FINAL REPORT: TASK 2

LITERATURE REVIEW OF *CHEMICALS OF INTEREST* RELATED TO THE REUSE OF PRODUCED WATERS FOR AGRICULTURAL IRRIGATION OF EDIBLE CROPS

Prepared for:

The California Central Valley Region Regional Water Quality Control Board

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ADBAC - Alkyldimethylbenzylammonium chloride

AGR - Agricultural

AMES - Ames II mutagenicity assay

atm - atmosphere

ATP - Adenosine triphosphate

ATSDR - Agency for Toxic Substance Disease Registry

BIW - Blended Irrigation Water

BLIA - BioLuminescence Inhibition Assay

BMD - Benchmark Dose

Bq - Becquerel

BTEX - Benzene, Toluene, Ethyltoluene, Xylene

CA - California

CASRN - Chemical Abstract Service Registration Number

CCR - California Code of Regulations

CDPH - California Department of Public Health

CDPR - California Department of Pesticide Regulation

CEDEN - California Environmental Data Exchange Network

CFR - Code of Federal Regulations

cm - Centimeters

CVRWQCB - Central Valley Regional Water Quality Control Board

Da - Daltons

DARTIC - Developmental and Reproductive Toxicant Identification Committee

DOGGR - Division of Oil, Gas, and Geothermal Resources

dpm - Decays per minute

DRI - Dietary Reference Intake

dS - DeciSiemans

EDTA - Ethylenediaminetetraacetate

EOR - Enhanced Oil Recovery

FDA - Food and Drug Administration

GAMA - Groundwater Ambient Monitoring and Assessment Program

GSI - GSI Environmental

HSDB - Hazardous Substances Data Bank

IARC - International Agency for Research on Cancer

IND - Industrial service

IRIS - Integrated Risk Information System

KBD - Kashin-beck disease

kg - Kilogram

Koc - Organic Carbon Partitioning Coefficient

Kow - Octanol-Water Partitioning Coefficient

L - Liter

LC/MS - Liquid Chromatography Mass Spectrometry

LD50 - Lethal Dose for 50% of Population

LOAEL - Lowest Observed Adverse Effect Level

LOEL - Lowest Observed Effect Level

LS/UV - Liquid Chromatography with Ultraviolet Detection

m - Meters

m3 - Cubic meters

MADL - Maximum Allowable Dose Level

mBq - MilliBecquerel

MCL - Maximum Contaminant Level

mg - Milligram

mmol - Millimolar

MN - Molecular Number

MOU - Memorandum of Understanding

MRL - Minimal Risk Level

MTBE - Methyl tert-butyl ether

MUN - Municipal and domestic water

ND - Non-detect

ng - Nanograms

NIH - National Institutes of Health

nL - Nanoliters

NOAEL - No Observed Adverse Effect Level

NOEL - No Observed Effect Level

NORM - Naturally Occurring Radioactive Material

NPDES - National Pollutant Discharge Elimination System

NSF - National Science Foundation

NTP - National Toxicology Program

OECD - Organisation for Economic Co-operation and Development

OEHHA - California Office of Environmental Health Hazards Assessment

PAH - Polyaromatic Hydrocarbon

PAM - Polyacrylamide copolymer

pCi – Picocurie

PEF - Potency Equivalency Factor

PMX - Particulate Matter with an average aerodynamic diameter less than "x" microns

PPAR-γ - Peroxisome proliferator-activated receptor gamma

ppb - Parts per billion

ppm - Parts per million

PPRTV - Provisional Peer Reviewed Toxicity Value

PRO - Industrial process

PTTIL - Provisional total tolerable intake level

QSAR - Quantitative Structure-Activity Relationship

REC-1 - Water contact recreation

REL - Reference Exposure Level

RfD - Reference Dose

RFG - Reactive Functional Groups

RO - Reverse Osmosis

SDS - Safety Data Sheet

SN1 - Unimolecular nucleophilic substitution reaction

SWAMP - Surface Water Ambient Monitoring Program

TDS - Total Dissolved Solids

TMAB - Tetramethylammonium bromide

TOC - Total Organic Carbon

Tox21 - Toxicology in the 21st Century

TOXNET - Toxicology Data Network

TPW - Treated Produced Water

TSCA - Toxic Substances Control Act

US EPA - United States Environmental Protection Agency

USGS - United States Geologic Survey

WD - Water District

WDR - Water Discharge Requirement

WET - Whole Effluent Toxicity

WQO - Water Quality Objective

YES - Yeast Estrogen Screen

µg - Microgram

µM - Micromol

µmhos - Micromhos

EXECUTIVE SUMMARY

Introduction and Methods

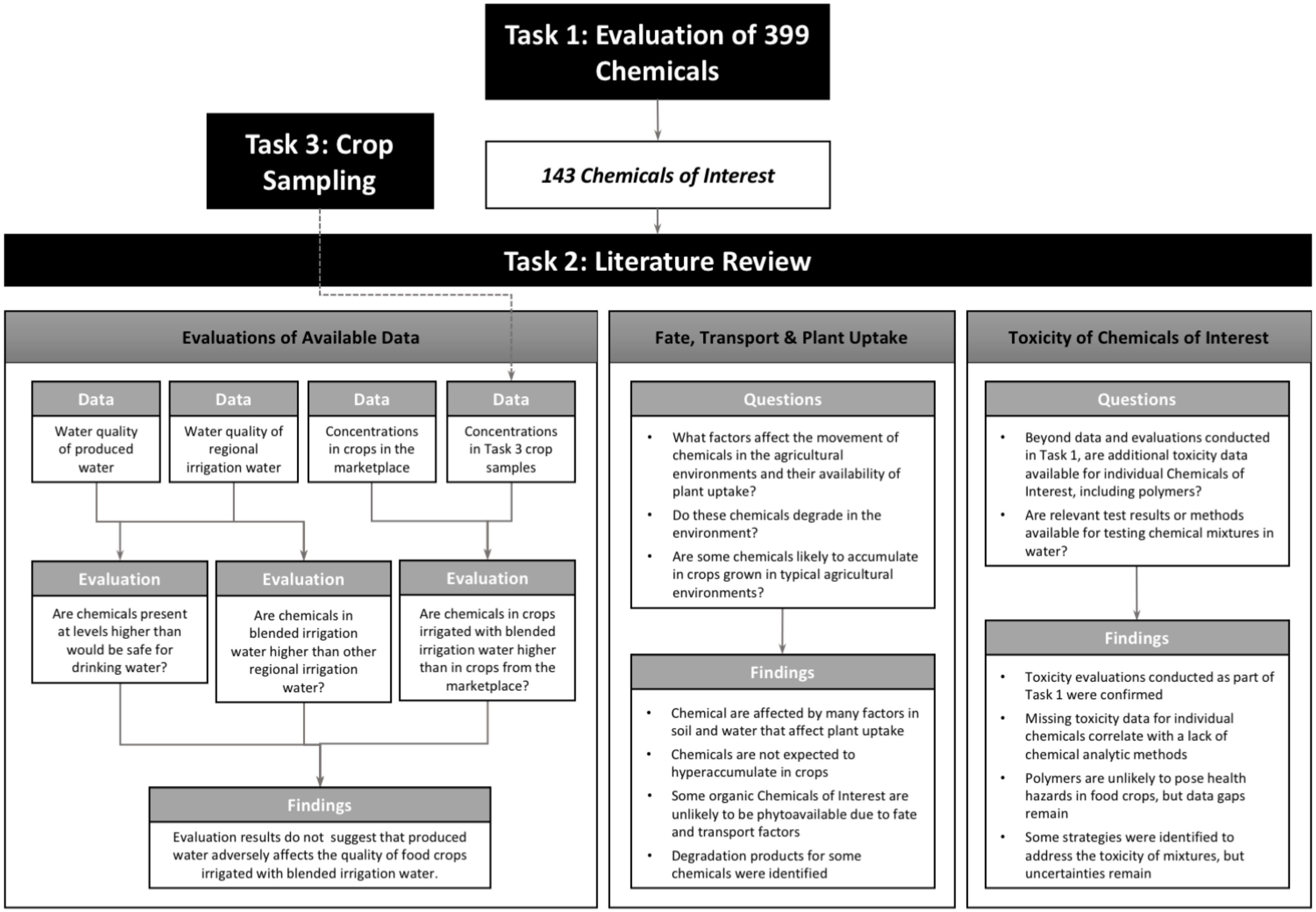
Task 2 was one of three tasks comprising the Food Safety Project which focused on the reuse of produced water for irrigation. The overarching goal of the project was to investigate and develop additional knowledge to address public concerns regarding the safety of irrigating food crops with treated produced water. In Task 1, 399 chemicals were identified as having the potential to be present in produced water from the San Joaquin Valley, and 143 of these were identified as “Chemicals of Interest” to be further evaluated in Task 2. The criteria used to select the Chemicals of Interest were chronic oral toxicity and expected persistence in irrigation water. The goal of the selection process was to assure that the data collection and evaluations performed under Task 2 were focused on chemicals with the greatest likelihood of posing a health risk via irrigation of food crops. Task 3 was a study in which chemicals potentially originating from produced water were measured in crops irrigated with produced water and crops irrigated with conventional irrigation water.

Task 2 included a literature review directed toward developing a better understanding of the occurrence of chemicals in produced water and the potential for those chemicals to accumulate in food crops when irrigated with produced water. The review also helped to identify uncertainties and knowledge gaps in the safety evaluation. Figure ES-1 illustrates the relationship between work completed for this report and work completed under Tasks 1 and 3.

Information developed under Task 2 was also used to evaluate the crop sampling data collected for Task 3, which included a comparison of chemical concentrations detected in produced water to levels that would be safe for drinking water (e.g., drinking water standards and risk-based concentration limits). In addition, Task 2 compared levels of chemicals found in produced water to levels of the same chemicals measured in other sources of water suitable for irrigation, which included surface water and groundwater sources.

Task 2 included a review of the general factors, as well as chemical specific factors, affecting the fate and transport of the chemicals in an agricultural setting, plant uptake, and migration of chemicals within a plant. Additional sources of toxicity data, alternative approaches to developing chronic toxicity values beyond those included in Task 1, and the application of whole effluent testing were also discussed as part of Task 2.

The text below summarizes the key findings of each of the sections of this report.



Evaluations of Available Data

Evaluation: Are chemicals present at levels higher than would be safe for drinking water?

Evaluation: Are chemicals in blended irrigation water higher than other regional irrigation water?

Evaluation: Are chemicals in crops irrigated with blended irrigation water higher than in crops from the marketplace?

Findings: Evaluation results do not suggest that produced water adversely affects the quality of food crops irrigated with blended irrigation water.

Fate, Transport & Plant Uptake

Questions

- What factors affect the movement of chemicals in the agricultural environments and their availability of plant uptake?
- Do these chemicals degrade in the environment?
- Are some chemicals likely to accumulate in crops grown in typical agricultural environments?

Findings

- Chemical are affected by many factors in soil and water that affect plant uptake
- Chemicals are not expected to hyperaccumulate in crops
- Some organic Chemicals of Interest are unlikely to be phytoavailable due to fate and transport factors
- Degradation products for some chemicals were identified

Toxicity of Chemicals of Interest

Questions

- Beyond data and evaluations conducted in Task 1, are additional toxicity data available for individual Chemicals of Interest, including polymers?
- Are relevant test results or methods available for testing chemical mixtures in water?

Findings

- Toxicity evaluations conducted as part of Task 1 were confirmed
- Missing toxicity data for individual chemicals correlate with a lack of chemical analytic methods
- Polymers are unlikely to pose health hazards in food crops, but data gaps remain
- Some strategies were identified to address the toxicity of mixtures, but uncertainties remain

Figure ES-1: Conceptual approach of the Task 2 literature review

Review of Produced Water Reuse for Agricultural Irrigation

When crude oil or natural gas is pumped from the ground, it is usually accompanied by large volumes of water that must be separated from the petroleum product and then managed. Common practices for managing the water have included pumping the water back into the ground, discharging it to evaporation/percolation ponds, and treatment/reuse. Varying levels of treatment can be applied to produced water, which can then be reused for industrial or agricultural purposes. Largely due to the cost of treatment and transportation, only a small percentage of produced water is reused for purposes other than petroleum production. Agricultural irrigation is one of several water reuse applications. While there are many examples in the United States and around the world of the reuse of treated produced water for agricultural irrigation, only a small fraction of produced water has salinity levels low enough for use as irrigation water.

Produced water from Kern County (areas east and north of Bakersfield) has sufficiently low salinity that it is suitable for reuse in agriculture and has been used over the last 30 years to irrigate food crops. Depending on the individual oil production facility, this produced water is treated by at least two of three processes, including: gravity separation, dissolved air flotation, and/or filtration, prior to being blended with surface water or groundwater. Reuse of the treated produced water for irrigation is regulated by the Central Valley Regional Water Quality Control Board through Waste Discharge Requirements that specify the volume of produced water each facility can discharge, the crops that may be irrigated with treated produced water, and water quality criteria for water reused for irrigation. In addition, Waste Discharge Requirements prohibit the reuse of produced water from wells containing “well stimulation treatment,” as defined by California Code of Regulations, title 14, section 1761. In other words, produced water from wells that undergo hydraulic fracturing are not permitted to be reused for irrigation.

Many case studies of the reuse of produced water for agricultural irrigation have been published, and many of these involve complex water treatment process. While successful examples of agricultural reuse of produced water have been identified in the literature, there are also reports of cases where the technical challenges of removing salinity, boron, metals, hydrocarbons, or other chemicals could not be overcome; and the reuse program was discontinued. Research and practical experience have shown that the treated produced waters with lower organic and total dissolved solids content are best suited to long-term agricultural irrigation and that mixing treated produced water with other suitable sources of irrigation water can expand the total volume of water acceptable for irrigation.

Chemicals of Interest

The Task 1 report identified 399 chemicals that could be present in produced water. Included in the list of 399 chemicals are: (1) chemical additives reported by oil producers who provide produced water used for agricultural irrigation in the San Joaquin Valley; (2) naturally occurring chemicals resulting from the contact of resident water with oil and rock in the reservoir; and (3) other chemicals that have previously been detected in raw produced water that are not directly related to additives or naturally occurring compounds.

The inorganic chemicals largely come from the geological formation surrounding the oil reservoir, but some can come from chemicals used in the production of oil. Similarly, organic chemicals in produced water largely come from contact of the water with oil; but others can come from chemicals used in the production of oil or from contact with materials used during production.

In Task 1, 143 of the 399 identified chemicals were selected for further evaluation in Task 2. The selection was based primarily on consideration of chronic oral toxicity and expected persistence in irrigation water. The emphasis on chronic oral toxicity was intended to maximize the likelihood that the most toxic chemicals were not overlooked. Limiting the Task 2 assessment to the 143 “Chemicals of Interest” also served to focus the data collection and evaluations to chemicals that current knowledge suggests have the greatest likelihood of posing a health risk via irrigation of food crops.

It is recognized that the Task 2 evaluation is based on a subset of the 399 chemicals identified as potentially present in produced water. This approach includes uncertainties associated with the fact that exposure and toxicity information is not available for all 399 chemicals and recognizes that all 399 chemicals were not necessarily present in the produced water used for irrigation of the crops studied under Task 3. Of necessity, Task 2 is biased toward chemicals that historically have been studied and evaluated. Reliance on such “indicator chemicals” as the basis for environmental risk assessments is a typical, if not the most common, way in which health risks of mixtures of chemicals in the environment are evaluated. Occasional updated reviews of the published literature for new information on the toxicity and fate and transport properties of these chemicals would be a way to address and reduce the uncertainty associated with the reliance on a subset of chemicals. Similarly, updated reviews of ongoing water quality monitoring data from the produced water may help confirm the presence or absence of chemicals identified as potentially present in produced water reused locally for irrigation.

Chemicals of Interest in Produced Water and Other Environmental Media

The Central Valley Regional Water Quality Control Board (CVRWQCB) regulates the use of produced water as part of its responsibility to enable existing and future beneficial uses of surface water and ground water. One tool used to regulate the reuse of treated produced water is the requirement for water quality testing and establishing maximum effluent limitations for produced water, which are used to ensure that chemicals do not exceed background levels or reach a level that causes a nuisance or otherwise adversely affects the beneficial reuse of groundwater.

Most Water Quality Objectives are associated with drinking water standards, and a few chemicals are regulated with the specific goal of protecting agricultural uses of the water. Many of the Chemicals of Interest, however, do not have associated Water Quality Objectives. As a point of reference for the chemicals without Water Quality Objective concentrations, we developed risk-based concentrations, which were concentrations that would not pose a health risk if the water were to be used as drinking water.

To help evaluate the potential for health risks associated with the reuse of blended produced water (i.e., treated produced water blended with other suitable irrigation water) for irrigating food crops and the potential for Chemicals of Interest to accumulate in food crops irrigated with blended produced water, we performed several water quality evaluations and compared the observed concentration of the Chemicals of Interest in Task 3 crop samples to those in similar crops found in the marketplace. These evaluations were designed to address the question of whether Chemicals of Interest accumulated in crops to higher levels as a result of the use of produced water, given that water quality data for conventional irrigation water used to irrigate Task 3 “control” samples was not collected. Summaries of the concentrations of the Chemicals of Interest in the various environmental media, including blended produced water, surface water, groundwater, marketplace food crops, and Task 3 crop samples, are reported in Table 10.

Water quality evaluations consisted of comparing chemical concentration in treated produced water and blended produced water to drinking water standards and other risk-based levels, as well as comparisons to chemical concentrations observed in surface and groundwater that would be suitable for agricultural irrigation. In evaluating the potential for the reuse of blended produced water to cause chemical concentrations to accumulate in crops, we attempted to determine if findings from the water quality analyses were correlated with several comparisons made using results from the Task 3 sampling. We attempted to determine if differences between treated and control crops were correlated with the following: exceedances of drinking water standards or other toxicity risk-based levels in blended produced water; differences between blended produced water and other sources of surface water and groundwater suitable for irrigation, in Kern County or nationally; and differences between chemical concentrations in Task 3 samples and food crops available in the marketplace.

