MANUAL

FOR

DOMENICO NON-STEADY STATE

SPREADSHEET ANALYTICAL MODEL

(FOR CONTINUOUS SOURCE RELEASE)

Tom Shih and Yue Rong

Underground Storage Tank Section
California Regional Water Quality Control Board - Los Angeles Region
320 West 4th Street, Suite 200, Los Angeles, CA 90013

May 15, 2001

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1. Introduction

The Domenico non-steady state analytical model (1987) presented in this manual is an analytical solution to the advection-dispersion partial-differential equation of organic contaminant transport processes in groundwater for a continuous release source as described below. The model contains one dimensional groundwater velocity, longitudinal, transverse, and vertical dispersion, the first order degradation rate constant, finite contaminant source dimensions, and can estimate travel time to a receptor at contaminant plume centerline, given a continuous release source. Since the plume concentration is a function of travel time in the model, the analytical model can be applied to estimate the plume travel time to a given distance for dissolved organic contaminants in groundwater. The use of the analytical model requires contaminant temporal concentration data at a minimum of one source and one downgradient monitoring well. The groundwater temporal concentration data for the downgradient monitoring well must show a reasonable pattern, in which contaminant concentrations over time resemble a sigmoidal curve. The model is calibrated by adjusting four model-input parameters to fit the pattern of groundwater temporal concentration distribution at the downgradient monitoring well. The model after calibration is then used to estimate the plume travel time to a given distance (e.g., to a drinking water well). The analytical solution form is programmed into a Microsoft Excel Spreadsheet. Prior to applying the spreadsheet model and interpreting the model results, understanding of model assumptions and uncertainties associated with model calibration with field data is strongly advised.

2. Domenico Non-Steady State Analytical Model

The Domenico non-steady state analytical model is based on the advection-dispersion partial-differential equation for organic contaminant transport processes in groundwater as described below (Domenico and Robbins, 1985):

$$\frac{\partial C}{\partial t} = D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} + D_z \frac{\partial^2 C}{\partial z^2} - v \frac{\partial C}{\partial x} \qquad (1)$$

Where C is the contaminant concentration in groundwater (mg/L); *t* is the time (day); *v* is the groundwater seepage velocity (ft/day); x, y, z are the coordinates to the three dimensions (ft); D_x, D_y, D_z are the dispersion coefficients for the x, y, z dimensions (ft^2/day), respectively.

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In an attempt to incorporate natural degradation factor, Domenico (1987) introduced a first order degradation rate constant to approximate the original analytical solution to equation (1). To evaluate transient plume behavior, the transient, centerline analytical solution derived by Domenico (1987) is applied. Under conditions of a continuous source and finite source dimensions with one-dimensional groundwater velocity, longitudinal, transverse, and vertical dispersion, and a first order degradation rate constant, equation (2) shown below represents the Domenico transient solution for the centerline concentration as a function of time (Domenico, 1987):

$$C(x,0,0,t) = \frac{C_0}{2}\exp\left\{\frac{x}{2\alpha_x}\left[1-\left(1+\frac{4\lambda\alpha_x}{v}\right)^{\frac{1}{2}}\right]\right\}\times\left\{erfc\left[\frac{x-vt\left(1+\frac{4\lambda\alpha_x}{v}\right)^{\frac{1}{2}}}{2(\alpha_x vt)^{\frac{1}{2}}}\right]\right\}$$

$$\times erf\left[\frac{Y}{4(\alpha_y x)^{\frac{1}{2}}}\right]\times erf\left[\frac{Z}{4(\alpha_z x)^{\frac{1}{2}}}\right] \qquad (2)$$

Where C(x,0,0,*t*) is the contaminant concentration (μg/L) in a downgradient well at time *t* along the plume centerline at a distance x (x,0,0); C_0 is the steady state contaminant concentration in the source well; x is the centerline distance between the downgradient well and source well (ft); α_x, α_y, and α_z are the longitudinal, transverse, and vertical dispersivity (ft), respectively; λ is the degradation rate constant (1/day) and equals to $0.693/t_{1/2}$ (where $t_{1/2}$ is the degradation half-life of the contaminant); *v* is the groundwater velocity (ft/day); Y is the source width (ft); Z is the source depth (ft); *erf* and *erfc* are the error and complementary error functions, respectively; and exp is the exponential function.

The Domenico non-steady state analytical equation (2) assumes:

a. Transient or non steady state (concentration is a function of time),
b. A continuous release source,
c. Homogeneous aquifer properties,
d. One dimensional groundwater flow,
e. No change in groundwater flow direction and velocity,
f. First order degradation rate,
g. Contaminant concentration estimated at the centerline of the plume,
h. Molecular diffusion based on concentration gradient is neglected, and
i. Adsorption in transport process is neglected.

Key Limitations:

a. The model should not be applied where vertical flow gradients affect contaminant transport.

b. The model should not be applied where hydrogeologic conditions change dramatically over the simulation domain.

Understanding model assumptions and limitations is crucial to simulate transport process for a specific contaminant in groundwater. For example, methyl tertiary butyl ether (MTBE) has a very low potential of being sorbed onto soil particles due to its low K_{oc} value and high solubility in water and therefore adsorption in transport process may be neglected. Conversely, perchloroethylene (PCE) has a relatively high retardation potential and the model described in this manual need to be modified before it can be applied for estimating PCE transport process in groundwater. In addition, when compared to other petroleum hydrocarbons (e.g., benzene, toluene, ethylbenzene, and total xylenes [BTEX]), MTBE does not naturally degrade to a significant degree.

