *Handbook of Chemical Property Estimation Methods*, edited by W. J. Lyman, W. F. Reehl, and D. H. Rosenblatt (McGraw-Hill, New York, 1982), Chap. 15.

[35] G. W. Bailey and J. L. White, J. Agric. Food Chem. **12**, 324 (1964).

[36] C. R. Harris, J. Econ. Entomol. **59**, 1221 (1966).

[37] P. J. Doherty and G. F. Warren, Weed Res. **9**, 20 (1969).

[38] C. I. Harris and T. J. Sheets, Weeds **13**, 215 (1965).

[39] R. P. Upchurch and D. D. Mason, Weeds **10**, 9 (1962).

[40] R. P. Upchurch, Weeds **6**, 161 (1958).

[41] R. P. Upchurch, F. L. Selman, D. D. Mason, and E. J. Kamprath, Weeds **14**, 42 (1966).

[42] J. B. Weber and C. J. Peter, Weed Sci. **30**, 14 (1982).

[43] E. M. Watkin and G. R. Sagar, Weed Res. **11**, 1 (1971).

[44] E. M. Watkin and G. R. Sagar, Weed Res. **11**, 247 (1971).

[45] R. G. Burns and L. J. Audus, Weed Res. **10**, 49 (1970).

[46] L. A. Gaston, M. A. Locke, and R. M. Zablotowicz, J. Environ. Qual. **25**, 120 (1996).

[47] J. G. Konrad, G. Chesters, and D. E. Armstrong, Soil Sci. Soc. Am. Proc. **33**, 259 (1969).

[48] F. J. Stevenson, J. Environ. Qual. **1**, 333 (1972).

[49] B. G. Oliver and M. N. Charlton, Environ. Sci. Technol. **18**, 903 (1984).

[50] J. E. Baker, P. D. Capel, and S. J. Elsenreich, Environ. Sci. Technol. **20**, 1136 (1986).

[51] H. B. Pionke and G. Chesters, J. Environ. Qual. **2**, 29 (1973).
[52] S. W. Karickhoff, J. Hydraul. Eng. **110**, 707 (1984).
[53] J. A. Smith, P. J. Witkowski, and C. T. Chiou, Rev. Environ. Contam. Toxicol. **103**, 127 (1988).
[54] W. J. Weber, P. M. Mc Ginley, and L. E. Katz, Environ. Sci. Technol. **26**, 1955 (1992).
[55] C. T. Chiou, P. E. Porter, and D. W. Schmedding, Environ. Sci. Technol. **17**, 227 (1983).
[56] *OECD-Guidelines for Testing of Chemicals*, TG-106, revised version (OECD, Paris, 1983).
[57] B. Von Oepen, W. Kördel, and W. Klein, Chemosphere **18**, 1495 (1989).
[58] P. G. J. De Maagd, T. L. Sinnige, S. M. Schrap, A. Opperhuizen, and D. T. H. M. Sijm, Environ. Toxicol. Chem. **17**, 1899 (1998).
[59] C. A. Black, editor, *Methods of Soil Analysis*, No. 9 in the Series Agronomy (ASA, Madison, WI, 1965).
[60] A. Klute, editor, *Methods of Soil Analysis*, Agron. Monogr. 9 (ASA and SSSA, Madison, WI, 1986).
[61] A. L. Page, R. H. Miller, and D. R. Keeny, editors, *Methods of Soil Analysis*, Argon. Monogr. 9 (ASA and SSSA, Madison, WI, 1988).
[62] G. Kuhnt and H. Muntau, editors, *EURO-SOILS: Identification, Collection, Treatment, Characterization* (JRC Ispra, European Commission Special Pub. No. 1.94.60, 1994).
[63] B. Gawlik, N. Sotiriou, G. Kuhnt, W. Karcher, A. Kettrup, and H. Muntau, Fresenius Environ. Bull. **5**, 610 (1996).
[64] European Directive 79/831/EEC, Annex V. Official Journal No L251 (19th September 1984), and No L133 (30th May 1988).
[65] W. P. Ball, C. H. Buehler, T. C. Harmon, D. Mackay, and P. V. Roberts, J. Contam. Hydrol. **5**, 253 (1990).
[66] S. Brunauer, P. H. Emmett, and E. Teller, J. Am. Chem. Soc. **60**, 309 (1938).
[67] G. L. Gaines, Jr. and P. Cannon, J. Phys. Chem. **62**, 997 (1960).
[68] J. Thomas, Jr. and R. R. Frost, Illinois Acad. Sci. Trans. **64**, 248 (1971).
[69] D. L. Carter, M. D. Heilman, and C. L. Gonzales, Soil Sci. **100**, 356 (1965).
[70] C. A. Bower and F. B. Gschwend, Soil Sci. Soc. Am. Proc. **16**, 342 (1952).
[71] Z. Ekler, Pestic. Sci. **22**, 145 (1988).
[72] J. Kozak and J. B. Weber, Weed Sci. **31**, 368 (1983).
[73] K. S. La Fleur, Soil Sci. **121**, 212 (1976).
[74] L. E. Allison, in *Methods of Soil Analysis*, edited by A. Black, No 9 in the Series of Agronomy, Part 2 (ASA, Madison, WI, 1965), pp. 1367–1378.
[75] D. W. Nelson and L. E. Sommers, in *Methods of Soil Analysis*, edited by A. L. Page, R. H. Miller, and D. R. Keeny, Agron. Monogr. 9, Part 2 (ASA and SSSA, Madison, WI, 1988), pp. 539–577.
[76] R. M. Gershey, M. D. Mackinnon, P. J. Williams, and R. M. Moore, Mar. Chem. **7**, 289 (1979).
[77] J. I. Hedges and J. H. Stern, Limnol. Oceanogr. **29**, 657 (1984).
[78] S. A. Waksman and L. J. Hutchings, Soil Sci. **40**, 347 (1953).
[79] C. H. Giles, D. Smith, and A. Huitson, J. Colloid Interface Sci. **47**, 755 (1974).
[80] C. H. Giles, D. Smith, and A. Huitson, J. Colloid Interface Sci. **47**, 766 (1974).
[81] T. C. Voice and W. J. Weber, Jr., Water Res. **17**, 1433 (1983).
[82] I. Langmuir, J. Am. Chem. Soc. **40**, 1361 (1918).
[83] J. W. Gibbs, I. Trans. Conn. Acad. **3**, 108 (1876).
[84] J. W. Gibbs, I. Trans. Conn. Acad. **3**, 343 (1876).
[85] H. Freundlich, *Colloid and Capillary Chemistry* (Methuen & Co. Ltd., London, 1926), pp. 110–114.
[86] D. J. O'Connor and J. P. Connolly, Water Res. **14**, 1517 (1980).
[87] P. S. C. Rao and J. M. Davidson, in *Environmental Impact of Nonpoint Source Pollution*, edited by M. R. Overcash and J. M. Davidson (Ann Arbor Sci., Inc., Ann Arbor, MI, 1980), pp. 23–67.
[88] W. P. Ball and P. V. Roberts, Environ. Sci. Technol. **25**, 1223 (1991).
[89] S. W. Karickhoff and D. S. Brown, J. Environ. Qual. **7**, 246 (1979).
[90] B. A. G. Knight and T. E. Tomlinson, J. Soil Sci. **18**, 233 (1967).
[91] C. T. Miller and W. J. Weber, J. Contam. Hydrol **1**, 243 (1986).
[92] J. A. Smith and P. R. Jaffé, Environ. Sci. Technol. **25**, 2054 (1991).
[93] J. A. Smith, P. R. Jaffé, and C. T. Chiou, Environ. Sci. Technol. **24**, 1167 (1990).
[94] Z. Wang, D. S. Gamble, and C. H. Langford, Environ. Sci. Technol. **26**, 560 (1992).
[95] R. W. Walters and R. G. Luthy, Environ. Sci. Technol. **18**, 395 (1984).
[96] S. W. Karickhoff, Chemosphere **10**, 833 (1981).
[97] J. J. Hassett, W. L. Banwart, S. G. Wood, and J. C. Means, Soil Sci. Soc. Am. J. **45**, 38 (1981).
[98] J. Farrell and M. Reinhard, Environ. Sci. Technol. **28**, 53 (1994).
[99] R. Haque and W. R. Coshow, Environ. Sci. Technol. **5**, 139 (1971).
[100] P. J. Isaacson and C. R. Frink, Environ. Sci. Technol. **18**, 43 (1984).
[101] J. L. Young and G. Spycher, Soil Sci. Soc. Am. J. **43**, 324 (1979).
[102] P. S. C. Rao and J. M. Davidson, Water Res. **13**, 375 (1979).
[103] R. D. Wauchope and W. C. Koskinen, Weed Sci. **31**, 504 (1983).
[104] J. M. Davidson, L. T. Ou, and P. S. C. Rao, EPA Rep. EPA-600/9-78-016, 1978, pp. 233–244.
[105] W. J. Lyman, in *Handbook of Chemical Property Estimation Methods*, edited by W. J. Lyman, W. F. Reehl, and D. N. Rosenblatt (McGraw-Hill, New York, 1982), Chap. 4, pp. 4.1–4.33.
[106] P. Lafrance, L. Marineau, L. Perreault, and J. P. Villeneuve, Environ. Sci. Technol. **28**, 2314 (1994).
[107] D. R. Burris, C. P. Antworth, and T. B. Stauffer, Environ. Toxicol. Chem. **10**, 433 (1991).
[108] S. W. Karickhoff, D. S. Brown, and T. A. Scott, Water Res. **13**, 241 (1979).
[109] R. W. Walters, S. A. Ostazeski, and A. Guiseppi-Elie, Environ. Sci. Technol. **23**, 480 (1989).
[110] W. P. Ball and P. V. Roberts, Environ. Sci. Technol. **25**, 1237 (1991).
[111] P. Lagas, Chemosphere **17**, 205 (1988).
[112] P. V. Roberts, M. N. Goltz, and D. Mackay, Water Resour. Res. **22**, 2047 (1986).
[113] D. F. Young and W. P. Ball, Environ. Progress **13**, 9 (1994).
[114] K. S. La Fleur, Soil Sci. **127**, 94 (1979).
[115] P. L. Mc Carty, M. Reinhard, and B. E. Rittmann, Environ. Sci. Technol. **15**, 40 (1981).
[116] S. M. Lambert, J. Agric. Food Chem. **15**, 572 (1967).
[117] K. E. Savage, Weed Sci. **24**, 525 (1976).
[118] K. E. Savage and R. D. Wauchope, Weed Sci. **22**, 106 (1974).
[119] R. S. Adams and P. Li, Soil Sci. Soc. Am. Proc. **35**, 78 (1971).
[120] G. G. Briggs, J. Agric. Food Chem. **29**, 1050 (1981).
[121] R. D. Carringer, J. B. Weber, and T. J. Monaco, J. Agric. Food Chem. **23**, 568 (1975).
[122] A. Felsot and P. A. Dahm, J. Agric. Food Chem. **27**, 557 (1979).
[123] J. W. Hamaker and J. M. Thompson, in *Organic Chemicals in the Soil Environment*, edited by C. M. Goring and J. W. Hamaker (Marcel Dekker, New York, 1972), Vol. 1, pp. 49–143.
[124] M. Hermann, in *EURO-SOILS: Identification, Collection, Treatment, Characterization*, edited by G. Kuhnt and H. Muntau (European Commission, JRC Ispra, 1994), Spec. Publ. No. 1.94.60.
[125] S. U. Khan, Can. J. Soil Sci. **53**, 429 (1973).
[126] M. S. Sharom and K. R. Solomon, J. Agric. Food Chem. **29**, 1122 (1981).
[127] R. A. Swanson and G. R. Dutt, Soil Sci. Soc. Am. Proc. **37**, 872 (1973).
[128] P. D. Vowles and R. F. C. Mantoura, Chemosphere **16**, 109 (1987).
[129] P. A. Wahid and N. Sethunathan, J. Agric. Food Chem. **26**, 101 (1978).
[130] D. S. Brown and E. W. Flagg, J. Environ. Qual. **10**, 382 (1981).
[131] H. Løkke, Ecotoxicol. Environ. Safety **8**, 395 (1984).
[132] R. T. Podoll, K. C. Irwin, and H. J. Parish, Chemosphere **18**, 2399 (1989).
[133] S. M. Schrap and A. Opperhuizen, in *Organic Micropollutants in the Aquatic Environment*, edited by G. Angeletti and A. Biorseth, Proc. 5th European Symp., 20–22 October 1987 (Kluwer, Dordrecht, 1988).
[134] J. T. Coates and A. W. Elzerman, J. Contam. Hydrol **1**, 191 (1986).
[135] P. J. Mc Call and G. L. Agin, Environ. Toxicol. Chem. **4**, 37 (1985).
[136] B. G. Oliver, Chemosphere **14**, 1087 (1985).
[137] R. E. White, J. S. Dyson, Z. Gerstl, and B. Yaron, Soil Sci. Soc. Am. J., **50**, 277 (1986).
[138] B. Yaron, A. R. Swoboda, and G. W. Thomas, J. Agric. Food Chem. **15**, 671 (1967).
[139] B. Yaron and S. Saltzman, Soil Sci. Soc. Am. Proc. **36**, 583 (1972).
[140] G. Dios Cancela, E. Romero Taboada, and F. Sanchez-Rasero, Soil Sci. **150**, 836 (1990).
[141] N. Senesi and C. Testini, Soil Sci. **130**, 314 (1980).
[142] D. R. Narine and R. D. Gui, Soil Sci. **133**, 356 (1982).
[143] R. S. Kookana, L. A. G. Aylmore, and R. G. Gerritse, Soil Sci. **154**, 214 (1992).
[144] R. J. Hance, Weed Res. **7**, 29 (1967).
[145] R. E. Talbert and O. H. Fletchall, Weeds **13**, 46 (1965).

[146] R. Haque, F. T. Lindstrom, V. H. Freed, and R. Sexton, Environ. Sci. Technol. **2**, 207 (1968).

[147] J. A. Leenheer and J. L. Ahlrichs, Soil Sci. Soc. Am. Proc. **35**, 700 (1971).

[148] M. Th. van Genuchten and P. J. Wierenga, Soil Sci. Soc. Am. J. **40**, 473 (1976).

[149] L. A. Gaston and M. A. Locke, J. Environ. Qual. **24**, 29 (1995).

[150] J. C. Huang and C. S. Liao, J. Saint. Eng. Dev. ASCE **96**, 1057 (1970).

[151] S. W. Karickhoff, in *Contaminants and Sediments: Analysis, Chemistry, and Biology*, edited by R. A. Baker (Ann Arbor Science, Ann Arbor, MI, 1980), Vol. 2, pp. 193–205.

[152] B. R. Larsen, M. Loekke, and L. Rasmussen, Oikos **44**, 423 (1985).

[153] A. B. Paya-Perez, M. Riaz, and B. R. Larsen, Ecotoxicol. Environ. Safety **21**, 1 (1991).

[154] J. J. Pignatello, in *Reactions and Movement of Organic Chemicals in Soils*, edited by B. L. Sawhney and K. Brown, SSSA Special Publ. No. 22 (Soil Science Society of America, Madison, VI, 1989), pp. 45–80.

[155] S. Wu and P. M. Gschwend, Environ. Sci. Technol. **20**, 717 (1986).

[156] S. W. Karickhoff and K. R. Morris, Environ. Toxicol. Chem. **4**, 469 (1985).

[157] W. P. Ball and P. V. Roberts, in *Organic Substances and Sediments in Water*: Vol. 2, Processes and Analytical, edited by R. A. Baker (Lewis, Chelsea, MI, 1991), Chap. 13, pp. 273–310.

[158] S. A. Clay and W. C. Koskinen, Weed Sci. **38**, 74 (1990).

[159] M. A. Locke, J. Environ. Qual. **21**, 558 (1992).

[160] N. Senesi, G. Brunetti, P. La Cava, and T. M. Miano, Soil Sci. **157**, 176 (1994).

[161] S. K. Xue and H. M. Selim, J. Environ. Qual. **24**, 896 (1995).

[162] R. Calvet, in *Interaction between Herbicides in the Soil*, edited by R. J. Hance (Academic, London, 1980), pp. 1–30.

[163] B. Von Oepen, W. Kördel, and W. Klein, Chemosphere **22**, 285 (1991).

[164] W. C. Koskinen, Weed Sci. **32**, 273 (1984).

[165] D. M. Mackay, W. P. Ball, and M. G. Durant, J. Contam. Hydrol. **1**, 119 (1986).

[166] M. L. Brusseau, T. Larsen, and T. H. Christensen, Water Resour. Res. **27**, 1137 (1991).

[167] W. F. Bradley, J. Am. Chem. Soc. **67**, 975 (1945).

[168] R. W. Hoffmann and G. W. Brindley, Geochim. Cosmochim. Acta **20**, 15 (1960).

[169] G. W. Brindley, R. Bender, and S. Ray, Geochim. Cosmochim. Acta **27**, 1129 (1963).

[170] R. D. Rogers, J. C. Mc Farlane, and A. J. Cross, Environ. Sci. Technol. **14**, 457 (1980).

[171] Y. Li and G. Gupta, Chemosphere **28**, 627 (1994).

[172] G. W. Bailey and J. L. White, Residue Rev. **32**, 29 (1970).

[173] R. H. Pierce, C. E. Olney, and G. T. Felbeck, Jr., Geochim. Cosmochim. Acta **38**, 1061 (1974).

[174] A. C. Mills and J. W. Biggar, J. Agric. Food Chem. **17**, 604 (1969).

[175] R. A. Griffin and S. F. J. Chou, Water Sci. Technol. **13**, 1153 (1981).

[176] S. M. Lambert, J. Agric. Food Chem. **16**, 340 (1968).

[177] S. U. Khan and M. Schnitzer, Geochim. Cosmochim Acta **36**, 745 (1972).

[178] R. Haque and D. Schmedding, J. Environ. Sci. Health, **B11**, 129 (1976).

[179] J. J. Hassett, J. C. Means, W. L. Banwart, S. G. Wood, S. Ali, and A. Khan, J. Environ. Qual. **9**, 184 (1980).

[180] J. C. Means, S. G. Wood, J. J. Hassett, and W. L. Banwart, Environ. Sci. Technol. **14**, 1524 (1980).

[181] G. Rippen, M. Ilgenstein, W. Klöpffer, and H. J. Poremski, Ecotoxicol. Environ. Safety **6**, 236 (1982).

[182] R. Lara and W. Ernst, Environ. Technol. **11**, 83 (1990).

[183] R. Lara and W. Ernst, Environ. Technol. **11**, 93 (1990).

[184] Y. Shin, J. J. Chodan, and A. R. Walcott, J. Agric. Food Chem. **18**, 1129 (1970).

[185] P. A. Wahid and N. Sethunathan, J. Agric. Food Chem. **27**, 1050 (1979).

[186] P. A. Wahid and N. Sethunathan, J. Agric. Food Chem. **28**, 623 (1980).

[187] R. L. Wershaw, P. J. Burcar, and M. C. Goldberg, Environ. Sci. Technol. **15**, 271 (1969).

[188] T. H. Gauthier, W. R. Seitz, and C. L. Grant, Environ. Sci. Technol. **21**, 243 (1987).

[189] Y. Hiraizumi, M. Takahashi, and H. Nishimura, Environ. Sci. Technol. **13**, 580 (1979).

[190] W. W. Choi and K. Y. Chen, Environ. Sci. Technol. **10**, 782 (1976).

[191] E. M. Richardson and E. Epstein, Soil Sci. Soc. Am. Proc. **35**, 884 (1971).

[192] P. Nkedi-Kizza, P. S. C. Rao, and J. W. Johnson, J. Environ. Qual. **12**, 195 (1983).

[193] D. R. Garbarini and L. W. Lion, Environ. Sci. Technol. **19**, 1122 (1985).

[194] D. R. Garbarini and L. W. Lion, Environ. Sci. Technol. **20**, 1263 (1986).

[195] C. T. Chiou, L. J. Peters, and V. H. Freed, Science **206**, 831 (1979).

[196] C. T. Chiou, L. J. Peters, and V. H. Freed, Science **213**, 683 (1981).

[197] C. T. Chiou, in *Reactions and Movements of Organic Chemicals in Soils*, edited by B. L. Sawhney and K. Brown (Soil Science Society of America, Inc., and American Society of Agronomy, Inc., Madison, WI, 1989), Chap. 1, pp. 1–29.

[198] C. T. Chiou, T. D. Shoup, and P. E. Porter, Org. Geochem. **8**, 9 (1985).

[199] A. S. Abdul and T. L. Gibson, Hazard. Waste Hazard. Mater. **3**, 125 (1986).

[200] P. J. Flory, J. Chem. Phys. **10**, 51 (1942).

[201] M. L. Huggins, Ann. N. Y. Acad. Sci. **43**, 1 (1942).

[202] F. C. Spurlock and J. W. Biggar, Environ. Sci. Technol. **28**, 989 (1994).

[203] P. J. Flory, Discuss. Faraday Soc. **49**, 7 (1970).

[204] F. C. Spurlock and J. W. Biggar, Environ. Sci. Technol. **28**, 996 (1994).

[205] F. C. Spurlock and J. W. Biggar, Environ. Sci. Technol. **28**, 1003 (1994).

[206] Y. P. Chin and W. J. Weber, Jr., Environ. Sci. Technol. **23**, 978 (1989).

[207] R. P. Schwarzenbach and J. Westall, Environ. Sci. Technol. **15**, 1360 (1981).

[208] T. Larsen, P. Kjeldsen, and T. H. Christensen, Chemosphere **24**, 979 (1992).

[209] S. M. Schrap and A. Opperhuizen, Chemosphere **18**, 1883 (1989).

[210] A. Khan, J. J. Hassett, W. L. Banwart, J. C. Means, and S. G. Wood, Soil Sci. **128**, 297 (1979).

[211] J. J. Hassett, J. C. Means, W. L. Banwart, and S. G. Wood, EPA Rept. 600/3-80-041 (1980).

[212] R. J. Hance, Can. J. Soil Sci. **49**, 357 (1969).

[213] T. B. Stauffer, W. G. Mac Intyre, and D. C. Wickman, Environ. Toxicol. Chem. **8**, 845 (1989).

[214] H. Kishi, N. Kogure, and Y. Hashimoto, Chemosphere **21**, 867 (1990).