Overall, the concentration of most Chemicals of Interest in treated produced water and blended produced water were consistently lower than drinking water standards or risk-based concentrations that would be suitable for drinking water. One exception was arsenic, which was regularly detected above its drinking water standard. When comparing blended produced water to surface and groundwater sources suitable for agricultural irrigation, however, the concentrations all monitored chemicals were consistent with the range of concentrations observed in other sources of water, including the concentrations of arsenic. Another possible exception was phenanthrene, which was detected in 18% of blended produced water samples with a detected range of 0.029 – 0.29 ppb. That range of concentrations was higher than the detected levels seen in raw surface water samples across the US. Phenanthrene, however, is not expected to accumulate in plants as a result of irrigating crops with such levels because it would be tightly bound to organic matter in soil. Copper was also higher than local sources of water suitable for irrigation, but it was below the drinking water standard level. Overall, there is little evidence that the Chemicals of Interest in blended produced water are higher than other suitable sources of local irrigation water. For those few chemicals where differences have been observed, we do not observe higher accumulation of these chemicals in crops irrigated with blended produced water.

For most chemicals, blending the treated produced water with other sources of water reduced the detected concentrations. In a few cases, concentration of the Chemicals of Interest increased with blending. Changes in the frequency of detection with blending were not pronounced, and no systematic pattern was observed. Some chemicals had higher detection frequencies in treated produced water than in blended produced water, and some chemicals had the reverse.

In general, the concentrations of the Chemicals of Interest in Task 3 samples were similar between treated and control groups and/or were similar to other food crops found in the marketplace. Crop-specific results, however, were not available in the literature for antimony and chromium; but the detected levels of these two elements were the same in crops irrigated with blended produced water and those irrigated with conventional water (see Task 3 Report). Accordingly, the comparison of chemical concentrations measured in the crops irrigated with blended produced water to concentrations reported in the literature does not indicate higher accumulation of chemicals in crops irrigated with blended produced water.

An additional approach to evaluating the accumulation of chemicals in crops irrigated with blended produced water was to ask if any chemicals detected in the crops sampled in Task 3 were unique to blended produced water. The Chemicals of Interest detected in crops irrigated with blended irrigation are not unique to Task 3 samples and have also been found in crops grown in other geographic areas. All the Chemicals of Interest detected in the Task 3 crop samples have also been found in samples of soil, air, and suitable irrigation water, other than treated produced water. Thus, the chemicals detected in crops irrigated with blended produced water could have come from other sources in addition to irrigation water.

As many of the Chemicals of Interest were not analyzed in previous water quality and food crop sampling, a review of the available analytic methods was conducted to identify methods that could be applied to future water quality monitoring. Most of the Chemicals of Interest that have approved analytic methods are currently being reported in the required water quality sampling of produced water. This literature review identified analytic methods for the group of ethoxylated alkylphenol surfactants used in oil production, four of which are Chemicals of Interest. This group of surfactants is not part of any regular monitoring program for produced water or blended produced water (or conventional irrigation water). After accounting for the chemicals currently monitored and the previously discussed surfactants, there are still 86 chemicals that do not have analytical methods; toxicity information is also not available for these 86 chemicals.

Fate, Transport, and Plant Uptake: Inorganic Chemical

The behavior of metallic and other inorganic chemicals in soil, is complex and is governed by a number of factors that can affect mobility, availability for uptake by plants, and distribution within a plant. While the state of the science is not sufficient to support the development of models to predict concentrations of metals in the edible portions of plants based on levels in soil or irrigation water, the literature on the uptake of metals from soil and their distribution within a plant does point to some predictable patterns. For example, some inorganics were more likely to be found in the roots; others were more likely to be found in aerial portions of the plant, including the fruit. There was no evidence suggesting that the inorganic Chemicals of Interest highly accumulate in the kinds of crops irrigated with blended produced water; however, information on soil uptake factors for the specific crops and specific inorganic Chemicals of Interest is limited.

Nitrite is the only inorganic Chemical of Interest that could be eliminated from any further evaluation because it is converted to an important nutrient for food crops; and in blended produced water, it is present at levels likely to be encountered in many agricultural settings.

Fate, Transport, and Plant Uptake: Radionuclides

Radionuclides are affected by many of the same fate and transport factors that affect other inorganic chemicals, and the available information suggests that radionuclides tend to be poorly absorbed from soil and do not bioaccumulate in crops. As is true for other inorganic chemicals, the current state of the science is not sufficient to support the prediction of concentrations of radionuclides in crops based on the concentrations in irrigation water. However, available monitoring data for blended produced water used to irrigate food crops in the San Joaquin Valley has shown that levels of radionuclides in the blended produced water are low and generally comply with drinking water standards.

Fate, Transport, and Plant Uptake: Organic Chemicals

A great deal is understood about the factors affecting the fate and transport of organic chemicals in soil, in general. For the individual Chemicals of Interest, however, fate and transport and plant uptake data are only available for some of the chemicals. In addition to a review of the available literature addressing the fate and transport and plant uptake factors that affect the accumulation of the Chemicals of Interest in irrigated food crops, a screening evaluation of 45 Chemicals of Interest was conducted to identify those chemicals with the greatest likelihood to be available for plant uptake, should they be present in blended produced water.

The literature review found reports that some of the Chemicals of Interest are unlikely to be taken up by plants from the soil. Polycyclic aromatic hydrocarbons (PAHs) were identified as one group of chemicals that are less available for plant uptake from soil due to their tendency to strongly bind onto organic material in soil and water and to degrade in sunlight, for example. Many of the biocides used by oil and gas producers are likely to biodegrade into compounds of limited concern. Some of the surfactants used in oil production, however, may degrade into compounds that are endocrine disruptors.

Much less is known about the root uptake and distribution of organic chemicals within plants than is known about the inorganic or radionuclide chemicals. The available information shows that plants can take up organic chemicals through the roots and leaves. More soluble organic chemicals are primarily taken up through the roots, while lipophilic and gas-phase organic chemicals can be taken up through the leaves. Lipophilic organic chemicals may also be taken up by root tissues that have higher lipid content, as is seen in the peels of potatoes and carrots.

Results from the screening evaluation of 45 organic Chemicals of Interest identified a few Chemicals of Interest with relatively high potential for availability for plant uptake. The other organic Chemicals of Interest reviewed in this screening evaluation had at least some characteristics that suggest their uptake by roots from soil would be attenuated. Many of the organic Chemicals of Interest were not included in this evaluation because data needed to support the evaluation were not available

Supplemental Toxicity Evaluation

Under Task 2, we searched for additional data on the chronic toxicity for the Chemicals of Interest, including exploring such methods as quantitative structure activity relationships or read-across toxicity evaluations to supplement the information found as part of Task 1. These efforts did not produce substantive improvement in our understanding of the chronic toxicity of these chemicals beyond that gained in Task 1. Our search for additional information was limited, in part, by the ambiguous identification of “aromatic amines” and missing characteristic information of the “polymeric materials” used as oil field additives. Polymeric materials have generally low toxicity and because of their widespread use in water treatment, they or their degradation products are likely to be present in some conventional irrigation water at some level, as well. The information that is available suggests these materials pose little risk from exposure via consumption of irrigated crops if they meet criteria based on the size of the molecule, the biological activity of reactive functional groups, and concentration of residual monomer.

Another question related to the toxicity of oil field chemicals is the possible toxicity of mixtures due to the presence of breakdown products, effects of individual chemicals without toxicity data, effects of unidentified chemical constituents, or chemical interactions. One way to approach this question is through whole effluent testing methods. Whole effluent testing of wastewater is a common practice and has involved the exposure of cell cultures or zebra fish embryos, for example, to wastewater effluent. Such testing has been explored in various water recycling projects, including testing of produced water from hydraulic fracturing, and to a lesser degree on produced water from conventional oil production. While adverse responses were seen in some of these screening tests, the relevance of the test results to irrigation water are difficult to evaluate; and the degree to which the components of the tested mixtures correspond to the component in the blended produced water addressed by this study is not known. While whole effluent testing is growing in use for monitoring wastewater discharged to surface waters supporting aquatic life and for water reused for drinking water, its value in evaluating the suitability of water for the irrigation of edible crops is not as clear.

Discussion and Conclusions

The literature review performed under Task 2 focused on collecting and evaluating information related to the reuse of produced water for agricultural irrigation and on summarizing general fate and transport principles relevant to chemicals in agricultural settings. Task 2 also evaluated factors that could be expected to enhance the accumulation of irrigation water chemicals in crops. Another objective of Task 2 was to check whether the findings from Task 2 were consistent with the results of the Task 3 crop testing.

The evaluations performed included a search for chemicals that might be present at elevated levels in blended produced water, a comparison of the levels of chemicals in blended produced water to levels in other water suitable for irrigation, and a comparison of levels of chemicals detected in crops irrigated with blended produced water to the levels detected in crops grown in other geographic areas. In addition, we searched the literature for information on the fate and transport of Chemicals of Interest in water and soil, plant uptake tendency, and chemical movement patterns within plants.

The results of the evaluations (summarized in Table ES-1, below) were consistent with the conclusions of the crop sampling analysis performed under Task 3. The fundamental finding of the Task 3 crop testing was that there were no significant differences between “treated” and “control” crops. While the mean or median concentration in 5 of 89 sample comparisons were statistically higher for crops irrigated with produced water ($p < 0.05$), these differences were small and not of toxicological significance. In addition, the concentrations of the five metals were not higher than those seen in the same crops found in the U.S. marketplace. These five chemical/crop differences between “treated” and “control” crops were observed for barium and zinc in almonds, and for strontium in garlic, grapes, and lemons. In addition, the information on the fate and transport in soil and plant uptake of the Chemicals of Interest suggest crops irrigated with blended produced water will accumulate chemicals to a similar degree as crops irrigated with conventional irrigation water.

While each evaluation completed as part of Task 2 had data gaps and associated uncertainties, the result of each evaluation was consistent with the finding that the Chemicals of Interest are unlikely to accumulate in crops irrigated with blended produced water to a higher degree than in crops irrigated with other suitable sources of irrigation water in the area. The fact that all evaluations were consistent with the finding that there were no significant differences in the chemical concentrations measured in crops irrigated with blended produced water and conventional irrigation water provides an additional degree of confidence to the finding from both Task 2 and Task 3.

While a great deal of research has been conducted on the fate and transport of chemicals in water and soil, as well as on plant uptake of chemicals, and the transport of chemicals to various plant parts, the current state of science does not support the ability to predict concentrations in the edible portions of plants based on concentrations of chemicals in irrigation water. Accordingly, the current state of science does not support the ability to set chemical-specific concentration limits for irrigation water designed to limit chemical concentrations in the edible portions of crops.

Table ES-1:
Summary of evaluation of the likelihood that Chemicals of Interest detected in crops Irrigated with blended produced water came from the oil production activities

Chemical of Interest	Does blended produced water regularly exceed drinking water quality standards or other toxicity screening values?	Are concentrations in blended produced water higher than other water suitable for irrigation in Kern County?	Are chemical concentrations higher in crops grown with produced water?	Are crops irrigated with blended produced water different than food crops in the marketplace?
Antimony	No	Unknown[1]	No	Unknown[2]
Arsenic	Yes	No	No	No
Barium	No	No	Yes	No
Cadmium	No	No	No	No
Chromium (VI)	No	No	Unknown[3]	Unknown[4]
Copper	No	Yes[5]	No	No
Lead	No	No	No	No
Molybdenum	No	No	No	No
Nickel	No	No	No	No
Strontium	No	No	Yes	No
Zinc	No	No	Yes	No

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[1] There is no data on the concentration of antimony in water suitable for irrigation in Kern County. Comparison of the concentration of antimony in blended produced water with surface water data across the US suggests levels in blended produced water are higher, see Section 5.4.2.

[2] Antimony was detected in almonds and garlic as part of the Task 3 crop sampling. No data was found on antimony levels in garlic or almond levels in samples collected from the marketplace.

[3] Results are reported for total chromium, not hexavalent chromium. Hexavalent chromium was not measured in Task 3 food crops.

[4] Data are limited in the literature for typical concentrations of hexavalent chromium in food crops in the marketplace.

[5] Concentrations of copper in blended produced water was higher than observed concentrations in other sources of water suitable for irrigation in Kern County, however, concentration of copper in blended produced water were below the Maximum Contaminant Level water quality standard.

1.0 INTRODUCTION

GSI Environmental Inc., (GSI) has been commissioned as a third-party consultant to perform technical work in support of an evaluation of the hazards associated with the reuse of produced water for irrigating food crops. The work is being performed in accordance with a Memorandum of Understanding (MOU) between (1) the Central Valley Regional Water Quality Control Board (CVRWQCB), (2) a group of permit holders that generate produced water as a result of their oil and gas extraction activities, and (3) a group of permit holders that accepts treated, produced water for beneficial reuse as agricultural irrigation water[1]. The MOU stipulates that the suppliers and users fund the technical work to support the scientific review of using produced water for irrigating agriculture and that the CVRWQCB direct the technical work performed by the third-party consultant. GSI's technical work was disseminated to the Food Safety Expert Panel, Science Advisor to the CVRWQCB, and CVRWQCB staff via draft reports and presentations during public Food Safety Meetings. The Food Safety Expert Panel, Science Advisor to the CVRWQCB, and CVRWQCB staff provided comments and recommendations on GSI's technical work, which were updated as appropriate.

The Scope of Work, developed in response to the MOU, is available on the CVRWQCB website[2],and includes three tasks:

1. Selection of “Chemicals of Interest,” from a list of known chemical additives and naturally occurring chemicals in produced water, for further evaluation (Task 1)
2. Literature review focusing on the “Chemicals of Interest” in the context of produced water reuse in agricultural irrigation and other potential sources of these chemicals in the agricultural water supply (Task 2)
3. Sampling and chemical analysis of crops irrigated with produced water and crops grown nearby using conventional sources for irrigation (Task 3)

The Scope of Work document proposed that Task 2 include a rigorous and thorough review of the available literature on existing studies and practices involving the use of produced water for the irrigation of food crops. This report describes the methods and data sources that have been evaluated under Task 2; and includes a discussion of the results of that literature review. The literature review also includes a summary of several chemical-specific topics of information that support an evaluation of the safety of using produced water for irrigating food crops. The topics all focus on the Chemicals of Interest, and address ambient levels, the identification of other potential sources, their environmental fate and transport, the formation of degradation and reaction products, and known plant uptake properties. A summary of the key knowledge gaps associated with the use of produced water is also presented.

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[1] https://www.waterboards.ca.gov/centralvalley/water_issues/oil_fields/food_safety/2017_0627_offs_mou.pdf
[2] https://www.waterboards.ca.gov/centralvalley/water_issues/oil_fields/food_safety/meetings/2018_0725_offs_mtg_sows.pdf

2.0 METHODS

This literature review focused on key technical issues associated with the reuse of produced water for irrigating food crops, and addresses the question, “What is currently known about the water quality of the blended produced water[1] that is currently being used to irrigate food crops in the context of the Chemicals of Interest?” More specifically, the literature review considers:

- What is known about the concentration of the Chemicals of Interest in the ambient environment, and do concentrations differ from those measured in blended produced water?
- Are there other sources of these chemicals, especially agricultural sources, that may contribute to their presence in an agricultural setting where food crops are grown, or otherwise affect the quality of food?
- Are there fate and transport factors that can enhance or attenuate the uptake of these Chemicals of Interest in food crops?
- Do the environmental degradation or transformation products of the Chemicals of Interest potentially attenuate or enhance the toxicity of blended produced water?
- Is there sufficient information to understand how plants take up these chemicals from the water and soil, and will plant uptake affect the resulting quality of food crops that were irrigated with blended produced water?
- Are there toxicities associated with the Chemicals of Interest that were not otherwise identified or previously considered?
- Do radionuclides potentially present in produced water create hazards associated with food crops irrigated with blended produced water?

In coordination with the Food Safety Expert Panel, CVRWQCB staff, and its scientific advisor Dr. William Stringfellow, we addressed these questions through a review of the literature focused on the following areas:

1. The reuse of produced water for agricultural irrigation
2. Water quality data collected as a result of CVRWQCB staff-issued Orders pursuant to California Water Code sections 13267 and 13267.5 to oil companies and chemical manufacturers and distributors, in the context of the Chemicals of Interest
3. Known ambient levels of the Chemicals of Interest
4. Other sources of the Chemicals of Interest, especially other agricultural sources
5. Factors affecting environmental fate and transport of the Chemicals of Interest that may be found in produced water used for agricultural irrigation

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[1] The term ‘blended produced water’ refers to treated produced water that is blended with other suitable sources of irrigation water.

6. The potential breakdown products of the Chemicals of Interest
7. Plant uptake of the Chemicals of Interest
8. Further review of the toxicity of the Chemicals of Interest and their degradation products to supplement the work completed in Task 1

We defined inclusion criteria to assist in identifying literature for this review; see Table 1. One important criterion was the applicability of the study to agricultural environments. This consideration was important in the selection of fate and transport and plant uptake studies because many of these were performed under conditions that would not provide valid results under agricultural conditions. A large fraction of plant uptake studies, for example, were soil phytoremediation studies conducted at chemical concentrations typical of contaminated industrial sites, rather than the lower concentrations typically found in agricultural soil. This selection criterion was important because the uptake of chemicals from soil by plants varies with the concentration of the chemical in soil, especially when concentrations approach levels toxic to a plant (Sharma et al., 2016; Singh et al., 2010). While systematic soil sampling has not been performed on any of the fields irrigated with blended produced water addressed in this study, we note that all are in active agricultural use, and we expect that the levels of chemicals in the fields addressed in this study are typically much lower than the levels of chemicals in the soils addressed in phytoremediation studies.

Some studies of produced water coming from hydraulic fracturing operations were included in this review, even though all of the produced water used for irrigation in the Central Valley of California (the focus area of this review) comes from oil wells that have not been hydraulically fractured (as defined by the California Code of Regulations (CCR), title 14, section 1761). Information from selected studies of produced water reuse from hydraulic fracturing operations were included in this review because there is overlap between chemicals used in hydraulic fracturing and chemicals used in conventional oil production during routine operations, such as well development, well maintenance, enhanced oil recovery, and other activities. Based on data from the South Coast Air Quality Management District, Stringfellow et al. (2017) reported there is significant overlap between chemicals used in hydraulic fracturing and conventional oil production. Only 4.2% of the chemicals used in hydraulic fracturing are unique to hydraulic fracturing methods (Stringfellow et al., 2017). Information from studies of chemicals in produced water from hydraulic fracturing was included in this review if the information was relevant to the use of produced water from conventional oil production.