3. Estimation of Centerline Distance

One of the conditions for using the Domenico Non-Steady State Analytical Model is that the selected downgradient monitoring well must be along the plume centerline. In most contamination cases, downgradient monitoring wells may be off the centerline. In order to apply the Domenico Analytic Model to these cases, the distance between these off-centerline wells and source wells must be converted to the centerline distance.

In this manual, an ellipse trigonometry method is used to convert an off-centerline distance to a centerline distance (Tong and Rong, 2001). The method is based on an assumption about the contaminant plume geometry, which can be described as an ellipse shape (Figure 1). This ellipse shape is idealized and assumed based on the observations that the plume migrates fastest along groundwater flow direction and the longitudinal dispersivity is greater than transverse dispersivity in general. This assumption is consistent with the shape in a similar study by Martin-Hayden and Robbins (1997).

Based on the assumption of the ellipse plume shape, the following offers the calculation of converting a distance from an off-centerline well to a centerline well. The assumptions are: (1) the ellipse width = 0.33 ellipse length (most studies assume $\alpha_y = 0.33\alpha_x$) (the ellipse length/width ratio can be adjusted based on the field data collected from every individual site) and (2) the ellipse is the contaminant iso-concentration line.
The equation for an ellipse with a horizontal major axis:

$$\frac{X^2}{a^2} + \frac{Y^2}{b^2} = 1 \qquad (3)$$

Where, a = the length of the major axis, b = the length of the minor axis, a > b > 0. X and Y are the coordinates to the x and y dimension, respectively. If the source well is assumed at close to one end of the ellipse and one downgradient well located on the ellipse (see Figure 1) with an off-centerline distance L', the centerline distance can be calculated as follows.

Since b = 0.33 × a, x_1 = Cos θ × L' – a, y_1 = Sin θ × L', where θ = the angle between off-centerline and centerline (θ < 90°) and 2*a* = the distance (x) between source well and projected downgradient centerline well.

Therefore,

$$\frac{(Cos\ \theta \times L' - a)^2}{a^2} + \frac{(Sin\ \theta \times L')^2}{(0.33 \times a)^2} = 1$$

$$(Cos\,\theta \times L' - a)^2 + 9.18 \times (Sin\,\theta \times L')^2 = a^2$$

$$(Cos\,\theta \times L')^2 + 9.18 \times (Sin\,\theta \times L')^2 = 2 \times a \times Cos\,\theta \times L'$$

$$X = 2a = \frac{Cos^2\ \theta \times L' + 9.18 \times Sin^2\ \theta \times L'}{Cos\,\theta} = L'(Cos\ \theta + 9.18 \times tg\ \theta \times Sin\ \theta)$$

(θ < 90°)

(4)

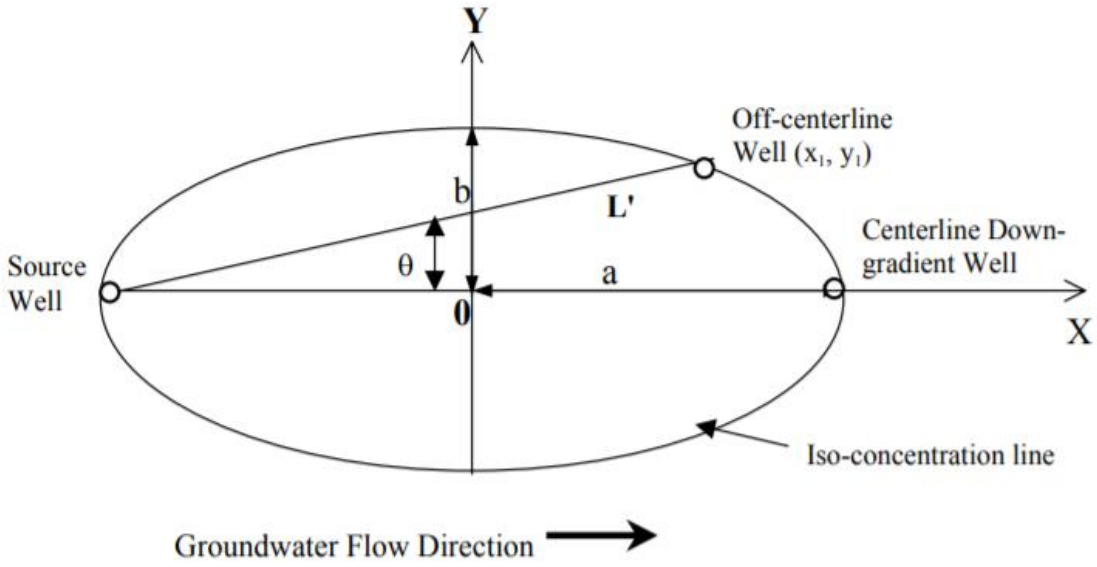

Figure 1: Plane view of regular plume geometry and groundwater monitoring system (Tong & Rong, 2001).

4. Uncertainties Regarding Initial Time (T0) of Release and Source Concentration (C0)

As in most contamination cases, the initial time of release (T_0) and the mass discharged are usually unknown. It is thus difficult to determine the exact source concentration (C_0). Since one of the assumptions in this analytical model is a continuous source, so ideally the temporal concentration profile at the source well should be constant over time. However, this is rarely the case. Due to a variety of factors such as changing groundwater levels, inherent variability of environmental quantification, instrumentation inexactness, sampling error, heterogeneous and varying subsurface environmental conditions, etc., the contaminant concentration at the source well will not show a constant over time. In order to select one contaminant concentration that best represents the source concentration over the period of time, an intuitive solution is to select an average (i.e., the mean) or median concentration.