[215] M. C. Lee, R. A. Griffin, M. L. Miller, and E. S. K. Chian, J. Environ. Sci. Health **A14**, 415 (1979).

[216] U. Mingelgrin and Z. Gerstl, J. Environ. Qual. **12**, 1 (1983).

[217] E. E. Kenaga and C. A. I. Goring, in *Aquatic Toxicology*, Proc. 3rd Ann. Symp., Publ. No. STP 707, edited by J. C. Eaton, P. R. Parrish, and A. C. Hendricks (American Society for Testing and Materials, Philadelphia, PA, 1980), pp. 78–115.

[218] J. M. Brannon, J. C. Pennington, V. A. Mc Farland, and C. Hayes, Chemosphere **31**, 3465 (1995).

[219] C. T. Chiou, D. E. Kile, T. I. Brinton, R. L. Malcolm, J. A. Leenheer, and P. Mc Carthy, Environ. Sci. Technol. **21**, 1231 (1987).

[220] C. T. Chiou, R. L. Malcolm, T. I. Brinton, and D. E. Kile, Environ. Sci. Technol. **20**, 502 (1986).

[221] R. J. Hance, Weed Res. **5**, 108 (1965).

[222] J. F. Lee, J. R. Crum, and S. A. Boyd, Environ. Sci. Technol. **23**, 1365 (1989).

[223] S. A. Boyd, J. F. Lee, and M. M. Mortland, Nature (London) **333**, 345 (1988).

[224] S. A. Boyd, M. M. Mortland, and C. T. Chiou, Soil Sci. Soc. Am. J. **52**, 652 (1988).

[225] W. F. Jaynes and S. A. Boyd, Soil Sci. Soc. Am. J. **55**, 43 (1991).

[226] P. Grathwohl, Environ. Sci. Technol. **24**, 1687 (1990).

[227] A. B. Paya-Pérez, A. Cortés, M. N. Sala, and B. Larsen, Chemosphere **25**, 887 (1992).

[228] E. M. Murphy, J. M. Zachara, and S. C. Smith, Environ. Sci. Technol. **24**, 1507 (1990).

[229] D. W. Rutherford, C. T. Chiou, and D. E. Kile, Environ. Sci. Technol. **26**, 336 (1992).

[230] D. E. Kile, C. T. Chiou, H. Zhou, H. Li, and O. Xu, Environ. Sci. Technol. **29**, 1401 (1995).

[231] M. J. Frissel and G. H. Bolt, Soil Sci. **94**, 284 (1962).

[232] R. J. Hance, Weed Res. **17**, 197 (1977).

[233] T. M. Ward and R. P. Upchurch, J. Agric. Food Chem. **13**, 334 (1965).

[234] D. C. Bouchard and T. L. Lavy, J. Environ. Qual. **14**, 181 (1985).

[235] Z. Gerstl and B. Yaron, J. Agric. Food Chem. **26**, 569 (1977).

[236] B. Yaron and S. Saltzman, Residue Rev. **69**, 1 (1979).

[237] B. T. Bowman, R. S. Adams, Jr., and S. W. Fenton, J. Agric. Food Chem. **18**, 723 (1970).
[238] W. F. Spencer and M. M. Cliath, Soil Sci. Soc. Am. Proc. **34**, 574 (1970).
[239] W. F. Spencer, M. M. Cliath, and W. J. Farmer, Soil Sci. Soc. Am. Proc. **33**, 509 (1969).
[240] I. J. Graham-Brice, J. Sci. Food Agric. **20**, 489 (1969).
[241] T. H. Dao and T. L. Lavy, Weed Sci. **26**, 303 (1978).
[242] G. Mac Namara and S. J. Toth, Soil Sci. **109**, 234 (1970).
[243] W. J. Farmer and J. L. Ahlrichs, Soil Sci. Soc. Am. Proc. **33**, 254 (1969).
[244] R. Van Bladel and A. Moreale, Soil Sci. Soc. Am. Proc. **38**, 244 (1974).
[245] E. González-Pradas, M. Villafranca-Sánchez, V. Pérez-Cano, M. Socias-Viciana, and A. Valverde-Garcia, Sci. Total Environ. **123/124**, 551 (1992).
[246] B. T. Bowman and W. W. Sans, Soil Sci. Soc. Am. J. **41**, 514 (1977).
[247] J. B. Weber, Am. Mineral, **51**, 1657 (1966).
[248] J. B. Weber, Soil Sci. Soc. Am. Proc. **34**, 401 (1970).
[249] J. B. Weber, P. W. Perry, and R. P. Upchurch, Soil Sci. Soc. Am. Proc. **29**, 678 (1965).
[250] G. W. Bailey, J. L. White, and T. Rothberg, Soil Sci. Soc. Am. Proc. **32**, 222 (1968).
[251] C. I. Harris and G. F. Warren, Weeds **12**, 120 (1964).
[252] B. A. G. Knight and P. J. Denny, Weed Res. **10**, 40 (1970).
[253] J. B. Weber and S. B. Weed, Soil Sci. Soc. Am. Proc. **32**, 485 (1968).
[254] M. H. B. Hayes, M. E. M. Pick, and B. A. Toms, Residue Rev. **57**, 1 (1975).
[255] Q. H. Yuen and H. W. Hilton, J. Agric. Food Chem. **10**, 386 (1962).
[256] L. C. Liu, H. Cibes-Viade, and F. K. S. Koo, Weed Sci. **18**, 470 (1970).
[257] D. E. Peck, D. L. Corwin, and W. J. Farmer, J. Environ. Qual. **9**, 101 (1980).
[258] T. C. Mueller, T. B. Moorman, and C. E. Snipes, J. Agric. Food Chem. **40**, 2517 (1992).
[259] R. J. Hance, Weed Res. **5**, 98 (1965).
[260] R. Grover, Can. J. Soil Sci. **55**, 127 (1975).
[261] J. R. W. Miles, B. T. Bowman, and E. R. Harris, J. Environ. Sci. Health **B16**, 309 (1981).
[262] I. J. Graham-Brice, J. Sci. Food Agric. **18**, 72 (1967).
[263] K. Kawamoto and K. Urano, Chemosphere **19**, 1223 (1989).
[264] M. S. Sharom, J. R. W. Miles, C. R. Harris, and F. L. Mc Ewen, Water Res. **14**, 1095 (1980).
[265] A. Felsot and J. Wilson, Bull. Environ. Contam. Technol. **24**, 778 (1980).
[266] P. Jamet and M. A. Piedaller, Phytiatrie-Phytopharmacie **24**, 279 (1975).
[267] S. Saltzman, L. Kliger, and B. Yaron, J. Agric. Food Chem. **20**, 1224 (1972).
[268] A. R. Swoboda and G. W. Thomas, J. Agric. Food Chem. **16**, 923 (1968).
[269] J. W. Biggar, U. Mingelgrin, and M. W. Cheung, J. Agric. Food Chem. **26**, 1306 (1978).
[270] R. J. Hance, Weed Res. **9**, 108 (1969).
[271] M. A. Mustafa and Y. Gamar, Soil Sci. Soc. Am. Proc. **36**, 561 (1972).
[272] C. W. Coggins and A. S. Crafts, Weeds **7**, 349 (1959).
[273] H. R. Sherburne and V. H. Freed, J. Agric. Food Chem. **2**, 937 (1954).
[274] K. E. Savage, Weed Sci. **21**, 416 (1973).
[275] H. W. Hilton and Q. H. Yuen, J. Agric. Food Chem. **11**, 230 (1963).
[276] H. Elabd, W. A. Jury, and M. M. Cliath, Environ. Sci. Technol. **20**, 256 (1986).
[277] Z. Gerstl and B. Yaron, J. Environ. Qual. **47**, 474 (1983).
[278] C. H. Wu, N. Buehring, and J. M. Davidson, Weed Sci. **23**, 454 (1975).
[279] J. Kozak, J. B. Weber, and T. J. Sheets, Soil Sci. **136**, 94 (1983).
[280] C. J. Peter and J. B. Weber, Weed Sci. **33**, 874 (1985).
[281] T. Obrigawitch, F. M. Hons, J. R. Abernathy, and J. R. Gipson, Weed Sci. **29**, 332 (1981).
[282] L. Guo, T. J. Bicki, A. S. Felsot, and T. D. Hinesly, J. Environ. Qual. **22**, 186 (1993).
[283] N. Senesi, Sci. Total Environ. **123/124**, 63 (1992).
[284] J. B. Weber, S. B. Weed, and T. M. Ward, Weed Sci. **17**, 417 (1969).
[285] D. C. Bouchard, T. L. Lavy, and D. B. Marx, Weed Sci. **30**, 629 (1982).
[286] M. D. Mc Glamery and F. W. Slife, Weeds **14**, 237 (1966).
[287] J. B. Weber, Weed Sci. **28**, 478 (1980).
[288] S. S. Harper, Weed Sci. **36**, 84 (1988).
[289] J. S. Ladlie, W. F. Meggitt, and D. Penner, Weed Sci. **24**, 477 (1976).
[290] D. C. Peek and A. P. Appleby, Weed Sci. **37**, 419 (1989).
[291] C. J. Peter and J. B. Weber, Weed Sci. **33**, 868 (1985).
[292] C. A. Seybold, K. Sweeney, and B. Lowery, J. Environ. Qual. **23**, 1291 (1994).
[293] Z. Wang, B. C. Pant, and C. H. Langford, Anal. Chim. Acta **232**, 43 (1990).
[294] Z. Wang, D. S. Gamble, and C. H. Langford, Anal. Chim. Acta **244**, 135 (1991).
[295] M. I. Haniff, R. H. Zienius, C. H. Langford, and D. S. Gamble, J. Environ. Sci. Health **B20**, 215 (1985).
[296] P. M. Huang, R. Grover, and R. B. Mc Kercher, Soil Sci. **138**, 20 (1984).
[297] O. Francioso, E. Bak, N. Rossi, and P. Sequi, Sci. Total Environ. **123/124**, 503 (1992).
[298] A. J. Beck and K. C. Jones, Chemosphere **32**, 2345 (1996).
[299] D. S. Murray, P. W. Santelmann, and J. M. Davidson, J. Agric. Food Chem. **23**, 578 (1975).
[300] J. R. Abernathy and J. M. Davidson, Weed Sci. **19**, 517 (1971).
[301] W. C. Koskinen, D. M. Stone, and A. R. Harris, Chemosphere **32**, 1681 (1996).
[302] D. Zierath, J. J. Hassett, W. L. Banwart, S. G. Wood, and J. C. Means, Soil Sci. **129**, 277 (1980).
[303] W. L. Banwart, J. J. Hassett, S. G. Wood, and J. C. Means, Soil Sci. **133**, 42 (1982).
[304] L. C. Liu and H. R. Cibes-Viade, J. Agric. Univ. P.R. **57**, 286 (1973).
[305] B. V. Tucker, D. E. Pack, and J. N. Ospenson, J. Agric. Food Chem. **15**, 1005 (1967).
[306] M. Damanakis, D. S. H. Drennan, J. D. Fryer, and K. Holly, Weed Res. **10**, 264 (1970).
[307] J. A. Best, J. B. Weber, and S. B. Weed, Soil Sci. **114**, 444 (1972).
[308] Y. Gamar and M. A. Mustafa, Soil Sci. **119**, 290 (1975).
[309] I. G. Burns and M. H. B. Hayes, Residue Rev. **52**, 117 (1974).
[310] S. U. Khan, Can. J. Soil Sci. **53**, 199 (1973).
[311] B. J. Brownawell, H. Chen, J. M. Collier, and J. C. Westall, Environ. Sci. Technol. **24**, 1234 (1990).
[312] Y. Angemar, M. Rebhun, and M. Horowitz, J. Environ. Qual. **13**, 321 (1984).
[313] J. D. Gaynor and V. V. Volk, Weed Sci. **24**, 549 (1976).
[314] J. W. Hamaker, C. A. I. Goring, and C. R. Youngson, Adv. Chem. Ser. **60**, 23 (1966).
[315] J. W. Biggar and M. W. Cheung, Soil Sci. Soc. Am. Proc. **37**, 863 (1973).
[316] W. J. Farmer and Y. Aochi, Soil Sci. Soc. Am. Proc. **38**, 418 (1974).
[317] R. Grover, Weed Sci. **19**, 417 (1971).
[318] D. C. Nearpass, Soil Sci. **121**, 272 (1976).
[319] J. S. Arnold and W. J. Farmer, Weed Sci. **27**, 257 (1979).
[320] R. Grover and A. E. Smith, Can. J. Soil Sci. **54**, 179 (1974).
[321] A. J. Krzyszowska, R. D. Allen, and G. F. Vance, J. Environ. Qual. **23**, 1051 (1994).
[322] M. R. Murray and J. K. Hall, J. Environ. Qual. **18**, 51 (1989).
[323] S. A. Clay, W. C. Koskinen, R. R. Allmaras, and B. H. Dowdy, J. Environ. Sci. Health **B23**, 559 (1988).
[324] H. Zhao, W. F. Jaynes, and G. F. Vance, Chemosphere **33**, 2089 (1996).
[325] J. R. Abernathy and L. M. Wax, Weed Sci. **21**, 224 (1973).
[326] P. J. Shea, Weed Sci. **34**, 474 (1986).
[327] O. K. Borggaard and J. C. Streibig, Weed Sci. **36**, 530 (1988).
[328] K. Thirunarayanan, R. L. Zimdahl, and D. E. Smika, Weed Sci. **33**, 558 (1985).
[329] W. Mersie and C. L. Foy, Weed Sci. **33**, 564 (1985).
[330] K. N. Reddy, M. A. Locke, S. C. Wagner, R. M. Zablotowicz, L. A. Gaston, and R. J. Smeda, J. Agric. Food Chem. **43**, 2752 (1995).
[331] K. N. Reddy, R. M. Zablotowicz, and M. A. Locke, J. Environ. Qual. **24**, 760 (1995).
[332] R. Grover, Weed Res. **13**, 51 (1973).
[333] A. Moreale and R. Van Bladel, J. Environ. Qual. **9**, 627 (1980).
[334] M. C. Hermosin and J. Cornejo, Chemosphere **24**, 1493 (1992).
[335] S. A. Boyd, Soil Sci. **134**, 337 (1982).
[336] J. Artiola-Fortuny and W. H. Fuller, Soil Sci. **133**, 18 (1982).
[337] K. Schellenberg, C. Leuenberger, and R. P. Schwarzenbach, Environ. Sci. Technol. **18**, 652 (1984).
[338] C. A. Bellin, G. A. O'Connor, and Y. Jin, J. Environ. Qual. **19**, 603 (1990).
[339] L. S. Lee, P. S. C. Rao, P. Nkedi-Kizza, and J. J. Delfino, Environ. Sci. Technol. **24**, 654 (1990).
[340] J. C. Westall, C. Leuenberger, and R. P. Schwarzenbach, Environ. Sci. Technol. **19**, 193 (1985).

[341] K. Yoshida, T. Shigeoka, and Yamauchi, Chemosphere **16**, 2531 (1987).

[342] C. T. Jafvert, Environ. Toxicol. Chem. **9**, 1259 (1990).

[343] M. G. Stapleton, D. L. Sparks, and S. K. Dentel, Environ. Sci. Technol. **28**, 2330 (1994).

[344] H. M. Seip, J. Alstad, G. E. Carlberg, K. Martinsen, and P. Skaane, Sci. Total Environ. **50**, 87 (1986).

[345] G. L. Jacques and R. G. Harvey, Weed Sci. **27**, 450 (1979).

[346] B. Xing, W. B. Mc Gill, and M. J. Dudas, Chemosphere **28**, 145 (1994).

[347] S. Dousset, C. Mouvet, and M. Schiavon, Chemosphere **28**, 467 (1994).

[348] J. Amonette and G. A. O'Connor, Soil Sci. Soc. Am. J. **44**, 540 (1980).

[349] L. W. Smith and D. E. Bayer, Soil Sci. **103**, 328 (1967).

[350] E. Iglesias-Jiménez, M. J. Sánchez-Martin, and M. Sánchez-Camazano, Chemosphere **32**, 1771 (1996).

[351] R. G. Harvey, Weed Sci. **22**, 120 (1974).

[352] W. Ehlers, J. Letey, W. F. Spencer, and W. J. Farmer, Soil Sci. Soc. Am. Proc. **33**, 501 (1969).

[353] W. Ehlers, J. Letey, W. F. Spencer, and W. J. Farmer, Soil Sci. Soc. Am. Proc. **33**, 505 (1969).

[354] F. Call, J. Sci. Food Agric **8**, 630 (1957).

[355] H. L. Hollist and C. L. Foy, Weed Sci. **19**, 11 (1971).

[356] W. F. Spencer and M. M. Cliath, J. Agric. Food Chem. **22**, 987 (1974).

[357] P. Wade, J. Sci. Food Agric. **5**, 184 (1954).

[358] S. Brunauer, L. S. Deming, W. E. Deming, and E. Teller, J. Am. Chem. Soc. **62**, 1723 (1940).

[359] J. J. Jurinak and D. H. Volman, Soil Sci. **86**, 6 (1958).

[360] F. Call, J. Sci. Food Agric. **8**, 137 (1957).

[361] F. Call, J. Sci. Food Agric. **8**, 143 (1957).

[362] C. T. Chiou and T. D. Shoup, Environ. Sci. Technol. **19**, 1196 (1985).

[363] C. T. Chiou, D. E. Kile, and R. L. Malcolm, Environ. Sci. Technol. **22**, 298 (1988).

[364] M. S. Peterson, L. W. Lion, and C. A. Shoemaker, Environ. Sci. Technol. **22**, 571 (1988).

[365] S. R. Thomas and L. W. Lion, Chemosphere **25**, 1707 (1992).

[366] R. D. Rhue, P. S. C. Rao, and R. E. Smith, Chemosphere **17**, 727 (1988).

[367] P. S. C. Rao, R. A. Ogwada, and R. D. Rhue, Chemosphere **18**, 2177 (1989).

[368] R. D. Rhue, K. D. Pennell, P. S. C. Rao, and W. H. Reve, Chemosphere **18**, 1971 (1989).

[369] S. M. Steinberg, J. S. Schmeltzer, and D. K. Kreamer, Chemosphere **33**, 961 (1996).

[370] J. A. Smith, C. T. Chiou, J. A. Kammer, and D. E. Kile, Environ. Sci. Technol. **24**, 676 (1990).

[371] S. K. Ong and L. W. Lion, J. Environ. Qual. **20**, 180 (1991).

[372] L. W. Petersen, P. Moldrup, Y. H. El-Farhan, O. H. Jacobsen, T. Yamaguchi, and D. E. Rolston, J. Environ. Qual. **24**, 752 (1995).

[373] K. Goss, Environ. Sci. Technol. **26**, 2287 (1992).

[374] K. Goss, Environ. Sci. Technol. **28**, 640 (1994).

[375] K. D. Pennell, R. D. Rhue, P. S. C. Rao, and C. T. Johnston, Environ. Sci. Technol. **26**, 756 (1992).

[376] S. M. Steinberg and D. K. Kreamer, Environ. Sci. Technol. **27**, 883 (1993).

[377] C. Thibaud, C. Erkey, and A. Akgerman, Environ. Sci. Technol. **27**, 2373 (1993).

[378] S. Batterman, A. Kulshrestha, and H. T. Cheng, Environ. Sci. Technol. **29**, 171 (1995).

[379] C. Y. Chen and S. C. Wu, Chemosphere **31**, 4225 (1995).

[380] S. M. Steinberg, J. J. Pignatello, and B. L. Sahwney, Environ. Sci. Technol. **21**, 1201 (1987).

[381] J. J. Pignatello, Environ. Toxicol. Chem. **9**, 1107 (1990).

[382] J. J. Pignatello, Environ. Toxicol. Chem. **9**, 1117 (1990).

[383] S. M. Steinberg, Chemosphere **24**, 1301 (1992).

[384] C. A. Shoemaker, T. B. Culver, L. W. Lion, and M. G. Peterson, Water Resour. Res. **26**, 745 (1990).

[385] J. P. Hassett and W. L. Banwart, in *Reactions and Movements of Organic Chemicals in Soils*, edited by B. L. Sawhney and K. Brown (Soil Science Society of America, Inc. and America Society of Agronomy, Inc., Madison, WI, 1989), Chap. 1, pp. 31–44.

[386] Th. E. M. ten Hulscher and G. Cornelissen, Chemosphere **32**, 609 (1996).

[387] J. J. Kipling, *Adsorption from Solution of Non-Electrolytes* (Academic, London, 1965).

[388] Y. He, A. Yediler, T. Sun, and A. Kettrup, Chemosphere **30**, 141 (1995).

[389] R. P. Schwarzenbach, P. M. Gschwend, and D. M. Imboden, *Environmental Organic Chemistry* (Wiley, New York, 1993).

[390] A. C. Mills and J. W. Biggar, Soil Sci. Soc. Am. Proc. **33**, 210 (1969).

[391] Z. Gerstl and U. Mingelgrin, Clays Clay Miner. **27**, 285 (1979).

[392] R. D. Wauchope, K. E. Savage, and W. C. Koskinen, Weed Sci. **31**, 744 (1983).

[393] M. A. T. Jota and J. P. Hassett, Environ. Toxicol. Chem. **10**, 483 (1991).

[394] F. Lüers and Th. E. M. ten Hulscher, Chemosphere **33**, 643 (1996).

[395] M. Bosetto, P. Arfaioli, and P. Fusi, Soil Sci. **155**, 105 (1993).

[396] S. U. Khan and R. Mazurkewich, Soil Sci. **118**, 339 (1974).

[397] F. C. Spurlock, J. Environ. Qual. **24**, 42 (1995).

[398] J. S. Graham and J. S. Conn, Weed Sci. **40**, 155 (1992).

[399] R. D. Wijayaratne and J. C. Means, Mar. Environ. Res. **11**, 77 (1984).

[400] J. F. Mc Carthy and B. D. Jimenez, Environ. Sci. Technol. **19**, 1072 (1985).

[401] S. Johnsen, Sci. Total Environ. **67**, 269 (1987).

[402] C. W. Carter and I. H. Suffet, Environ. Sci. Technol. **16**, 735 (1982).

[403] Z. Liu, S. A. Clay, D. E. Clay, and S. S. Harper, J. Agric. Food Chem. **43**, 815 (1995).