A variety of sources of information were used in this review, with preference given to peer-reviewed publications. We also relied on many government publications, which included evaluations and conclusions prepared by various agencies. Much of the data summarized in the government reports was from peer-reviewed journals, and most of the government reports underwent peer review and/or public review. Information from scientific letters were considered as possible data sources, but they may not have been subject to peer-review even though they have been published in peer-reviewed journals. Publications from professional and trade associations knowledgeable about practices and procedures in oil production and in the use of produced water were also reviewed and relied upon as information sources for this report.

Literature was identified by searching the following sources and indexes: Google Scholar, other internet searches, University of California Melvyl search index, University of California Berkeley OskiCat search index, PubMed (US National Library of Medicine, National Institutes of Health), PubChem (US National Library of Medicine, National Institutes of Health), Hazardous Substances Data Bank [HSDB] (US National Library of Medicine, National Institutes of Health), Toxicology Data Network [TOXNET] (US National Library of Medicine, National Institutes of Health), Haz-Map (US National Library of Medicine, National Institutes of Health), CompTox (USEPA), European Chemicals Agency: Search for Chemicals, Organisation for Economic Co-operation and Development (OECD) databases, Pharos Project databases, Integrated Risk Information System (USEPA), Toxicological Profiles (Agency for Toxic Substance Disease Registry, Centers for Disease Control), COSMOS toxicological database, USEPA National Library Catalog (USEPA), The Endocrine Disruptor Exchange (TEDX), California State Water Resources Control Board website, USEPA Inert Finder, FracFocus, California Department of Pesticide Regulation (CDPR) chemical ingredient database and California Office of Environmental Health Hazards Assessment (OEHHA) chemical databases.

As part of the literature review, we attempted to identify published concentrations of Chemicals of Interest in air, soil, and surface water. Ambient concentrations in drinking water were sometimes included as comparison to surface water concentrations. We attempted to identify the most geographically representative environmental data by following a geographic search hierarchy. We first searched for data in the San Joaquin Central Valley area and expanded the search to include California, followed by the United States. To the extent practical, search results were limited to research conducted within the last 20 years, although sometimes that was not possible given the paucity of data.

3.0 REVIEW OF PRODUCED WATER REUSE FOR AGRICULTURAL IRRIGATION

Produced water refers to the aqueous fluid pumped to the surface along with crude oil or natural gas (Veil et al., 2004, OTEG, 2011). It is typically produced in larger volumes than the oil or gas from a well, and its composition varies. After being pumped to the surface, oil and gas are separated from the produced water, which is a by-product of virtually all oil and gas production. National estimates of produced water exceed approximately 2.57 million acre-feet of water (Clark and Veil, 2009; Chittick and Srebotnjak, 2017). During production, produced water is brought to the surface as a mixture of reservoir fluids that can include injection fluids, and any chemicals added during exploration, production, or treatment (Echchelh et al., 2018). Much of the naturally occurring water in produced water exists because hydrocarbon reservoirs consist of subsurface geologic formations naturally permeated with a combination of fluids (water, oil, or gas) (Echchelh et al., 2018).

The ratio of water to oil/gas in a petroleum well is generally greater than three; it can be more than 20 in some locations (WEF, 2018).

Produced water can be managed in a few different ways. A large fraction of this water is pumped back into Class II injection wells for reuse or disposal (USEPA, 2019a). Produced water may also be discharged to percolation/evaporation ponds or treated and reused (Echchelh et al., 2018). Reuse of this water may take the form of reinjecting it into Class II wells to enhance recovery of hydrocarbons (USEPA, 2019a), or for irrigation (Echchelh et al., 2018). In most cases, produced water requires treatment for salinity and/or sodicity in order to be reused for agriculture. Echchelh et al. (2018) reviewed over 474 produced water samples from the US, Australia, South Africa, and Qatar and determined that only 8.4% of samples met agricultural irrigation water quality guidelines[1] for electrical conductivity and sodium absorption ratio. In treating produced water for salts, the literature cites the two most common solutions as dilution/blending with low-salinity freshwater and desalination with reverse osmosis (Echchelh et al., 2018). Produced water from some of the wells in the Central Valley of California has been used to irrigate food crops because of its low salinity and dissolved solid content.

This section presents a summary of the current state of information on the beneficial re-use of produced water for agricultural irrigation. This section begins with a discussion of management of produced water reuse in the United States, followed by discussions of management of produced water reuse in the Central Valley and examples of reuse of produced water for agricultural irrigation.

3.1 Management of Produced Water Reuse in the United States

Most produced water is disposed of by underground reinjection or in percolation/evaporation ponds; and a small, but increasing, fraction of this water is being put to beneficial reuse after treatment (Jimenez et al., 2018). A miniscule fraction of produced water is used to augment US agricultural water withdrawals, which in 2000, totaled 153.4 million (acre-feet for irrigation and 6.12 million acre-feet for livestock water and aquaculture (Clark and Veil, 2009). Historically, produced water has been managed as waste via underground injection control disposal wells (regulated under the Safe Drinking Water Act) or disposal in onsite evaporation pits (USEPA, 2019b). Although underground disposal remains the predominant management approach for US produced water, produced water is increasingly being recycled and reused within the oil and gas field for enhanced oil recovery, drilling, and hydraulic fracturing activities (USEPA, 2019b). Opportunities for beneficial reuse exist outside the oil and gas industry but are rarely implemented due to treatment costs and unknown environmental and human health risks. Currently, less than one percent of produced water is reused outside the oil field (NAS, 2017). Only a few states use produced water for agriculture and road-spreading, to control dust and ice (Veil et al. 2004, Clark and Veil, 2009, USEPA 2019b). The Clean

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[1] The comparisons in Echchelh et al., (2018) are based on agricultural water quality guidelines reported in, "Ayers, R.S. and Westcot, D.W., 1985. Water quality for agriculture (Vol. 29). Rome: Food and Agriculture Organization of the United Nations."

Water Act prohibits discharges of produced water to surface water east of the 98th meridian. Operators of conventional oil fields west of the 98th meridian may discharge produced water directly to surface water for agriculture or livestock watering after securing a permit under the National Pollutant Discharge Elimination System (NPDES) and after achieving effluent concentrations specified in the permit. NDPES permit specifications require the effluent to contain oil and grease concentrations of 35 mg/L or less than (40 CFR 435 Subpart E), though state-specific discharge requirements may impose more stringent parameters. Produced water discharges to surface water have been documented in California, Colorado, Utah, and Wyoming for agriculture and wildlife (Veil 2015, USEPA 2019b; CWB, CVRWQCB). A NPDES permit is not required for irrigation uses that do not discharge to surface water. In Wellington, Colorado, treated produced water is used in an aquifer storage and recovery project to maintain groundwater supplies in the region (AGI, 2018). In California, low salinity produced water is reused for groundwater recharge and agricultural irrigation of crops for human consumption (AGI, 2018).

Prior to most reuse applications, produced water is typically treated to meet effluent standards and other requirements for general surface discharge or reuse for agricultural irrigation. After the raw oil stream is dewatered through a series of separators, coalescers, or other devices, the produced water is typically sent to a water treatment system (USEPA, 1996). After primary treatment, the effluent is typically sent through a secondary treatment, such as a floater, to separate residual oil and gas (Jimenez et al., 2018). In most cases, however, the combination of primary and secondary treatment is unable to produce an effluent that meets water quality requirements for beneficial reuse (Dores et al., 2012).

After the initial separation of oil and/or natural gas, the produced water may need to undergo polishing treatment to meet effluent standards for reuse (Jimenez et al., 2018). There are three main classes of polishing treatment technologies used to treat produced water beyond primary and secondary treatment, including physical, biological, and chemical treatment technologies. Physical treatment technologies may include adsorption, cyclones, enhanced flotation, membrane filters, and thermal evaporation or distillation. Biological technologies include phytoremediation, aerobic and anaerobic biodegradation, and bioflocculation. Chemical technologies include chemical precipitation, electrochemical processes, room temperature ionic liquids, demulsifiers, ion exchange, macro-porous polymer extraction technology, and advanced oxidation processes (Jimenez et al., 2018).

The effectiveness of the polishing treatment classes and specific technologies can vary depending on water quality. In addition, some have reported high-quality water resulting from treatment, while most individual treatment methods only remove specific contaminant groups. For example, Daigle et al. (2012) reports that absorption treatment can result in residual chemical concentrations in the ppb or lower concentration range. In contrast, cyclones perform poorly for removal of dissolved hazardous chemicals and had low removal efficiency of dispersed oil when compared to other treatment methods (Van den Broek et al., 2013). Some biological treatment technologies have shown effective removal of hydrocarbons (Gurden and Cramwinckel, 2013) and metals (Al Mahruki et al., 2013). However, high salinity can dramatically reduce biodegradation rates (Tellez et al., 2012). Chemical treatment methods are also similarly selective and can be affected by the initial water quality. For example, demulsifiers counteract the effect of additive surfactant and allow oil droplets to coalesce, which are then separated from the water (Almarouf et al., 2015). Demulsification can be affected by other water quality issues, such as the presence of iron sulfides, silts, clay, drilling mud, and paraffin (Holloway, 2013).

Effective treatment of produced water may call for a combination of different treatment technologies selected for specific kinds of compounds found in the produced water. Selection of polishing treatment technologies will depend on contaminant type and removal efficiency, energy and reagent consumption, environmental impacts, and economic costs (Jimenez et al., 2018).

3.2 Produced Water Reused for Agricultural Irrigation in the Central Valley

In 2017, more than 300 million cubic meters of produced water (more than 240,000 acre-feet) were produced in the Central Valley along with approximately 131 million barrels of oil (1 barrel of oil is equal to approximately 42 gallons) (CWB, 2019). Some of this produced water is used for agricultural irrigation, with the remainder reused in oil operations, disposed in permitted underground injection wells, or disposed to the surface (CWB, 2019). Produced water from Kern County (areas east and north of Bakersfield) has low salinity so that it is suitable for reuse in agriculture and has been used over the last 30 years to irrigate food crops (CWB, 2019).

The CVRWQCB regulates and permits the discharge and reuse of produced water for irrigation. Recycling of water is encouraged by State policy as a means to supplement California's limited water supply, provided the water is suitable for the intended use. This is regulated under waste discharge requirements (WDRs) that require the analyses of produced water for a variety of chemicals, including chemicals that are associated with additives used during petroleum exploration, production, and treatment. Cawelo Water District (WD), North Kern Water Storage District, Jasmin Ranchos Mutual Water Company, and Kern-Tulare WD are the four Districts that received produced water during the collection of crop samples for Task 3. Cawelo WD and parts of Kern-Tulare WD, including operation of the Jasmin Ranchos Mutual Water Company reservoir, have the longest history reusing produced water for irrigation. Cawelo WD receives approximately 32,000 acre-feet of produced water a year from regional oil producers under Waste Discharge Requirements Order Nos. R5-2012-0058 and R5-2012-0059 adopted by the CVRWQCB. The produced water is received into Cawelo WD's water distribution facilities and blended with water sources (surface and/or groundwater) prior to being delivered to agricultural fields for irrigation (Enviro-Tox Services, 2017). Per Waste Discharge Requirements Order R5-2015-0127 adopted in 2015, the North Kern Water Storage District also has authorization to use treated produced water from the Kern Front Oil Field blended with other irrigation water for irrigation and groundwater recharge. The Order allows produced water to be used on 55,000 acres of irrigated farmland and 608 acres of spreading basins for groundwater recharge. Kern-Tulare WD and the Jasmin Ranchos Mutual Water Company are partnered with Hathaway LLC, and permitted under Waste Discharge Requirements Order No. R5-2019-0043, to receive a maximum of 2,640 acre-feet per year of produced water from the Jasmin oil field (US Bureau of Reclamation, 2017). The order allows that the maximum volume may increase to 3,320 acre-feet upon written approval by the CVRWQCB. On June 6, 2019, the CVRWQCB adopted order R5-2019-0043, which are the previously mentioned waste discharge requirements for: Hathaway, LLC; Kern-Tulare Water District; and Jasmin Ranchos Mutual Water Company. These orders expressly state that, "The discharge of fluids used in 'well stimulation treatment,' as defined by CCR, Title 14, Section 1761 (including hydraulic fracturing, acid fracturing, and acid matrix stimulation), to land is prohibited" and "The discharge of produced wastewater from wells containing well stimulation treatment fluids, as defined by CCR, title 14, section 1761, is prohibited." These provisions clearly prohibit the discharge of produced water from hydraulic fracturing projects to the surface, and ostensibly for reuse on agricultural fields as irrigation waters.

Produced water reused for irrigating food crops in the Central Valley of California comes from conventional oil wells in Kern County. These wells produce oil under primary, secondary, or enhanced oil recovery, but do not use hydraulic fracturing or other well stimulation techniques described under CCR, Title 14, Section 1761. Primary oil recovery takes place during the natural rise of hydrocarbons or when oil is pumped to the surface (Schlumberger, 2020). Secondary recovery happens when water or gas is injected into a formation to displace the oil, which is then pumped to the surface (Schlumberger, 2020). Tertiary recovery, also known as enhanced oil recovery (EOR), is when heat, gas, and/or chemicals are injected into the geologic formation to change physical properties or availability of the oil to make recovery easier. Enhanced oil recovery may take place during any stage of the production lifecycle of an oil well (Schlumberger, 2020). Based on WDRs adopted by the CVRWQCB, suppliers of produced water for irrigating food crops in Kern County are allowed to use a variety of EOR techniques, with the exception of those described under CCR, Title 14, Section 1761. Some of the techniques that Kern County producers may use include cyclic steaming, steam flooding, and water flooding; in addition, these methods may be combined with additive chemicals, such as acids, alkalis, surfactants, and polymers.

Produced water coming from oil wells in Kern County that is used for irrigating food crops is treated by at least two of the following: gravity separation, dissolved air flotation, traditional filters, or walnut shell filters (CWB, 2019). After treatment, it may be blended with surface and groundwater before being delivered for irrigation. The blended produced water distributed by Cawelo WD is used to irrigate food crops that include citrus, nuts, grapes, apples, and row crops (e.g., garlic and carrots). During periods of low demand for irrigation water, blended produced water from Cawelo WD may be discharged to the Famoso Basins (recharge basins regulated under the WDRs) in addition to reducing the volume of surface water and groundwater that is blended with produced water (Wood, 2019). The produced water supplied by Kern-Tulare WD and Jasmin Ranchos Mutual

Water Company is blended and used to irrigate citrus. Blended produced water coming from the North Kern Water Storage District is used to irrigate nuts, grapes, and fruit grown within the water district. The WDRs that regulate the use of these irrigation waters also set out requirements to protect water quality, which includes extensive monitoring (CWB, 2019). These water quality data are reported later, in Section 5 of this report.

3.3 Other Examples of Reuse of Produced Water for Agricultural Irrigation in the United States

Aside from the reuse of produced water for agricultural irrigation in the Central Valley of California, US case-studies testing the feasibility of reusing produced water for agricultural reuse have taken place in other parts of California and in Wyoming. In California's Monterey County, produced water from the San Ardo Field treatment system yielded irrigation-quality effluent to recharge a shallow aquifer for agricultural reuse (Myers, 2014, Tao et al., 1993). Produced water from the San Ardo Field was treated by using oil/water separation, dissolved gas flotation, walnut shell filtration, reverse osmosis (RO), and phytoremediation in treatment wetlands (Myers, 2014). In California's Los Angeles County, researchers tested a pilot plant at the Placerita Oil Field to treat produced water for irrigation reuse (Doran et al., 1998; Funston et al., 2002). The Placerita pilot plant treated produced water with walnut shell filtration, warm precipitative softening with caustic soda and magnesium chloride, cooling, fixed-film biological oxidation (trickling filter), pressure filtration, ion-exchange softening, and RO. The primary goals of this treatment were the removal of hardness and silica, total dissolved solids (TDS), boron, ammonia, and total organic carbon (TOC). Due to fundamental operational conflicts in removing both boron and ammonia simultaneously with RO, the study authors advised considering an alternative conceptual design that involved blending the treated effluent with another non-potable supply to produce an acceptable non-potable water supply for irrigation (Doran et al., 1998).

In Wyoming, Jackson and Myers (2002) completed a pilot study that demonstrated the feasibility of using untreated produced water with 3,220 mg/L TDS and 4,740 µmhos/cm conductivity for aquaculture and hydroponically grown crops. When they compared tomatoes grown in control potable water to the tomatoes grown in produced water, those grown in produced water were generally smaller, tasted saltier, and more acidic. The tomatoes grown hydroponically in produced water also contained twice as much sodium and chloride as those grown in potable water (Jackson and Myers, 2002). In another study in Wyoming, researchers found that diluted produced water from coal bed methane production could be used to grow camelina over short time periods but use of the water could adversely affect soil sodium concentrations (Sintim et al., 2017). Burkhardt et al. (2015) report similar results in a 2-year study growing corn, switchgrass, and other biofuel feedstocks where they reported that produced water from coal bed methane production could adversely affect both plants and soil if the produced water isn't diluted with good-quality water.

3.4 Examples of Reuse of Produced Water for Agricultural Irrigation in Other Countries

There are case-studies in Mexico, Brazil, Oman, and Yemen where produced water was reused for agricultural irrigation. Martel-Valles et al. (2014) used produced water from Sabinas-Piedras Negas, in northern Mexico, to cultivate tomatoes in pots of peat moss and perlite in a greenhouse. They used produced waters from three different natural gas producers. The water was diluted to reduce electrical conductivity down to 1.5 deciSiemans per meter (dS/m). Produced water from two of the three producers could be used for irrigation, while the third source of produced water induced plant toxicity with its high levels of copper, chloride, and middle-fraction hydrocarbons (Martel-Valles et al., 2014).

In Brazil, Sousa et al. (2016) irrigated sunflowers with produced water filtered through a sand filter and cation resin, and produced water treated with post-filtration steps of pH correction, flocculation, and RO. They found that filtered produced water reduced nutrient accumulation in plants due to the effects of salinity and that RO treated produced water enhanced nutrient content and promoted plant growth (Sousa et al. 2016).

In Oman, Hirayama et al. (2002), created a pilot treatment system that consisted of air floatation, anthracite filtration, and activated carbon absorption. The treated produced water was used to irrigate planted beds of alfalfa, barley, and Rhodes grass. Compared to freshwater controls, the treated produced water reduced the growth of alfalfa due to salinity. Hirayama et al. (2002) also observed increases in soil sodicity resulting from treated produced water (8 dS/m electrical conductivity and 3,000-6,000 ppm salt content) and warned that long-term irrigation would require proper management of soil conditions.