The uncertainties associated with T_0 would affect the calibration of model-input parameters for predicting plume travel time. As the model parameter sensitivity analysis indicates in the later section, the analytical model is sensitive to changes made to T_0 (see Table I). Furthermore, changes made to T_0 as well as groundwater velocity (v) would shift horizontally the time (x-axis) versus normalized concentration (C/C_0) plot (y-axis) for the model predicted and field measured curves relative to each other. The collective impacts from T_0 and v would thus generate large uncertainties in the calibration of model-input parameters and the prediction of the plume travel time. This problem may be dealt with in two ways during the model calibration: (1) to obtain relatively accurate site-specific

information regarding the initial time of release (e.g., time of underground tank leaking, or history of contaminant usage), or (2) to use a more conservative value of groundwater seepage velocity (faster), estimated by the range of groundwater velocities typically associated with certain soil types, formations, and hydrology. Since relatively accurate site-specific information regarding the time of release is generally unavailable or unknown, the latter approach is more useful and thus is the one applied in this model.

5. Spreadsheet Analytical Model

The analytical model can be applied to estimate the travel time to a receptor for contaminants in groundwater. Figure 1 shows the model setting. Figure 2 presents a flowchart of the analytical model application. The downgradient well used to calibrate the model must be downgradient of the source well and has the maximum concentration less than source concentration C0. Step one, groundwater monitoring data provide temporal concentrations at one source and one downgradient well with known C(Ti), Ti, and X1 (i = 1,…,n) where C(Ti) = concentration at downgradient well at time Ti, X1 = downgradient well distance from the source well (Figure 1). As was discussed in Section 4, the source concentration C0 may be selected as the mean or median concentration of the temporal concentration profile. T0 is the initial time of contaminant release. T1 is the time for the first monitoring data point used to calibrate the model. The groundwater monitoring is conducted periodically. Since T0 is usually unknown in most cases, T1 or time of the first monitoring data point relative to T0 will also be unknown. However, time T2,…,Tn relative to T1 is known. Thus an educated judgement for T1 must be made first, and T2,…,Tn are directly related to T1. Step two, the ellipse trigonometry method presented in Section 3 is used to convert off-centerline distance to centerline distance for the downgradient well location. Step three, the field data are plotted (Ti vs. C(Ti)/C0, i = 1,…,n for the downgradient well). The field data must show a temporal pattern of a “sigmoidal” shape. Step four, the known C(Ti) and Ti, and selected source concentration C0 are used to choose values for model parameters αx, v, λ, and T1, by trial-and-error to fit the data points on the plot generated in step three. Step five, the calibrated values of the parameters αx, v, λ, and T1 are to be used to predict the travel time to a receptor at a downgradient distance X.

The Domenico Non-Steady State Analytical Model solution form has been programmed into a user-friendly spreadsheet in Microsoft Excel (version 7.0). The groundwater monitoring data from a specific site provide $C(T_i)$ and T_i (i = 1,…,n) which are plotted ($C(T_i)/C_0$ vs. T_i). By trial and error method, the model parameters α_x, *v*, λ, and T_1 are altered within the reasonable ranges until a best-fit curve to the temporal concentration distribution field data is visually identified (see example in Section 8). For example, changes made to T_1 and groundwater velocity (*v*) would shift horizontally the time (x-axis) versus normalized concentration (C/C_0) plot for the model predicted and field measured curves relative to each other; changes made to α_x would primarily affect the spreading of the curve; and changes made to λ would primarily affect the height of the curve. After a “best-fit” curve is established, the calibrated values of α_x, *v*, λ, and T_1 are used to predict

the travel time *t* at a downgradient distance X. An example of Excel spreadsheet is demonstrated in Tables V and VI, Section 8.