[404] Y. A. Madhun, J. L. Young, and V. H. Freed, J. Environ. Qual. **15**, 64 (1986).

[405] R. D. Wijayaratne and J. C. Means, Environ. Sci. Technol. **18**, 121 (1984).

[406] J. C. Means and R. D. Wijayaratne, Science **215**, 968 (1982).

[407] J. Y. Ding and S. C. Wu, Chemosphere **30**, 2259 (1995).

[408] P. M. Gschwend and S. C. Wu, Environ. Sci. Technol. **19**, 90 (1985).

[409] B. J. Eadie, N. R. Morehead, and P. F. Landrum, Chemosphere **20**, 161 (1990).

[410] B. J. Eadie, N. R. Morehead, J. V. Klump, and P. F. Landrum, J. Great Lakes Res. **18**, 91 (1992).

[411] J. M. Brannon, J. C. Pennington, W. M. Davis, and C. Hayes, Chemosphere **30**, 419 (1995).

[412] D. M. Di Toro, C. S. Zarba, D. J. Hansen, W. J. Berry, R. C. Swartz, C. E. Cowan, S. P. Pavlou, H. E. Hallen, N. A. Thomas, and P. R. Paquin, Environ. Toxicol. Chem. **10**, 1541 (1991).

[413] R. Lara and W. Ernst, Chemosphere **19**, 1655 (1989).

[414] P. F. Landrum, S. R. Nihart, B. J. Eadie, and W. A. Gardner, Environ. Sci. Technol. **18**, 187 (1984).

[415] T. D. Gauthier, E. C. Shane, W. F. Guerin, W. R. Seitz, and L. Grant, Environ. Sci. Technol. **20**, 1162 (1986).

[416] J. P. Hassett and E. Milicic, Environ. Sci. Technol. **19**, 638 (1985).

[417] C. Yin and J. P. Hassett, Environ. Sci. Technol. **20**, 1213 (1986).

[418] G. R. B. Webster, D. H. Muldrew, J. J. Graham, L. P. Sarna, and D. C. G. Muir, Chemosphere **15**, 1379 (1986).

[419] Y. P. Chin and P. M. Gschwend, Environ. Sci. Technol. **26**, 1621 (1992).

[420] C. S. Ragle, R. R. Engebretson, and R. Von Wandruszka, Soil Sci. **162**, 106 (1997).

[421] G. Caron, I. H. Suffet, and T. Belton, Chemosphere **14**, 993 (1985).

[422] F. C. Spurlock and J. W. Biggar, Environ. Sci. Technol. **24**, 736 (1990).

[423] D. Y. Lee and W. J. Farmer, J. Environ. Qual. **18**, 468 (1989).

[424] B. Whitehouse, Estuarine Coastal Shelf Sci. **20**, 393 (1985).

[425] F. De Paolis and J. Kukkonen, Chemosphere **34**, 1693 (1997).

[426] J. P. Hassett and M. A. Anderson, Water Res. **16**, 681 (1982).

[427] T. M. Ballard, Soil Sci. Soc. Am. Proc. **35**, 145 (1971).

[428] A. S. Abdul, T. L. Gibson, and D. N. Rai, Environ. Sci. Technol. **24**, 328 (1990).

[429] C. G. Enfield, G. Bengtsson, and R. Lindquist, Environ. Sci. Technol. **23**, 1278 (1989).

[430] B. R. Magee, L. W. Lion, and A. T. Lemley, Environ. Sci. Technol. **25**, 323 (1991).

[431] F. M. Dunnivant, P. M. Jardine, D. L. Taylor, and J. F. Mc Carthy, Environ. Sci. Technol. **26**, 360 (1992).

[432] A. T. Kan and M. B. Tomson, Environ. Toxicol. Chem. **9**, 253 (1990).

[433] P. Nkedi-Kizza, J. W. Biggar, H. M. Selim, M. T. van Genuchten, P. J. Wierenga, J. M. Davidson, and D. R. Nielsen, Water Resour. Res. **20**, 1123 (1984).

[434] J. F. Mc Carthy and M. C. Black, in *Aquatic Toxicology and Hazard Assessment*, edited by W. J. Adams, G. A. Chapman, and W. G. Landis, ASTM STP 971 (American Society for Testing and Materials, Philadelphia, 1988), Vol. 10, pp. 233–246.

[435] M. C. Black and J. F. Mc Carthy, Environ. Toxicol. Chem. **7**, 593 (1988).

[436] J. F. Mc Carthy and B. D. Jimenez, Environ. Toxicol. Chem. **4**, 511 (1985).

[437] J. F. Mc Carthy, B. D. Jimenez, and T. Barbee, Aquat. Toxicol. **7**, 15 (1985).

[438] J. F. Mc Carthy, Adv. Chem. Ser. **219**, 263 (1989).

[439] J. Kukkonen and A. Oikari, Sci. Total Environ. **62**, 399 (1987).

[440] J. Kukkonen and A. Oikari, Sci. Total Environ. **79**, 197 (1989).

[441] J. Kukkonen, J. F. Mc Carthy, and A. Oikari, Arch. Environ. Contam. Toxicol. **19**, 551 (1990).

[442] J. Kukkonen and A. Oikari, Water Res. **25**, 455 (1991).

[443] J. Kukkonen, J. F. Mc Carthy, and A. Oikari, in *Organic Substances and Sediments in Water*, Vol. 1, Humics and Soils, edited by R. A. Baker (Lewis, Chelsea, MI, 1991), pp. 111–127.

[444] K. B. Woodburn, P. S. C. Rao, M. Fukui, and P. Nkedi-Kizza, J. Contam. Hydrol. **1**, 227 (1986).

[445] P. S. C. Rao, A. G. Hornsby, D. P. Kilcrease, and P. Nkedi-Kizza, J. Environ. Qual. **14**, 376 (1985).

[446] G. L. Amidon, S. H. Yalkowsky, and S. Leung, J. Pharm. Sci. **63**, 1858 (1974).

[447] S. H. Yalkowsky, G. L. Amidon, G. Zografi, and G. L. Flinn, J. Pharm. Sci. **64**, 48 (1975).

[448] S. H. Yalkowsky, S. C. Valvani, and G. L. Amidon, J. Pharm. Sci. **65**, 1488 (1976).

[449] J. T. Rubino and S. H. Yalkowsky, Pharm. Res. 4, 220 (1987).

[450] J. T. Rubino and S. H. Yalkowsky, Pharm. Res. **4**, 231 (1987).

[451] K. R. Morris, R. Abramowitz, R. Pinal, P. Davis, and S. H. Yalkowsky, Chemosphere **17**, 285 (1988).

[452] P. Nkedi-Kizza, P. S. C. Rao, and A. G. Hornsby, Environ. Sci. Technol. **21**, 1107 (1987).

[453] P. S. C. Rao and L. S. Lee, in *Health and Environmental Research on Complex Organic Mixtures*, edited by R. H. Gray, E. K. Chess, P. J. Mellinger, R. G. Riley, and D. L. Springer, 24th Hanford Life Sciences Symposium (Pacific Northwest Laboratory, Richland, WA, 1988), pp. 457–471.

[454] K. J. Fu and R. G. Luthy, J. Environ. Eng. ASCE **112**, 346 (1986).

[455] P. Nkedi-Kizza, P. S. C. Rao, and A. G. Hornsby, Environ. Sci. Technol. **19**, 975 (1985).

[456] R. W. Walters and A. Guiseppi-Elie, Environ Sci. Technol. **22**, 819 (1988).

[457] A. L. Wood, D. C. Bouchard, M. L. Brusseau, and P. S. C. Rao, Chemosphere **21**, 575 (1990).

[458] R. Pinal, P. S. C. Rao, L. S. Lee, P. V. Cline, and S. H. Yalkowsky, Environ. Sci. Technol. **24**, 639 (1990).

[459] P. S. C. Rao, L. S. Lee, and P. Pinal, Environ. Sci. Technol. **24**, 647 (1990).

[460] L. S. Lee, P. S. C. Rao, and M. L. Brusseau, Environ. Sci. Technol. **25**, 722 (1991).

[461] W. J. M. Hegeman, C. H. van der Weijden, and J. P. G. Loch, Environ. Sci. Technol. **29**, 363 (1995).

[462] R. Grover and R. J. Hance, Soil Sci. **109**, 136 (1970).

[463] E. G. Lotse, D. A. Graetz, G. Chesters, G. B. Lee, and L. W. Newland, Environ. Sci. Technol. **2**, 353 (1968).

[464] T. C. Voice, C. P. Rice, and W. J. Weber, Jr., Environ. Sci. Technol. **17**, 513 (1983).

[465] W. J. Weber, Jr., T. C. Voice, M. Pirbazari, G. E. Hunt, and D. M. Ulanoff, Water Res. **17**, 1443 (1983).

[466] D. M. Di Toro, J. S. Jeris, and D. Clarcia, Environ. Sci. Technol. **19**, 1169 (1985).

[467] L. M. Horzempa and D. M. Di Toro, J. Environ. Qual. **12**, 373 (1983).

[468] M. R. Servos and D. C. G. Muir, Environ. Sci. Technol. **23**, 1302 (1989).

[469] J. A. Celorie, S. L. Woods, T. S. Vinson, and J. D. Istok, J. Environ. Qual. **18**, 307 (1989).

[470] D. M. Di Toro, J. D. Mahony, P. R. Kirchgraber, A. L. O'Byrne, L. R. Pasquale, and D. C. Piccirilli, Environ. Sci. Technol. **20**, 55 (1986).

[471] D. M. Di Toro and L. M. Horzempa, J. Great Lakes Res. **8**, 336 (1982).

[472] P. Friesel, G. Milde, and B. Steiner, Fresenius Z. Anal. Chem. **319**, 160 (1984).

[473] J. J. Pignatello, Environ. Toxicol. Chem. **10**, 1399 (1991).

[474] B. C. Fairbanks and G. A. O'Connor, J. Environ. Qual. **13**, 297 (1984).

[475] R. Grover, Weed Sci. **22**, 405 (1974).

[476] A. G. Hornsby and J. M. Davidson, Soil Sci. Soc. Am. Proc. **37**, 823 (1973).

[477] J. R. Moyer, R. B. Mc Kercher, and R. J. Hance, Can. J. Soil Sci. **52**, 439 (1972).

[478] R. D. Wauchope and R. S. Myers, J. Environ. Qual. **14**, 132 (1985).

[479] W. R. Roy and I. G. Krapac, J. Environ. Qual. **23**, 549 (1994).

[480] S. A. Clay and W. C. Koskinen, Weed Sci. **38**, 262 (1990).

[481] J. J. Pignatello and L. Q. Huang, J. Environ. Qual. **20**, 222 (1991).

[482] E. Barriuso, W. C. Koskinen, and B. Sorenson, Sci. Total Environ. **123/124**, 333 (1992).

[483] L. Ma, L. M. Southwick, G. H. Willis, and H. M. Selim, Weed Sci. **41**, 627 (1993).

[484] G. A. O'Connor, P. J. Wierenga, H. H. Cheng, and K. G. Doxtader, Soil Sci. **130**, 157 (1980).

[485] T. M. van Genuchten, J. M. Davidson, and P. J. Wierenga, Soil. Sci. Soc. Am. Proc. **38**, 29 (1974).

[486] B. T. Bowman and W. W. Sans, J. Environ. Qual. **14**, 265 (1985).

[487] B. T. Bowman and W. W. Sans, J. Environ. Qual. **14**, 270 (1985).

[488] P. S. C. Rao, J. M. Davidson, and D. P. Kilcrease, *Agron. Abstracts* (American Society of Agronomy, Madison, WI, 1978), p. 34.

[489] H. D. Scott, D. C. Wolf, and T. L. Lavy, J. Environ. Qual. **11**, 107 (1982).

[490] D. M. Di Toro and L. M. Horzempa, Environ. Sci. Technol. **16**, 594 (1982).

[491] L. M. Horzempa and D. M. Di Toro, Water Res. **17**, 851 (1983).

[492] J. M. Santana-Casiano and M. González-Dávila, Environ. Sci. Technol. **26**, 90 (1992).

[493] A. A. Koelmans and L. Lijklema, Chemosphere **25**, 313 (1992).

[494] T. C. Voice and W. J. Weber, Jr., Environ. Sci. Technol. **19**, 789 (1985).

[495] S. M. Schrap, M. Haller, and A. Opperhuizen, Environ. Toxicol. Chem. **14**, 219 (1995).

[496] D. M. Di Toro, Chemosphere **14**, 1503 (1985).

[497] D. Mackay and B. Powers, Chemosphere **16**, 745 (1987).

[498] K. B. Lodge and P. M. Cook, Chemosphere **19**, 439 (1989).

[499] S. M. Schrap and A. Opperhuizen, Chemosphere **24**, 1259 (1992).

[500] R. L. Curl and G. A. Keoleian, Environ. Sci. Technol. **18**, 916 (1984).

[501] P. J. Witkowski, P. R. Jaffe, and R. A. Ferrara, J. Contam. Hydrol. **2**, 249 (1987).

[502] P. S. C. Rao, J. M. Davidson, R. E. Jessup, and H. M. Selim, Soil Sci. Soc. Am. J. **43**, 22 (1979).

[503] J. J. T. I. Boesten and J. T. van der Pas, Soil Sci. **146**, 221 (1988).

[504] J. J. Pignatello, C. R. Frink, P. A. Marin, and E. X. Droste, J. Contam. Hydrol. **5**, 195 (1990).

[505] J. Farrell and M. Reinhard, Environ. Sci. Technol. **28**, 63 (1994).

[506] B. D. Kay and D. E. Elrick, Soil. Sci. **104**, 314 (1967).

[507] J. M. Davidson and J. R. Mc Dougal, J. Environ. Qual. **2**, 428 (1973).

[508] J. M. Davidson and R. K. Chang, Soil Sci. Soc. Am. Proc. **36**, 257 (1972).

[509] M. Th. van Genuchten, P. J. Wierenga, and G. A. O'Connor, Soil Sci. Soc. Am. J. **41**, 278 (1977).

[510] K. H. Coats and B. D. Smith, J. Soc. Pet. Eng. **4**, 73 (1964).

[511] C. T. Miller and W. J. Weber, Water Res. **22**, 465 (1988).

[512] C. T. Miller and W. J. Weber, Ground Water **22**, 584 (1984).

[513] M. L. Brusseau and P. S. C. Rao, CRC Crit. Rev. Environ. Control **19**, 33 (1989).

[514] H. M. Selim, J. M. Davidson, and R. S. Mansell, in *Proceedings Summer Computer Simulation Conference* (Simulation Councils, Inc., Washington, D. C., July 12–14, 1976), pp. 444–448.

[515] L. Ma and H. M. Selim, Water Resour. Res. **30**, 447 (1994).

[516] M. L. Brusseau and P. S. C. Rao, Chemosphere **18**, 1691 (1989).

[517] M. L. Brusseau, R. E. Jessup, and P. S. C. Rao, Environ. Sci. Technol. **24**, 727 (1990).

[518] M. L. Brusseau, R. E. Jessup, and P. S. C. Rao, Environ. Sci. Technol. **25**, 134 (1991).

[519] M. L. Brusseau, Environ. Sci. Technol. **25**, 1747 (1991).

[520] L. S. Lee, P. S. C. Rao, M. L. Brusseau, and R. A. Ogwada, Environ. Toxicol. Chem. **7**, 779 (1988).

[521] M. L. Brusseau and P. S. C. Rao, Environ. Sci. Technol. **25**, 1501 (1991).

[522] M. L. Brusseau, Environ. Toxicol. Chem. **12**, 1835 (1993).

[523] J. T. Angley, M. L. Brusseau, W. L. Miller, and J. J. Delfino, Environ. Sci. Technol. **26**, 1404 (1992).

[524] T. Larsen, T. H. Christensen, and M. L. Brusseau, Chemosphere **24**, 141 (1992).

[525] P. Nkedi-Kizza, M. L. Brusseau, P. S. C. Rao, and A. G. Hornsby, Environ. Sci. Technol. **23**, 814 (1989).

[526] M. L. Brusseau, A. L. Wood, and P. S. C. Rao, Environ. Sci. Technol. **25**, 903 (1991).

[527] A. P. Gamerdinger, A. T. Lemley, and R. J. Wagenet, J. Environ. Qual. **20**, 815 (1991).

[528] G. Singh, W. F. Spencer, M. M. Cliath, and M. Th. van Genuchten, J. Environ. Qual. **19**, 520 (1990).

[529] J. A. Johnson and W. J. Farmer, Soil Sci. **155**, 92 (1993).

[530] S. M. Schrap, P. J. De Vries, and A. Opperhuizen, Chemosphere **28**, 931 (1994).

[531] S. A. Boyd and R. King, Soil Sci. **137**, 115 (1984).

[532] H. D. Scott, D. C. Wolf, and T. L. Lavy, J. Environ. Qual. **12**, 91 (1983).

[533] R. E. Green and V. K. Yamane, Soil Sci. Soc. Am. Proc. **34**, 353 (1970).

[534] J. J. T. I. Boesten, Pestic. Sci. **30**, 31 (1990).

[535] R. A. Dobbs, L. Wang, and R. Govind, Environ. Sci. Technol. **23**, 1092 (1989).

[536] B. T. Bowman, Can. J. Soil Sci. **59**, 435 (1979).

[537] Z. Ou, A. Yediler, Y. He, A. Kettrup, and T. Sun, Chemosphere **30**, 313 (1995).

[538] R. E. Green and J. C. Corey, Soil Sci. Soc. Am. Proc. **35**, 561 (1971).

[539] B. H. Ketelle and G. E. Boyd, J. Am. Chem. Soc. **69**, 2800 (1947).

[540] R. Grover, Weed Sci. **25**, 159 (1977).

[541] J. T. Wilson, C. G. Enfield, W. J. Dunlop, R. L. Crosby, D. A. Foster, and L. B. Baskin, J. Environ. Qual. **10**, 501 (1981).

[542] I. Hashimoto, K. B. Deshpande, and H. C. Thomas, Ind. Eng. Chem. Fundam. **3**, 213 (1964).

[543] D. Mackay, W. Y. Shiu, and R. P. Sutherland, Environ. Sci. Technol. **13**, 333 (1979).

[544] S. L. Kayal and D. W. Connell, Aust. J. Mar. Freshwater Res. **41**, 443 (1990).

[545] D. A. Backhus and P. M. Gschwend, Environ. Sci. Technol. **24**, 1214 (1990).

[546] P. F. Landrum, M. D. Reinhold, S. R. Nihart, and B. J. Eadie, Environ. Toxicol. Chem. **4**, 459 (1985).

[547] G. A. Harkey, P. F. Landrum, and S. J. Klaine, Chemosphere **28**, 583 (1994).

[548] D. S. Gamble and S. U. Khan, Can. J. Chem. **66**, 2605 (1988).

[549] R. Collander, Acta Chem. Scand. **5**, 774 (1951).

[550] J. C. Mc Gowan, J. Appl. Chem. **4**, 41 (1954).

[551] J. C. Mc Gowan, Nature (London) **200**, 1317 (1963).

[552] R. J. Hance, J. Agric. Food Chem. **17**, 667 (1969).

[553] D. A. Dzombak and R. G. Luthy, Soil Sci. **137**, 292 (1984).

[554] W. J. Lyman, in *Environmental Exposure from Chemicals*, Vol. 1, edited by W. Brock Neely and G. E. Blau (CRC, Boca Raton, FL, 1986), pp. 13–47.

[555] B. M. Gawlik, N. Sotiriou, E. A. Feicht, S. Schulte-Hostede, and A. Kettrup, Chemosphere **34**, 2525 (1997).

[556] A. Leo, C. Hansch, and D. Elkins, Chem. Rev. **71**, 525 (1971).

[557] J. C. Means, S. G. Wood, J. J. Hassett, and W. L. Banwart, Environ. Sci. Technol. **16**, 93 (1982).

[558] G. G. Briggs, Austr. J. Soil Res. **19**, 61 (1981).

[559] K. A. Lord, C. G. Helene, M. M. De Andrea, and E. F. Ruegg, Arq. Inst. Biol., Sao Paulo **45**, 47 (1978).

[560] Y. P. Chin, W. J. Weber, Jr., and T. C. Voice, Water Res. **20**, 1443 (1986).

[561] A. Sabljić, H. Güsten, H. Verhaar, and J. Hermens, Chemosphere **31**, 4489 (1995).

[562] Z. Gerstl, J. Contam. Hydrol. **6**, 357 (1990).

[563] Z. Gerstl and U. Mingelgrin, J. Environ. Sci. Health **B19**, 297 (1984).

[564] E. E. Kenaga, Ecotoxicol. Environ. Safety **4**, 26 (1980).

[565] J. C. Means, J. J. Hassett, S. G. Wood, W. L. Banwart, S. Ali, and A. Khan, in *Polynuclear Aromatic Hydrocarbons: Chemistry and Biological Effects*, edited by A. Bǿrseth and A. J. Dennis (Battelle, Columbus, OH, 1980), pp. 395–404.

[566] S. H. Yalkowsky, Ind. Eng. Chem. Fundam. **18**, 108 (1979).

[567] S. H. Yalkowsky, R. J. Orr, and S. C. Valvani, Ind. Eng. Chem. Fundam. **18**, 351 (1979).

[568] D. Mackay and W. Y. Shiu, J. Chem. Eng. Data **22**, 399 (1977).

[569] C. T. Chiou, D. W. Schmedding, and M. Manes, Environ Sci. Technol. **16**, 4 (1982).

[570] G. R. Southworth and J. L. Keller, Water Air Soil Pollut. **28**, 239 (1986).

[571] R. A. Rapaport and S. J. Eisenreich, Environ. Sci. Technol. **18**, 163 (1984).

[572] C. Hovarth and W. J. Melander, J. Chromat. Sci. **15**, 393 (1977).

[573] R. L. Swann, D. A. Laskowski, P. J. Mc Call, K. Vander Kuy, and H. J. Dishburger, Residue Rev. **85**, 17 (1983).

[574] K. B. Woodburn, L. S. Lee, P. S. C. Rao, and J. J. Delfino, Environ. Sci. Technol. **23**, 407 (1989).