In Yemen, Rambeau et al. (2004) constructed artificial wetlands to remove hydrocarbons from low salinity produced water for use in irrigating of cotton and hemp. They reported that the treated produced water could be used for cotton plants, but not for hemp plants, which exhibited salinity stress (Rambeau et al., 2004).

3.5 Examples of Reuse of Hydraulic Fracturing Produced Water or Simulated Hydraulic Fracturing Produced Water in Greenhouse Settings

There are a few examples of experiments investigating the reuse of actual and simulated produced water from hydraulic fracturing. Sedlacko et al. (2019) evaluated the morphophysiological response of greenhouse-grown spring wheat irrigated with diluted produced water from a hydraulically fractured well in the Denver-Julesburg basin of Colorado. The study had four water treatments: municipally treated tap water as a control, produced water diluted 1:9 with municipally treated tap water (and designated as “PW10”), produced water diluted 1:1 with municipally treated tap water (and designated as “PW50”), and a salinity control that mimicked the salinity of PW50. The salinity control contained the same average TDS as raw produced water and was diluted 1:1 with municipally treated tap water. The study results showed no difference in grain yields between PW10 and the salinity control, despite the salinity control containing five-times more TDS than PW10. Furthermore, the growth of crops irrigated with PW50 was severely stunted with no grain produced. The results comparing the high salinity water to the PW10 group suggest the influence of factors other than salinity in produced water were affecting crop health (Sedlacko et al., 2019). These factors may have included plant toxicity due to metals and/or organic chemicals in produced water as well as additive effects with salinity, drought, and oxidative stress (Sedlacko et al., 2019).

Shariq (2019) conducted a greenhouse experiment with simulated flowback water containing arsenic, cadmium, and tetrasodium ethylenediaminetetraacetic acid (EDTA) to irrigate wheat. The results indicated that EDTA did not significantly increase plant uptake of the applied metals; however, grain samples irrigated with the simulated flow back water contained 6.5 times higher arsenic and 1.4 times higher cadmium than control samples (Shariq, 2019).

3.6 Summary of Reuse of Produced Water for Agricultural Irrigation

Produced water is a large by-product stream from oil and gas exploration and production (Veil et al., 2014). This water may be pumped back into wells for reuse by oil and gas producers during secondary and enhanced oil recovery, or disposal (USEPA, 2019a), used to recharge aquifers (Tao et al., 1993; Myers, 2014; AGI, 2018; Wood, 2019), and for agricultural irrigation or watering livestock (Hirayama et al., 2002; Rambeau et al., 2004; Martel-Valles et al., 2014; Sousa et al. 2016; Enviro-Tox Services, 2017; AGI, 2018; CWB, 2019; Echchelh et al, 2018; Clark and Veil, 2009).

Prior to most reuse for agricultural irrigation, produced water needs to be treated to address the presence of residual oil, hazardous chemicals, and dissolved inorganics (Echchelh et al., 2018; Jimenez et al. 2018). Treatments may include primary and secondary treatment to initially separate oil and gas from the water, but polishing steps may be required to meet water quality levels needed for agricultural irrigation. These polishing methods include physical, biological, and chemical treatment methods (Jimenez et al., 2018). Treatment methods need to be selected to address the initial quality of the water, regulatory water quality requirements, and water quality requirements for their intended usage. Other factors to consider when selecting treatment methods are removal efficiency, energy and reagent consumption, environmental impacts, and economic costs (Jimenez et al., 2018).

For over the last 30 years, blended treated produced water has been used in the Central Valley of California for irrigating food crops (CWB, 2019). These crops include tree fruit, tree nuts, tomatoes, grapes, and root crops. There are other examples of reuse of produced in the US (Jackson and Myers, 2002; Tao et al., 1993; Myers, 2014; Burkhardt et al., 2015; Sintim et al., 2017) and throughout the world (Hirayama et al., 2002; Rambeau et al., 2004; Martel-Valles et al., 2014; Sousa et al. 2016). Few of these, however, have reported on reuse for food crops like those grown in the Central Valley of California.

The examples presented above highlight the complexity of reusing produced water for agricultural irrigation. Research has suggested that blending treated produced water, that by itself is not usable for irrigation, with other sources of water that are suitable for irrigation can expand the total volume of acceptable irrigation waters (Myers, 2014, Tao et al., 1993; Martel-Valles et al., 2014; Sousa et al. 2016). The results from these studies, however, also reported that under some conditions, there were noticeable effects on irrigated fruit (Jackson and Meyer, 2002), water induced plant toxicity (Martel-Valles et al., 2014), or plant nutrient uptake was adversely affected when the water was insufficiently treated (Sousa et al., 2016). Other research also reports that issues related to soil salinity may need to be addressed when produced water is used as a long-term source of irrigation water (Hirayama et al., 2002; Burkhardt et al., 2015; Sintim et al., 2017). Overall, these studies suggest that treated produced water with lower organic and total dissolved solids content is better suited to long term agricultural irrigation.

4.0 CHEMICALS OF INTEREST

As discussed in the Task 1 report, the Chemicals of Interest are a prioritized list of chemicals selected as being the best indicators of potential health hazard associated with the reuse of produced water for irrigating crops in the San Joaquin Valley of California. The Chemicals of Interest were selected for further evaluation based primarily on consideration of chronic oral toxicity and, to a lesser extent, the likelihood of being taken up by irrigated crops. The candidate chemicals considered in Task 1 were potentially present in produced water, which included naturally occurring chemicals found in produced water and chemical additives used in oil production in the San Joaquin Valley. The chemical additives were those disclosed to the CVRWQCB as being used during oil exploration, production, and treatment by oil producers that supply produced water to water districts for agricultural irrigation. The naturally occurring chemicals were identified from a variety of published sources addressing the composition of produced water.

To provide background material for later sections of this report, the text below presents a number of summaries. Section 4.1 presents a summary of the composition of produced water. Section 4.2 presents the methods used to select the Chemicals of Interest from the candidate list of 399 chemicals. Section 4.3 presents the uses of the additive Chemicals of Interest in oil production, along with the uses of the Chemicals of Interest that may contribute to other human exposures, including agricultural exposures. Section 4.3 provides context for evaluating the significance of potential exposures from food crops and the significance of data gaps.

4.1 Composition of Produced Water

The chemical composition of produced water is highly variable, with the physical and chemical characteristics of produced water depending on multiple factors, including the oil field's geographic location, geological host formation, type of hydrocarbon being produced, and the production well's life-stage (Veil et al., 2004; OTEG, 2011). Generally, produced water contains several chemical groups that may present environmental and/or health concerns. Some of these chemicals that pose environmental and/or health hazards are naturally occurring inorganic chemicals, radionuclides, and organic chemicals. Also included in the chemicals that potentially pose environmental and/or health hazards are chemical additives that are used during oil production. The lists of naturally occurring chemicals and chemical additives are not mutually exclusive as some of the naturally occurring chemicals found in produced water are also used as additives. The inorganic chemicals, including radionuclides, and organic chemicals that are typically found in produced water and the source or sources of these chemicals are discussed below.

Naturally occurring inorganic chemicals in produced water are primarily derived from contact of the petroleum formation water with the field's geological formations (Benko and Drewes 2008). Collectively, the inorganic content of produced water is typically described by its salt content, which is usually quantified as TDS or electrical conductivity (EC) (Veil et al. 2004, Fillo et al.,1992). In general, the TDS in produced water can range from less than 100 ppm to over 300,000 parts per million (ppm), with most of the salt content consisting of sodium chloride (Fillo et al.,1992). Cations (e.g. Na+, K+, Ca+, Mg+) and anions (e.g. Cl-, SO_4^{2-}, CO_3^{2-}) affect produced water chemistry in terms of buffering capacity, salinity, and scale potential (Hansen and Davies, 1994). Produced water also typically contains trace amounts of heavy metals (e.g., lead, arsenic, cadmium, mercury) with concentrations that may reach 100 to 100,000 times those in seawater (Jimenez et al., 2018, Chittick et al., 2017, Shepherd et al., 1992).

Naturally occurring radioactive materials (NORMs) have been reported in produced water (Smith, 1992; Bretz et al., 1994; DOGGR, 1996; Zielinski and Otton, 1999; Veil et al., 2004; Guerra et al., 2011; Neff, 2011; Rowan et al., 2011). The concentration of NORMs in produced water are variable and depend on the geologic formation, often correlating with TDS and the salinity of the water (DOGGR, 1996; Fisher, 1995; Rosenblum et al., 2017; Zielinski and Otton, 1999). They can originate in geological formations, dissolve in produced water, and can precipitate into scale or sludge when produced water is brought to the surface and water temperatures decrease (Jimenez et al., 2018). The most abundant NORM compounds in produced water are radium (isotopes 226 and 228) (Veil et al., 2004; Jimenez et al., 2018), and to a lesser extent, uranium, and thorium[1] (Smith, 1992). It has also been noted that thorium-232 (Th-232) is not typically a major component of produced water, due to its limited solubility (Platford and Joshi, 1986). Outside of the United States, it has been reported that Th-232 and U-238 were identified in produced water samples (Ali et al., 2015), suggesting the potential for its dissolution into formation waters.

There are only a few studies reporting on NORM content of produced water in California (DOGGR, 1996; McMahon et al., 2018). A study by the Division of Oil, Gas, and Geothermal Resources (DOGGR, 1996) reported on radioactivity levels in multiple process streams from oil production, including produced water. In this study, radionuclide concentrations were reported for produced water samples collected within Kern and Tulare Counties. Concentrations were reported for potassium-40 (K-40), radium-226 (Ra-

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[1] Thorium was not originally reviewed during the Task 1 assessment. Work conducted under this literature review identified thorium-232 as a potential radionuclide in produced water. We added thorium-232 to the list of Chemicals of Interest to the radionuclide reviewed in this report.

226), radium-228 (Ra-228), uranium-235 (U-235), and uranium-238 (U-238), and cesium-137 (Cs-137) in eight samples. Potassium-40 was detected in nearly all samples of produced water with a maximum reported concentration of 270 ± 71 pCi/L.[1] In one sample, both Ra-226 and Ra-228 were detected at concentrations of 19.2 ± 14.8 pCi/L and 19.0 ± 6.1 pCi/L, respectively. In another sample, Ra-228 was detected at a concentration of 67.4 ± 13.8 pCi/L; there were no other detections of radionuclides in the produced water samples (DOGGR, 1996). McMahon et al. (2018) reported on radium concentrations in oil-field water from wells in the Southern San Joaquin Valley of California, using some of the same data that is reported in Section 5 of this report. They reported that oil-field water from western formations (Lost Hills and Belridge fields) have statistically higher concentrations of radium than water from the eastern formation (Fruitvale Field); the western formation also has higher salinity than does the eastern formation. Median total concentration of radium for the Lost Hills and Belridge fields are reported as 1.3 Bq/L (1Bq = 27 pCi) and 3.5 Bq/L, respectively, while waters from the Fruitvale Field has a median concentration of 1.1 Bq/L (McMahon et al., 2018). Their research also seems to indicate that radium-224 is a predominant radionuclide in produced water from oil wells in southern San Joaquin Valley of California (McMahon et al., 2018).[2]

Produced water can also contain naturally occurring organic chemicals that are not removed during the separation of target hydrocarbon products. The composition and concentration of organic constituents in produced water vary according to the type of hydrocarbon in contact with the water, volume of water production, artificial lift technique, and length of production in the lifecycle of the well (Benko and Drewes, 2008). The organic constituents within produced water exist as either dissolved organic compounds or suspended, dispersed oil droplets (Benko and Drewes, 2008). Dissolved organic compounds are water-soluble and include aliphatic hydrocarbons, carboxylic acid, and low-weight aromatic hydrocarbons (e.g., benzene, toluene, ethylbenzene, and xylene) (Utvik et al., 2002). Dispersed oil consists of small drops of oil suspended in produced water and can include polyaromatic hydrocarbons (PAHs) and some of the heavier alkyl phenols that are less soluble in produced water (e.g., C6-C9 alkylated phenols) (Faksness et al., 2004). The low-molecular weight aromatic hydrocarbons (e.g., benzene, toluene, ethylbenzene, and toluene) are found in higher concentrations in natural gas-produced water than oil-produced water; semi-volatile organic compounds are more

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[1] Potassium-40 was not considered further as a potential Chemicals of Interest: it is a radionuclide to which we are commonly exposed. Typical daily intake of potassium-40 is 2,300 pCi, which mostly comes from foodstuff (NRC, 1977). Translating these food exposures to drinking water suggests that a water equivalent concentration would need to be over 1000 pCi/L to approximate food exposures, based on an assumption of 2 liter per day consumption of water. Concentrations in produced water are a near order of magnitude lower, suggesting they are of limited concern for human health.

[2] Ra-224 has similar radioactivity to Ra-226, but is short lived with a half-life of 3.6 days where it emits alpha radiation. If present in produced water, Ra-224 is unlikely to go unnoticed because gross alpha radiation (CASRN # 12587-46-1) is an analyte in the laboratory analyses of water samples collected under the WDRs. Given its short half-life and the ongoing monitoring for gross-alpha radiation, Ra-224 was not further considered for its addition to the list of Chemicals of Interest.

prevalent from oil-produced water and are rarely found in natural gas-produced water (Utvik et al., 2002; Benko and Drewes, 2008). Over time though, the organic constituents in produced water may undergo biodegradation, which will change the composition and concentration of the organic constituents (Stromgen et al., 1995). Most US agency regulatory requirements for monitoring in water are focused on oil & grease content using USEPA Method 1664 (Jimenez et al., 2018). USEPA Method 1664 defines oil & grease content as "a mixture of those components that are extractable in hexane at pH <2 and remain after vaporization of hexane." This definition would include dispersed oil and some water-soluble organics, but would exclude low-weight phenols, low-weight acids, and BTEX.

Produced water may can also contain chemical additives used during exploration, production, and treatment (Veil et al., 2004; Echchelh et al., 2018). These chemical additives typically consist of: corrosion inhibitors and oxygen scavengers to limit equipment corrosion; scale inhibitors to reduce mineral scale deposits; biocides to mitigate bacterial fouling; emulsion breakers and clarifiers to break water-in-oil emulsions; reverse emulsion breakers to break oil-in-water emulsions; coagulants, flocculants, and clarifiers to remove solids; and solvents to reduce paraffin deposits (Veil et al., 2004; Stringfellow et al., 2017). Oil producers in the San Joaquin Valley of California that provide produced water for the reuse of agricultural irrigation are required to declare oil field additives that they use during exploration, production, and treatment activities. The list of declared oil field additives are reported on the CVRWQCB website.[1]

4.2 Summary of Task 1: Selecting the Chemicals of Interest

The primary objective of Task 1 was to develop the list of Chemicals of Interest to be reviewed further with a literature review focused on understanding the context of health hazards associated with the reuse of produced water for agricultural irrigation. The Chemicals of Interest are a prioritized list of chemicals that were selected as being the best indicators of potential health hazard associated with the reuse of produced water for irrigating food crops. The Chemicals of Interest were selected from a list of 399 chemicals that were initially identified as potentially being present in produced water from San Joaquin Valley oilfields. The list of 399 chemicals includes likely naturally occurring chemicals in produced water and chemical additives declared by oil producers, as discussed above in Section 4.1.

As discussed in greater detail in the Task 1 report, the selection of Chemicals of Interest was based on a screening-level hazard assessment. In brief, the hazard assessment was based on two primary factors: chronic oral toxicity and the potential for the chemicals to be taken up into irrigated crops, including consideration of loss from irrigation water due to such processes as biodegradation, hydrolysis, and volatilization. Oral toxicity was the only toxicity route considered because we were interested in the safety of consumption of the irrigated crops. The potential for exposure by inhalation and dermal contact was considered to be insignificant in comparison to ingestion. Chemicals were not included in

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[1] https://www.waterboards.ca.gov/centralvalley/water_issues/oil_fields/food_safety/#data

the list of Chemicals of Interest if the chemicals had very low toxicity and if it was clear that exposure at levels that might cause adverse health effects was not plausible as a result of ingesting irrigated produce. Chemicals were also not included in the list of Chemicals of Interest if there was evidence that their concentration in water would rapidly and substantially reduce and, therefore, not be available for significant plant uptake following irrigation.

Because the toxicity of the 399 chemicals had not been studied to the same degree across all chemicals, a variety of sources of information and approaches to assess their toxicity was used during Task 1 (See Figure 1). To assess the toxicity hazards associated with each chemical, we used agency-derived screening values, identified chemicals of low concern for toxic effects, identified chemicals with available toxicity data that could be used to develop project-specific surrogate toxicity values, and identified data gaps associated with the toxicity of the 399 chemicals. Agency derived toxicity values included non-cancer and cancer outcome toxicity values. Chemicals of low concern for toxicity included food additives, chemicals considered essentially non-toxic, chemicals with therapeutic oral use and low toxicity, inert compounds, and compounds that break down into one of the previously identified essentially non-toxic chemicals. We developed project-specific surrogate toxicity values using published toxicity studies and applying uncertainty factors consistent with those used by the Office of Environmental Health Hazard Assessment (OEHHA, 2008). The surrogate toxicity values were mostly based on animal studies. Finally, all chemicals for which we identified data gaps in toxicity were added to the list of Chemicals of Interest.

Upon completing the Task 1 screening of the 399 chemicals, 143 chemicals were identified as Chemicals of Interest for further evaluation in Task 2. There were 53 chemicals with agency-derived toxicity values, 12 with project-specific surrogate toxicity values, 59 with no toxicity data, and 15 with incomplete information to assess their toxicity based on chronic oral exposure. We also identified five radionuclides: Ra-226, Ra-228, U-238, krypton-85 (Kr-85), and xenon-133 (Xe-133).

For this report, Th-232 and strontium were added to the list of Chemicals of Interest. Thorium-232 was added to the list of Chemicals of Interest because literature found while researching this task reported that Th-232 was identified in samples of produced water outside of the United States (Ali et al., 2015), and Th-232 is a decay product of radium (Fisher, 1998). And while strontium was evaluated in Task 1 and screened out because of its low toxicity, we have included it as a Chemical of Interest because it was detected at high frequency in crop samples collected as part of this study.

Appendix D of the Task 1 Report provides the list of 143 Chemicals of Interest, not including Th-232 or strontium.