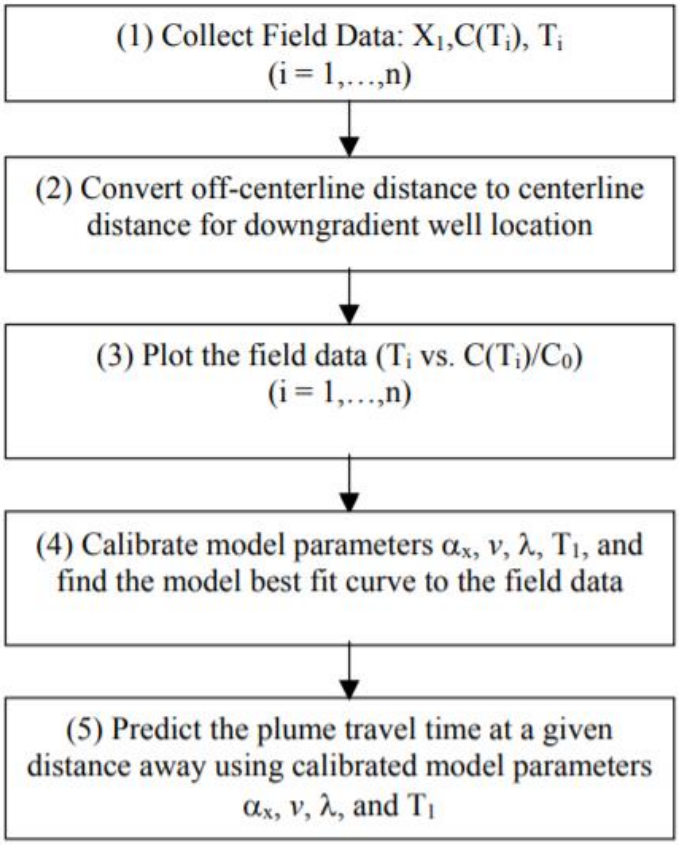

Figure 2: Domenico Non-Stready State Spreadsheet Analytical Model Flowchart

6. Sensitivity Analysis

A sensitivity analysis as presented in Table I is conducted for the Domenico Non-Steady State Analytical Model in the same way as presented in Rong et al. (1998). Model runs under the condition of varying input parameter values, one at a time, within reasonable ranges. Then model outputs from various input values are compared with the respective "baseline" cases. The sensitivity analysis results indicate that model output *t* (time for plume to reach 5 μg/L in downgradient receptor) is relatively sensitive to model input parameters α_x, *v*, and X. The concentration 5 μg/L is used here since it's the secondary maximum contaminant level for MTBE. Model output *t* is not as sensitive to model input parameters Y, Z, or λ. However, since model output $C(T_i)$ is sensitive to λ, λ is included along with α_x, *v*, and X to calibrate the model by changing the values of these parameters to fit in the field data.

Table I: Sensitivity Analysis Results for Domenico Analytical Model

Input Parameter	*Factor of Input Change from Baseline*	*Model Output t (years)*	*Factor of t Difference from Baseline*	*Relative Sensitivity S[1]*
α_x (ft)				0.09
1 (baseline)	---	3.1	---	
0.1	0.1	3.7	1.16	
4	4	2.6	0.84	
v (ft/day)				0.19
0.1 (baseline)	---	3.1	---	
0.25	2.5	1.3	0.42	
0.5	5.0	0.7	0.23	
X (ft)				1.23
150 (baseline)	---	3.1	---	
100	0.67	1.9	0.61	
300	2.0	7	2.26	
Y (ft)				0.03
20 (baseline)	---	3.1	---	
10	0.5	3.2	1.03	
30	1.5	3.1	1.0	
Z (ft)				0.036
5 (baseline)	---	3.1	---	
1	0.2	3.3	1.06	
10	2	3.1	1	
λ (1/day)				0.032
0.0005 (baseline)	---	3.1	---	
0.001	2	3.2	1.03	
0.002	4	3.4	1.10	

[1] Note Table 1: Relative sensitivity (S) is calculated using the following equation:

$$S = \left| \left(\frac{df}{f} \right) \left(\frac{x}{dx} \right) \right|$$

Where x and f are baseline input and model output values, dx and df are input and model output range, respectively.

7. Model Input Parameters

7.1. Dispersivity (α_x)

One of the primary parameters that control the fate and transport of contaminant is dispersivity of the aquifer. The Domenico non-steady state analytical model uses the longitudinal (α_x), transverse (α_y), and vertical (α_z) dispersivities to describe the mechanical spreading and mixing caused by dispersion. The spreading of a contaminant caused by molecular diffusion is assumed to be small relative to mechanical dispersion in groundwater movement and is ignored in the model. Various dispersivity values have been reported in studies. Most of existing studies traditionally use α_y and α_z as a fraction of α_x. For this relationship, we only calibrate α_x, which relates α_y and α_z. Table II is a summary of the three dimensional dispersivity values in literatures.

Table II: Dispersivity Values in Literature

Dispersivity Valves	Reference
α_x[2]= 0.1 X[3]	Gelhar and Axness (1981)
α_y[4]= 0.33 α_x	Gelhar and Axness (1981)
α_z [5]= 0.056 α_x	Gelhar and Axness (1981)
α_x= 0.1 X	Gelhar et al. (1992)
α_y= 0.1 α_x	Gelhar et al. (1992)
α_z= 0.025 α_x	Gelhar et al. (1992)
α_x= 14 – 323 (ft)	USEPA (1996)
α_y= 0.13 α_x	USEPA (1996)
α_z= 0.006 α_x	USEPA (1996)
α_x= 16.4 (ft)	Martin-Hayden and Robbins (1997)
α_y= 0.1 α_x	Martin-Hayden and Robbins (1997)
α_z= 0.002 α_x	Martin-Hayden and Robbins (1997)
α_x= 0.33 – 328 (ft)	AT123D (1998)
α_y= 0.1 α_x	AT123D (1998)
α_z= 0.1 α_x	AT123D (1998)

[2] α_x = the longitudinal dispersivity (ft)
[3] X = the distance to the downgradient well (ft)
[4] α_y = the transverse dispersivity (ft)
[5] α_z = the vertical dispersivity (ft)

7.2. Groundwater Velocity (*v*)

Groundwater velocity in the geologic material is controlled by hydraulic conductivity, hydraulic gradient in the vicinity of the study area, and effective porosity of the geologic material. Based on the Darcy's Law, the average groundwater velocity can be calculated using the following equation:

$$v = K \times \frac{dh}{dx} \times \frac{1}{n_e} \quad (5)$$

Where,

v - Groundwater velocity (ft/day)

K- Hydraulic conductivity (ft/day)

dh/dx - Hydraulic gradient (ft/ft)

n_e - Effective porosity (dimensionless)

The groundwater hydraulic gradient can be determined from field data. The hydraulic conductivity and effective porosity are also preferably obtained from site-specific testing. The hydraulic conductivity and effective porosity are mainly affected by the geologic material grain size. In cases where site-specific data are absent (i.e., pumping test or slug test), to estimate groundwater velocity, the lithologic boring logs can be reviewed to identify the predominant aquifer materials needed to estimate hydraulic conductivity and effective porosity to be consistent with value ranges from published references (see Tables III and IV).