[575] P. J. Mc Call, R. L. Swann, D. A. Laskowski, S. M. Unger, S. A. Vrona, and H. J. Dishburger, Bull. Environ. Contam. Toxicol. **24**, 190 (1980).

[576] J. W. Hamaker, in *Dynamics of Pesticides in the Environment*, edited by R. Haque and V. H. Freed (Plenum, New York, 1975), pp. 21–30.

[577] H. Hong, L. Wang, and S. Han, Chemosphere **32**, 343 (1996).

[578] D. A. Bahnick and W. J. Doucette, Chemosphere **17**, 1703 (1988).

[579] J. Hodson and N. A. Williams, Chemosphere **17**, 67 (1988).

[580] W. Kördel, J. Stutte, and G. Kotthoff, Chemosphere **27**, 2341 (1993).

[581] W. Kördel, G. Kotthoff, and J. Müller, Chemosphere **30**, 1373 (1995).

[582] M. Müller and W. Kördel, Chemosphere **32**, 2493 (1996).

[583] B. M. Gawlik, E. A. Feicht, W. Karcher, A. Kettrup, and H. Muntau, Chemosphere **36**, 2903 (1998).

[584] G. Szabó, Chemosphere **21**, 729 (1990).

[585] G. Szabó, Chemosphere **21**, 777 (1990).

[586] G. Szabó, G. Farkas, and R. A. Bulman, Chemosphere **24**, 403 (1992).

[587] G. Szabó, and J. Guczi, Chemosphere **30**, 1717 (1995).

[588] L. Pussemier, G. Szabó, and R. A. Bulman, Chemosphere **21**, 1199 (1990).

[589] J. H. Hildebrand and R. L. Scott, *Solubility of Non-Electrolytes* (Reinhold, New York, 1950).

[590] L. Pussemier, R. De Borger, P. Cloos, and R. van Bladel, Chemosphere **18**, 1871 (1989).

[591] A. Sabljić, J. Agric. Food Chem. **32**, 243 (1984).

[592] N. Nirmalakhandan and R. E. Speece, Environ. Sci. Technol. **22**, 606 (1988).

[593] M. Randić, J. Am. Chem. Soc. **97**, 6609 (1975).

[594] L. B. Kier and L. H. Hall, *Molecular Connectivity in Chemistry and Drug Research* (Academic, New York, 1976).

[595] L. B. Kier and L. H. Hall, *Molecular Connectivity in Structure-Activity Analysis* (Research Studies Press Ltd., Letchworth, Hertfordshire, England, 1986).

[596] R. Koch, Toxicol. Environ. Chem. **6**, 87 (1983).

[597] A. Sabljić, Environ. Sci. Technol. **21**, 358 (1987).

[598] W. Meylan, P. H. Howard, and R. S. Boethling, Environ. Sci. Technol. **26**, 1560 (1992).

[599] A. Sabljić, R. Lara, and W. Ernst, Chemosphere **19**, 1665 (1989).

[600] Q. Hu, X. Wang, and M. L. Brusseau, Environ. Toxicol. Chem. **14**, 1133 (1995).

[601] M. T. Saçan and I. A. Balcioglu, Chemosphere **32**, 1993 (1996).

[602] J. H. Park and H. J. Lee, Chemosphere **26**, 1905 (1993).

[603] M. J. Kamlet, J. L. M. Abboud, M. H. Abraham, and R. W. Taft, J. Org. Chem. **48**, 2877 (1983).

[604] M. J. Kamlet and R. W. Taft, Acta Chem. Scand. **B39**, 611 (1985).

[605] S. A. Boyd, J. Xiang Can, and J. F. Lee, J. Environ. Qual. **19**, 734 (1990).

[606] B. T. Walton, M. S. Hendricks, T. A. Anderson, W. H. Griest, R. Merriweather, J. J. Beauchamp, and C. W. Francis, J. Environ. Qual. **21**, 552 (1992).

[607] R. A. Kango and J. G. Quinn, Chemosphere **19**, 1269 (1989).

[608] G. R. Southworth and J. L. Keller, Environ. Toxicol. Chem. **3**, 575 (1984).

[609] W. G. MacIntyre and T. B. Stauffer, Chemosphere **17**, 2161 (1988).

[610] C. W. Carter and I. H. Suffet, in *Fate of Chemicals in the Environment*, ACS Symposium Series 225, edited by R. L. Swann and A. Eschenroder (American Chemical Society, Washington, D.C., 1983), pp. 215–230.

[611] D. W. Lickfeldt and B. E. Branham, J. Environ. Qual. **24**, 980 (1995).

[612] S. B. Socha and R. Carpenter, Geochim. Cosmochim. Acta **51**, 1273 (1987).

[613] J. M. Brannon, C. B. Price, F. J. Reilly, Jr., J. C. Pennington, and V. A. Mc Farland, Bull. Environ. Contam. Toxicol. **51**, 873 (1993).

[614] G. P. Curtis, P. V. Roberts, and M. Reinhard, Water Resour. Res. **22**, 2059 (1986).

[615] F. T. Phillips, J. Sci. Food Agric. **15**, 444 (1964).

[616] J. J. Deitsch and J. A. Smith, Environ. Sci. Technol. **29**, 1069 (1995).

[617] W. P. Ball, C. Liu, G. Xia, and D. F. Young, Water Resour. Res. **33**, 2741 (1997).

[618] P. H. Howard, *Handbook of Fate and Exposure Data for Organic Chemicals* (Lewis, Chelsea, MI, 1989).

[619] M. R. Anderson and J. F. Pankow, Water Resour. Res. **22**, 1051 (1986).

[620] B. G. Oliver, in *QSAR in Environmental Toxicology*, Vol. 2, Proceedings of 2nd International Workshop, 1986, edited by K. L. E. Kaiser (Riedel, Dordrecht, Netherlands, 1987), pp. 251–260.

[621] W. C. Steen, D. F. Paris, and G. L. Baughman, Water Res. **12**, 655 (1978).

[622] B. J. Eadie, C. P. Rice, and W. A. Frez, in *Physical Behavior of PCBs in the Great Lakes*, edited by D. Mackay, S. Paterson, S. J. Eisenreich, and M. S. Simmons (Ann Arbor Science, Ann Arbor, MI, 1983), pp. 213–228.

[623] G. M. Nau-Ritter, C. F. Wurster, and R. G. Rowland, Water Res. **16**, 1615 (1982).

[624] G. M. Nau-Ritter and C. F. Wurster, Water Res. **17**, 383 (1983).

[625] M. T. Halter and H. E. Johnson, in *Aquatic Toxicology and Hazard Evaluation*, ASTM STP-634, edited by F. L. Mayer and J. L. Hamelink (American Society for Testing and Materials, Philadelphia, 1977), pp. 178–195.

[626] K. Ballschmiter and M. Zell, Fresenius Z. Anal. Chem. **302**, 20 (1980).

[627] D. Broman, C. Näf, C. Rolff, and Y. Zebühr, Environ. Sci. Technol. **25**, 1850 (1991).

[628] T. Mill, in *Dioxins in the Environment*, edited by M. A. Kamrin and P. W. Rogers (Hemisphere, Washington, D.C., 1985), pp. 173–193.

[629] A. T. Lemley, R. J. Wagenet, and W. Z. Zhong, J. Environ. Qual. **17**, 408 (1988).

[630] N. Burkhard and J. A. Guth, Pestic. Sci. **12**, 45 (1981).

[631] H. D. Scott and R. E. Phillips, Soil Sci. Soc. Am. Proc. **36**, 714 (1972).

[632] H. Ghadiri, P. J. Shea, G. A. Wicks, and L. C. Haderlie, J. Environ. Qual. **13**, 549 (1984).

[633] C. I. Harris, Weeds **14**, 6 (1966).

[634] J. M. Novak, T. B. Moorman, and D. L. Karlen, J. Agric. Food Chem. **42**, 1809 (1994).

[635] E. A. Rochette and W. C. Koskinen, Soil Sci. Soc. Am. J. **60**, 453 (1996).

[636] G. Wehtje, L. N. Mielke, J. R. C. Leavitt, and J. S. Schepers, J. Environ. Qual. **13**, 507 (1984).

[637] E. Barriuso, U. Baer, and R. Calvet, J. Environ. Qual. **21**, 359 (1992).

[638] R. Grover and R. J. Hance, Can. J. Plant Sci. **49**, 378 (1969).

[639] R. C. Wietersen, T. C. Daniel, K. J. Fermanich, B. D. Girard, K. Mc Sweeney, and B. Lowery, J. Environ. Qual. **22**, 811 (1993).

[640] R. Celis, J. Cornejo, M. C. Hermosín, and W. C. Koskinen, Soil Sci. Soc. Am. J. **61**, 436 (1997).

[641] R. C. Rhodes, I. J. Belasco, and H. L. Pease, J. Agric. Food Chem. **8**, 524 (1970).

[642] J. Kanazawa, Environ. Toxicol. Chem. **8**, 477 (1989).

[643] S. A. Clay, R. R. Allmaras, W. C. Koskinen, and D. L. Wyse, J. Environ. Qual. **17**, 719 (1988).

[644] J. T. Majka and T. L. Lavy, Weed Sci. **25**, 401 (1977).

[645] K. N. Reddy, M. A. Locke, and L. A. Gaston, Soil Sci. **162**, 501 (1997).

[646] A. P. Mallawatantri and D. J. Mulla, J. Environ. Qual. **21**, 546 (1992).

[647] G. A. O'Connor, B. C. Fairbanks, and E. A. Doyle, J. Environ. Qual. **10**, 510 (1981).

[648] H. M. Selim, R. S. Mansell, and A. Elzeftawy, Soil Sci. **121**, 176 (1976).

[649] S. U. Khan, Environ. Sci. Technol **8**, 236 (1974).

[650] A. J. A. Vinten, B. Yaron, and P. H. Nye, J. Agric. Food Chem. **31**, 662 (1983).

[651] M. Arienzo, M. Sánchez-Camazano, T. Crisanto Herrero, and M. J. Sánchez-Martín, Chemosphere **27**, 1409 (1993).

[652] M. Arienzo, T. Crisanto, M. J. Sánchez-Martín, and M. Sánchez-Camazano, J. Agric. Food Chem. **42**, 1803 (1994).

[653] P. W. Lee, S. M. Stearns, H. Hernandez, W. R. Powell, and M. V. Naidu, J. Agric. Food Chem. **37**, 1169 (1989).

[654] T. C. Herrero and L. F. L. Martin, Toxicol. Environ. Chem. **31/32**, 63 (1991).

[655] B. A. Brown, R. M. Hayes, D. D. Tyler, and T. C. Mueller, Weed Sci. **42**, 629 (1994).

[656] C. B. Rogers, R. E. Talbert, J. D. Mattice, T. L. Lavy, and R. E. Frans, Weed Sci. **34**, 122 (1985).

[657] F. Huggenberger, J. Letey, and J. Farmer, Soil Sci. Soc. Am. Proc. **36**, 544 (1972).

[658] R. C. Rhodes, J. Agric. Food Chem. **28**, 311 (1980).

[659] M. J. Sánchez-Martín and M. Sánchez-Camazano, Soil Sci. **152**, 283 (1991).

[660] J. B. Weber and L. R. Swain, Soil Sci. **156**, 171 (1993).

[661] L. S. Wood, H. D. Scott, D. B. Marx, and T. L. Lavy, J. Environ. Qual. **16**, 251 (1987).

[662] M. A. Locke, S. S. Harper, and L. A. Gaston, Soil Sci. **157**, 279 (1994).

[663] M. Leistra, L. G. M. Th. Tuinstra, A. M. M. van der Burg, and S. J. H. Crum, Chemosphere **13**, 403 (1984).

[664] H. M. Gaber, S. D. Comfort, W. P. Inskeep, and H. A. El-Attar, Soil Sci. Soc. Am. J. **56**, 1392 (1992).

[665] K. S. La Fleur, Soil Sci. **121**, 9 (1976).

[666] G. Wehtje, R. Dickens, J. W. Wilcut, and B. F. Hajek, Weed Sci. **35**, 858 (1987).

[667] W. C. Koskinen, G. A. O'Connor, and H. H. Cheng, Soil Sci. Soc. Am. J. **43**, 871 (1979).

[668] W. C. Koskinen and H. H. Cheng, J. Environ. Qual. **12**, 325 (1983).

[669] G. A. O'Connor and J. U. Anderson, Soil Sci. Soc. Am. Proc. **38**, 433 (1974).

[670] S. S. Chang and J. F. Stritzke, Weed Sci. **25**, 184 (1977).

[671] P. Jamet and M. A. Piedaller, Phytiatrie Phytopharmacie **27**, 111 (1978).

[672] W. A. Jury, R. Grover, W. F. Spencer, and W. J. Farmer, Soil Sci. Soc. Am. J. **44**, 445 (1980).

[673] W. L. Banwart, A. Khan, and J. J. Hassett, J. Environ. Sci. Health **B15**, 165 (1980).

[674] C. R. Worthing, *The Pesticide Manual*, 8th ed. (British Crop Protection Council, Thornton Heath, U.K., 1987).

[675] V. P. Kozak, G. V. Simsiman, G. Chester, D. Stensby, and J. Harkin, EPA-600/1-79-0.12, U.S. Environmental Protection Agency, Washington, DC (1979).

[676] K. Ugland, T. Lundales, T. Greinbrokk, and A. Bjorseth, J. Chromatogr. **213**, 83 (1981).

[677] A. Albert and E. P. Sergeant, in *Ionization Constants of Acid and Bases* (Methuen and Co., Ltd., London, 1962).

[678] M. A. Callahan, M. W. Slimak, N. W. Gabel, I. P. May, C. Fowler, J. R. Freed, P. Jennings, R. L. Durfee, F. C. Whitmore, B. Maestri, W. R. Mabey, B. R. Holt, and C. Gould, EPA-440/4-79-029a and EPA-440/4-79-029b, U.S. Environmental Protection Agency, Washington, DC (1979).

[679] J. B. Weber, Adv. Chem. Series **111**, 55 (1972).

[680] J. B. Weber, in *Research Methods in Weed Science*, edited by B. Truelove (Southern Weed Sci. Soc., Auburn Print., Inc., Auburn, AL, 1977), pp. 109–118.

[681] R. C. Weast, editor, *Handbook of Chemistry and Physics*, 50th ed. (CRC, Cleveland, OH, 1969–70).

Environ. Sci. Technol. **1997,** *31,* 597−602

Volatile Loss of PCB Aroclors from Subaqueous Sand

JEFFREY R. CHIARENZELLI,*
RONALD J. SCRUDATO, AND
MICHELE L. WUNDERLICH
Environmental Research Center, 319 Piez Hall,
SUNY at Oswego, Oswego, New York 13126

A series of experiments were conducted to measure the rate of volatile loss of PCBs from subaqueous quartz sand spiked with Aroclors 1242, 1248, 1254, and 1260 under laboratory conditions (20 C, 25% relative humidity). Volatilized PCBs were trapped on Florisil columns attached to a 1.5-L evaporation chamber through which 1.2 L/min of filtered air was drawn for a 24-h period. PCB losses ranged from 20 to 65% and were inversely correlated with the chlorine percentage of the aroclors ($R^2 = 0.97$). Congeners with the fewest number of chlorines in each aroclor were preferentially lost. In comparison, sediment from a Federal Superfund site along the St. Lawrence River, originally contaminated with Aroclor 1248, lost 19% of its PCB total during a similar experiment. Several orthochlorinated congeners, produced by anaerobic biodegradation, were preferentially lost, and four of these (2/2; 2/6; 2; 26/2) accounted for >55% of the total loss. This work suggests that under certain conditions the volatile loss of PCBs and other hydrophobic compounds from wet soils and sediments may be rapid and substantial. Further work is needed to elucidate the implications for analytical procedures, remedial actions, and the global mass balance of PCBs.

Introduction

Numerous studies have documented the occurrence of PCBs and other organochlorine compounds in various media, including moss and lichen (*1−6*), higher plants (*5*), snow and rain (*7, 8*), lake sediments (*9, 10*), and biota (*11, 12*), in locations considerably removed from their use and manufacture. Transfer by atmospheric processes is inferred, and PCBs have been identified in air samples from many locations (*13−15*). Atmospheric deposition and loss through volatilization from water (*13, 16−18*) have been noted as primary factors in the mass balance and transfer of PCBs in the Great Lakes and other water bodies, including the oceans (*19*).

Conflicting information on the rate of volatile loss of PCBs from solid media exists. Larsson (*20*) found only 0.5−0.7% of the PCBs originally spiked into lake sediments in artificial ponds were lost after 15 months, presumably by volatilization, and half-lives of ~10−20 years have been estimated for PCBs in soils (*21*). In contrast, PCB Aroclor (1254 and 1260) half-lives as brief as 1.1 years have been measured from experimental plots in the Canadian Arctic (*22*) despite low temperatures, and Haque et al. (*23*) measured significant volatile losses of Aroclor 1254 (~30% tetrachlorinated congeners; ~20% pentachlorinated congeners) from dry sand after 1 week. Even more rapid rates of loss (half-lives of a few days) have been measured during the drying of small samples (0.25−1.0 g) of PCB contaminated, anaerobically biodegraded, river sediment under ambient laboratory conditions (*24*). These studies suggest that rapid PCB volatile losses can take place from soil and sediment under some conditions.

Numerous studies have confirmed that PCB concentrations in air and water bodies have declined (*25, 26*) since efforts to reduce their escape into the environment were enacted in the 1970s. With falling PCB fugacities in the air (*21*), soils and sediments may release previously deposited PCBs to water bodies and the atmosphere (*27*). In an effort to learn which PCB congeners are likely to be released from submerged sediment and the potential differences between a range of Aroclors, we have conducted a series of experiments in which the PCBs released from spiked, subaqueous sand were captured and quantitated. Because the results cannot be directly extrapolated to 'real world' scenarios, a comparison is made with the PCB volatile loss from contaminated river sediment.

Analytical Methods

Reagents. All reagents utilized including hexane, sodium sulfate, sulfuric acid (Fisher Scientific), Florisil, and tetrabutylammonium sulfate (Sigma Chemical Company) were reagent grade and checked for contamination before use. Double-deionized water (DDI) was used throughout. Concentrated Aroclor 1248 in hexane was purchased from ChemService. Aroclors 1242, 1254, and 1260 in methanol were purchased from Supelco, Inc. Sediment consisting of ~70% fine-grained sand and containing ~63 ppm PCBs was obtained from the St. Lawrence River adjacent to a Federal Superfund site located near Massena, NY (*24*).

Experimental Procedures. A series of four experiments were conducted with Aroclors 1242, 1248, 1254, and 1260. For comparative purposes, a fifth experiment utilized contaminated St. Lawrence River sediment. A 1.5-L jacketed, glass evaporation chamber with two sample ports was utilized for all experiments. A flat glass lid was held securely to the upper flange of the chamber using a Teflon gasket and spring-loaded horseshoe clamp, which allowed rapid opening and air-tight sealing of the chamber. Prior to each experiment, the chamber was cleaned, and a blank consisting of a hexane rinse of all interior surfaces, including the lid, was analyzed. Approximately 0.25 g of dry, precleaned, medium-grained, quartz sand was weighed and placed in a shallow, preweighed, precleaned, glass beaker. A milliliter of aroclor spike with a known PCB concentration in methanol (~20 μg of Aroclors 1242, 1254, and 1260) or hexane (~25 μg of Aroclor 1248) was added to the sand. The solvent was allowed to evaporate to dryness (1−2 h) within the sealed chamber under experimental conditions. After solvent drying, the outlet Florisil column ($t = 0$ h column) was removed and eluted with hexane to monitor the loss of PCBs during spike evaporation. For Aroclors 1242 and 1248, the interior of the chamber was also rinsed with hexane and analyzed. Once the solvent evaporated, 25 mL of double deionized water (DDI) was added to the beaker and allowed to evaporate, under laboratory conditions (25% relative humidity and 20 C), for a period of 24 h. For the experiment utilizing St. Lawrence River sediment, ~0.25 g of sediment (dry weight) was added to the glass beaker and submersed in 25 mL of DDI water.

Inlet and outlet columns were fitted to ports on the evaporation chamber and filled with sodium sulfate (for water absorption) and 100% activated Florisil (10 g). Air was withdrawn through the outlet column with a vacuum pump at a rate of 1.2 L/min. Outlet Florisil columns were changed after solvent evaporation ($t = 0$) and $t = 1, 2, 4, 8,$ and/or 24

---

* Corresponding author telephone: (315) 341-3639; fax: 341-5346; e-mail: chiarenz@oswego.edu.

S0013-936X(96)00555-X CCC: $14.00

TABLE 1. Summary of Aroclor Volatilization Experiments[a]

experiment	Aroclor 1242	Aroclor 1248	Aroclor 1254	Aroclor 1260	St. L. River sediment
initial loss during spiking (ng)					
spike drying column	1 590	732	84	259	na
post-spike chamber rinse	56	171	nd	nd	na
recovered on columns (ng)					
1 h	2 427	1 991	432	153	310
2 h	1 305	1 435	432	190	241
4 h	1 493	2 455	nd	nd	643
8 h	2 241	2 138	nd	nd	nd
24 h	4 467	5 257	4 317	1 987	1 998
chamber rinse (ng)	57	106	1 545	1 368	130
remained on sand or sediment (ng)	3 754	9 388	9 569	13 802	12 320
total recovered (ng)	17 390	23 673	16 379	17 759	15 642
amount spiked (ng)	20 899	25 000	19 580	18 720	na
initial concentration (ppm)	83.6	100.0	78.3	74.9	63.0
mass balance (%)	83.2	94.7	83.7	94.9	na
PCBs volatilized (%)	62.3	55.5	34.5	20.0	19.2

[a] na, not applicable; nd, not determined.

h. During each column change, the beaker containing the sand– or sediment–water mixture was removed and weighed to monitor water loss.

Data Analysis. At the end of each experiment, the outlet Florisil columns were eluted with 100 mL of hexane, the entire interior of the chamber was rinsed with hexane, and the sediment or quartz sand and remaining water was extracted. The inlet column was also eluted and analyzed. Initial PCB concentrations spiked onto the sand were determined by GC analysis of Aroclor standards. The total recovered (Table 1) was calculated by adding the amount of PCBs volatilized during spike drying, the amount captured on columns during the experiment, the post-experiment chamber rinse, and the amount recovered from the sediment. The mass balance (Table 1) was determined by dividing the total recovered by the amount spiked. The amount of PCBs volatilized (Table 1) was calculated by summing the amount recovered from the columns and the post-experimental chamber rinse and dividing by the amount spiked minus the amount released during spike drying. For the St. Lawrence River sediment experiment, the amount of PCBs volatilized was calculated by dividing the amount recovered on the columns and in the post-experimental rinse by the total recovered as above; however, no PCBs were added.