4.3 Uses of the Chemicals of Interest

Although the health risk posed by a chemical is not dependent on the source of a chemical, there is value in understanding the likely source of chemicals in produced water and in crops irrigated with produced water. Many of the Chemicals of Interest are likely to originate from more than one source. As discussed below, however, information about the source(s) of all the Chemicals of Interest is not complete. Information about sources of Chemicals of Interest can help us evaluate the likelihood that any one source of chemicals is a dominant source of chemicals in produced water or irrigated produce, or if there are any unexpected sources of chemicals. If any chemical warranted reduction of concentrations in produced water or irrigated crops, understanding the source(s) of chemicals would be useful in identifying control measures.

We identified the source(s) of most of the Chemicals of Interest through an extensive literature review, by reviewing the list of oil production additives reported to the CVRWQCB, and with the professional advice of Dr. Iliana Rhodes[1], a chemist with decades of experience in the oil industry and with chemicals used in oil production. Dr. Rhodes also has experience performing chemical analysis on produced water and other process streams associated with oil and gas production. She helped us fill data gaps in the published literature by bringing a working knowledge of industry practices in the use of oil field chemicals to the identification of uses of some of the Chemicals of Interest in oil field operations. We also identified many uses of the Chemicals of Interest in conventional petroleum production through searches of the National Library of Medicine's PubChem database, Schlumberger's Oilfield Glossary database, and general internet searches (which included chemical distributors). To identify the agricultural uses of these chemicals, the literature review process involved searching for possible associations with pesticides, fertilizer, or general agricultural applications. Searches were conducted of pesticide registration databases for pesticide ingredients maintained by the California Department of Pesticide Regulation (CDPR, 2019) and inert pesticide ingredients maintained by the USEPA (USEPA, 2019c). To identify commercial/consumer and other industrial uses of the Chemicals of Interest, we searched the National Library of Medicine's PubChem database and performed general internet searches when PubChem yielded limited information. Tables 2 and 3 summarize the results of these searches.

Table 2 reports uses of the 111 declared additives on the list of Chemicals of Interest as they are often used in conventional oil and gas production. Eleven of the chemical additives declared by the oil producers did not have a CASRN. A specific use in oil and gas production could not be found for 13 of the chemicals. Eight of the chemicals were elements that did not have specific uses by themselves but are thought to have been components of chemical mixtures used in oil and gas production. Of these elements, Dr. Rhodes reported that nickel and zinc could be used as an oxygen scavenger and anti-corrosion agent, respectively. For 51 of the chemicals, Dr. Rhodes was also able to identify a usage based on her professional experience; however, little other literature was identified that was able to confirm their specific use in petroleum production. The remainder of the chemicals were identified based on available literature. Their reported uses were consistent with production chemicals reported by Stringfellow et al. (2017) and use in petroleum production: biocides; corrosion and scale inhibitors; lubricants and

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[1] Ileana Rhodes, PhD [https://www.gsi-net.com/en/people/principals/ileana/ileana-a-l-rhodes-bio/file.html]

friction reducers; proppants; oxygen scavengers; agents for adjusting/controlling foam, emulsification, surface tension, viscosity, flocculation, and pH; and radionuclides as tracers and measurement aids. A few chemicals were identified as ingredients for specific processes from environmental summary plans that reported the general usage of these chemicals (drilling, well working over, system integrity fluid[1]). These summary plans did not report the usage of the specific chemical, but instead reported the usages of declared chemicals in a mixture used in a specific production system.

Table 3 presents a summary of reported uses of the Chemicals of Interest in agriculture and other applications. Eighty-three of the original 143 Chemicals of Interest have agricultural uses, including uses in pesticides, agrochemicals, fertilizer, and some are natural components of soil. Sixty-four chemicals were historically or are currently used as pesticide ingredients, with 15 of these chemicals currently registered for use in California (CDPR, 2019) and 34 approved as inert pesticide ingredients at the national level (USEPA, 2019c). We could not find a known agricultural use for 60 of the Chemicals of Interest. We were also able to identify other common uses for 112 of the 143 Chemicals of Interest; these uses cover a broad range of applications, from use in industrial manufacturing to consumer pharmaceuticals and personal care products. A number of these chemicals are used in processing materials or products, ranging from food, plastics, dyes, pharmaceuticals, and sanitizers. The two radionuclides that were identified as additives (Krypton-85 and Xenon-133) have medical imaging applications. Thorium-232 is used in thoriated welding electrodes and some ceramics (PubChem). No common uses could be identified for 22 of the 143 Chemicals of Interest. Of these 22 chemicals, Radium-228 has uses that are apparently limited to research. The remaining 21 chemicals also lacked data that could support an evaluation of chronic oral toxicity.

Of the 15 chemicals noted above as being registered for use in California by the Department of Pesticide Regulation (CDPR), 10 of the Chemicals of Interest are actively registered for agricultural use in California as pesticide ingredients, the others are approved for other uses, including uses in pools, in manufacturing setting, in treating lumber, and other industrial/institutional applications (CDPR, 2019). Only one of the Chemicals of Interest approved for agricultural use in California is specifically registered for use with food crops, and two are registered for use in drinking water systems. There are a similarly varied number of uses for chemicals approved by the USEPA as pesticide ingredients, which include use as surfactants, coating agents, buffering agents, and fragrance ingredients (USEPA, 2019c). Of the 34 Chemicals of Interest approved for use in pesticides by the USEPA, 16 are approved for use on food crops, while the remainder are restricted to non-food applications. There are also other ingredients such as “Polyoxyalklenes”, “Amine derivative”, and “Polyglycol ether” that are approved for use on food crops by the USEPA, but not currently registered in California.

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[1] Based on the environmental summary plans used as reference for these chemicals, system integrity fluid is a mixture of components that are used to control bacterial growth, fouling, corrosion, and scale build up.

There are 17 Chemicals of Interest that are produced by microorganisms, are naturally occurring in plants/soils, or are associated with fertilizers. The majority of these 17 chemicals include metals with known toxicities and environmental fate and transport factors that may affect their impact on food crops (e.g., antimony, mercury, uranium), described later in this literature review. There are other chemicals, such as nitrite, polyhydroxyalkanoates, steranes, and fulvic acid, that are produced by microorganisms or ubiquitous in organic soils and water.

Table 3 also reports general uses for 112 of the 143 Chemicals of Interest. These 112 Chemicals of Interest are used in a wide range of products and processes including consumer products, industrial products and processes, and medical applications. A few of the Chemicals of Interest are approved as food additives including: isoquinoline, which is used as a food flavoring/adjuvant (PubChem); ethylenediaminetetraacetates (EDTA) and sulfur dioxide, which are used as food preservatives (PubChem); and “POE (20) sorbitan trioleate” and sorbitan esters, which are used as emulsifying agents in preparing foods (Ankit Polymers Industries, Sorbitan Esters; Venus Ethoxyethers, 2020).

The Chemicals of Interest have a wide range of uses both within and outside of petroleum production, and the presence of most of these chemicals in produced water may come from more than one source. More than half of the Chemicals of Interest have known agricultural applications and, accordingly, may be present in any irrigated crop. We also found that some of the Chemicals of Interest are used as food additives and occur naturally. Several of the Chemicals of Interest appear to be used only in industrial processes or in petroleum production. We were unable to identify specific petroleum-related uses or other common uses for 21 of the Chemicals of Interest. These were also chemicals identified in Task 1 as lacking chronic oral toxicity data.

5.0 REVIEW OF CONCENTRATION DATA OF THE CHEMICALS OF INTEREST IN PRODUCED WATER USED FOR IRRIGATION AND OTHER ENVIRONMENTAL MEDIA

In accordance with the Scope of Work for Task 2, GSI collected published information on the levels of the Chemicals of Interest in soil, air, groundwater, surface water, and food crops. Additionally, an important purpose of this section is to present an evaluation of the observed concentrations of the Chemicals of Interest in produced water used to irrigate food crops in the San Joaquin Valley. To that end, the evaluation of produced water quality data includes a comparison of concentrations of the Chemicals of Interests in produced water to Water Quality Objectives (WQOs) that are regulated by the CVRWQCB and also to concentrations of the same chemicals in surface and groundwater that could be used for agricultural irrigation. As part of this evaluation, we present a discussion of the general authorities and tools available to the CVRWQCB to regulate water quality and in the San Joaquin Valley, as well as a discussion of how these authorities and tools are used to regulate produced water reused for agricultural irrigation.

One of the objectives for the review and evaluation of the concentration of the Chemicals of Interest in other sources of irrigation water, soil, and air was to provide background information for the interpretation of the produce sampling results presented in the Task 3 report. Among the pertinent background questions was whether the Chemicals of Interest were present in blended irrigation or treated produced water (also referred to as effluent water in this report) at levels higher than they are found in other irrigation water. The answer to that question could alert us to look at the crop sampling data, collected under Task 3, more closely to see if higher levels of chemicals in blended produced water corresponded to higher levels of the same chemical in crops irrigated with blended produced water. A second question was whether chemicals present in produced water were also present in other environmental media that could have been a source of the chemicals detected in the crop samples. Seeing chemicals in produced water that were not seen in other environmental media might have suggested taking a closer look at crop data for any such chemicals in produced water. We also wanted to know if the Chemicals of Interest were typically present in the same crops grown in other locations, and, if so, were the chemical levels in crops grown in other areas present at levels comparable to those seen in this study? Seeing higher levels of chemicals in crops irrigated with produced water than were seen in crops grown in other regions could also trigger concern that produced water was the source of such chemicals. We found that test results and other relevant information are available on all of these topics; and while the available information was useful, it certainly was not complete. We provide additional discussions about the observed concentrations in food crops sampled in this project beyond those presented in the Task 3 report due to the potential relationships between the concentrations of the Chemicals of Interest in various environmental media and the concentrations of the Chemicals of Interest observed in the crops sampled as part of this project. For a few chemicals, we discuss whether differences between chemical concentrations in produced water used for irrigation and other suitable sources of irrigation water explain differences between the concentrations of chemicals in food crops sampled in this project and concentrations of chemicals in food crops published in the literature. We also present a review of the standard laboratory analytical methods that are available to measure concentrations of the Chemicals of Interest. The review of these analytical methods was conducted to determine if there are methods available to measure Chemicals of Interest in water that are not currently being monitored in produced water used for irrigation.

The remainder of this section in the report is divided into seven subsections. In Section 5.1, a discussion of the administration of produced water reused for agricultural irrigation in the San Joaquin Valley is presented. This discussion addresses the various beneficial uses of water that the CVRWQCB regulates (Table 4) and protects through its Water Quality Objectives (WQOs). The WQOs applicable to the Chemicals of Interest and their respective water concentrations are summarized in Table 5. Section 5.2 presents a discussion of the observed concentrations of the Chemicals of Interest in produced water and a comparison of these concentrations to WQO concentration levels. The sampling locations of treated produced water (also called effluent) and treated produced water blended with other irrigation water sources (referred to as blended produced water) are shown in Table 6. Table 7 and Table 8 report statistical summaries of the concentration of the Chemicals of Interest monitored in effluent and blended produced water, respectively. Also reported in Tables 7 and 8 are summaries of the comparisons of the observed concentrations of the Chemicals of Interest to WQO concentration levels. In addition, Table 9 compares the frequencies of detection and detected mean concentrations of the Chemicals of Interest between effluent and blended produced water samples. In section 5.3, we present a summary of published information on the levels of the Chemicals of Interest in several environmental media including soil, air, groundwater, surface water, and food other than the crops sampled as part of this study (Table 10). Section 5.4 includes a comparison of concentrations of chemicals detected in produced water to concentrations detected in surface water and groundwater. Section 5.5 includes a review of the levels of Chemicals of Interest detected in the crops sampled under Task 3 and presents a discussion of the levels detected in crops in relation to the levels of the same chemicals detected in irrigation waters. One of the things we learned over the course of collecting and reviewing the many studies of the levels of the Chemicals of Interest in various environmental media was that analytical methods are not available for many of the Chemicals of Interest, and this point is discussed in Section 5.6. Finally, Section 5.7 presents a summary and discussion of the findings presented in this section of the report.

5.1 Water Quality Requirements for the Discharge of Produced Water that is used for Agricultural Irrigation

The CVRWQCB regulates the discharge of wastes to San Joaquin Valley surface- and groundwaters (also referred to as receiving waters) to protect their quality and to enable existing and future beneficial uses and to minimize degradation. The primary regulatory document the CVRWQCB relies upon to perform this responsibility is the *Water Quality Control Plan for the Tulare Lake Basin* (3rd edition, revised May 2018; also referred to as the “Basin Plan”). The Basin Plan designates the beneficial uses (BUs) of the receiving waters within the Tulare Lake Basin and specifies water quality objectives (WQOs) to protect those uses. In the study area, the Basin Plan designated the BUs of surface waters and groundwater, that include, but are not limited to, municipal and domestic water supply (MUN), agricultural supply (AGR), industrial process supply (PRO), industrial service supply (IND), and water contact recreation (REC-1) (see Table 4). The California Water Code defines WQOs as “…the limits or levels of water quality constituents or characteristics which are established for the reasonable protection of beneficial uses of water or the prevention of nuisance within a specific area.” (WAT § 13050). Regarding WQOs:

1. WQOs are applied to regulate controllable water quality factors.
2. WQOs are achieved primarily through the adoption of waste discharge requirements and enforcement orders.
3. WQOs may be in numerical or narrative form.

The Basin Plan also contains specific effluent limits for discharges of oilfield produced water to receiving waters. These are discussed in more detail below.

The Basin Plan is not self-implementing; rather its requirements are implemented through the adoption by the CVRWQCB of waste discharge requirements (WDRs) for specific discharges. WDRs include effluent limits, discharge specifications, and receiving water limits that implement Basin Plan requirements. The CVRWQCB has adopted WDRs for the discharge of produced water to canals in the Tulare Lake Basin. The canals distribute produced water that is typically blended with surface water and groundwater that is then used to irrigate crops for human consumption.

5.1.1 Water Quality Objectives in The Basin Plan Applicable to the Reuse of Produced Water for Agricultural Irrigation

The Basin Plan contains a narrative WQOs stating that receiving waters shall not contain chemical constituents in concentrations that adversely affect beneficial uses. It specifically addresses issues related to toxicity, chemical constituents, radionuclides, other requirements to protect beneficial uses for surface waters and groundwaters.

Under the Basin Plan, toxicity is addressed in a few ways. The Basin Plan states that waters shall be maintained free of toxic substances in concentrations that produce detrimental physiological responses in human, plant, animal, or aquatic life associated with designated beneficial uses. The toxicity WQO applies regardless of whether the toxicity is caused by a single substance or the interactive effect of multiple substances. Discharges of wastes may not cause receiving waters that have MUN designated BUs to contain concentrations of chemical constituents in excess of the maximum contaminant levels (MCLs) as specified in 22 CCR § 64444. The CVRWQCB can also apply more stringent limits to protect beneficial uses of the surface and groundwater. Radionuclides, similarly, have MCLs stated as numeric WQOs. There is also a narrative WQO for radionuclides that states that they are not present in waters at concentrations that are deleterious to human, plant, animal, or aquatic life, or that result in the accumulation of radionuclides in the food web to an extent that presents a hazard to human, plant, animal or aquatic life.

The CVRWQCB has set both narrative and numeric limits in its WDRs for the discharge of produced water to receiving waters. Under the narrative requirements, the discharge of produced water for irrigation cannot degrade the water quality of other sources of water beyond that required to maintain their designated BUs. This narrative water quality requirement does not set strict effluent limits for the water quality of irrigation water that contains produced water. For example, it is permissible to discharge wastewaters with chemical concentrations above MCLs into drinking water aquifers as long as the discharge doesn't degrade the aquifer beyond requirements necessary for its use as a drinking water source. The numeric effluent limits in the WDRs include electrical conductivity, chloride, and boron, and oil and grease.

Numeric limits for electrical conductivity, chloride, and boron are meant to protect beneficial uses that may be impacted by salt and boron. Generally, the water quality limits for electrical conductivity and chloride in both treated produced water and blended produced water are 1,000 μΩ/cm and 200 mg/L, respectively. For most of the treated produced water and all blended produced water, the water quality limit for boron is 1.0 mg/L (annual average); this is the same as set out in the Basin Plan. The CVRWQCB can set higher effluent limits to facilitate beneficial use (including irrigation), so long as it does not cause an exceedance of a WQO. For some treated produced water, boron concentrations are allowed to be higher than 1.0 mg/L (annual average), but boron concentrations in blended produced water are not allowed to exceed 1.0 mg/l. In WDR R5-2012-0058, Discharge 001 (unblended treated produced water) has an annual average effluent limit for boron of 1.3 mg/L. Historically, other WDRs have also allowed treated produced water to contain boron above 1.0 mg/L. For example, R-2007-0170 allowed Discharge 001 to contain up to 1.6 mg/L. It should be noted that the boron water quality limits are set to protect plants that are sensitive to the phytotoxic effects of boron. The Basin Plan, however, also requires that any effluent limit also protects human health. Any higher limits set by the Water Board for boron in unblended treated produced water take into account the amount of water that is used for irrigation and the sensitivity of the crops that are intended to be irrigated with the respective blended produced water.

The CVRWQCB must comply with the Basin Plan’s implementation of the State’s Antidegradation Policy (State’s Resolution No. 68-16: Statement of Policy with Respect to Maintaining High Quality of Waters in California) when setting limits. The Antidegradation Policy states that where waters have higher quality than necessary for beneficial use, the quality is to be maintained at that high level unless it can be demonstrated that the change is to the maximum benefit to the people of the State. The CVRWQCB can authorize some degradation of high-quality waters by discharges of waste if the following conditions are met: the degradation maximizes benefit to the people of the State; the degradation does not unreasonably affect present and anticipated beneficial uses; and related WDRs require implementation of the best practicable treatment/control that assures pollution or nuisance will not occur and the highest water quality is maintained, consistent with the maximum benefit to the people of the State.

5.2 Evaluation of Water Quality Sampling of Produced Water Used for Agricultural Irrigation

Evaluating the health risks posed by chemicals in irrigation water would ideally have been performed by comparing concentrations of Chemicals of Interest in blended produced water to concentrations that would be considered safe for irrigating food crops. As previously noted, however, there are no published water quality standards for irrigation water. In theory, it would be possible to calculate risk-based irrigation water quality standards using a two-step process, including: 1) using published crop consumption levels and toxicity limits for chemicals to calculate chemical-specific concentration limits for each chemical in each crop; and 2) calculating the concentration of each chemical in irrigation water that translates to the concentration limit of each chemical in each crop. As is discussed in later sections of this report (Sections 6-8), however, there are too many site-specific factors and too many gaps in the understanding of chemical fate and transport, plant uptake, and chemical translocation within a plant to support the second step of that process.