Table III: Hydraulic Conductivity Range for Various Classes of Geologic Materials

Material	*Todd 1980 (ft/day)*	*Bower 1978 (ft/day)*	*Freeze & Cherry 1979 (ft/day)*	*Dawson & Istok 1991 (ft/day)*
Gravel	$5 \times 10^{2} - 1 \times 10^{3}$	$3 \times 10^{2} - 3 \times 10^{3}$	$3 \times 10^{2} - 3 \times 10^{5}$	$3 \times 10^{3} - 3 \times 10^{5}$
Coarse Sand	1×10^{2}	$7 \times 10^{1} - 3 \times 10^{2}$	$3 \times 10^{-2} - 3 \times 10^{3}$	$3 \times 10^{3} - 3 \times 10^{5}$
Medium Sand	4×10^{1}	$2 \times 10^{1} - 7 \times 10^{1}$	$3 \times 10^{-2} - 3 \times 10^{3}$	$3 - 3 \times 10^{3}$
Fine Sand	10^{1}	$3 - 2 \times 10^{1}$	$3 \times 10^{-2} - 3 \times 10^{3}$	$3 \times 10^{-2} - 3$
Silt and Clay	$10^{-3} - 3 \times 10^{-1}$	$3 \times 10^{-8} - 3 \times 10^{-2}$	$3 \times 10^{-7} - 3 \times 10^{-3}$	$3 \times 10^{-6} - 3 \times 10^{-1}$

Table IV: Total Porosities and Effective Porosities of Well-sorted, Unconsolidated Formations[6]

Material	Diameter (mm)	Total Porosity (%)	Effective Porosity (%)
Gravel - Coarse	64.0 – 16.0	28	23
Gravel - Medium	16.0 – 8.0	32	24
Gravel - Fine	8.0 – 2.0	34	25
Sand - Coarse	2.5 – 0.5	39	27
Sand - Medium	0.5 – 0.25	39	28
Sand -Fine	0.25 – 0.162	43	23
Silt	0.162 – 0.004	46	8
Clay	<0.004	42	3

8. Case Study

A case study example is included in this manual to demonstrate the modeling procedures for estimating MTBE plume travel time. The case study is a real case from an underground storage tank (UST) release site in the City of Los Angeles, California. Figure 3 depicts the site layout (USTs, dispenser islands, buildings, and well locations) and site groundwater contour map with gradient and approximate direction of groundwater flow. The modeling procedures are described in detail as the following steps:

Step 1:

Find the groundwater contour map for the site. Identify the area of the USTs, dispenser islands, piping, or any other likely source(s) of release that will be designated as the source area(s). Locate one source monitoring well (usually in the source area with the highest MTBE concentration) and one or two downgradient well(s) along or in close proximity to the plume centerline with sufficient data that support a temporal sigmoid curve of contaminant concentration profile.

As shown on Figure 3, the groundwater flow direction is towards the southwest with a gradient of 0.0077 ft/ft across the site. The USTs are the suspected source of release. Monitoring well MW-2 lies near the area of the former USTs and has the highest MTBE concentration and so will be designated as the source well. The MTBE concentration for MW-2 fluctuated somewhat over time, from 150,000 to 250,000 μg/L, with outliers of 27,000 and 970,000 μg/L, but generally cluster around the concentration level of 250,000 μg/L (Table V). Either mean or median MTBE value may be used. The source well concentration is selected as 250,000 μg/L. Monitoring well MW-6 is downgradient of the source well MW-2, and has 7 quarters of MTBE groundwater concentration data with a temporal MTBE concentration profile that resembles a sigmoidal curve (Table V). The

[6] SOURCE: Roscoe Moss Company, 1990

boring logs for these monitoring wells indicate that soil materials are composed predominantly of silty sand.

Step 2:

Measure the distance between the source area and the downgradient well(s). Measure the off-centerline angle (if any). Use the ellipse trigonometry method presented in this manual to estimate centerline distance. Use equation (4): given L' = 92 ft, θ = 10°,

$$X = 2a = \frac{Cos^2\ \theta \times L' + 9.18 \times Sin^2\ \theta \times L'}{Cos\,\theta} = L'(Cos\ \theta + 9.18 \times tg\ \theta \times Sin\ \theta)$$

= 116 ft

Tables V and VI are the case field data entry and model parameter entry, respectively.

Table V: Field Data Entry

Case Name: ABC Oil Company **Address:** XYZ Rd. Los Angeles, CA **Case ID Number:** 123456789			
Source Well No.	*Concentration (μg/L)*	Date	Selected Source Concentration C_0 (μg/L)
MW-2	250,000	1/19/95	
	240,000	4/17/95	
	250,000	8/21/95	
	150,000	11/29/95	250,000
	27,000	5/2/96	
	270,000	7/22/96	
	240,000	11/15/96	
	970,000	1/27/97	

Down-gradient well MW-6 at Time T_i	Concentration $C(T_i)$ (μg/L)	Time (day)	C/C_0
T_1	570	980	0.0023
T_2	16,000	1,070	0.064
T_3	25,000	1,190	0.1
T_4	65,000	1,280	0.26
T_5	59,000	1,631	0.236
T_6	59,000	1,783	0.236
T_7	58,000	2,134	0.232

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The actual field monitoring data usually provide the time (month, day, year) and the corresponding MTBE groundwater concentration. Hence, the real time between the monitoring events is known, and can be linked together by adding the difference in time elapsed between monitoring events from the previous event. For example, three months or one quarter had elapsed between T_1 and T_2, and then $T_2 = T_1 + 90$ (days), and so on. However, field-monitoring data would not typically provide information on the initial time of release (T_0). Consequently, T_1 from the above data entry is unknown and an educated judgement for T_1 must be made first. Here, we choose $T_1 = 800$ days to start with. T_1 will be adjusted during the model calibration.