PCB Extraction and Gas Chromatography. Water was separated from subaqueous sand and sediment by pipetting and was extracted by three sequential liquid/liquid separations with acetone, acetone/hexane (1:1), and hexane. The remaining wet sand and sediment were extracted by three sequential sonications with acetone, acetone/hexane (1:1), and hexane and recombined with the hexane extracts of their respective liquid fractions. Decachlorobiphenyl was added to the sand and sediment samples before extraction as a surrogate standard. The extracts were combined and dried using sodium sulfate, and sediment samples were oxidized with sulfuric acid and cleaned using tetrabutylammonium sulfate and 4% activated Florisil columns. Extracts from precleaned spiked sand samples were analyzed without cleanup. Aroclor standards in methanol were solvent switched to hexane and diluted before GC analysis. The hexane extract was condensed and stored at 4 C until analyzed. Congener-specific PCB analysis was performed on an HP5890 gas chromatograph using an electron capture detector and an Ultra DB-5 column. The gas chromatograph was calibrated every six samples using a mixed Aroclor standard prepared by the New York State Department of Health Wadsworth Laboratory enabling accurate quantitation of 69 congeners (Table 2). Volatilized PCBs were removed from Florisil columns by elution with hexane. The hexane was concentrated for GC analysis without further treatment. The interior of the glass drying chamber was also rinsed with hexane, condensed, and analyzed.

Quality Assurance/Quality Control. Inlet columns and chamber blanks were used to monitor possible contamination by laboratory air or reagents or other organic compounds. PCB accumulation rates on inlet columns ranged from 0.7 to 2.3 ng/h and averaged 1.6 ng/h ($n = 4$), which provided an estimate of laboratory air PCB concentrations during the period that this work was conducted. All possible sources of contamination were found to be insignificant in comparison to the amount of PCBs volatilized during the aroclor experiments ($>2\ \mu g$). The initial level of PCB contamination in the drying chamber was estimated by rinsing the interior of the chamber thoroughly with hexane before use. The total recovered before each experiment ranged from 1 to 4 ng of PCBs. The average concentration of the chamber blank was 2.5 ng of PCBs ($n = 5$). A blank experiment utilizing 'uncontaminated' (measured PCB concentration 76 ppb) archived soil obtained from the Geneva Agricultural Experimental Station of Cornell University yielded 6.5 ng of PCBs during a 24-h period. Decachlorobiphenyl (DCB) recovery from sediment and sand ranged from 95% (St. Lawrence River sediment) to 120% (sand spiked with Aroclor 1260) and averaged 108%. The recovery for Aroclor 1260 is elevated because of the presence of DCB in the original aroclor mixture.

Results

Table 1 summarizes the key parameters of the five experiments conducted with subaqueous sand and St. Lawrence River sediment. The loss of PCBs during each 24-h experiment ranged from 19% (sediment) to 62% (sand spiked with Aroclor 1242). Mass balances for the four Aroclor experiments ranged from 83 to 95%. A table summarizing congener-specific recovery, volatile loss percentage, and normalized volatile loss percentage for each aroclor experiment is available in the microfilm edition of the journal (see paragraph at end of paper on Supporting Information). In general, lower chlorinated congeners show lower recoveries than more highly chlorinated congeners. The loss of PCBs during evaporation of the spike solution (methanol or hexane) ranged from 12% (Aroclor 1242) to 1% (Aroclor 1254) of the total volatilization loss during the experiment. Significantly more PCBs (>10 times) were recovered from the final chamber rinse of experiments with Aroclors 1254 and 1260 than from Aroclors 1242 and 1248, suggesting that volatilized higher chlorinated congeners are transported shorter distances than lower chlorinated congeners before redeposition.

TABLE 2. PCB Congener Identification, IUPAC Numbers, and Assigned Peak Numbers for Figures 2 and 3

congener	IUPAC No.	assigned no.
2	1	1
4	3	2
2/2+2/6	4+10	3
24+25	7+9	4
2/3	6	5
2/4+23	8+5	6
HCB		7
26/2	19	8
25/2	18	9
4/4+24/2	15+17	10
236+26/3	24+27	11
23/2+26/4	16+32	12
25/3	26	13
24/3	25	14
25/4	31	15
24/4	28	16
34/2	33	17
23/4	22	18
236/2	45	19
25/25	52	20
24/25	49	21
24/24+245/2	47+48	22
23/25	44	23
236/2+23/24+34/4	59+42+37	24
236/4	64	25
23/23	40	26
235/26+245/4	94+74	27
25/34	70	28
24/34	66	29
234/4+34/23	60+55	30
245/25	101	31
245/24	99	32
245/23	97	33
234/25	87	34
DDE		35
236/236	136	36
34/34+236/34	77+110	37
2356/25+34/23	151+82	38
235/236	135	39
2356/24	147	40
236/245	149	41
245/34	118	42
2356/23	134	43
235/245	146	44
245/245+234/236	153+132	45
234/34	105	46
2345/25	141	47
2356/236	179	48
234/235	130	49
2346/236+2356/34	176+163	50
234/245	138	51
2346/34	158	52
2345/23	129	53
2356/245+2345/246	187+181	54
2346/245	183	55
234/234+245/345	128+167	56
23456/25	185	57
2345/236	174	58
2356/234	177	59
2346/234+2345/34	171+156	60
2346/2356	201	61
2345/235	172	62
2345/245	180	63
23456/236	200	64
MIREX		65
2345/234+23456/34	170+190	66
2345/2356	199	67
23456/245+2345/2346	203+196	68
23456/234	208	69
2345/2345	194	70
23456/2345	206	71
decachlorobiphenyl	209	72

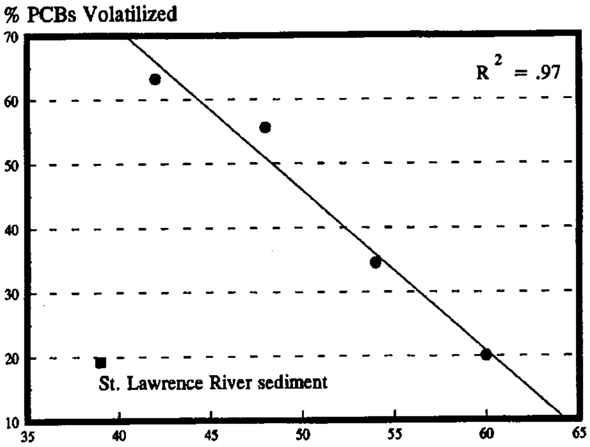


FIGURE 1. Plot of PCBs lost via volatilization from subaqueous sand versus the chlorine percentage of each Aroclor (1242, 1248, 1254, 1260) during evaporation experiments. Loss from St. Lawrence River sediment shown for comparative purposes. All experiments conducted at 20 C and 25% relative humidity for a period of 24 h.

Discussion

Correlation of PCB Loss with Aroclor Chlorine Content. Figure 1 shows that the percentage of PCBs lost during each experiment is negatively correlated with the weight percent of chlorine in the spiked aroclor. Note that the St. Lawrence River sediment sample, despite having undergone substantial anaerobic biodegradation as evidenced by its large percentage of lower orthochlorinated congeners (*28*) and its lower chlorine percentage (~40%), lost the least amount of PCBs during the experimental period. The retarded PCB loss from river sediment is believed to be related to its age (*29*), composition (organic rich), and/or grain-size distribution (30% clay and silt); all of which differ significantly from the uniform quartz sand used in the Aroclor experiments. The magnitude of PCB loss from the sediment is analytically indistinguishable from Aroclor 1260, which has 20% more chlorine and more highly chlorinated congeners; however, different congeners were volatilized in each experiment (Table 3).

Which Congeners Are Volatilized? Table 3 lists the 10 most abundant PCB peaks collected on the outlet column in each of the experiments by percentage of the normalized volatile loss. Note that many of the peaks are actually composed of two co-eluting congeners that cannot be resolved on the capillary column used for this study (Ultra DB-5). The 10 largest peaks account for 62.0–69.1% of the total volatile loss in each Aroclor experiment. The experiments conducted with Aroclors 1242 and 1248 are dominated by congeners containing only two or three chlorines, whereas the majority of those volatilized from Aroclors 1254 and 1260 have four to seven chlorines. Note that with the exception of congener 24/34, lower chlorinated congeners are either absent or not abundant enough to significantly influence the total volatile loss shown in Table 3 for Aroclor 1260. This progressive shift toward a pattern dominated by higher chlorinated congeners with increasing chlorine percentage is shown schematically in Figure 2 and is thought to be a function of the reduced abundance of lower chlorinated congeners, which would dominate the volatilized fraction if present.

Supporting Information (Tables 1a–1d and Figure 1) indicate that all four Aroclors display a progressive decrease in volatilization of individual congeners with increasing

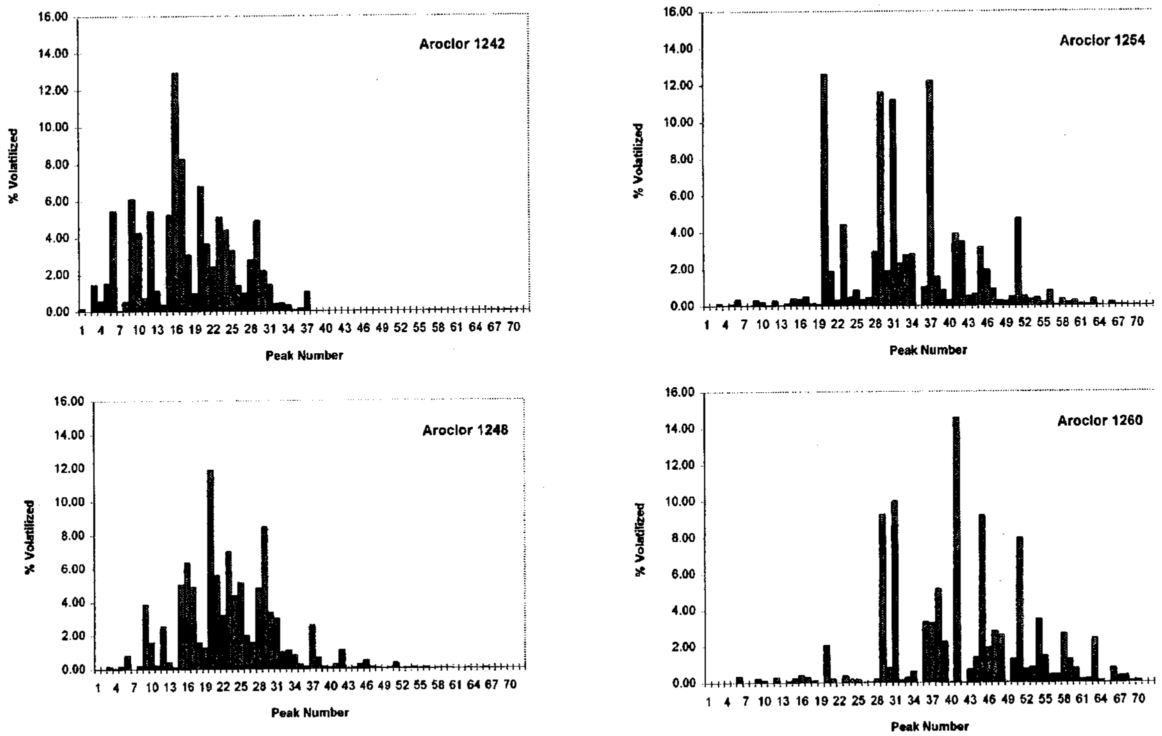


FIGURE 2. Percentage of total volatile loss by PCB congener for each aroclor experiment. Note the progressive shift to the right (more highly chlorinated congeners) with increasing levels of Aroclor chlorination and the range of congeners lost in each experiment. See Table 2 for peak identification.

TABLE 3. 10 Most Abundant (% of Normalized Volatile Loss) Congeners Volatilized in Each Experiment

Aroclor 1242		Aroclor 1248		Aroclor 1254		Aroclor 1260		St. L. River sediment	
congener	%	congener	%	congener	%	congener	%	congener	%
24/4	12.57	25/25	11.89	25/25	12.58	236/245	14.56	2/2+2/6	35.72
34/2	8.03	24/34	8.48	236/34+34/34	12.23	245/25	10.01	2	13.07
25/25	6.59	23/25	7.02	24/34	11.61	24/34	9.28	26/2	7.74
25/2	5.92	24/4	6.37	234/235	4.74	245/245+234/236	9.19	236+26/3	7.10
2/4+23	5.30	236/4	5.16	23/25	4.43	234/245	7.95	4/4+24/2	5.50
26/4+23/2	5.29	25/4	5.03	236/245	3.92	2356/25+2345/23	5.16	2/4+23	4.18
25/4	5.06	34/2	4.91	245/34	3.49	2356/245+2345/246	3.50	24/4	3.83
23/25	4.98	25/34	4.82	245/245+234/236	3.17	236/236	3.35	23/2+26/4	3.64
24/34	4.79	236/3	4.40	25/34	2.96	236/34+34/34	3.30	4	2.18
236/3	4.30	25/2	3.87	234/25	2.81	2345/25	2.83	25/25	1.90
total	62.83		61.95		61.94		69.13		84.86

retention time (chlorine content). In addition, a progressive steepening of the relative difference in the amount of volatile loss between lower and higher chlorinated congeners is noted as chlorine percentage increases. Aroclor 1260 lost >90% of its lower chlorinated congeners and almost none of the more highly chlorinated congeners, whereas Aroclor 1242 lost between ~60 and 70% of all congeners measured. Shifts in homologue distribution are apparent between the original Aroclor and the volatilized PCBs trapped on the Florisil columns (Table 4). The volatilized PCBs have a progressive increase in chlorine/biphenyl ratio from 3.41 (Aroclor 1242) to 5.65 (Aroclor 1260); however, for Aroclors 1248, 1254, and 1260, the volatilized PCBs are less chlorinated than the original Aroclor, while the converse is true for Aroclor 1242.

PCB Loss versus Time. The lower the chlorination of an Aroclor, the faster it lost PCBs via volatilization (Figure 3). Further, as illustrated by Figure 3, the initial rapid PCB loss in experiments with lighter Aroclors (1242 and 1248) begins to slow after several hours. Aroclor 1260, however, had a near linear loss throughout the duration of the experiment (24 h). These data suggest that when the most soluble and volatile PCBs are depleted, other less soluble and less volatile PCBs begin to dominate the volatilized fraction and the rate of loss via volatilization slows considerably. Further evidence of the influence of PCB aqueous solubility on volatile loss is evident in comparison of the ratio of PCBs (~2–13 μg) vs water (~7 g) lost in these experiments (equivalent to 0.3–1.9 ppm of PCBs), which varies within the reported range of PCB aqueous solubilities (*24*). Figure 3 implies that the greatest rate of PCB loss will occur during the first few hours of drying of contaminated media.

Comparison with PCB Loss from St. Lawrence River Sediment. As previously mentioned, St. Lawrence River sediment lost considerably less PCBs than would have been predicted based on its PCB chlorine percentage alone. Table 3 shows orthochlorinated congeners with one to three chlorines were lost primarily, and two co-eluting congeners 2/2 and 2/6 account for over 35% of the total loss measured. These orthochlorinated congeners are not found in great abundance in any of the Aroclors and are believed to be produced by anaerobic microbial degradation (*28*) of the original PCB mixture (Aroclor 1248). The 10 peaks reported in Table 3 account for approximately 85% of the PCB volatile loss from the sediment in this experiment. In Table 4, the

TABLE 4. Comparison of Homologue, Mole Percentage, and Cl/biphenyl Calculations for Aroclors and Volatilized Congeners in Evaporation Experiments

no. of chlorine	Aroclor 1242	Aroclor 1248	Aroclor 1254	Aroclor 1260	columns 1242	columns 1248	columns 1254	columns 1260	columns St. L. River
1	0.73	0.00	0.00	0.00	0.15	0.00	0.00	0.00	18.32
2	15.15	2.16	0.26	0.12	10.84	1.99	0.67	0.40	48.08
3	44.58	25.12	1.21	0.56	46.06	27.59	2.48	1.82	26.82
4	34.63	58.65	31.91	5.52	34.47	58.02	43.57	14.98	5.63
5	4.34	11.79	34.43	8.25	4.23	10.09	31.66	17.23	0.51
6	0.50	2.10	26.34	35.42	1.81	1.98	19.11	47.88	0.54
7	0.06	0.19	4.98	33.63	0.43	0.32	2.33	16.46	0.10
8	0.00	0.00	0.84	16.16	0.01	0.01	0.19	1.22	0.00
9	0.00	0.00	0.03	0.35	0.00	0.00	0.00	0.01	0.00
Cl per biphenyl	3.28	3.87	5.04	6.46	3.41	3.83	4.74	5.65	2.24
ortho	45.47	41.22	35.34	38.19	43.96	41.49	36.89	40.29	80.50
meta	27.56	33.58	38.87	39.42	33.58	33.18	38.81	37.22	9.26
para	26.96	25.20	25.79	22.39	25.33	25.33	24.30	22.49	10.24

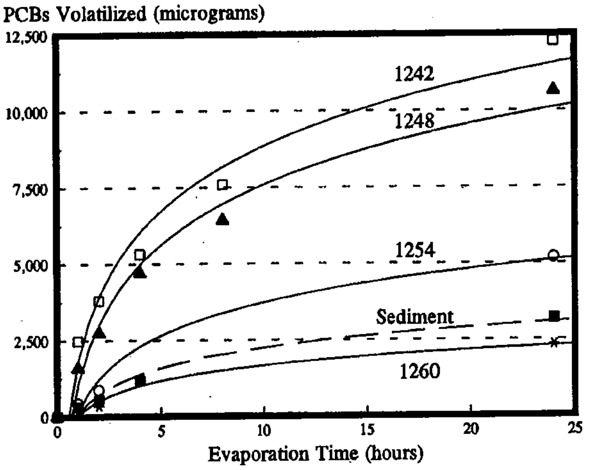


FIGURE 3. Temporal trends of PCB volatile loss in each Aroclor experiment. All regressions are logarithmic and R^2 values range from 0.97 to 0.98. Symbols used: (□) Aroclor 1242 (initial concentration 20.9 μg); (▲) Aroclor 1248 (25.0 μg); (○) Aroclor 1254 (19.6 μg); (*) Aroclor 1260 (18.7 μg); and (■) St. Lawrence River sediment (15.6 μg).

predominance of the lower orthochlorinated congeners is readily apparent in the volatilized mixture. Congeners with one (18.3%) and two chlorines (48.1%) are enriched in comparison to the Aroclor volatilization mixtures. In addition, the percentage of orthochlorination (80.5%) is higher than the Aroclor experiments that contained 37–44% *o*-chlorines.

Possible Implications. The rate of loss reported in these experiments (half-lives ranging from ~1 day to 1 week) from subaqueous sand is rapid in comparison with other studies on PCB volatilization (*20, 21*). Our results are approximately an order of magnitude faster than rates of loss reported by Haque et al. (*23*), who in a similar study found the volatile loss of Aroclor 1254 from dry sand at ambient laboratory conditions (34.5% of total Aroclor in 1 day vs ~30% of tetrachlorinated congeners in 1 week, respectively). The key difference between the two studies is the presence and evaporation of water. Water facilitates the transfer of PCBs from grain surfaces into the aqueous phase and transports the PCBs to the air–water interface where they can be lost by evaporative processes (*24*). It is therefore likely that the rate of loss will vary with factors that control evaporation (e.g., temperature, air flow, or surface area). By extension, contaminated shallow lakes, rivers, estuaries, harbors, and marine tidal environments may release significant quantities of PCBs and other hydrophobic organics to the air via volatilization enhanced by evaporative processes (*30*).

This work also suggests that there is a direct correlation between Aroclor chlorine percentage and the amount of PCBs that will be lost during water evaporation. However, despite extensive biodegradation resulting in the production of soluble and volatile orthochlorinated congeners, St. Lawrence River sediment originally contaminated with Aroclor 1248 lost PCBs at a rate similar to Aroclor 1260. This appears to support the work of Hatzinger and Alexander (*29*) on the effects of aging on contaminant availability in soils; note, however, that recent work by McGroddy et al. (*31*) suggests that other factors besides age may influence PCB retention. Temporal trends suggest that PCB volatile loss is initially rapid but slows with depletion of the most volatile and soluble congeners, suggesting that the greatest rates of contaminant loss will be during the first few hours of exposure to evaporative processes. The volatilized fraction from anaerobically biodegraded sediment may be dominated by highly volatile orthochlorinated congeners with one to three chlorines which were not part of the original Aroclor mixture (*24*).

The results of these experiments are thought to be most applicable to PCB analysis of soil and sediment or other media where relatively small quantities are handled in a laboratory setting. Moist media with moderate or high levels of PCBs may experience significant volatile loss during drying, even for short durations at ambient conditions. However, some recent studies indicate that media with low levels of contamination may uptake PCBs during exposure to contaminated laboratory air with greater PCB levels (*3*). Remedial technologies that employ dewatering of contaminated sediments prior to additional treatment or containment may contribute significant amounts of PCBs and similar compounds to the local environment (*24, 30*). Further work is needed to evaluate the applicability of this loss mechanism to natural sediments and soils, to estimate the magnitude of the transfer of PCBs from these reservoirs to the air and water, and to determine the potential role in local and global PCB mass balance calculations.

Acknowledgments

We would like to acknowledge the analytical support and expertise of J. Pagano. We are grateful to Dr. Brian Bush for relevant discussions on PCB transfer and analytical considerations. Ken Jock and Dave Arquette of the St. Regis Mohawk Tribe Environmental Division are thanked for their help with sample collection. Critical review and suggestions by three anonymous reviewers are gratefully acknowledged. Funding for this work came from the New York Sea Grant Institute and the National Institute of Environmental Health Sciences Basic Research Program.