In the absence of agricultural water standards or risk-based concentration levels for irrigation water designed to protect human health, we compared the concentrations of the Chemicals of Interest in blended produced water to concentration limits associated with WQOs and to other risk-based concentration limits calculated for drinking water, when WQO concentration limits were not available. Most of the WQO concentration levels we used in evaluating treated produced water and blended produced water are the same as drinking water Maximum Contaminant Levels (MCL), with the exception of boron[1]. This evaluation had the purpose of identifying chemicals that might be present at elevated levels in blended produced water and, thus, might be elevated in crops irrigated with this water. We also present summaries of the concentration of the Chemicals of Interest in treated produced water, with the understanding that this water is not directly used as irrigation water. As such, we restrict the comparison of the reported concentration levels in treated produced water to the WQO concentration limits that are used in the regulation of the water. The concentrations of chemicals in treated produced water provides us a point of reference to understand which water source—produced water or blending water—contributes most to the observed concentration levels in blended produced water.

When WQO concentration limits were not available for the Chemicals of Interest monitored in blended produced water, we compared the observed concentrations of chemicals in blended produced water to toxicity risk-based concentration limits assuming that water considered safe to drink would also be safe to use as irrigation water. Because it is difficult to gauge the degree of health risk implied by chemical toxicity values without an understanding of potential exposures to the chemicals, we decided to apply the assumption that the irrigation water was consumed as drinking water with the understanding that such an exposure assumption would likely overstate the exposure from crop consumption. Closer scrutiny is subsequently applied to the chemicals identified as potentially posing a health hazard by virtue of their concentration in blended produced water exceeding the estimated screening level.

Of the 143 Chemicals of Interest, 47 of the Chemicals of Interest are represented by the target analytes; some of these Chemicals of Interest are compounds measured by total metals in water rather than for the specific form listed as a Chemical of Interest (e.g., antimony for antimony trioxide, lithium for lithium chlorate, copper for copper sulphate pentahydrate, etc.).

Aniline, 2-naphthylamine, and acrylamide have been added to the list of reported analytes related to the Chemicals of Interest reported in Table 5, even though they are not specifically named Chemicals of Interest. Aniline and 2-naphthylamine were added to the table because they are members of the group of chemicals known as “aromatic amines,” which was identified as used in oil production. It should be noted that 2-naphthylamine is

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[1] Boron doesn’t have an MCL; the concentration limit in blended produced water was set at an annual average of 1 mg/L to protect against its phytotoxic effects. The WQO regulatory limits for unblended treated produced water ranges between 1.0 and 1.6 mg/L (as an annual average), discussed in more detail in Section 5.1.

no longer used or produced (HSDB, 2019), and aniline is readily biodegradable in water (ECHA, Aniline). Acrylamide was evaluated during Task 1, and not initially included on the list of Chemicals of Interest, because it is readily biodegradable in water. Literature identified here during work conducted under Task 2 reported that residual acrylamide in polyacrylamide soil amendments similar to some of the Chemicals of Interest can be taken up by plants (Bologna et al., 1999; Mroczek et al., 2014). It was for this reason that it was included in the review of the treated produced water and blended produced water sampling data.

5.2.1 Drinking Water Toxicity Risk-Based Screening Levels for Chemicals without Maximum Contaminant Levels or Water Quality Objectives

Drinking water screening values used in this evaluation were based on the toxicity values developed during Task 1, which are the lowest available published toxicity values for each of the Chemicals of Interest. To estimate drinking water consumption, we used point estimates of consumption provided in the OEHHA *Air Toxics Hot Spots Program Risk Assessment Guidelines Technical Support Document for Exposure* (OEHHA, 2012). From this guidance document, we used average water consumption for children aged 2-9 years (26 mL/kg/day) and adults (18 mL/kg/day), depending on whether the toxicity value was associated with a cancer outcome, or not. For outcomes associated with cancer, we assumed a lifetime exposure, and hence an average adult exposure. For non-cancer outcomes, we assumed a shorter chronic exposure period associated with children aged 2-9 years. Exposures estimated for children are also protective for reproductive/developmental effects in pregnant women due to the higher water consumption rate for children.

While guidance for risk-assessments in the OEHHA guidance document prescribes an approach that uses estimates of both the mean and the 95th percentile of exposure, the 95th percentile represent drinking water exposure for those living/working in hot climates or who are highly physically active (OEHHA, 2012). Exposure scenarios for those who are highly active or who are living/working in hot climate, however, are not applicable to a hazard assessment of irrigation water used for irrigating food crops. As such, we have only used mean estimates of drinking water exposure. Additionally, we did not address drinking water exposures for those less than 2 years old because mean estimates in the guidance document represent drinking water exposures associated with reconstituted formula.

The risk-based screening concentrations in water were calculated using Equation 1, below:

$$Screening\ Concentration = \frac{Toxicity\ Value\ Dose}{Drink.Water\ Consump.} = \frac{Tox.Val. * Body\ Weight}{Drink.Water\ Consump.Level * Body\ Weight} \qquad \text{Equation 1}$$

Table 5 reports the MCLs, the boron WQO equal to 1 mg/L, and the screening concentrations based on Equation 1 used to evaluate chemicals without MCLs or other WQOs.

5.2.2 Results of the Evaluation of Water Quality Sampling of Produced Water Used for Agricultural Irrigation

Samples of treated produced water and blended produced water relevant to this project were collected from the nine sampling locations listed in Table 6. The treated effluent water and the blended produced water have been sampled since 1967; but the treated effluent data summarized in Table 7, and the blended produced water data summarized in Table 8 were collected between 1985 and September 2019. Data prior to 1985 did not include any of the Chemicals of Interest. Figure 2 shows the number of effluent and blended produced water sample events by calendar year and illustrates the fact that the majority of the water samples summarized in Tables 7 and 8 were collected in recent years.

In Table 7 and Table 8, we report basic statistical summaries that include the minimum detected concentration, mean concentration, and maximum of the detected values. The mean concentration reported in these tables were estimated from detected values. Given that detection and reporting limits have changed over the years in the supporting datasets, using substitution methods (e.g., assuming values reported as non-detected were half the detection limit) to estimate a mean concentration would not have been informative to readers. The tables also show the number and proportion of samples that exceeded the concentration level associated with the WQO.

Concordant with how the WQO for radium is evaluated, the combined concentration of Ra-226 and Ra-228 isotopes was reported in some of the water quality sampling results. In the remainder of the sampling results, however, Ra-226 and Ra-228 were reported separately. In Tables 7 and 8, we reported the added concentrations of Ra-226 and Ra-228 when they were reported separately so the sum could be compared to the WQO. Summaries of these later summed concentrations are shown as separate table entries from those that were already reported as summed concentrations in the analytic results. Additionally, when a reported concentration of radium was less than zero, we assumed this indicated that the concentration of radium was below the detection limit. While this assumption is not how radionuclide results are typically assessed, the standard method requires an estimate of the counting error, which was not provided in the data tables. Without estimates of the counting errors, we are unable to control for negative bias in the radionuclide concentrations. By implementing the assumption that negative values were below the detection limit, the averages that we calculated using only detected values provided more conservative estimates of radium concentration in produced water.

Two rows of data are presented in Tables 7 and 8 for boron. The first row is like the data presented for all the other chemicals listed in Tables 7 and 8—a summary and evaluation of all the individual samples collected between 1985 and 2019[1]. The second rows of boron results in Tables 7 and 8 are a presentation of annual average boron concentrations at the various sampling locations collected over that period. The annual average concentrations were evaluated because the WQO is expressed as an annual average concentration. Unlike other analytes where the reported mean value is calculated from only the detected values, the annual average for boron is calculated by using a substitution method where ½ the detection limit is used to substitute for results reported as non-detect.

As shown in Table 9, the mean concentrations for the majority of the chemicals listed in Tables 7 and 8 were lower in blended produced water than in treated produced water. The mean concentrations of most of the chemicals detected in treated produced water were higher than the mean concentrations of chemicals detected in blended irrigation, but the ratios of the means were roughly two or less. As can be seen in Table 9, the inorganic chemicals with the much higher mean concentrations in treated produced water were manganese, chromium VI, and mercury. Four polycyclic aromatic hydrocarbons (including acenaphthene, chrysene, phenanthrene and pyrene) were also detected at a higher mean concentration in treated produced water than in blended produced water, and the mean concentration of 1,4-dioxane in treated produced water was nearly double (1.7 times higher) the mean level in blended produced water.

The mean concentrations of beryllium, cobalt, copper, lead, nitrite, and vanadium were higher, however, in blended produced water than in treated produced water; and the frequency of detection of these chemicals was higher in blended produced water than in treated produced water. Other than these six chemicals, there was no systematic pattern in the frequency of detection. Some chemicals had higher detection frequencies in treated produced water than in blended produced water, and some chemicals had the reverse pattern.

While there were differences for some chemicals in the mean concentrations and frequencies of detections of chemicals in treated produced water and blended produced water, there were few consistent exceedances of the WQOs in either treated produced water or blended produced water. Arsenic exceeded the WQO in 75% of treated produced water samples and 53% of blended produced water samples. The boxplots of the detected arsenic concentrations in treated produced water and blended produced water presented in Figure 3 illustrate the higher mean of arsenic concentrations found in the treated produced water and the higher upper range of the arsenic levels found in the treated produced water.

As discussed later in this section (Section 5), concentrations of arsenic in blended produced water are similar to other conventional sources of water in the Central Valley that are used for food crop irrigation (see discussion on Fujii and Swain (1995) and CEDEN (2020)). Given the similarities between arsenic concentrations in blended

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[1] Over these 35 years, sampling data were not available for 1990 and 1993.

produced water and in conventional irrigation water, there is no evidence of a difference in the level of exposure to blended produced water or other irrigation water in the San Joaquin Valley. This observation is consistent with the fact that among the 13 crops sampled in Task 3, carrots was the only crop in which arsenic was detected; and the detected levels were below reporting limits (i.e., detected at trace levels).

The only other analytes that exceeded the current narrative WQOs or current Basin Plan WQOs in more than 10% of samples were boron in treated produced water (16 of 66 annual sample averages = 24% exceedance rate – see Table 7) and nitrite in blended produced water (1 of 5 samples = 20% exceedance rate – see Table 8). As discussed above, the effluent limit for boron can be set higher than the limit in the Basin Plan by the CVRWQCB to facilitate beneficial use.

As allowed by the Basin Plan to facilitate reuse, some of the most recent WDRs (R5-2012-0058, R5-2012-0059, R-2015-0127, R5-2019-0043), have effluent limits for boron that are set higher than the numeric limits in the Basin Plan. Under WDRs R5-2012-0058 and R5-2012-0059, the effluent limits are set at an annual average concentration level of 1.3 mg/L. In 2016, WDR R5-2016-0093 amended WDR R-2015-0127 and set the effluent limit for 'Discharge 001 - Section 23 Treatment Facility' to 1.5 mg/L. We compared, below, the treated produced water sample results of annual average boron concentrations that exceeded the Basin Plan boron WQO of 1.0 mg/L with these higher effluent limits outlined in the WDRs.

Six of the 16 reported exceedance of the Basin Plan boron effluent limit of 1.0 mg/L were measured under the current WDRs and do not represent exceedances of the prescribed effluent limits. Three of the sample results are attributable to WDRs R5-2012-0058 and R5-2012-59 and are below 1.3 mg/L. 'Discharge 001 - Kern River Station 36' reported a 2016 annual average boron concentration of 1.2 mg/L. In 2012 and 2019, 'Discharge 001 - Kern Front No. 2 Treatment Facility' reported annual average boron concentrations of 1.25 mg/L and 1.01[1] mg/L, respectively. The other three reported annual averages that exceeded 1 mg/L were at 'Discharge 001 - Section 23 Treatment Facility' with reported concentrations of 1.03 mg/L in 2016, 1.05 mg/L in 2017, and 1.05 mg/L in 2019[2]; these reported concentrations do not exceed the effluent limit of 1.5 mg/L set out in the WDR amendment R5-2016-0093. One earlier reported concentration at the 'Quinn Lease – Pond No. 7' was reported in 2007 with annual average boron concentration of 1.1 mg/L; this represents an apparent exceedance of the effluent limits set in WDR 98-205 of 1.0 mg/L.

We were unable to conduct a similar audit of the remaining exceedances between 1986 and 2003 as electronic copies of the earlier WDRs were not available for our review. The remaining nine reported exceedances ranged between 1.05 and 2.2, with all but two being less than 1.3 mg/L. In 1986 and 1988, the annual average boron concentrations in 'EFF

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[1] 2019 estimates for annual average boron concentration are based on partial year reporting
[2] 2019 estimates for annual average boron concentration are based on partial year reporting

- 001 (Discharge to Reservoir B)' were 2.2 and 1.4 mg/L and were sampled under WDRs 85-063 and 85-065, respectively. In addition, the annual average boron concentration in blended produced water only exceeded the current Basin Plan effluent limit of 1.0 mg/L in two samples, collected in 1985 and 1986. These exceedances were reported in 'Receiving Water - Sample Station #2 (Outfall from Reservoir B)' and sampled under WDR 85-063.

Table 8 shows that 20% of blended produced water samples exceed the MCL for nitrite. A review of the available environmental water quality data, toxicological literature, and use of nitrite by plants suggest that the observed nitrite concentrations pose little or no health hazard. When compared to other environmental water quality data, typical concentrations of nitrite in surface waters not impacted by agricultural activities are less than 0.3 mg/L, while concentrations up to 8.7 mg/L have been reported in waters that have been impacted by agricultural activity (USEPA, 1990). Additionally, nitrite in untreated groundwater used for drinking water in Kern County is detected at a frequency of 0.92 with a mean of 3.5 mg/L and range of 0.07 – 12.1 mg/L (GAMA, USGS).

There were only two detections of nitrite in five samples of blended produced water with reported concentrations of 0.8 mg/L and 19 mg/L. In contrast, nitrite was only detected in a single sample of treated produced water, and the detected level was 1 mg/L. Typical concentrations of nitrite in surface waters not impacted by agricultural activities are less than 0.3 mg/L, while concentrations up to 8.7 mg/L have been reported in waters that have been impacted by agricultural activity (USEPA, 1990). Additionally, nitrite in untreated groundwater used for drinking water in Kern County is detected at a frequency of 0.92 with a mean of 3.5 mg/L and range of 0.07 – 12.1 mg/L (GAMA, USGS).

The MCL used as a comparison value for blended produced water is based on the epidemiological evidence that infants presented with methemoglobinemia when fed baby formula mixed with water containing nitrate concentrations greater than 10 mg/L (USEPA, IRIS; Walton, 1951). The NOAEL of 10 mg/L identified in the Walton (1951) study is also supported by more recent studies (NAS, 1977; Winton, 1971; Calabrese, 1978). In infants, nitrate is more likely to be converted to nitrite by nitrate reducing bacteria in the gut than in older children and adults, as they have lower levels of methemoglobin reductase activity (Power et al., 2007). There was no evidence of methemoglobinemia in children between 1-8 years old who consumed water with nitrate concentrations up to 111 mg/L (Craun et al., 1981). Blended produced water is also not directly consumed and nitrite is expected to be metabolized by plants as a source of essential nitrogen for growth (Yoneyama et al., 1980; Breteler & Luczak, 1982; Ibarlucea et al., 1983., Agüera et al., 1990; as discussed in Section 6). Overall, the evidence suggests that nitrite in blended produced water poses little or no health hazard: nitrite was only observed in one sample at concentrations above the MCL but appears to be related to water used for blending; the major risk of methemoglobinemia is for children less than one year old, but nitrite in blended produced water will—at least in part—be metabolized by plants and converted into amino acids and used for photosynthesis.

5.3 Chemicals of Interest in Soil, Air, Groundwater, Surface Water, and Food

As discussed above, GSI collected data on the concentration of Chemicals of Interest in soil, air, groundwater, surface water, and food in accordance with the Scope of Work for Task 2. These data are reported in Table 10 and illustrate a couple of key points about the data available on the levels of Chemicals of Interest in the environment. One is the fact that environmental measurement data is not widely available for many of the chemicals selected as Chemicals of Interest for purposes of this study. Many of the Chemicals of Interest are not specifically addressed by environmental regulatory programs. Accordingly, they are not part of environmental testing programs and tend not to be analytes searched for in routine monitoring programs. Test results for many other chemicals are missing because analytical methods are not available for many of the Chemicals of Interest. A second key point is that—where data were available—the observed concentrations of the Chemicals of Interest in blended produced water are generally similar to the concentrations observed in surface water, municipal groundwater, and other groundwater sources that are likely suitable for agricultural irrigation. Only a few differences between concentrations in blended produced water and the range of concentrations observed in surface and groundwaters were noted. These differences do not point to any chemicals being present in blended produced water at levels notably higher than had been seen in other water sources, and the observed concentrations were below water quality standards. For phenanthrene, whose concentration was higher in blended produced water than reported in surface water, fate and transport factors would cause significant attenuation of the chemical’s phytoavailability (discussed in Section 8). A third key point illustrated by this research is that the Chemicals of Interest detected in crops sampled as part of this project, and in the blended produced water, are reported in the literature as being present in soil, air, surface water, groundwater, and other crops. The Chemicals of Interest detected in the crops sampled as part of this study are found throughout the environment and were not uniquely detected in those that are either irrigated with conventional or blended produced water.

Although the focus of this project is the potential accumulation of chemicals from irrigation water in crops, it is important to recognize that irrigation water is not the only potential source of chemicals detected in crops. The potential for deposition of chemicals in the air onto crops and the uptake of chemicals present in soil for reasons other than the fact that they were carried there by irrigation cannot be ignored. In addition, potential differences between fields in the contribution of these potential sources of chemicals in produce to levels seen in crops cannot be overlooked.

While studies discussed later in this report have shown that chemicals can deposit onto food crops from the air, the kind and amount of information needed to estimate the fraction of each chemical detected in a crop that came from aerial deposition is not available. The data presented in Table 10 shows that many of the Chemicals of Interest are known be present in air, even if the presence and specific concentration of each chemical in the air above the fields from which the samples collected as part of this study are not known. Because of such factors as proximity of fields to sources of chemicals in the air and difference in wind patterns at different fields, it is possible that different fields will have different levels of aerial deposition of any specific chemical.