Table VI: Spreadsheet Model Parameter Entry

Parameter	Notation	Value	Unit
X axis dispersivity	α_x	0.6	ft
Y axis dispersivity	α_y	0.198	ft
Z axis dispersivity	α_z	0.0336	ft
Groundwater velocity	*v*	0.1	ft/day
Source dimension Y	Y	20	ft
Source dimension Z	*Z*	5	ft
First order attenuation rate	λ	0.00062	1/day
Centerline distance from source well to well 1	X_1	116	ft
Centerline distance from source well to well 2	X_2	N/A	ft
Centerline distance from source well to receptor	X_3	1,000	ft

The choice of parameter values in Table VI is dependent upon the "best-fit" with field data plot by trial-and-error. For the best fitting in the plot, experience is needed. Parameters α_x, *v*, and λ as in boldface are those "fitting" parameters. The general guidance on how the model parameters are calibrated is provided in Section 5 of this manual (page 7). Changes made to groundwater velocity *v* and T_1 would shift horizontally the model predicted and the field measured peak, respectively, in the plot of concentration versus time. As was discussed in Section 4 on uncertainties, the approach of using a more conservative value of groundwater seepage velocity that is estimated by the range of groundwater velocities typically associated with certain soil types, formations, and hydrology will be used in this model to estimate the groundwater seepage velocity. The estimated *v* will then be used to readjust T_1 until the model best-fit curve is established relative to the measured field data.

Changes made to α_x and λ affect primarily the spreading and height, respectively, of the model prediction curve. Initial values for α_x and λ are entered first in order to "match" the spreading and height of the model prediction curve to the observed field data. In any case, groundwater seepage velocity *v* should be estimated first, with the other parameters (i.e., T_1, α_x, and λ) to follow. Repeat this sequence until the best-fit model prediction curve to the field data is obtained. The range of values for the calibration of these parameters is derived from literature sources and appears in the Microsoft Excel Spreadsheet Cell H2-H8 next to the model parameters in the "Domenico" Model Spreadsheet File.

Step 3:

A. Open the Microsoft Excel file "Domenico Model Manual."

B. Use "distance" sheet to calculate the centerline distance from source well to downgradient well.

C. Use "Domenico Non-Steady State" sheet to find the best-fit curve on the plot of time vs. MTBE concentration C/C_0:

- Enter case information: case name, address and case ID number.

- Enter case data: X_1 = 116 ft, $C(T_1)$ = 570 μg/L, T_1 = 980 days, $C(T_2)$ = 16,000 μg/L, T_2 = 1,070 days, $C(T_3)$ = 25,000 μg/L, T_3 = 1,190 days, and so on (see Table V). Enter an initial temporary value for T_1. T_1 will be modified to fit the field data during the model calibration process. This can be done by entering the formula into the Excel worksheet. In this case, click on cell E23 to enter the formula for T_2. A formula of "= E22 + 90" should be displayed in the formula bar. Change the default value 90 to whatever the difference in time in days between the two monitoring events. Repeat the same procedure for all subsequent monitoring events, replacing the part of the formula of "= E22" with E23, E24, E25, and so on to correspond to the previous monitoring event. Enter the date of the first and last monitoring event, and record (roughly) the time differences (days) between the last monitoring event and present, in Cell D33. This will allow for the calculation of time remaining for the plume to reach the receptor.

- Manipulate model parameters α_x, *v*, λ, and T_1 to find best-fit curve. The general guidance on how these parameters affect the curve shape is provided in Section 5 of this manual (page 7). Table VI shows the spreadsheet model data entry and Figure 1 in Microsoft Excel File shows the plot of field data versus model fitting curve. The model parameters are in Cells colored in red in the Microsoft Excel File and in Table V and VI. The field data are in Cells colored in pink. Based on references in Table II and the approximate ratio of the contaminant plume

width to its length, the following value ranges are used in this case study: α_x = [0.1 ft, 10 ft], α_y = [0.33α_x, 0.65α_x] and α_z = 0.056α_x. For instance, from the contaminant (i.e., TPHg, benzene, or MTBE) iso-concentration plots, the width of the plume for this particular case is approximately one-third of its length. Based on this finding the value of 0.33*C3 is entered into Cell C4. Cells G1-G8 and H1-H8 contains the individual soil types and the range of groundwater velocities typically associated with them. Based on the soil boring logs, the predominant soil type is silty sand. Apply conservative groundwater velocity value associated with this soil type. In this case, the maximum groundwater velocity should be 0.1 ft/day, corresponding to the conservative groundwater velocity value associated with this soil type.