Supporting Information Available

One figure and four tables detailing the congener-specific recovery, volatile loss percentage, and normalized volatile loss percentage for each Aroclor experiment (5 pp) will appear following these pages in the microfilm edition of this volume of the journal. Photocopies of the Supporting Information from this paper or microfiche (105 × 148 mm, 24× reduction, negatives) may be obtained from Microforms Office, American Chemical Society, 1155 16th St. NW, Washington, DC 20036. Full bibliographic citation (journal, title of article, names of authors, inclusive pagination, volume number, and issue number) and prepayment, check or money order for $15.00 for photocopy ($17.00 foreign) or $12.00 for microfiche ($13.00 foreign), are required. Canadian residents should add 7% GST. Supporting Information is available to subscribers electronically via the Internet at http://pubs.acs.org (WWW) and pubs.acs.org (Gopher).

Literature Cited

(1) Focardi, S.; Gaggi, C.; Chemello, G.; Bacci, E. *Polar Rec.* 1991, *162*, 241–244.

(2) Villeneuve, J.-P.; Holmes, E. *Chemosphere* 1984, *13*, 1133–1138.

(3) Lead, W.; Steinnes, E.; Jones, K. *Environ. Sci. Technol.* 1996, *30*, 524–530.

(4) Bacci, E.; Calamari, D.; Gaggi, C.; Fanelli, R.; Focardi, S.; Morosini, M. *Chemosphere* 1986, *15*, 747–754.

(5) Thomas, W.; Simon, H. *Sci. Total Environ.* 1985, *46*, 83–94.

(6) Muir, D.; Segstro, M.; Welbourn, P.; Toom, D.; Eisenreich, S.; Macdonald, C.; Whelpdale, D. *Environ. Sci. Technol.* 1993, *27*, 1201–1210.

(7) Gregor, D.; Gummer, W. *Environ. Sci. Technol.* 1989, *23*, 561–565.

(8) Welch, H.; Muir, D.; Billeck, B.; Lockhart, W.; Bruskill, G.; Kling, H.; Olson, M.; Lemoine, R. *Environ. Sci. Technol.* 1991, *25*, 280–286.

(9) Mudroch, A.; Allan, R.; Joshi, S. *Arctic* 1992, *45*, 10–19.

(10) Swackhammer, D.; Armstrong, D. *Environ. Sci. Technol.* 1986, *20*, 879–883.

(11) Andersson, O.; Linder, C.-E.; Olsson, M.; Reutergardh, L.; Uvemo, U.-B.; Wideqvist, U. *Arch. Environ. Contam. Toxicol.* 1988, *17*, 755–765.

(12) Muir, D.; Ford, C.; Grift, N.; Metner, D.; Lockhart, W. *Arch. Environ. Contam. Toxicol.* 1990, *19*, 530–542.

(13) Hornbuckle, K.; Achman, D.; Eisenreich, S. *Environ. Sci. Technol.* 1993, *27*, 87–98.

(14) Manchester-Neesvig, J.; Andren, A. *Environ. Sci. Technol.* 1989, *23*, 1138–1148.

(15) Bush, B.; Smith, R.; O'Keefe, P.; Fitzgerald, E. In *Sharing Knowledge, Linking Sciences: An International Conference on the St. Lawrence Ecosystem. Conference Proceedings. Vols. 1 and 2*; Needham, R. D., Novakowski, E. N., Eds.; Institute for Research on Environment and Economy, University of Ottawa: Ottawa, 1996; p 731.

(16) Achman, D.; Hornbuckle, K.; Eisenreich, S. *Environ. Sci. Technol.* 1993, *27*, 75–86.

(17) Pearson, R.; Hornbuckle, K.; Eisenreich, S.; Swackhammer, D. *Environ. Sci. Technol.* 1996, *30*, 1429–1436.

(18) Crane, J.; Sonzogni, W. *Chemosphere* 1992, *24*, 1921–1941.

(19) Loganathan, B.; Kannan, K. *Ambio* 1994, *23*, 187–191.

(20) Larsson, P. *Nature* 1985, *317*, 347–349.

(21) Harner, T.; Mackay, D.; Jones, K. *Environ. Sci. Technol.* 1995, *29*, 1200–1209.

(22) Grundy, S.; Bright, D.; Dushenko, W.; Reimer, K. *Environ. Sci. Technol.* 1996, *30*, 2661–2666.

(23) Haque, R.; Schmedding, D.; Freed, V. *Environ. Sci. Technol.* 1974, *8*, 139–142.

(24) Chiarenzelli, J.; Scrudato, R.; Arnold, G.; Wunderlich, M.; Rafferty, D. *Chemosphere* 1996, *33*, 899–911.

(25) Jones, K.; Duarte-Davidson, R.; Cawse, P. *Environ. Sci. Technol.* 1995, *29*, 272–275.

(26) Jeremaison, J.; Hornbuckle, K.; Eisenreich, S. *Environ. Sci. Technol.* 1994, *28*, 903–914.

(27) Alcock, R.; Johnston, A.; McGrath, S.; Berrow, M.; Jones, K. *Environ. Sci. Technol.* 1993, *27*, 1918–1923.

(28) Sokol, R.; Kwon, O.; Bethoney, C.; Rhee, G.-Y. *Environ. Sci. Technol.* 1994, *28*, 2054–2064.

(29) Hatzinger, P.; Alexander, M. *Environ. Sci. Technol.* 1995, *29*, 537–545.

(30) Cullen, A.; Vorhees, D.; Altshul, L. *Environ. Sci. Technol.* 1996, *30*, 1581–1588.

(31) McGroddy, S.; Farrington, J.; Gschwend, P. *Environ. Sci. Technol.* 1996, *30*, 172–177.

Received for review June 25, 1996. Revised manuscript received September 20, 1996. Accepted September 24, 1996.[⊗]

ES960555N

[⊗] Abstract published in *Advance ACS Abstracts*, December 1, 1996.

APPLIED AND ENVIRONMENTAL MICROBIOLOGY, May 1991, p. 1576–1578
0099-2240/91/051576-03$02.00/0

Vol. 57, No. 5

Reductive *ortho* and *meta* Dechlorination of a Polychlorinated Biphenyl Congener by Anaerobic Microorganisms

HEIDI M. VAN DORT AND DONNA L. BEDARD*

Biological Sciences Laboratory, GE Research and Development Center, P.O. Box 8, Schenectady, New York 12301

Received 18 December 1990/Accepted 25 February 1991

We used gas chromatography-mass spectrometry to study the metabolic fate of 2,3,5,6-tetrachlorobiphenyl (2356-CB) (350 μM) incubated with unacclimated methanogenic pond sediment. The 2356-CB was dechlorinated to 25-CB (21%), 26-CB (63%), and 236-CB (16%) in 37 weeks. This is the first experimental demonstration of *ortho* dechlorination of a polychlorinated biphenyl by anaerobic microorganisms.

The fate of polychlorinated biphenyls (PCBs) in aquatic sediments is a public concern because PCBs are relatively persistent and tend to bioaccumulate. Environmental dechlorination of PCBs via losses of *meta* and *para* chlorines has been reported for freshwater, estuarine, and marine sediments, including those from the Acushnet Estuary, the Hudson River, the Sheboygan River, and Waukegan Harbor (2–5), and via *ortho*, *meta*, and *para* dechlorination in Silver Lake (Pittsfield, Mass.) (5). Reductive dechlorination of PCBs by anaerobic microorganisms from Hudson River and Silver Lake sediments has recently been confirmed in the laboratory, but only losses of *meta* and *para* chlorines were observed (1, 6–8). Here we report the first experimental demonstration of biologically mediated *ortho* dechlorination of a PCB and stoichiometric conversion of a PCB congener to less-chlorinated forms.

Core samples (45 cm) of sediment were collected from the west side of Woods Pond (Lenox, Mass.), a shallow impoundment on the Housatonic River located 10.5 miles (ca. 16.9 km) downstream from Silver Lake. The pond's sediments are a mixture of black humic matter, sand, and silt contaminated with a hydrocarbon oil and Aroclor 1260. The sediment PCBs exhibited slight environmental dechlorination via loss of *meta* and *para* chlorines.

Methanogenic slurries were prepared under nitrogen in an anaerobic chamber by mixing wet sediment (2 volumes) with reduced anaerobic mineral medium (3 volumes) (9) and L-cysteine-HCl (0.1%). The slurries were dispensed into serum bottles, and 2,3,5,6-tetrachlorobiphenyl (2356-CB) (350 μM, 99% purity; AccuStandard, North Haven, Conn.) was added from a concentrated stock solution (70 mM in acetone). The bottles were crimp-sealed with teflon-lined butyl rubber septa (Wheaton). Sterile controls were prepared by sequential pasteurization (75°C, 20 min), incubation (23 to 25°C, 24 h), and autoclaving (121°C, 3 h). Duplicate samples and controls were incubated in the dark at 23 to 25°C. Aliquots (1 ml) of the slurries were sampled weekly and extracted by vigorous shaking (24 h) with anhydrous ether (5 volumes) and elemental mercury (1/4 volume, to remove sulfur) in vials with Teflon-lined foam-backed screw caps. Samples were analyzed by gas chromatography (GC) with an electron capture detector and a DB-1 capillary column (J & W Scientific; 30 m by 0.25-mm [inside diameter] by 0.25 μm) as previously described (5). PCBs that were formed as dechlorination products were initially identified by matching GC retention times with those of authentic standards (99% purity; AccuStandard). The identifications were subsequently confirmed by GC-electron capture detection with a C-87 capillary column (Chrompac; 60 m by 0.32 mm [inside diameter] by 0.2 μm) and by GC-mass spectrometry with a Hewlett-Packard 5890/5971A GC-mass spectrometer. An 18-point calibration curve (third order, not forced through zero) was used to determine the relative molar distribution of 2356-CB and its dechlorination products throughout the experiment.

Autoclaved controls (Fig. 1, top panel) showed no change throughout the experiment. Small amounts of three transformation products, tentatively identified as 25-CB, 235-CB, and 236-CB, were first detected at 21 weeks (Fig. 1, center panel). At later times a fourth product, identified as 26-CB, was also present (Fig. 1, bottom panel).

All transformation products were analyzed by GC-mass spectrometry to confirm their identifications. A sample containing the products tentatively identified as 25-CB, 26-CB, and 236-CB was ionized by electron impact (70 eV) and was scanned from 50 to 550 mass units. The observed molecular ions (*m/z* 222 and *m/z* 256), isotope patterns, and fragments (M^+, -70) were those expected for di- and trichlorobiphenyls, respectively. We confirmed our identification of 235-CB by selective ion monitoring at *m/z* 256. Collectively, these data indicate that the 2356-CB was reductively dechlorinated by anaerobic microorganisms in the sediment.

Figure 2 shows the relative molar distribution of 2356-CB and its dechlorination products over the course of the experiment. Small amounts of 25-CB, 235-CB, and 236-CB were first detected at 21 weeks. Both 25-CB and 236-CB increased with time, concomitant with a decrease in 2356-CB, but 235-CB never increased beyond 0.2 mol%. The 236-CB peaked at 64 mol% at 28 weeks, then steadily declined, and was replaced by 26-CB, which eventually increased to 58 mol%. Hence, the major route of dechlorination was 2356-CB → 236-CB → 26-CB (Fig. 3, pathway 1). There are several possible routes of formation of 25-CB. The simultaneous loss of both chlorines is theoretically possible, but there is no biological precedent for this type of dechlorination. It is more likely that the chlorines were removed sequentially by one or both of two possible routes: 2356-CB → 235-CB → 25-CB (Fig. 3, pathway 2) or 2356-CB → 236-CB (identical to 256-CB) → 25-CB (pathway 1A). To

---

* Corresponding author.

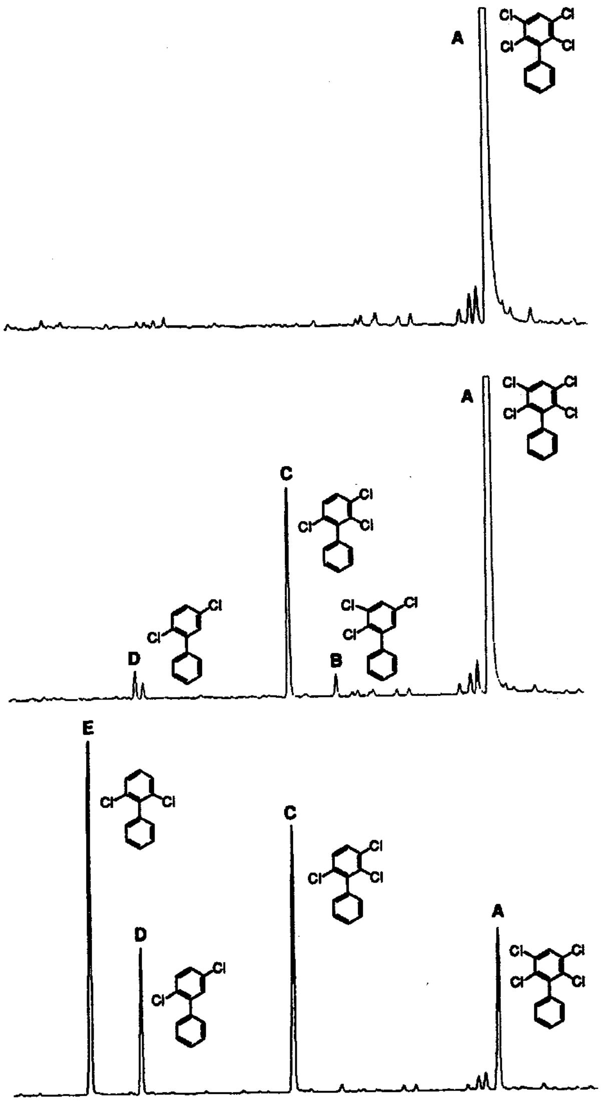


FIG. 1. GC-electron capture detector profile (DB-1 column) of 2356-CB and dechlorination products. (Top) Autoclaved control (37 weeks) showing 2356-CB. (Center) Live sample (21 weeks) showing 2356-CB (A), 235-CB (B), 236-CB (identical to 256-CB) (C), and 25-CB (D). (Bottom) Live sample (37 weeks) showing 2356-CB (A), 236-CB (C), 25-CB (D), and 26-CB (E). The vertical scale was 120 Hz for the top and center panels and 480 Hz for the bottom panel.

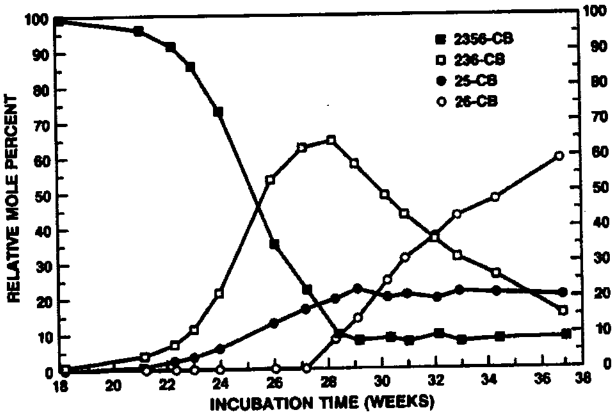


FIG. 2. Relative molar distribution of 2356-CB and its dechlorination products as a function of time. The data shown are from one of duplicate samples. The second sample was essentially identical except for a 1-week shift in the time frame.

gain a better understanding of how the 25-CB was formed, the duplicate cultures were combined at 37 weeks and were then used to inoculate autoclaved sediment slurries. The slurries were amended with 2356-CB, 236-CB, or 235-CB (350 μM, 99% purity). Dechlorination of 236-CB to 26-CB was detected at 3 weeks and was complete at 9 weeks of incubation. No dechlorination of 2356-CB or 235-CB occurred despite incubation for 21 weeks.

Although our results do not unequivocally establish the route of formation of 25-CB, we favor pathway 2 for several reasons. (i) Low levels of 235-CB were detected as soon as dechlorination of 2356-CB began. (ii) The formation of 25-CB appeared to be coupled to the depletion of 2356-CB (both ceased simultaneously at 29 weeks) but not to the presence of 236-CB. No 25-CB was formed during the last 8 weeks of incubation despite the nearly linear dechlorination of 236-CB to 26-CB. (iii) The transfer culture amended with 236-CB was dechlorinated exclusively to 26-CB. We have consistently seen the same transformation in unacclimated slurries of this sediment after only 2 to 3 weeks of incubation but have never observed the formation of 25-CB from

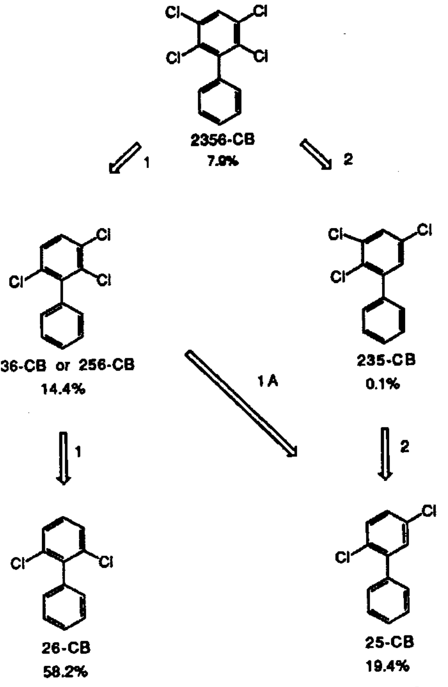


FIG. 3. Proposed routes of dechlorination of 2356-CB, showing all dechlorination products and giving their molar distribution at 37 weeks.

236-CB. (iv) In other experiments, we have observed the dechlorination of 235-CB to 25-CB in unacclimated slurries of this sediment after a long incubation (14 weeks).

Collectively, our observations support the proposal that the dechlorination of 2356-CB occurred in two separate stages. In the first stage (between 21 and 29 weeks of incubation), approximately 92% of the 2356-CB was dechlorinated; of this total, 79% was converted to 236-CB by loss of a *meta* chlorine and 21% was converted to 25-CB, via 235-CB, by sequential loss of an *ortho* chlorine and then a *meta* chlorine (Fig. 3). In the second stage, which began at 28 weeks, the 236-CB was rapidly dechlorinated to 26-CB. We speculate that these two stages may reflect a shift in the microbial population. We propose that the first population has a long acclimation time and can dechlorinate 2356-CB and 235-CB but not 236-CB. The second population has a shorter acclimation time and can dechlorinate 236-CB to 26-CB, but it has no activity against 2356-CB or 235-CB. This would explain why transfers of inocula collected at 37 weeks (stage 2) were able to dechlorinate 236-CB but not 2356-CB or 235-CB.

It has already been demonstrated that anaerobes from the Hudson River remove virtually all *meta* and *para* chlorines from Aroclors 1242 and 1248, leaving predominantly *ortho*-substituted mono- and dichlorobiphenyls (7). Our data clearly establish that anaerobic microorganisms from Woods Pond are capable of removing chlorine from the *ortho* position of at least one PCB congener. If this capability can be extended to 2-CB, 2,2′-CB, and 26-CB, the major products of PCB dechlorination by Hudson River microorganisms (2, 5, 7), then it may be possible to totally dechlorinate PCBs to biphenyl. Experiments with these congeners are in progress.

We thank Ralph J. May for expert GC and GC-mass spectrometry analyses and John A. Bergeron and John F. Brown, Jr., for helpful discussions and comments on the manuscript.

REFERENCES

1. **Abramowicz, D. A., M. J. Brennan, H. M. Van Dort, and E. L. Gallagher.** Anaerobic microbial dechlorination of polychlorinated biphenyls. *In* J. Glasser (ed.), Chemical and biochemical detoxification of hazardous waste II, in press. Lewis Publishers, Inc., Chelsea, Mich.
2. **Brown, J. F., Jr., D. L. Bedard, M. J. Brennan, J. C. Carnahan, H. Feng, and R. E. Wagner.** 1987. Polychlorinated biphenyl dechlorination in aquatic sediments. Science **236:**709–712.
3. **Brown, J. F., Jr., and R. E. Wagner.** 1990. PCB movement, dechlorination and detoxication in the Acushnet Estuary. Environ. Toxicol. Chem. **9:**1215–1233.
4. **Brown, J. F., Jr., R. E. Wagner, D. L. Bedard, M. J. Brennan, J. C. Carnahan, R. J. May, and T. J. Tofflemire.** 1984. PCB transformations in upper Hudson sediments. Northeast. Environ. Sci. **3:**167–179.
5. **Brown, J. F., Jr., R. E. Wagner, H. Feng, D. L. Bedard, M. J. Brennan, J. C. Carnahan, and R. J. May.** 1987. Environmental dechlorination of PCBs. Environ. Toxicol. Chem. **6:**579–593.
6. **Nies, L., and T. M. Vogel.** 1990. Effects of organic substrates on dechlorination of Aroclor 1242 in anaerobic sediments. Appl. Environ. Microbiol. **56:**2612–2617.
7. **Quensen, J. F., III, S. A. Boyd, and J. M. Tiedje.** 1990. Dechlorination of four commercial polychlorinated biphenyl mixtures (Aroclors) by anaerobic microorganisms from sediments. Appl. Environ. Microbiol. **56:**2360–2369.
8. **Quensen, J. F., III, J. M. Tiedje, and S. A. Boyd.** 1988. Reductive dechlorination of polychlorinated biphenyls by anaerobic microorganisms from sediments. Science **242:**752–754.
9. **Shelton, D. R., and J. M. Tiedje.** 1984. General method for determining anaerobic biodegradation potential. Appl. Environ. Microbiol. **47:**850–857.