While soil uptake of chemicals appears to be much better understood than plant uptake following aerial deposition, our understanding of plant uptake from soil does not support the quantification of the fraction of any specific chemical detected in a crop that would have originated from soil. Soil properties that can affect chemical uptake can vary within relatively short distances and between agricultural fields. The concentrations of chemicals in soil can also vary within short distances and between agricultural plots as a result of differences in such factors as soil type and agricultural practices. Differences in concentrations of chemicals in soil and soil structure are likely attenuated by management practices that tend to manage soil for optimal crop production and, thus, tend to reduce differences between fields growing the same crop. Nonetheless, differences in soil conditions between fields are still to be expected.

The evaluation of the variation of chemical concentrations in crops and the attribution of the differences in concentrations to the irrigation with blended produced water (i.e., “treated” samples) or with other irrigation water (i.e., “control” samples) is based on the assumption that the only difference between the “treated” and “control” samples is the use of blended produced water. As discussed above, however, differences in aerial deposition and soil conditions between fields from which crops were sampled could affect the concentrations of chemicals measured in crops. Additionally, variations in the chemical content of irrigation water coming from sources other than treated produced water are another potential source of variation in the concentration of chemicals measured in crop samples collected as part of this study.

In the Task 3 report, we compared levels of chemicals detected in crops sampled as part of this study to levels of chemicals reported in the literature for the same crops and chemicals. The fundamental finding of the Task 3 crop testing was that there were no significant differences between “treated” and “control” crops. While the mean or median concentration in 5 of 89 sample comparisons were statistically higher for crops irrigated with produced water ($p < 0.05$), these differences were small and not of toxicological significance. In addition, the concentrations of the five metals were not higher than those seen in the same crops found in the U.S. marketplace. These five chemical/crop differences between “treated” and “control” crops were observed for barium and zinc in almonds, and for strontium in garlic, grapes, and lemons. Some of that discussion is summarized below to facilitate the discussion of the presence of Chemicals of Interest in various environmental media, including food crops. For some crop-chemical combinations, we were able to identify studies for the same crop-chemical combinations for crops grown in other geographic areas. The concentrations reported in the literature helped us understand if the levels of chemicals detected in this study were typical of levels seen in the crops grown in other geographic areas. In a few cases, concentrations reported in the Task 3 report differed from concentrations reported in the literature. Factors that may have played a role in these differences are also discussed in later sections of this report.

Below, we report comparisons and related discussions about similarities and differences observed in the reported concentrations of the Chemicals of Interest in the published literature and publicly available databases when compared with concentration observed in blended produced water and food crops sampled as part of this study. While we were also tasked with collecting concentration data of the Chemicals of Interest in soil and air, we were unable to make comparisons similar to those reported for irrigation water and food crops because these data were not collected in the fields where food crops were sampled as part of this study.

5.4 Comparison of Produced Water Quality Data with Surface Water and Groundwater Concentrations

The surface water and groundwater concentration data for the Chemicals of Interest (Table 10) provide another point of reference for evaluating the degree to which Chemicals of Interest may be present at elevated levels in blended produced water. We compared the levels in the blended produced water to levels measured in local sources of irrigation water, local groundwater, and local potable water supplies, for example. Water quality monitoring data was not uniformly available for all sources. In some cases, concentration data from other locations (e.g., national) are presented to provide perspective. Some of the comparisons discussed below reveal a higher concentration or higher frequency of detection of some chemicals in the blended produced water than in the water to which the comparison is being made. In such cases, we compared the levels in the blended water to drinking water standards to provide some sense of the significance of the concentrations detected in the blended produced water. In some cases, fate and transport factors that affect accumulation in plants is discussed as an approach to evaluating the significance of a chemical’s presence in blended produced water.

We identified water quality programs and other literature that reported concentrations for some of the Chemicals of Interest in both surface and groundwater. The data reported here represents surface and groundwater sources in the San Joaquin Valley that may be used for irrigation or as drinking water sources. Surface water data reported in Table 10 were collected from the Kaweah and Tule Rivers, both of which are used as sources of irrigation water. Surface water data was extracted from the CVRWQCB’s California Environmental Data Exchange Network (CEDEN), which reports data from many monitoring projects. The surface water data for the Kaweah and Tule rivers reported in Table 10 is from the Surface Water Ambient Monitoring Program (SWAMP). We also report summaries of Kern County groundwater data compiled by the USGS, California Department of Public Health, and CVRWQCBs as part of the Groundwater Ambient Monitoring and Assessment Program (GAMA). This dataset provides water quality analysis results for untreated samples collected from municipal supply wells that are analyzed for chemical, physical, and biological properties. Some of the surface water and groundwater water quality data were identified from various government agency publications, such as ATSDR Toxicological Profiles, and peer reviewed literature. Most of the data from the agency publications and peer reviewed literature reported surface water and groundwater concentration data at the national level, or in other states.

The review of the relevant literature and available water quality data identified concentration data for 44 analytes. These 44 analytes represent 66 of the 143 Chemicals of Interest because many of the Chemicals of Interest are metal-salts, compounds of metals, or belong to a class of chemicals that are measured as technical mixtures. For example, measurement of total lithium captures the potential presence of the six forms of lithium listed as Chemicals of Interest (i.e., Lithium, Li-carbonate, Li-chlorate,Li-chloride, Li-hydroxide, Li-hypochlorite). There are other similar examples of one analyte representing multiple Chemicals of Interest: antimony and antimony trioxide, nickel and nickel sulfate, and technical mixtures of ethoxylated alkylphenols for various ethoxylated alkylphenol Chemicals of Interest, to name a few.

Some of the organic Chemicals of Interest were only reported for surface waters. It is unlikely that the published reporting of chemical concentrations in surface water, but not in groundwater, is an indication that the chemical is absent from groundwater. It is more likely this is related to the general paucity of published groundwater data investigating organic compound concentrations that fits the selection criteria of this literature review.

Generally, the chemicals observed in blended produced water were detected at similar concentrations to those observed in surface water, municipal groundwater, and other groundwater sources. In comparing the concentrations of the Chemicals of Interest in blended produced water to those in surface water, we observe only a few notable differences that warranted additional evaluation: arsenic, boron, cobalt, copper, manganese, nitrite, phenanthrene, and radium. Similarly, when we compared concentrations of the Chemicals of Interest in blended produced water to municipal groundwater and other groundwater data, we noted that 1,4-dioxane, antimony, beryllium, cobalt, copper, and mercury were present at higher levels in blended produced water.

5.4.1 1,4 Dioxane

1,4-dioxane was detected in 22% of blended produced water samples with mean of detected samples equal to 0.75 µg/L [range: 0.52-0.98], but not in any Kern County municipal groundwater data collected by the GAMA program (GAMA, USGS). 1,4-dioxane did not, however, exceed the toxicity screening values discussed in Section 5.2. Additionally, concentrations of 1,4-dioxane in blended produced water are below California's notification level of 1 µg/L. Given that 1,4-dioxane was not detected in any of the Task 3 samples irrigated with blended produced water and the observed concentrations in blended irrigation are low, it does not appear that dioxane is impacting the quality of food crops irrigated with this water.

5.4.2 Antimony

Antimony was detected in 44% of blended produced water samples with a mean of detected levels of 1.36 µg/L [range: 0.1–11]. In groundwater used for municipal drinking water, it was detected at lower frequencies but with higher detected values. The California Department of Public Health (CDPH) aggregated raw water quality data from 918 groundwater wells used for drinking water systems serving 15 or more connections or more than 25 people per day. Antimony was detected in 27% of these wells with a sample detection frequency of 9%. The mean of detected samples was 4.7 µg/L [range: 0.002–62] (GAMA, CDPH). Making direct comparisons between sample detection frequencies, however, is not possible because of differences in reporting conventions with regard to reporting and detection limits. In the blended produced water data, estimated concentrations are provided when sample results are below the reporting limit but above the detection limit. In the CDPH data, all results below the reporting limit are indicated as such, but in 41% of those results, a reporting limit is not provided. Moreover, the reporting limits in the CDPH data span a range from 0.001 µg/L to 100 µg/L. In contrast, the reporting limit for the blended produced water is near uniformly set at 2 µg/L.

A more equal comparison between the blended produced water and the CDPH drinking water source data compares datasets where reported concentrations below 2 µg/L are treated as below reporting limits. This comparison, in addition to the comparison to concentrations in surface water, shows some difference and some similarities between concentrations of antimony in blended produced water and other water sources that may be suitable for irrigating food crops. When comparing antimony concentrations in blended produced water to other groundwater sources, we observe some small differences. Antimony in blended produced water is detected in 20% of samples above 2 µg/L with a detected sample mean of 3.7 µg/L; in the CDPH groundwater data, antimony is detected in 4% of samples above 2 µg/L with a detected sample mean of 11.7 µg/L (GAMA, CDPH). When comparing concentrations of antimony in surface water to those in blended produced water, we observe that tail-end distributions based on higher reporting limits are similar. In 1,077 surface water samples collected by the USGS Resource Division between 1960 and 1988, antimony was detected above the detection limit of 5 µg/L in about 6.5% of samples; the geometric mean and standard deviation of the 70 detected samples was 12 µg/L with a standard deviation of 1.93 (HSDB, 2019). In blended produced water, antimony concentrations above 5 µg/L are detected in 3% of samples with a geometric mean of 6.7 µg/L and standard deviation of 2.7 µg/L. Antimony in blended produced water may be detected at a higher frequency than in groundwater used for drinking water, but its detected concentrations are lower than those observed in both surface and groundwaters. The data also suggest that blended produced water is not substantially different than surface waters (discussed above) with respect to the detection frequency and concentration of samples with concentrations above 5 µg/L. The significance of identified differences in the concentrations of antimony in blended produced water compared to concentrations in municipal groundwater and its impact on the antimony concentrations in food crops irrigated with these waters is unknown. As an additional point of reference, antimony in blended produced water only exceeded the WQO concentration level in one of 54 samples. Together, the comparison of the concentration in blended produced water to other sources of water suitable for irrigation and its general compliance with WQO concentration levels suggest that antimony levels in blended produced water do not lead to the expectation of seeing high levels of antimony in crops irrigated with blended produced water.

5.4.3 Arsenic

Concentrations of arsenic in blended produced water, on average, were higher than in surface waters used for irrigation in Tulare County. Differences between the concentration of arsenic in blended produced water and surface water are difficult to characterize precisely because of differences in the way arsenic concentrations are reported from different monitoring programs. Even taking these differences into account and as discussed below, arsenic levels in blended produced water appear to be similar or even lower than arsenic in nearby groundwater suitable for irrigation or drinking water.

In blended produced water, total arsenic was detected in 86% of samples, with mean of detections of 13.85 µg/L (range: 0.2 – 65) (Table 8). Water quality samples collected from the Kaweah and Tule rivers provide what would appear to be relevant comparison data for the blended produced water because both rivers are sources of irrigation water in Tulare County. The value of the comparison is limited, however, because arsenic data from the Kaweah and Tule Rivers is for dissolved arsenic; and the data for the blended produced water is for total arsenic. Because total arsenic would measure arsenic sorbed to suspended sediments and organic materials within the water column in addition to dissolved arsenic, it would measure arsenic not captured by a measure of dissolved arsenic.

In these rivers, dissolved arsenic has been detected in 84% of samples with a mean concentration of 2.1 µg/L of dissolved arsenic [range: 0.15–29 µg/L] (CEDEN, 2020). For reasons noted above, total arsenic levels in these rivers are likely to be higher. In comparing blended produced water to groundwater, arsenic concentrations in Kern County municipal groundwater sources are similar, or even higher, than those reported for blended produced water. It is unclear from the database, however, whether arsenic in Kern County municipal groundwater is reported as dissolved or total arsenic. This uncertainty could only serve to under-report the concentration of arsenic in Kern County municipal groundwater when compared to blended produced water and make any conclusions derived from its comparison with blended produced water more conservative. Arsenic in Kern County municipal groundwater sources have a detection frequency of 100% with mean of 18 µg/L [range: 0.03–278] (GAMA, USGS). Additionally, a study in the Tulare Basin of the San Joaquin Valley reported that concentrations of arsenic in shallow groundwater aquifers vary with median concentrations ranging 1 to 20.5 µg/L and maximums ranging 12 to 2,600 µg/L (Fujii and Swain, 1995); the concentrations of arsenic in blended produced water fall within the reported ranges of these aquifers. These data, together, suggest that concentrations of arsenic in blended produced water are similar to other water sources in the Central Valley that can be used for irrigation.

5.4.4 Beryllium

Detected levels of beryllium appeared to be higher in blended produced water than in Kern County municipal water sources. Beryllium was detected in 4% of blended produced water samples with a mean of detected samples equal to 2.94 µg/L [range: 0.28-5.6]. In groundwater, beryllium was detected in 11% of samples with a mean in detected samples of 0.03 µg/L [range: 0.004 - 0.06], which is nearly two orders of magnitude lower than in blended produced water. The significance of this difference is not immediately apparent by itself. To provide a point of reference, the concentration of beryllium in blended produced water only exceeded the WQO concentration level in one of 53 samples with a total of two detections in all 53 samples. The low rate of exceedance of the WQO concentration level and the low detection frequency do not trigger an expectation of seeing high levels of beryllium in crops irrigated with blended produced water.

5.4.5 Boron

The concentration of boron in blended produced water is higher than we observe in surface waters in the US generally and, more specifically, in the Kaweah and Tule rivers. In blended produced water, boron is detected in 97% of samples with a mean of detected samples equal to 480 µg/L [range: 20-2200]. In comparison, the average concentration of boron in US surface water is 100 µg/L (ATSDR, 2010) and in the Kaweah and Tule rivers, it is detected in 91% of samples with a mean of detected samples equal to 49.56 µg/L [range: 1.8–340] (CEDEN, 2020), both of which are lower than in blended produced water. The significance of this difference is illuminated by comparing the concentration of blended produced water to its respective WQO and to other sources of nearby potable water. The concentrations of boron in blended produced water has not exceeded the WQO for over 20 years; there have only been two years where the annual average concentration exceeded 1 mg/L: 1985 and 1986. Additionally, boron in untreated Kern County municipal groundwater is very similar to blended produced water, where it is detected in 97% of water samples with a detected sample mean equal to 402.66 µg/L [range: 8–1790] (GAMA, USGS). Because the concentration of boron in blended produced water is similar to nearby potable sources of groundwater, and that the WQO has not been exceeded in 20 years, we would not expect to see elevated boron levels in crops irrigated with blended produced water.

5.4.6 Cobalt

The concentration of cobalt in blended produced water is higher than has been reported in some surface and groundwaters in the US and Kern County. The concentration of cobalt in blended irrigation has a detected sample mean equal to 1.26 µg/L with range of 0.092–10 (Table 8). The concentration in Kern County groundwater has a detected sample mean equal to 0.14 µg/L with range of 0.02–0.523 (GAMA, USGS). In the US, broadly, cobalt in surface water is observed only in trace amounts and most waters have no detectable cobalt, with concentrations rarely exceeding 10 µg/L (HSDB, 2019). While there is no WQO concentration level for cobalt, nor other relevant regulatory level, the concentrations of cobalt reported in drinking water suggest that the observed concentrations in blended produced water would not cause crops irrigated with blended produced water to have elevated levels of cobalt. In US drinking water, the average concentration of cobalt is 2 µg/L, with concentrations up to 107 µg/L (ATSDR, 1992); typically, concentrations in drinking water range between 0.1 and 5 µg/L (HSDB, 2019). These drinking water concentrations are similar, or higher, than that observed in blended produced water, suggesting the level of cobalt in blended produced water would not be considered to be elevated.

5.4.7 Copper

Concentrations of copper in blended produced water are higher than those observed in Kaweah and Tule rivers and in untreated Kern County groundwater used for drinking water. Copper was detected in 74% of blended produced water samples with a detected sample mean equal to 8.93 µg/L [range: 0.64–87] (Table 8). In contrast, copper was detected in 81% of Kaweah and Tule samples with a detected sample mean equal to 1.4 µg/L [range: 0.078-8.1] (CEDEN, 2020) and in 23% of Kern County groundwater with a detected sample mean equal to 2.9 µg/L [range: 1.8-5.3] (GAMA, USGS). Detected copper concentrations in blended produced water are about six times higher than concentrations in the Kaweah and Tule rivers and about three times higher than in Kern County groundwater. Additionally, the frequency of detection of copper in blended produced water is more than three-times greater than in these other water sources. As a point of reference, the concentration of copper in blended produced water did not exceed the WQO of 1300 µg/L, which is based on the drinking water MCL set to protect human health. Given that concentrations of copper in blended produced water did not exceed the MCL, we would not expect to see levels of copper in crops irrigated with blended produced water greater than crops irrigated with water that was safe to drink.

5.4.8 Manganese

Concentrations of manganese in blended produced water are higher than in some surface waters, including the Kaweah River, Tule Rivers, and other surface water in the US and California (CEDEN, 2020; HSDB, 2019). When compared against agricultural surface and groundwater and untreated Kern County groundwater used for drinking water, however, we observe that concentrations of manganese in blended produced water are not elevated above levels already observed in waters suitable for agricultural irrigation. Manganese was detected in 86% of blended produced water samples with a detected sample mean equal to 45.79 µg/L [range: 3 – 610] (Table 8). In the Kaweah and Tule rivers, manganese was detected in 97% of samples with a detected sample mean equal to 3.73 µg/L [range: 0.22 – 160] (CEDEN, 2020).

In contrast, when compared against agricultural waters the concentrations of manganese observed in blended produced water are more similar to agricultural surface and groundwater. In agricultural surface water sampled in the US, manganese concentrations are reported to have a median value of 19 µg/L with a 99th percentile value of 700 µg/L; 12.3% of the collected samples have a value above 300 µg/L[1] (ATSDR, 2012a). In

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[1] The 300 µg/L concentration level represents the EPA derived health reference level for manganese, which is a health-related benchmark for evaluating occurrence data of manganese in water. It is a concentration level meant to protect susceptible populations from the neurotoxic effects of manganese (USEPA, 2003). We only report this characteristic of the distribution of manganese concentrations as it was reported in the primary literature and serves as a point of reference to understand the distribution of values that are observed in these agricultural waters.

agricultural groundwater sampled in the US, manganese concentrations are reported to have a median value of 4 µg/L with a 99th percentile value of 1600 µg/L; 12.8% of the collected samples have a value above 300 µg/L (ATSDR, 2012a). The average concentration of manganese in surface water drainage basins in the Southeastern US, Pacific Northwest US, and CA was 2.8 µg/L (HSDB, 2019).