- The first step in the calibration process should consist of narrowing down the groundwater velocity *v*. Apply initial values of *v* = 0.1 ft/day, T_1 = 800 ft/day, α_x = 2 ft, and λ = 0.0005/day. The groundwater velocity *v* can be adjusted downwards later in the process of obtaining the best-fit model curve to the observed field data. As the time versus concentration plot for the model prediction curve (Figure 1 in Excel Spreadsheet File) is shifted to the right of the field data curve, T_1 has to be readjusted (increased). A readjusted value of 980 is entered. Compare to the model prediction curve, the field data curve has significantly less spreading. Readjust α_x (decreasing α_x has the effect of decreasing the spreading of the curve). A trial value of 1 ft is entered. Compare the two curves. The field data curve still has greater spreading. Enter the readjusted value of 0.6 ft for α_x. The height of the model prediction curve is now much higher than the field data curve. Readjust λ (increase). An initial value of 0.00062/day is entered. Repeat the same sequence of parameter calibration as above (i.e., readjust *v*, T_1, α_x, and lastly λ) until the best-fit model prediction curve to the observed field data curve is established. With everything else being equal, changing the groundwater velocity has the effect of "allowing more or less time for dispersion" and thus indirectly affects the spreading of the time versus concentration curve.

- Record plume parameters after the "best fit" curve is established:
- α_x = 0.60 ft; *v* = 0.1 ft/day; λ = 0.00062 1/day; T_1 = 980 days

D. Change distance X value in Cell C12 of this spreadsheet model (X_3 in Table IV) to correspond to the centerline distance to the receptor (e.g., a drinking water well). In this case, a hypothetical downgradient distance of 1,000 ft is entered.

E. Model prediction and solutions are presented in Cell B14-B19, and in Cell C14-C18. Record the times at which the MTBE plume front first appears (i.e., when MTBE concentration is greater 5 μg/L). The time is shown in Cell B16 (days) and

C16 (years). The maximum MTBE concentration predicted to appear in the drinking water well and the associated time at which it appears is shown in Cell B19 (μg/L) and C17 (years), respectively. Cell C18 shows the time (years) remaining for the plume to reach 5 μg/L in the drinking water well. The Microsoft Excel worksheet shows that given the monitoring data at MW-6, it would take approximately 25.8 and 37.0 years for the MTBE plume to travel to and reach maximum concentration, respectively, in the downgradient drinking water well 1,000 feet away. An approximate estimate for this time can also be obtained through visualizing Figure 4 in Excel file.

F. Save the file.

9. Troubleshooting for the Spreadsheet Analytical Model

Trouble 1: By changing the values of either α_x, ν, or λ, the model calculation and curve on the chart do not respond.

Solution: Go to "Add-In" option in Excel under the "Tools" menu bar and select the "Analysis Toolpak."

Trouble 2: Some field data do not show on the chart.

Solution: Change the Y-axis range by double clicking the Y-axis, and add one or two more decimals for minimum range in Scale sheet.

Trouble 3: The predicted plume travel times do not show on the chart.

Solution: Change the X-axis range by double clicking the X-axis, and add one or more digits for maximum range in Scale sheet.

10. Acknowledgments

The authors would like to thank David Bacharowski of the Los Angeles Regional Water Quality Control Board for his constructive criticism and support in the development of this work.

11. References

AT123D, Reference Guide and User's Guide (Version 3.0), (1998). General Sciences Corporation, 4600 Powder Mill Road, Suite 400, Beltsville, MD 20705.

Manual Domenico Non-Steady State Spreadsheet Analytical Model Manual

Bouwer H (1978). *Groundwater Hydrology*. McGraw-Hill Book, New York, 448 pp.

Dawson KJ and Istok JD (1991). *Aquifer Testing – Design and Analysis of Pumping and Slug Tests.* Lewis Publishers. Chelsea. 344 pp.

Domenico PA and Robbins GA (1985). A new method of contaminant plume analysis. *Ground Water* **23(4):** 476-485.
Domenico PA (1987). An analytical model for multidimensional transport of decaying contaminant species. *Journal of Hydrology* **91:** 49-58.

Environmental Resolutions, Inc. (2001). Quarterly Groundwater Monitoring Report – Fourth Quarter 2000.

Freeze RA and Cherry JA (1979). *Groundwater*. Prentice-Hall, Inc., Englewood Cliffs, NJ 07632. 604 pp.

Fried JJ (1975). *Developments in Water Science*. *Groundwater Pollution: Theory, Methodology, Modeling and Practical Rules*. American Elsevier, New York, 132 pp.

Gelhar LW and Axness CL (1981). *Stochastic analysis of macrodispersion in three-dimensionally heterogeneous aquifers.* Report H-8. Hydraulic Research Program. New Mexico Institute of Mining and Technology, Socorro, NM 87801.

Gelhar LW, Welty C, and Rehfeldt KR (1992). A critical review of data on field-scale dispersion in aquifers. *Water Resources Research* **28(7):**1955-1974.

Martin-Hayden JM and Robbins GA (1997). Plume distortion and apparent attenuation due to concentration averaging in monitoring wells. *Ground Water* **35(2):**339-346.