BOREAL ENVIRONMENT RESEARCH 4: 331–342
Helsinki 15 December 1999

ISSN 1239-6095

Characterization and fate of polychlorinated biphenyl contaminants in Kernaalanjärvi sediments

Taina S. Hurme and Jaakko A. Puhakka

Tampere University of Technology, Institute of Water and Environmental Engineering, P.O. Box 541, FIN-33101 Tampere, Finland

Hurme, T. S. & Puhakka, J. A. 1999. Characterization and fate of polychlorinated biphenyl contaminants in Kernaalanjärvi sediments. *Boreal Env. Res.* 4: 331–342. ISSN 1239-6095

Polychlorinated biphenyl (PCB) content and distribution of individual PCB congeners in sediment samples from Kernaalanjärvi, a lake in Finland, were determined with a gas chromatography-electron/capture detection (GC-ECD) technique. Three different extraction methods with hexane–acetone mixture were tested. Neither extended extraction time (1 day vs. 10 days) nor sonication increased the recovery of PCBs from the aged sediments. For freshly spiked PCBs the extraction efficiency was 93% ± 2% (w/w). Total PCB concentrations ranging from 0.5 to 10.7 mg kg^{-1} d.w. were measured in Kernaalanjärvi sediment samples from the 2–15 cm depth. Comparison of PCB discharge documentation to congener distribution patterns in sediments suggested selective removal of lower chlorinated PCBs by physical processes. There was no evidence of *in situ* biotransformations of PCBs by indigenous sediment microorganisms. Presence of potentially toxic mono- and di-*ortho* chlorinated coplanar PCBs in sediments resulted in estimated 2,3,7,8-TCDD (tetrachlorodibenzo-*p*-dioxin) toxic equivalents between 15 and 301 ng kg^{-1} d.w.

Introduction

Freshwater and marine sediments serve as sinks for many synthetic chemicals. Some contaminants are recalcitrant in sediments whereas others shift between different physical compartments or are transformed in various ways (Calmano *et al.* 1996). Contaminating substances are frequently technical mixtures of different homologs and isomers from the same chemical group (e.g. polychlorinated biphenyls, polyaromatic hydrocarbons). Each component in a mixture may move and be transformed at different rates, which results in changes in pollutant mixture profiles in a given sediment location over time.

Polychlorinated biphenyls (PCBs) are among more common organochlorine compounds that typically accumulate in sediments. PCBs were used as complex mixtures of individual congeners in various applications including heat transfer, dielec-

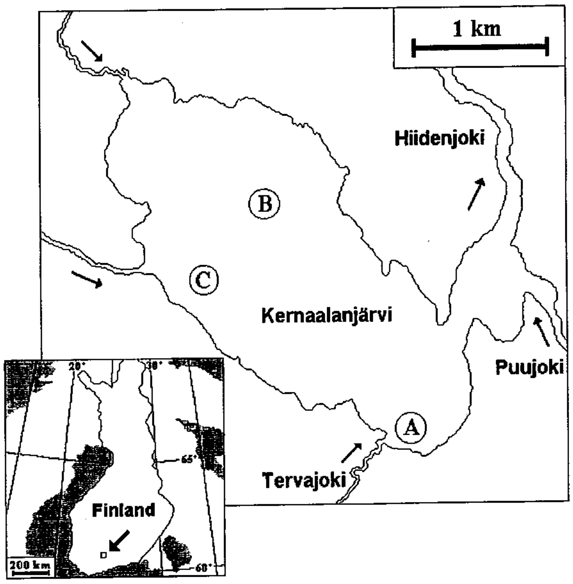


Fig. 1. Kernaalanjärvi and locations of sediment sampling sites.

tric, and hydraulic fluids, flame retardants, and plasticizers (Abramowicz 1990). PCBs were never introduced to nature by design as was the case with pesticides. Nevertheless, the environmental PCB load is estimated to exceed 350 000 tonnes which corresponds to one third of the total world production (Tanabe 1988).

PCBs are characterized by excellent oxidative and thermal stability, and were long believed to be recalcitrant in the environment. However, it has now been shown that both aerobic and anaerobic microorganisms can transform PCBs (for reviews, *see* e.g. Abramowicz 1990, Unterman 1996). Furthermore, there are several reports confirming *in situ* biotransformations of PCBs both in the presence and absence of oxygen (Brown *et al.* 1987, Brown and Wagner 1990, Flanagan and May 1993, Bedard and May 1996).

Physical phenomena such as sorption, desorption, dissolution, and volatilization affect PCB concentrations and distribution in contaminated sediments. The composition of the PCB mixture and the characteristics of the contaminated site determine the importance of these processes. For example, Kannan *et al.* (1997) reported extensive contamination of soil and marsh sediments with highly chlorinated Aroclor 1268. The PCB congener profile in sediment samples corresponded to Aroclor 1268 suggesting high stability of this PCB mixture. PCBs were strongly bound by the sediment environment; over a 50-fold decline in total PCBs with a distance of 500 meters away from the discharge point was reported.

Our goal was to characterize the PCB contamination of Kernaalanjärvi, a lake in Finland, using selected sediment samples, and to determine whether or not the composition of the original PCB mixture in the sediments has changed as a result of biological or other processes. Although the PCB content in Kernaalanjärvi sediments was previously studied, the distribution of individual PCB congeners is not reported (Kansanen and Pilke 1987, Kansanen *et al.* 1990, Kansanen *et al.* 1991). Previous observations concerning *in situ* biotransformations of PCBs were from sites under moderately temperate climate, i.e. between 40° and 50° northern latitude (Brown *et al.* 1987, Brown and Wagner 1990, Flanagan and May 1993, Bedard and May 1996). It was in our interest to study whether or not these *in situ* biotransformations occurred under boreal conditions (60–65° northern latitude), where water temperature approaches 4 °C.

Materials and methods

Site description and sample collection

Kernaalanjärvi is a lake located in southern Finland, in the municipality of Janakkala (Fig. 1). The surface area of the lake is 4.7 km^2 with a mean depth of 4 m. In 1956–1984, approximately 900 l (1 250 kg) of PCB oils were discharged into the lake from the research laboratory of a paper mill manufacturing dielectric paper (Waltari *et al.* 1987). The exact composition of the PCB load is not known, but it consisted of Clophen A50 mixture with pentachlorobiphenyls as the main PCB congeners and of several Pyralene and Aroclor mixtures with mostly tri- and tetrachlorinated PCB components. Use of Clophen A50 in test capacitors ceased in the 1960s when it was replaced by the lower chlorinated PCB mixtures. It has been estimated that 100 l of Clophen A50 and 800 l of the other PCB mixtures were discharged to Kernaalanjärvi (Waltari *et al.* 1987). Therefore, the main sediment contaminants were originally tri- and tetrachlorobiphenyls. Previous gas chromatographic

(GC) analyses, performed by comparison of sediment PCB profiles to standard chromatograms with known Aroclor compositions and contents, suggested that the total concentrations of extractable PCBs in Kernaalanjärvi sediments did not exceed 15 mg kg^{-1} d.w. (Kansanen *et al.* 1990). The concentrations of individual PCB congeners have not been previously reported.

Sediment samples were collected from three locations in Kernaalanjärvi (Fig. 1). Sampling site A was situated in the most contaminated region near the mouth of the Tervajoki, which is the original source of PCBs to the lake (Kansanen and Pilke 1987). Other main inflows to the lake have been shown to be noncontaminated with PCBs; thus reference site C was expected to contain relatively low PCB levels. The water depth at locations A and C was 2 m. The third sampling point (site B) was in the accumulation zone with a water depth of 8 m. The sedimentation rate in this accumulation zone is approximately 0.2 g cm^{-2} a^{-1} when neglecting the influence of resuspension (Kansanen *et al.* 1991).

Samples were taken in October 1995 when the water temperature was 10 °C. A plexiglass sampling tube (i.d. 45 mm) was used to collect approximately 15-cm sediment cores from the lake bottom. Three to five samples were taken from each sampling point to compose two separate combination samples. A 2-cm proportion from the top of each profile was separated for the enrichment of aerobic PCB degrading cultures (Hurme and Puhakka 1997). The remaining subsurface sediment (2–15 cm) from three parallel samples was combined to achieve a total sample volume of 0.6 l. This proportion was used in anaerobic degradation experiments (Hurme and Puhakka 1997) and for PCB quantification. Samples were collected in glass jars that were filled with the lake water and stored at 8 °C.

Sediment analyses

Sediment samples were analyzed for their organic carbon and PCB content. Organic carbon was measured according to the standard method SFS 3008 (Finnish Standards Association 1990) as a difference of total solids and total fixed residue. The organic carbon content in the three sediment samples ranged from 11% to 14%.

Extraction of PCBs from the sediment was conducted in 15-ml test tubes sealed with teflon lined rubber septa and screw-caps. Sediment samples were thoroughly mixed with the lake water and 10.0 or 12.5-ml subsamples were transferred into triplicate tubes. The amount of dry sediment in each tube was approximately 2 g. With the site A sediment, three different extraction techniques were tested and nine parallel tubes were used. After centrifuging (3 000 rpm, 3 min) the supernatant was discarded and octachloronaphthalene (OCN, 2.48 nmol) was added as an internal standard. In preliminary experiments using site A sediment, the supernatant was extracted with 2 ml of hexane and analyzed. No observable amounts of PCBs were found in the extract.

Sediment samples were extracted twice with 6 ml of hexane–acetone (1:1) mixture. In the first stage, triplicate samples from three sampling sites were set on a shaker for 16–20 h (method 1), whereas the additional samples of site A sediment were either shaken for 10 days (method 2) or sonicated for 5 min (method 3). In the second stage, all samples were shaken with solvent mixture for 5 min, and the solvent phases from the two steps were combined in a separatory funnel. Solids remaining after the extraction were dried at 105 °C, and the dry weight was measured for the normalization of PCB concentrations.

Acetone was removed from the extracts by reverse partitioning into distilled water (2 × 10 ml) in a separatory funnel. The remaining hexane fractions were concentrated to less than 2 ml under a nitrogen stream, and passed through a Florisil column (0.5 g in a Pasteur pipette). PCBs were eluted from the column into a weighed glass vial with 4 ml of hexane. The sample was further concentrated to approximately 1 ml, and the vial was weighed to determine the exact hexane volume. Elemental sulfur, which interferes during GC analysis, was removed with a reagent prepared by adding 3.39 g of tetrabutylammonium (TBA) hydrogen sulfate in 100 ml of distilled water and by saturating the solution with 25 g of sodium sulfite (Jensen *et al.* 1977). This TBA sulfite reagent (1 ml) was vigorously shaken with the extract, and the upper hexane fraction was collected for GC analysis.

PCB extraction efficiency from freshly spiked sediment was determined with method 1 alone. The PCB addition was 40 µg of either Aroclor 1242 or Aroclor 1254 to approximately 2 g (d.w.) of site C sediment. In these tests, PCBs were analyzed also from the supernatant. The PCB recovery (± SD) achieved for six samples was 93% ± 2% (w/w). As compared to the sediment samples with aged PCBs, there was a significant proportion (30% ± 4%) of PCBs present in the supernatant, and 63% ± 4% was recovered from the sediment. Proportions of individual congeners remained relatively unchanged in both extracts as compared to the original PCB mixtures. Most variation was observed in the sediment extracts of Aroclor 1242 spiked samples, where the relative proportions of penta- and hexa-CBs increased by 4.7%–4.9%, and the proportions of di-, tri-, and tetra-CBs decreased by 2.3%–4.6%. The extraction efficiency value was not used to correct the PCB results of Kernaalanjärvi sediments.

Congener-specific PCB analysis

PCBs were analyzed with a Hewlett-Packard 5890 Series II GC equipped with a HP-5 fused-silica column (length 25 m, i.d. 0.32 mm, film thickness 0.52 µm), a ^{63}Ni electron capture detector, and a HP 7673 automatic liquid sampler. Helium served as the carrier gas (5 ml min^{-1}) and argon–methane mixture (19:1) as the makeup gas (50 ml min^{-1}). The injector and detector temperatures were 250 °C and 320 °C, respectively. The initial oven temperature was 60 °C, from which it was ramped at 20 °C min^{-1} to 160 °C, 3 °C min^{-1} to 250 °C, and 10 °C min^{-1} to 270 °C, and finally held for 5 min.

Aroclor 1242 and Aroclor 1254 mixtures used separately served as standards for identification of PCB congeners. These commercial PCB mixtures were used by us as estimates of the contaminants discharged to Kernaalanjärvi. GC profiles of the two Aroclors were matched with the chromatograms published by Schulz *et al.* (1989), Bedard *et al.* (1987), and Ivanov and Sandell (1992). Single congeners 25-25-CB, 245-25-CB, and 245-245-CB were also used for the identification. Relative retention times of all peaks in relation to OCN were calculated and compared to those reported by Mullin *et al.* (1984). The PCB congener names and IUPAC numbers assigned for the GC peaks in this study are given in Table 1.

Sediment PCBs were quantified with four point calibration curves of both Aroclor 1242 and 1254 as described by Eisenreich (1987). The concentrations of individual congeners in standard samples were calculated from the total PCB content and the weight percent distribution of congeners in the Aroclor mixtures according to Schulz *et al.* (1989). The relation between the response area and concentration was determined, and for each chromatographic peak an individual linear estimation line was calculated. The total sediment PCB content was the sum of the concentrations assigned for single peaks.

Results and discussion

Extraction techniques

Desorption of PCBs from the site A sediment was studied with three different extraction techniques. In addition to simply shaking the sample overnight with hexane/acetone mixture (method 1), an extended extraction period of 10 days (method 2) or extraction in a sonicator for 5 min (method 3) were tested. Longer extraction time was expected to enhance the recovery of PCBs, since sorbed organic compounds often display biphasic desorption kinetics i.e. a labile portion is released more readily as compared to the resistant, slowly desorbing component (Pignatello and Xing 1996). Sonication, on the other hand, could improve extraction by dissociating the complex sediment matrix.

The total PCB yields of 10.7 ± 0.6, 9.2 ± 1.2, and 8.9 ± 0.5 mg kg^{-1} d.w. were achieved for triplicate site A samples extracted with methods 1, 2, and 3, respectively. In this study, neither longer extraction time nor the use of sonication enhanced the PCB recovery from aged sediment samples. Method 1 was most efficient for all PCB homologs from di- to octachlorinated congeners, and it was selected for further sediment characterization.

Quantification of sediment PCBs

Congener-specific PCB analysis was performed on the sediment samples from three different sampling locations of Kernaalanjärvi. The total PCB concentrations detected in triplicate samples from sites A, B, and C were 10.7 ± 0.6, 1.2 ± 0.1, and 0.53 ± 0.01 mg kg^{-1} d.w., respectively. These results, representing average PCB concentrations in the sediment depth of 2–15 cm, correspond with previous measurements of surface sediment PCB levels in different parts of Kernaalanjärvi (Fig. 2) (Kansanen *et al.* 1990).

Fig. 3 shows PCB congener distributions measured in the three sediment samples and, for comparison, the corresponding profiles for Aroclors 1242 and 1254. Aroclor mixtures do not represent the original PCB load, but are indicative of the type of PCB contamination. Considering the discharge history, the similarity of the site A profile with that of Aroclor 1254 was surprising. Homolog distribution of extractable PCB congeners in sediment samples, and in Aroclor 1242 and 1254 mixtures are presented in Fig. 4. Pentachlorinated PCBs were most abundant in all the sediment samples as well as in Aroclor 1254. Since tri- and tetrachlorinated PCBs were originally the main contaminant groups, then significant removal of

Table 1. PCB congener assignment for gas chromatographic peaks. The major constituents of peaks consisting of two congeners are indicated with bold IUPAC numbers and substitution patterns.

Peak	IUPAC no.	Chlorine substitution	Peak	IUPAC no.	Chlorine substitution
1	10 + **4**	26 + **2-2**	37	119	246-34
2	7 + 9	24 + 25	38	83	235-23
3	6	2-3	39	97	245-23
4	**8** + 5	**2-4** + 23	40	115 + **87**	2346-4 + **234-25**
5	19	26-2	41	85	234-24
6	18	25-2	42	136	236-236
7	15 + 17	4-4 + 24-2	43	77 + **110**	34-34 + **236-34**
8	24 + 27	236 + 26-3	44	82 + 151	234-23 + 2356-25
9	16 + 32	23-2 + 26-4	45	135	235-236
10	29	245	46	109	235-34
11	26	25-3	47	123 + **149**	345-24 + **236-245**
12	25	24-3	48	118	245-34
13	31	25-4	49	134	2356-23
14	28	24-4	50	131	2346-23
15	33 + 53	34-2 + 25-26	51	122	345-23
16	51	24-26	52	146	235-245
17	22	23-4	53	153	245-245
18	45	236-2	54	132 + 105	234-236 + 234-34
19	46	23-26	55	**141** + 179	**2345-25** + 2356-236
20	52	25-25	56	130	234-235
21	49	24-25	57	176 + 137	2346-236 + 2345-24
22	47 + 48	24-24 + 245-2	58	138	234-245
23	44	23-25	59	158	2346-34
24	59 + 42	236-3 + 23-24	60	129 + **178**	2345-23 + **2356-235**
25	41 + 64	234-2 + 236-4	61	175	2346-235
26	40	23-23	62	187	2356-245
27	100 + 67	246-24 + 245-3	63	183	2346-245
28	63	235-4	64	128	234-234
29	74	245-4	65	167	245-345
30	70	25-34	66	174	2345-236
31	66 + **95**	24-34 + **236-25**	67	177	2356-234
32	91	236-24	68	171 + **156**	2346-234 + **2345-34**
33	56 + 60	23-34 + 234-4	69	173 + **201**	23456-23 + **2346-2356**
34	92 + 84	235-25 + 236-23	70	172	2345-235
35	90 + **101**	235-24 + **245-25**	71	180	2345-245
36	99	245-24	72	**170** + 190	**2345-234** + 23456-34

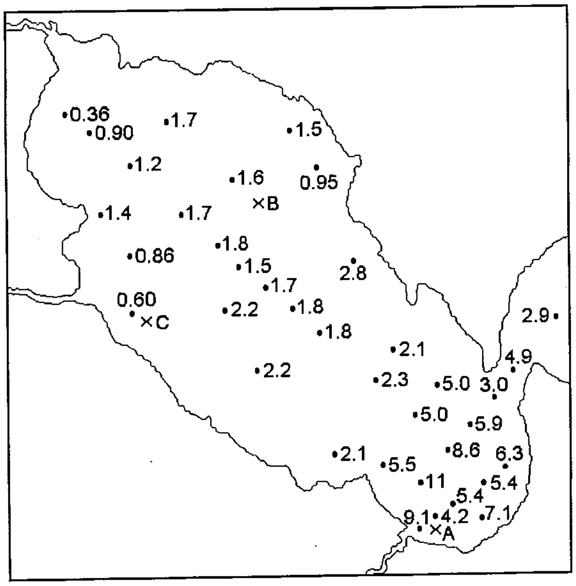


Fig. 2. Average PCB concentrations (mg kg^{-1} d.w.) in the surface sediment samples (0–2 cm) of Kernaalanjärvi as reported by Kansanen *et al.* (1990).

lower chlorinated PCBs has occurred from the sediments.

Fate of PCBs in Kernaalanjärvi

Several physical and biological processes may be responsible for the PCB patterns observed in Kernaalanjärvi sediment samples. Chemical transformations are unlikely for inert PCBs. The preferential loss of lower chlorinated congeners has likely resulted from congener-selective processes such as dissolution, volatilization, and biotransformation. To understand the fate of PCBs in Kernaalanjärvi, the PCB loads in different physical compartments of the lake were reviewed together with principal processes affecting PCBs.

Sediment

Kansanen *et al.* (1990) reported that the total amount of PCBs in Kernaalanjärvi sediment is 1 100–1 200 kg, which corresponds the overall discharge to the lake. This estimate was based on 34 surface sediment samples (0–2 cm) and three sediment profiles (0–30 cm) that were analyzed in 2-cm segments. PCB quantification was conducted by comparison of the total response areas in sediment samples and in certain Aroclor mixtures. Characterization of the PCB mixture composition in sediment samples was ignored. Although their calculations suggested high persistence of PCBs in Kernaalanjärvi, they also estimated that 100–200 kg of PCBs could be found in sediments downstream the lake. A higher number of sediment profiles is needed to accurately determine the total sediment PCB content in Kernaalanjärvi. In the absence of such information, we can only examine other possible fates of PCBs.

Water mass

PCBs may exist in the water mass in two forms: dissolved or adsorbed onto particles. The dissolved phase contains colloidal matter (e.g. humus) that binds PCBs (Eisenreich 1987, Kukkonen and Oikari 1991). The water solubility of PCBs inversely correlates with the chlorine content; therefore, dissolution may have resulted in selective removal of lower chlorinated PCBs from the sediment. With suspended solids concentrations less than 10 mg l^{-1}, the fraction of dissolved PCBs is typically higher than the amount of PCBs in the particulate phase (Eisenreich 1987). In Kernaalanjärvi, the suspended solids concentration is near 10 mg l^{-1}, and the particulate phase PCB concentrations range from 0.01 to 0.07 µg l^{-1} depending on the sampling site and the time of year (Kansanen *et al.* 1990, 1991). The average PCB concentration in the water phase of Kernaalanjärvi including both dissolved and particulate bound PCBs is thus roughly estimated to be at least 0.04 µg l^{-1}. On that basis, there may be about 1 kg of PCBs presently associated with the water.