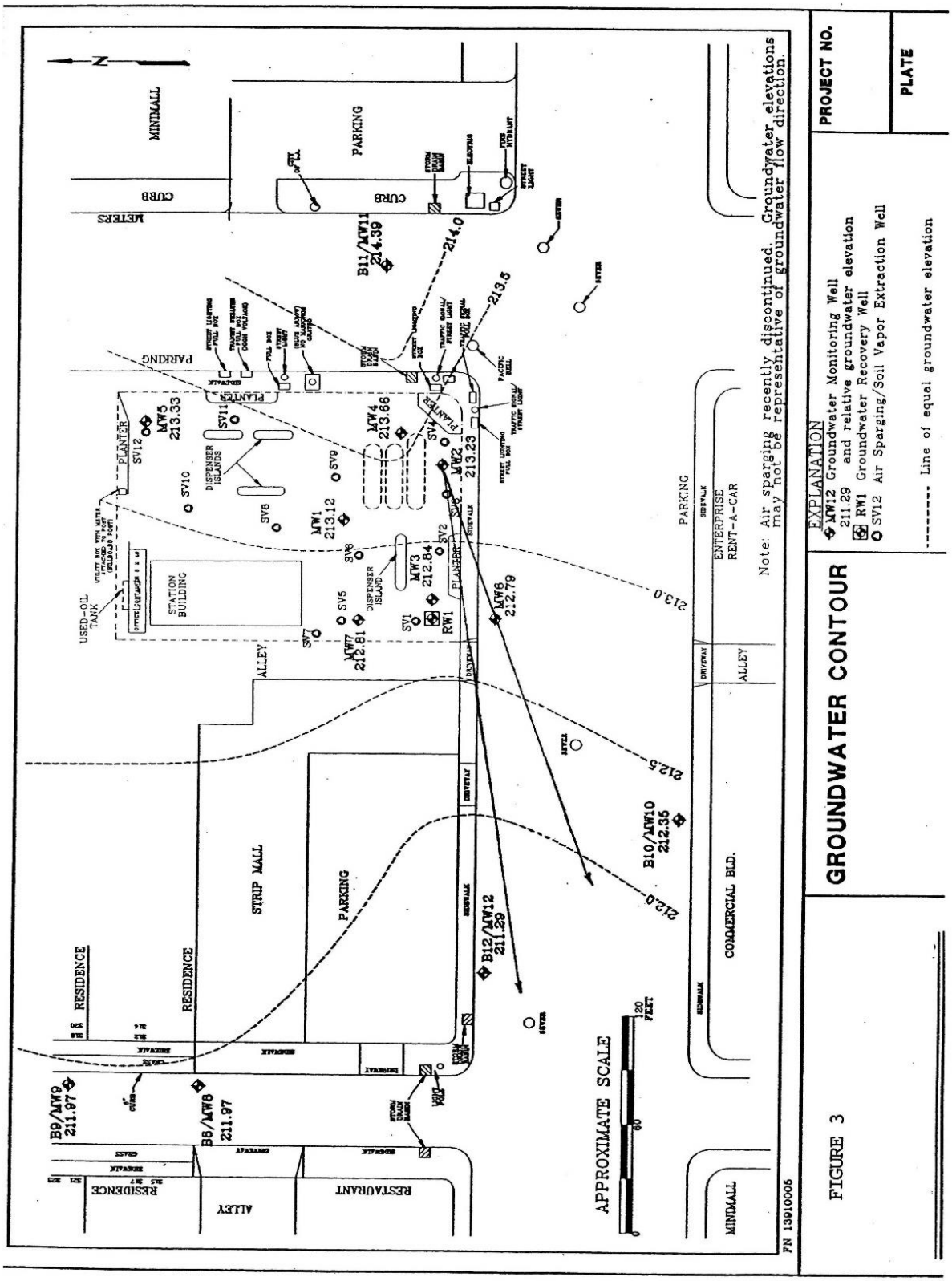
Rong Y, Wang RF, and Chou R (1998). Monte Carlo simulation for a groundwater mixing model in soil remediation of tetrachloroethylene. *Journal of Soil Contamination* **7(1):**87-102.

Roscoe Moss Company (1990). *Handbook of Ground Water Development*. John Wiley and Sons, New York. 493 pp.

Todd DK (1980). *Ground Water Hydrology*. John Wiley and Sons, New York.

Tong W and Rong Y (2001). Estimation of Methyl *tert*-Butyl Ether Plume Length Using the Domenico Analytical Model. *Journal of Environmental Forensics* **2(3),** Article No. enfo. 2001.0025.

United States Environmental Protection Agency (USEPA), (1996). Soil screening guidance: technical background document E-25pp EPA/540/R-95/128, PB96-963502


N
MINIMALL
PARKING
CURB
METERS
B11/MW11
214.39
214.0
213.5
PARKING
PLANTER
SV12
MW5
213.33
SV11
SV10
DISPENSER ISLAND
SV9
SV8
MW4
213.66
MW2
213.23
MW1
213.12
SV6
SV3
SV2
MW3
212.84
SV5
DISPENSER ISLAND
SV1
RW1
MW6
212.79
SV7
MW7
212.81
USED-OIL TANK
STATION BUILDING
ALLEY
213.0
212.5
212.0
PARKING
ENTERPRISE RENT-A-CAR
DRIVEWAY
ALLEY
Note: Air sparging recently discontinued. Groundwater elevations may not be representative of groundwater flow direction.
EXPLANATION
MW12 Groundwater Monitoring Well
211.29 and relative groundwater elevation
RW1 Groundwater Recovery Well
SV12 Air Sparging/Soil Vapor Extraction Well
Line of equal groundwater elevation
PROJECT NO.
PLATE
GROUNDWATER CONTOUR
B10/MW10
212.35
B12/MW12
211.29
STRIP MALL
PARKING
COMMERCIAL BLD.
RESIDENCE
RESIDENCE
B9/MW9
211.97
B8/MW8
211.97
RESIDENCE
ALLEY
RESTAURANT
APPROXIMATE SCALE
120
FEET
60
MINIMALL
FN 13910006
FIGURE 3