From the water phase PCBs may accumulate within living organisms or sorb back onto sediments at a less contaminated location. Moreover, run-off or volatilization may result in complete removal of water-bound PCBs from the lake. The outflow from Kernaalanjärvi is through Hiidenjoki, which during the years 1981–1990 had a mean discharge of 18.9 m s^{-1} (Hydrological Yearbook 1990, KVVY 1997). Kernaalanjärvi delivers two thirds of this water and the rest comes from the Puujoki (KVVY 1997). With the estimated PCB concentration of 0.04 µg l^{-1} in the Kernaalanjärvi

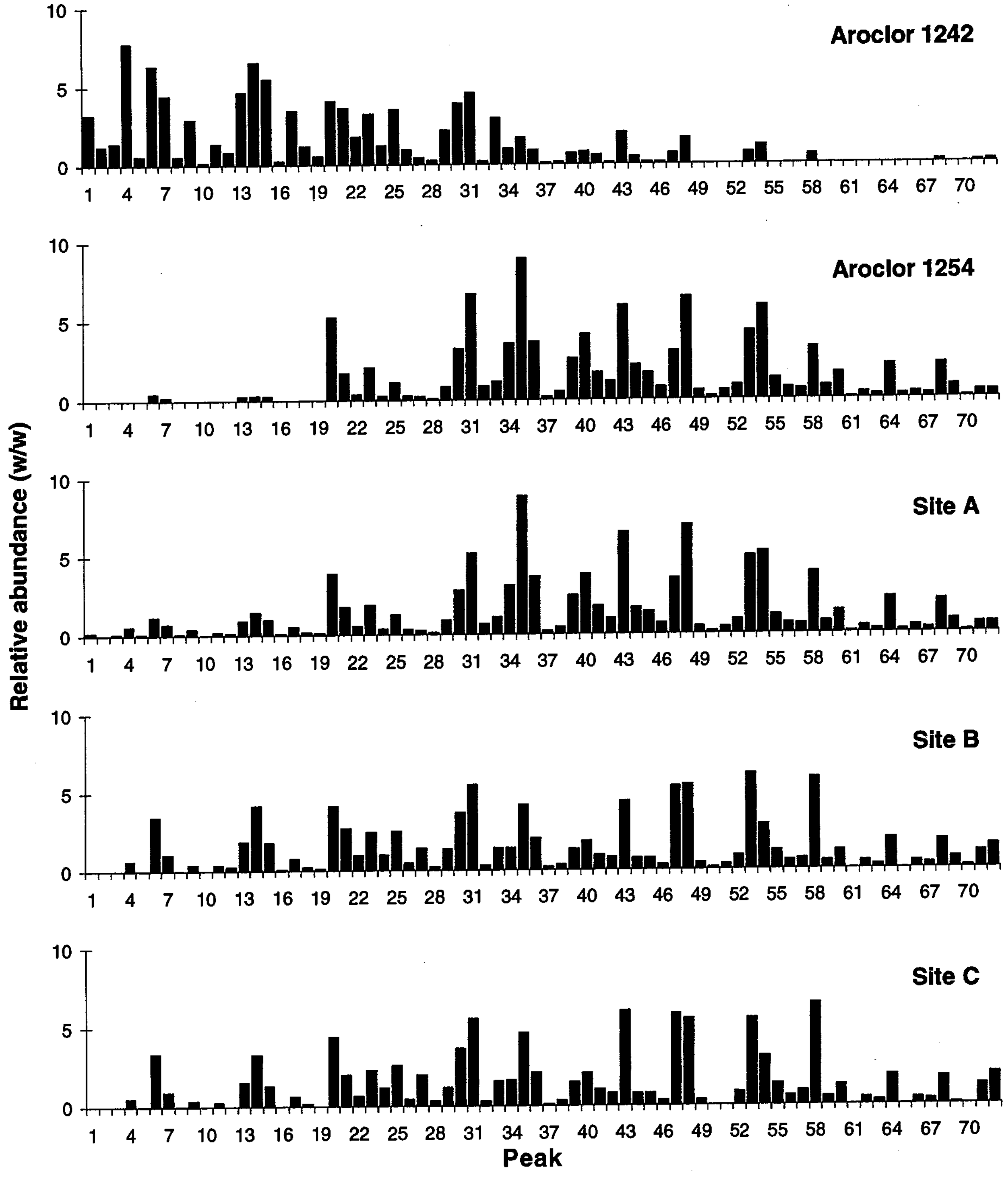


Fig. 3. Distribution of PCB congeners in Kernaalanjärvi sediment samples (2–15 cm) and in Aroclor 1242 and 1254 mixtures.

water mass, an annual PCB discharge of 16 kg from the lake is expected. Most of the PCBs were discharged to Kernaalanjärvi before 1970. If the prevailing conditions have been stable during the last 30 years, 480 kg of PCBs may have escaped the lake. This is considerably more than the estimate made by Kansanen *et al.* (1990), which was based on the PCB concentrations in three surface sediment samples downstream of Kernaalanjärvi.

Considering the initial 900-liter (1 250 kg) discharge of the PCB mixtures to the lake, the proposed run-off corresponds to over one third of this

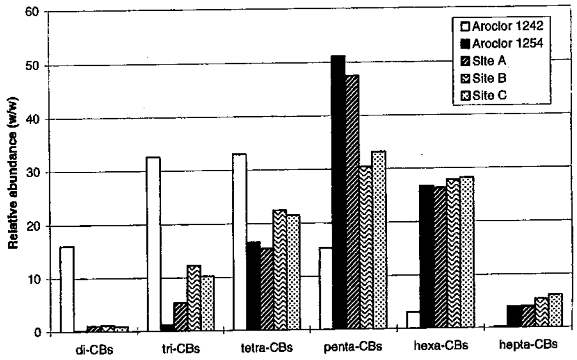


Fig. 4. PCB homolog distribution in Kernaalanjärvi sediment samples (2–15 cm) and in Aroclor 1242 and 1254 mixtures.

load. If a mixture of Aroclor 1242 and Aroclor 1254 (88:12 w/w) is regarded as an estimate of the original load, then the share of di- and trichlorobiphenyls would have initially been 535 kg. Dissolution followed by run-off could thus well explain the loss of lower chlorinated PCBs from the sediment.

Water-air interface

Henry's law constants for PCBs are independent of the degree of chlorine substitution (Burkhard *et al.* 1985). Therefore, individual PCB congeners are volatilized from solid state at approximately equal rates. In watercourses, however, volatilization of PCBs occurs from the dissolved state in the air-water interface, and is thus proportional to the solubility of congeners. Achman *et al.* (1993) studied volatilization of PCBs in natural aquatic conditions from Lake Michigan, where water column PCB concentrations are lower than in Kernaalanjärvi. Net volatilization rates between 10 and 1 000 ng m^{-2} d^{-1} were measured. In the case of Kernaalanjärvi this would result in an annual PCB loss of 0.02–1.7 kg. During a 30-year period, 1–50 kg of PCBs may have volatilized from the lake, which is minor as compared to the outflow. Main factors influencing the extent of PCB volatilization in the air-water interface are dissolved PCB concentrations, wind speed, and temperature (Achman *et al.* 1993).

Bioaccumulation

Aquatic organisms take up PCBs through ingestion and direct partitioning from water into lipids (Shaw 1993). Octanol-water partition coefficients (K_{ow}) describe the bioaccumulation potential of hydrophobic compounds. Lipophilicity increases with increasing degree of chlorine substitution, and coplanar PCBs and their mono- and di-*ortho* substituted congeners exhibit higher lipophilicity as compared to non-coplanar PCBs. These compounds possessing two *para* chlorines and at least one *meta* chlorine, are detected in significant levels in environmental samples although their proportion in PCB products is typically low (Shaw 1993). In this study, di-*ortho* coplanar PCBs assigned to peaks no. 53 (245-245-CB) and 58 (234-245) were present in relatively high proportions at sites B and C. Bioaccumulation of coplanar PCBs in fish tissue followed by death of the organisms may have resulted in these patterns. Total PCB concentrations in perch, bream, and pike in Kernaalanjärvi have been reported to be close to 1 mg kg^{-1} fresh weight (Kansanen *et al.* 1990). The distribution of individual PCB congeners in fish has not been reported.

Aerobic degradation

Verification of aerobic PCB biodegradation in sediments requires the detection of degradation products such as chlorobenzoic acids as reported by Flanagan and May (1993). In the absence of such evidence, it can be presumed that aerobic microbial degradation may have partially resulted in the loss of lower chlorinated PCBs from the sediments. In aqueous phase experiments with aerobic biphenyl degrading enrichment from Kernaalanjärvi sediment, di- and trichlorinated Aroclor 1242 congeners with less than two *ortho* chlorines and no double-*para* substitution were selectively removed at 20 °C (Hurme and Puhakka 1997). For example, PCBs assigned to chromatographic peaks no 4 (2-4-CB and 23-CB), 13 (25-4-CB), and 17 (23-4-CB) were all degraded in the laboratory tests. Nevertheless, the same peaks are present in sediment samples suggesting that the lower temperature, poor bioavailability, lack of oxygen, and the relatively low contaminant concentrations limit the *in situ* degradation of PCBs in sediments.

Reductive dechlorination

Microbial reductive dechlorination of PCBs does not remove the lower chlorinated PCBs but, on the contrary, increases the relative proportion of these congeners by replacing halogen substituents with hydrogen in higher chlorinated PCBs (Abramowicz 1990). In Kernaalanjärvi sediments, the *in situ* dechlorination of PCBs does not seem likely. A methanogenic enrichment culture from Kernaalanjärvi sediment dechlorinated Aroclor 1254 congeners assigned to peaks no. 35 (235-24-CB and 245-25-CB), 48 (245-34-CB), and 53 (245-245-CB) in laboratory experiments at 20 °C, but only after an enrichment period of 10 months (Hurme and Puhakka 1997). These congeners are major contaminants in all sediment samples, which together with long lag time indicates no *in situ* dechlorination. Furthermore, the overall sediment PCB concentrations at sites where *in situ* dechlorination has been detected have been considerably higher than in Kernaalanjärvi (Brown *et al.* 1987, Brown and Wagner 1990, Bedard and May 1996).

Toxicity of sediments

The toxicity of PCBs is usually presumed due to the presence of coplanar PCBs and some of their mono- and di-*ortho* substituted congeners (Safe 1990). The assessment of sediment toxicity based on total PCB content alone gives misleading results and thus a congener-specific analysis is always needed.

The concentrations of several mono- and di-*ortho* substituted coplanar congeners in Kernaalanjärvi sediment samples and their 2,3,7,8-TCDD toxic equivalents are given in Table 2. The most toxic PCB congeners, 345-345-CB and 345-34-CB, were not assigned to the Aroclor formula-

Table 2. Concentrations (mg kg^{-1} d.w.) and 2,3,7,8-TCDD toxic equivalents (ng kg^{-1} d.w.) of several non-, mono-, and di-*ortho* substituted coplanar PCBs in Kernaalanjärvi sediment samples (2–15 cm) and in Aroclor 1268 contaminated tidal creek sediment (Kannan *et al.* 1997).

		Conc. (mg kg^{-1} d.w.)/TEQ (ng kg^{-1} d.w.)			
IUPAC#	TEF[a]	Site A	Site B	Site C	T.c.sed.[c]
77	0.0005	ND	ND	ND	1.7/0.9
126	0.1	ND	ND	ND	0.8/82
169	0.01	ND	ND	ND	0.2/1.8
60[b]	0.001	57/57	7.9/7.9	4.0/4.0	12/12
105[b]	0.0001	279/28	16/1.6	8.1/0.8	35/3.5
118	0.0001	739/74	62/6.2	29/2.9	74/7.4
156	0.0005	221/111	21/11	9.0/4.5	17/8.5
128	0.00002	236/4.7	22/0.4	9.8/0.2	32/0.6
137[b]	0.00002	28/0.6	3.5/0.1	2.3/0.0	17/0.3
138	0.00002	413/8.3	67/1.3	34/0.7	131/2.6
153	0.00002	526/11	70/1.4	29/0.6	138/2.8
170	0.0001	57/5.7	17/1.7	10/1.0	32/3.2
180	0.00001	56/0.6	12/0.1	6.5/0.1	114/1.1
194	0.00002	ND	ND	ND	294/5.9
Total TEQ (ng kg^{-1} d.w.)		301	32	15	133

ND = Not detected

[a] TEFs for IUPAC nos. 60, 128, 137, 138, 153, and 194 from Safe (1990), others from Ahlborg *et al.* (1994).

[b] Peak constitutes two equal congeners and the concentration is half the total peak concentration.

[c] Tidal creek sediment from Kannan *et al.* (1997).

tions, so their presence in sediment samples was not verified. Third non-*ortho* substituted coplanar PCB, 34-34-CB, coeluted with 236-34-CB in peak no 43, and was ignored. Table 2 compares our results with the corresponding values of tidal creek sediment (Glynn County, Georgia, USA) contaminated with residues of Aroclor 1268 from a study by Kannan *et al.* (1997). This site was chosen for comparison since the total sediment PCB content (9.6 mg kg^{-1} d.w.) was similar to that of Kernaalanjärvi site A.

The estimated 2,3,7,8-TCDD toxic equivalents (TEQ) in Kernaalanjärvi sediment samples were between 15 and 301 ng kg^{-1} d.w., whereas toxic concentrations in sediment quality guidelines range from 0.014 to 210 ng kg^{-1} d.w. (Iannuzzi *et al.* 1995). Therefore, the PCB contaminated sediments likely pose a risk to organisms at least in the most contaminated parts of Kernaalanjärvi.

The sum concentrations of sediment PCBs in Kernaalanjärvi site A and in tidal creek sediment are at a same level, but the toxic equivalents differ considerably. This implies that the composition rather than the total amount of a PCB mixture determines its potential toxicity. The average chlorine content of PCB mixtures has also been used as a measure of product toxicity. In the tidal creek sediment, the chlorine content of PCBs was reported to average 64%, whereas in Kernaalanjärvi sediment samples it ranged from 54% to 56%.

Conclusions

The average contents of extractable PCBs in the 2–15 cm sediment layer in the most contaminated area of Kernaalanjärvi, the accumulation zone, and near the inflow of a noncontaminated river are 10.7, 1.2, and 0.53 mg kg^{-1} d.w., respectively. Principal contaminant isomers in the sediment are pentachlorinated PCBs and, as compared to the discharge documentation, the minor relative proportion of lower chlorinated PCBs indicates selective removal of these congeners. Approximately 1 kg of PCBs exists momentarily in the water mass. Outflow, volatilization, and aerobic degradation are the principal processes that may have resulted in the removal of di-, tri-, and tetrachlorinated PCBs from the lake. *In situ* biodegradation potential is limited, and volatilization is minor as compared to the proposed annual PCB outflow of 16 kg.

More information is needed on PCB concentrations in the water mass and in biota, before an overall fate estimation of PCBs in Kernaalanjärvi can be established. The distribution results of individual congeners are especially needed. The remaining PCBs in the sediment are more stable than the original PCB mixture because further dissolution is reduced. However, PCBs may still escape from the lake. The accumulation zone receives resuspended sediment material with sorbed PCBs until noncontaminated sediment covers the contaminated layers.

Toxicity risk of the PCB contaminated Kernaalanjärvi sediments was assessed as 2,3,7,8-TCDD toxic equivalents since total PCB content represents an insufficient indicator of toxicity. Considerable levels of several mono- and di-*ortho* substituted coplanar PCBs are present in sediment samples resulting in estimated 2,3,7,8-TCDD toxic equivalents between 15 and 301 ng kg^{-1} d.w. with the highest value exceeding the sediment quality criteria reported by Iannuzzi *et al.* (1995).

Acknowledgements: This work was financially supported by the Ministry of Education (Doctoral School for Environmental Ecology, Ecotoxicology, and Ecotechnology) and Maa- ja vesitekniikan tuki r.y. We also thank Kokemäenjoen vesistön vesiensuojeluyhdistys r.y. for the assistance in sampling.

References

Abramowicz D.A. 1990. Aerobic and anaerobic biodegradation of PCBs: a review. *Crit. Rev. Biotechnol.* 10: 241–251.

Achman D.R., Hornbuckle K.C. & Eisenreich S.J. 1993. Volatilization of polychlorinated biphenyls from Green Bay, Lake Michigan. *Environ. Sci. Technol.* 27: 75–87.

Ahlborg U.G., Becking G.C., Birnbaum L.S., Brouwer A., Derks H.J.G.M., Feeley M., Golor G., Hanberg A., Larsen J.C., Liem A.K.D., Safe S.H., Schlatter C., Wærn F., Younes M. & Yrjänheikki E. 1994. Toxic equivalency factors for dioxin-like PCBs. *Chemosphere* 28: 1049–1067.

Ballschmiter K. & Zell M. 1980. Analysis of polychlorinated biphenyls (PCB) by glass capillary gas chromatography. *Fresenius Z. Anal. Chem.* 302: 20–31.

Bedard D.L., Wagner R.E., Brennan M.J., Haberl M.L. &

Brown J.F.Jr. 1987. Extensive degradation of Aroclors and environmentally transformed polychlorinated biphenyls by Alcaligenes eutrophus H850. *Appl. Environ. Microbiol.* 53: 1094–1102.

Bedard D.L. & May R.J. 1996. Characterization of the polychlorinated biphenyls in the sediments of Woods Pond: evidence for microbial dechlorination of Aroclor 1260 in situ. *Environ. Sci. Technol.* 30: 237–245.

Brown J.F.Jr., Bedard D.L., Brennan M.J., Carnahan J.C., Feng H. & Wagner R.E. 1987. Polychlorinated biphenyl dechlorination in aquatic sediments. *Science* 236: 709–712.

Brown J.F.Jr. & Wagner R.E. 1990. PCB movement, dechlorination, and detoxication in the Acushnet Estuary. *Environ. Toxicol. Chem.* 9: 1215–1233.

Burkhard L.P., Armstrong D.E. & Andren A.W. 1985. Henry's law constants for the polychlorinated biphenyls. *Environ. Sci. Technol.* 19: 590–596.

Calmano W., Ahlf W. & Förstner U. 1996. Sediment quality assessment: chemical and biological approaches. In: Calmano W. & Förstner U. (eds.), *Sediments and toxic substances: environmental effects and ecotoxicity*, Springer-Verlag, Berlin, pp. 1–35.

Dunnivant F.M., Elzerman A.W., Jurs P.C. & Hasan M.N. 1992. Quantitative structure-property relationships for aqueous solubilities and Henry's law constants of polychlorinated biphenyls. *Environ. Sci. Technol.* 26: 1567–1573.

Eisenreich S.J. 1987. The chemical limnology of nonpolar organic contaminants: polychlorinated biphenyls in Lake Superior. In: Hites R.A. & Eisenreich S.J. (eds.), *Sources and fates of aquatic pollutants*, American Chemical Society, Washington, pp. 393–469.

Finnish Standards Association 1990. *SFS 3008: Determination of total residue and total fixed residue in water, sludge and sediment*, 3 pp.

Flanagan W.P. & May R.J. 1993. Metabolite detection as evidence for naturally occurring aerobic PCB biodegradation in Hudson River sediments. *Environ. Sci. Technol.* 27: 2207–2212.

Hawker D.W. & Connell D.W. 1988. Octanol-water partition coefficients of polychlorinated biphenyl congeners. *Environ. Sci. Technol.* 22: 382–387.

Hurme T.S. & Puhakka J.A. 1997. Polychlorinated biphenyl biotransformations by aerobic and anaerobic boreal lake sediment microorganisms. In: Alleman B.C. & Leeson A. (eds.), *In situ and on-site bioremediation: volume 2*, Battelle Press, Columbus, Ohio, pp. 427–432.

Hydrological Yearbook 1990. *National Board of Waters and the Environment*, Helsinki, Finland, 197 pp.

Iannuzzi T.J., Bonnevie N.L. & Wenning R.J. 1995. An evaluation of current methods for developing sediment quality guidelines for 2,3,7,8-tetrachlorodibenzo-p-dioxin. *Arch. Environ. Contam. Toxicol.* 28: 366–377.

Ivanov V. & Sandell E. 1992. Characterization of polychlorinated biphenyl isomers in Sovol and Trichlorodiphenyl formulations by high-resolution gas chromatography — mass spectrometry techniques. *Environ. Sci. Technol.* 26: 2012–2017.

Jensen S., Renberg L. & Reutergårdh L. 1977. Residue analysis of sediment and sewage sludge for organochlorines in the presence of elemental sulfur. *Anal. Chem.* 49: 316–318.

Kannan K., Maruya K.A. & Tanabe S. 1997. Distribution and characterization of polychlorinated biphenyl congeners in soil and sediments from a Superfund site contaminated with Aroclor 1268. *Environ. Sci. Technol.* 31: 1483–1488.

Kansanen P. & Pilke A. 1987. *Vanajaveden reitin PCB-tutkimus v. 1986*, Insinööri- ja limnologitoimisto Oy Vesitekniikka Ab, Hollola, 19 pp.

Kansanen P., Pilke A. & Hanski A. 1990. *Tutkimus PCB-yhdisteistä ja vesistön puhdistusmahdollisuuksista. Osa I: PCB:n nykyinen levinneisyys ja kulkeutuminen kaloihin Tervajoessa ja Kernaalanjärvessä*, Insinööritoimisto Paavo Ristola Oy, Hollola, 32 pp.

Kansanen P., Hanski A. & Pilke A. 1991. *Tutkimus PCB-yhdisteistä ja vesistön puhdistusmahdollisuuksista. Osa II: Mahdollisuudet PCB-haitan vähentämiseen kunnostustoimenpitein Kernaalanjärvessä*, Insinööritoimisto Paavo Ristola Oy, Hollola, 49 pp.

Kukkonen J. & Oikari A. 1991. Bioavailability of organic pollutants in boreal waters with varying levels of dissolved organic material. *Wat. Res.* 25: 455–463.

KVVY 1997. *Vuosiyhteenveto Sucros Oy:n jätevesien purkualueen velvoitetarkkailusta käyntikaudelta 1996*, Kokemäenjoen vesistön vesiensuojeluyhdistys r.y., Tampere.

Mullin M.D., Pochini C.M., McCrindle S., Romkes M., Safe S.H. & Safe L.M. 1984. High-resolution PCB analysis: synthesis and chromatographic properties of all 209 PCB congeners. *Environ. Sci. Technol.* 18: 468–476.

Pignatello J.J. & Xing B. 1996. Mechanisms of slow sorption of organic chemicals to natural particles. *Environ. Sci. Technol.* 30: 1–11.

Safe S. 1990. Polychlorinated biphenyls (PCBs), dibenzo-p-dioxins (PCDDs), dibenzofurans (PCDFs), and related compounds: environmental and mechanistic considerations which support the development of toxic equivalency factors (TEFs). *Crit. Rev. Toxicol.* 21: 51–88.

Schulz D.E., Petrick G. & Duinker J.C. 1989. Complete characterization of polychlorinated biphenyl congeners in commercial Aroclor and Clophen mixtures by multidimensional gas chromatography-electron capture detection. *Environ. Sci. Technol.* 23: 852–859.

Shaw G. 1993. Polychlorinated biphenyls (PCBs), effects on humans and the environment. In: Corn M. (ed.), *Handbook of Hazardous Materials*, Academic Press, Inc., pp. 611–625.

Tanabe S. 1988. PCB problems in the future: foresight from current knowledge. *Env. Pollut.* 50: 5–28.

Unterman R. 1996. History of PCB contamination. In: Crawford R. L. & Crawford D. L. (eds.), *Bioremediation —*

principles and applications, Cambridge University Press, England, pp. 209–253.

Waltari L., Pohjola H., Rossi E. & Ettala M. 1987. *Tervakoski Oy: kaatopaikkojen ympäristöriskiselvitys*, Insinööri- ja limnologitoimisto Oy Vesitekniikka Ab, Hollola, 5 pp.

Received 5 March 1999, accepted 18 August 1999