Additionally, concentrations of manganese in untreated Kern County municipal groundwater were detected in 74% of samples with a detected sample mean equal to 128.95 µg/L [range: 0.2 – 2250] (GAMA, USGS). Given that concentrations of manganese in blended produced water fall within the range of concentrations observed in other agricultural water and are lower than concentrations in nearby municipal groundwater, we would not expect concentrations of manganese in crops irrigated with blended produced water to be higher than crops irrigated with other suitable irrigation water sources from the area.

5.4.9 Mercury

Mercury detected in blended produced water had higher concentrations than mercury detected in Kern County municipal groundwater, but lower than levels in water samples from other local sources of irrigation water, the Kaweah River and Tule Rivers. Mercury was detected in 13% of blended produced water samples with a detected sample mean equal to 0.04 µg/L [range: 0.001-0.095] (Table 8). In Kern County municipal groundwater mercury was detected in one of 15 samples at a concentration of 0.02 µg/L (GAMA, USGS). Mercury was detected in 39% of samples of Kaweah River and Tule River water with a detected sample mean equal to 0.12 µg/L [range: 0.035 - 0.31], a level higher than was reported in blended produced water. Additionally, mercury concentrations in blended produced water did not exceed the WQO concentration level of 2 µg/L, and all samples had concentrations less than 0.1 µg/L. Based on its similarity to nearby sources of agricultural water and reported concentrations below the WQO concentration level, we would not expect to see elevated levels of mercury in crops irrigated with blended produced water.

5.4.10 Nitrite

The maximum reported concentrations of nitrite in blended produced water is higher than is reported in some US public drinking water supplies, but when compared to Kern County municipal groundwater we do not observe a significant difference. Nitrite was observed in two of five blended produced water samples with reported concentrations of 800 µg/L and 19,000 µg/L (Table 8). In the US public drinking water supply, the reported median concentration of nitrite is 20 µg/L with maximum reported concentrations of 8680 µg/L (USEPA, 1990). Nitrite (reported as nitrite-as-nitrogen) was also detected in 92% of untreated Kern County municipal groundwater samples with a detected sample mean of 3550 µg/L [range: 70-12,100] (GAMA, USGS). To compare observed concentrations in blended produced water to concentrations in Kern County municipal groundwater, nitrite-as-nitrogen needs to be converted to nitrite (1 µg/L as nitrite = 0.304 µg/L as nitrite-nitrogen). Using this conversion, the concentrations of observed nitrite in Kern County municipal groundwater have a detected sample mean of 11,680 µg/L [range: 260-39,800], which entirely covers the range of nitrite concentrations observed in blended produced water. Additionally, the large reported concentration of nitrite in blended produced water may not be attributable to the reuse of produced water. In treated produced water, nitrite was detected in only one of six samples with a reported concentration of 1,000 µg/L, which is nearly 20-times lower than the maximum reported in blended produced water. It is likely that the large maximum concentration observed in blended produced water is related to nitrite in the blending water, not the treated produced water.

5.4.11 Phenanthrene

Detected levels of phenanthrene are about ten-times higher in blended produced water than is reported in surface waters in the US.. Phenanthrene was detected in 18% of blended produced water samples with a detected sample mean equal to 0.11 µg/L [range: 0.029-0.29]. In contrast, raw surface water samples collected from various US sites are reported to have concentration of phenanthrene that range between 0.006 and 0.020 µg/L (HSDB, 2019). We expect phenanthrene to be of limited likelihood to accumulate in irrigated crops because of fate and transport factors that will attenuate its phytoavailability. That is, while levels of phenanthrene in blended produced water are higher than observed in surface waters, its impact on food crops is likely to be low as it binds to organic materials and sediments, making it immobile, and therefore, unavailable for plant uptake (Landrum et al., 1992).

5.4.12 Radium

The maximum reported concentrations of radium in blended produced water are higher than those reported in surface water. When compared to US and Kern County municipal groundwater, concentrations of radium in blended produced water are lower. In blended produced water, radium-226 and radium 228 were both detected in 97% of water quality samples. The detected sample mean concentrations are 0.86 pCi/L [range: 0-9.2] and 0.61 pCi/L [range: 0-4.7] for radium-226 and radium-228, respectively (Table 8). To compare, surface waters in the US generally have concentrations of radium that range between 0.1-0.5 pCi/L (HSDB, 2019). In Kern County municipal groundwater well data collected by California Department of Public Health (CDPH), radium is detected in all samples with a mean radium concentration (Ra-226 + Ra-228) of 2.6 pCi/L [range: 0.023–31]. Among 990 groundwater drinking water sources in the US, the population-weighted average concentration was 0.91 pCi/L for radium-226 and 1.41 pCi/L for radium-228 (ATSDR, 1990a). Additionally, more than 20% of these 990 groundwater sources of drinking water exceeded the MCL of 5 pCi/L; the average concentration of Ra-226 among these 200 groundwater sources was about 10 pCi/L (ATSDR, 1990a). A comparison of the radium concentration and exceedance frequency of the MCL in both blended produced water and groundwater drinking water sources suggest that blended produced water may have lower levels of radium than some drinking water sourced from groundwater in the US and Kern County. Mean concentrations of radium are lower in blended produced water than in untreated municipal groundwater in the US and Kern County. Additionally, blended produced water exceeded the MCL at a lower rate than the other two sources of municipal groundwater data. In blended produced water, the MCL is exceeded in 1 of 33 samples, or 3%; in the Kern County data, it is exceeded in 6% of other samples (GAMA, CDPH), while more than 20% of the US sources of drinking water in the US exceeded the MCL of 5 pCi/L (HSDB, 2019) for RA-226 + RA-228. Given that concentrations of radium in blended produced water are similar or lower than those observed in other suitable sources of irrigation water, we would not expect to see elevated levels of radium in crops irrigated with blended produced water.

In summary, the observed concentrations of the Chemicals of Interest in the blended produced water does not lead to the expectation of seeing elevated levels of the chemicals in blended produced water. The reasons identified above for this include observed concentrations of the Chemicals of Interest are similar to or lower than those observed in surface water, groundwater drinking water sources, and other groundwater that could ostensibly be suitable for agricultural irrigation; observed concentrations meet drinking water requirements, which implies their suitability for irrigating food crops; and one chemical is unlikely to be phytoavailable in soil due to fate and transport mechanisms. We were unable to make comparisons to some of the environmental water quality data identified for the Chemicals of Interest because corresponding blended produced water data were not available. These chemicals were not reported in routine water quality monitoring of produced water because standard USEPA methods do not exist. The Chemicals of Interest that have environmental water quality data but do not have corresponding produced water quality data include isoquinoline in rainwater and oxyalkalated alkylphenol (68412-54-4) and ethoxylated 4–nonphenol (26027-38-3) in surface waters.

5.5 Chemicals of Interest in Food Crops Irrigated with Treated Produced Water

Under Task 3, crops were tested for the presence of many different chemicals. The concentrations detected in “treated” vs “control” samples were compared to see if concentrations in crops irrigated with blended produced water (i.e., “treated” samples) were higher than the concentrations of chemicals in crops irrigated with conventional irrigation water (i.e., “control samples). As part of Task 3, we also compared concentrations measured in sampled crops to concentrations reported in the literature for the same chemicals and crops, when data to support such comparisons were available. Table 10 includes a summary comparison of the chemical concentrations for the 14 Chemicals of Interest that were detected in the crops sampled in Task 3 and a comparison of the concentrations of the same crop-specific concentrations reported in the literature.

As part of the cross-media evaluation performed as part of Task 2 for the Chemicals of Interest, we have included a summary of the comparison of the levels of chemicals detected in crops sampled as part of this study to the chemical levels reported in the literature for the same crops. This comparison was included in Task 2 as part of a search for any deviations from consistent patterns that might suggest chemicals are accumulating in crops irrigated with blended produced water. Finding chemicals in crops irrigated with blended produced water at levels higher than are reported in the literature might suggest the blended produced water is a source of the chemical.

The fourteen Chemicals of Interest detected in crops irrigated with blended produced water and sampled as part of this study included, antimony, arsenic, barium, cadmium, chromium, cobalt, copper, lead, molybdenum, nickel, selenium, strontium, vanadium, and zinc. The concentrations of these 14 chemicals in the crops sampled as part of this study were similar to the concentrations in food crops reported in the literature (ATSDR, 2004d; ATSDR, 2004e; ATSDR, 2007b; ATSDR, 2012e; ATSDR, 2017b; FDA, 2007; Thomas et al., 1974). Concentrations of antimony and chromium in crops sampled during Task 3, however, were detected at higher concentrations than have been reported in the literature.

5.5.1 Antimony

Concentrations of antimony detected in almonds and garlic in Task 3 samples from fields irrigated with blended produced water and from fields irrigated with conventional irrigation water were higher than the range of detected antimony concentrations reported in the literature for food, on the whole. Adding to the difficulty of comparing the concentrations in foods discussed in the literature to the concentrations reported in Task 3 was that concentrations from the literature were reported on a dry-weight basis, in some cases. In contrast, the results from Task 3 were reported as concentrations based on fresh-weight. In addition, other comparisons were difficult because results presented in the literature were reported by food class. We found that the reported concentration for antimony in nuts was based on a mixture of dried fruit, nuts, and seeds.

Reports of the concentrations of antimony in dried garlic and in mixtures of “dried fruit, nuts and seeds” is the nearest comparative data. We recognize that a mixture of “dried fruit, nuts, and seeds” is very different than raw almonds and thereby places large limits on our ability to draw conclusions from qualitative comparisons, but this data represents the nearest available data. From the Task 3 sampling, antimony was detected in almond and garlic crops irrigated with blended produced water. In almonds irrigated with blended produced water, antimony was detected in 7 of 20 samples with a mean concentration of 0.44 mg/kg (range: <0.20–1.8). In comparison, detected concentrations of antimony in a mixture of dried fruit, nuts, and seeds was much lower. In the French Total Diet Study, four samples of a mixture of dried fruit, nuts, and seeds were collected, and antimony was detected in only one sample at a concentration of 0.001 mg/kg fresh-weight (ANSES, 2011; Millour et al., 2011; Arnich et al., 2012). We were unable to find any other sampling results that reported the concentration of antimony in only almonds or in any other strict group of nuts. In garlic crops irrigated with blended produced water, antimony was detected in 1 of 5 samples at a concentration of 0.61 mg/kg. In comparison, Belzile et al. (2011) reported that concentrations of antimony in garlic range between 0.013-0.0227 mg/kg by dry-weight. An equivalent fresh-weight based on the assumption that garlic is 59% water would be 0.0053-0.0093 mg/kg. The detected concentrations of antimony in garlic reported in Belzile et al. (2011) are lower than are reported in the Task 3 sampling results. More generally, reported concentrations of antimony in fruits and vegetables do not exceed 0025 mg/kg (Millour et al., 2011).

Antimony was also detected in crops irrigated with conventional irrigation water that were sampled as part of this study. In almonds irrigated with conventional irrigation water, antimony was detected in 2 of 20 samples with reported concentrations of 0.64 mg/kg and 0.73 mg/kg. In garlic crops irrigated with conventional irrigation water, antimony was detected in 2 of 6 samples with detected concentrations of 0.55 mg/kg and 0.61 mg/kg. The detected concentrations in these samples are higher than the detected concentrations reported in the literature.

While antimony concentrations in crops irrigated with conventional irrigation water are slightly lower and are detected at a lower frequency than in crops irrigated with blended produced water, the detected concentrations of antimony in crop samples irrigated with conventional irrigation water are of a similar magnitude to those observed in samples irrigated with blended produced water when compared to concentrations reported in the literature.

Even though we were not able to make fair comparisons between detected antimony concentrations in Task 3 crops irrigated with blended produced water to concentrations in similar marketplace foods, there are some indications that antimony concentrations are higher in samples collected as part of this study. While the reasons for the apparent differences between Task 3 samples and marketplace foods are not clear, it is noteworthy that there were no significant differences in antimony concentration between Task 3 samples irrigated with blended produced water and conventional irrigation water. Differences between Task 3 samples and marketplace foods may be attributable to concentration of antimony in soil, irrigation water, or other agricultural reasons.

5.5.2 Chromium

Chromium levels[1] detected in carrots irrigated with blended produced water and conventional irrigation water and sampled as part of Task 3 appear to be higher than chromium levels reported in the literature for carrots. Chromium was reported to be present in one of six samples of carrots irrigated with blended produced water and in one of three carrot samples irrigated with conventional irrigation water. The reported concentration of chromium detected in both of the samples in which it was detected was 0.23 mg/kg.

The ATSDR Toxicological Profile for chromium reports that chromium concentrations in fruits and vegetables range from 0.02-0.14 mg/kg (ATSDR, 2012c). Chromium concentrations in carrots were reported in the range of 0.004-0.090 mg/kg (Thor et al.,

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[1] Chromium concentrations reported here refer to total chromium, while the Chemical of Interest is hexavalent chromium. We do not have sampling data or sufficient data from the literature to evaluate the potential presence or likely concentrations of hexavalent chromium that may be present in typical food crops.

2011). Thus, it appears that chromium levels in carrots collected as part of this study are higher than levels reported in the literature.

The reason for the difference is not clear. Because carrots are root crops, differences in sample preparation (e.g., washing) could have contributed to the differences between the values reported in the literature and the levels measured in the carrots sampled as part of this study. While the levels of chromium detected in two carrot samples collected as part of this study are higher than levels reported in the literature, the levels in carrots irrigated with blended produced water do not appear to be different than the levels in carrots irrigated with conventional irrigation water.

5.6 Review of Analytic Methods for Determining Concentrations of Chemicals of Interest in Chemicals Not Currently Being Monitored

As noted above, there were gaps in the availability of data on the presence of Chemicals of Interest in environmental media, and some of that gap stemmed from the lack of analytical methods for the Chemicals of Interest in water. We reviewed the available methods to identify Chemicals of Interest that are not currently being measured but have methods that can be used for future monitoring. Table 11 lists these 90 chemicals and shows that nearly all that can be monitored are currently monitored. A few chemicals, however, have applicable analytical methods that are not currently implemented in routine water quality monitoring of produced water. These methods measure the concentration of technical mixtures of ethoxylated alkylphenols and would allow us to quantify the combined concentration of ‘Ethoxylated 4-nonphenol’, ‘Nonylphenol ethoxylates’, ‘Nonylphenol polyethylene glycol ether’, and ‘Oxyalkylated alkylphenol’. These four chemicals are used as surfactants. The identified method uses LC/MS or LC/UV. If implemented in future water quality monitoring, water quality analytic methods would still not exist for 86 Chemicals of Interest.

Overall, the review of analytic methods has shown that routine water quality monitoring required by WDRs includes nearly all Chemicals of Interest for which analytical methods are available. Technical mixtures of ethoxylated alkylphenols are the only additional chemicals that could be added to future monitoring, using existing analytical methodology. Conversely, there are 86 Chemicals of Interest that cannot be monitored because standard analytic methods for these chemicals do not exist. This data gap for monitoring data corresponds to data gaps in our toxicological understanding of these chemicals. That is, these 86 chemicals are the same as those that do not have sufficient toxicologic information to evaluate their potential human health hazards from oral exposure.

5.7 Summary of Review of Concentration Data of the Chemicals of Interest in Irrigation Water and Other Environmental Media

In combination, the available data do not indicate that crops irrigated with blended produced water have higher levels of the Chemicals of Interest than would be seen in crops irrigated with conventional irrigation water. This conclusion is based on two key assumptions. First, if blended produced water quality complies with the WQO or other screening levels for a given chemical, use of that water for irrigating crops is unlikely to cause unusually high accumulation of the chemical in a crop. Second, by comparing observed concentrations of the Chemicals of Interest in blended produced water and/or in crops irrigated with blended produced water with the concentration of these chemicals reported in the literature in water suitable for irrigation and in typical food crops, we are able to draw conclusions about the impact that the use of produced water in irrigation water has on the quality of food crops.

In our review of the available data, we were able to show that blended produced water generally complied with WQO and other screening concentration levels and that most comparisons discussed above showed little difference between concentrations associated with blended produced water and those associated with conventional irrigation water sources. Our review of routine monitoring data required by WDRs showed that concentrations of measured chemicals in blended produced water do not routinely exceed WQO concentration levels, with the exception of arsenic.

Concentrations of the Chemicals of Interest in crops currently irrigated with blended produced water were mostly similar to the conventionally irrigated crops they were compared to in the San Joaquin Valley (reported in the Task 3 Report) and were also similar to typical concentrations of food crops published in the literature. We also observed that the concentrations of Chemicals of Interest in blended produced water are similar to those reported in surface and groundwaters that could be used for agricultural irrigation.

The few differences in the observed concentrations associated with blended produced water and those associated with conventional irrigation water sources did not point to patterns that indicate chemical levels would be higher in crops irrigated with blended produced water versus conventional irrigation water. We were able to show that the concentrations of most Chemicals of Interest in blended produced water were within the range of potential concentrations encountered in both surface water and groundwater suitable for agricultural irrigation, even though concentrations in blended produced water may have been higher than one of them. In cases where the concentrations of Chemicals of Interest in blended produced water were higher than both surface water and groundwater sources, concentrations in blended produced water were not above water quality standards, notification levels, or other screening levels used to evaluate the water quality. Also, when comparing concentrations of Chemicals of Interest in food crops sampled as part of this project, we found that both antimony and chromium levels may be higher in some food crop samples than is reported in the literature. Concentrations of antimony and chromium in these crops, however, were similar for both crops irrigated with blended produced water or with conventional irrigation water. The similar concentrations of both metals in both sample groups suggest that factors other than irrigation water may be contributing the observed concentration in food crops, for example, soil composition, air quality, or varietal of the crop.

Additionally, while the concentration of arsenic exceeded WQO levels in about 50% of blended produced water samples, the observed concentrations were not significantly different than other sources of water that may be suitable for irrigation in the San Joaquin Area. And to this point, arsenic was not observed in any of the food crop sampled in this study above levels reported in typical food crops. Arsenic was only detected in one crop (carrots) sampled as part of the crop sampling component of this project, and the reported levels were below laboratory quantification levels, but above detection limits.

Finally, the review of analytic testing methods for water quality monitoring revealed that most of the Chemicals of Interest that have analytic methods are being monitored in routine water quality testing required by the WDRs for produced water. Future monitoring could include the analysis of technical mixtures of ethoxylated alkylphenols through LC/MS or LC/UV. There are 86 Chemicals of Interest that cannot currently be monitored due to a lack of analytic methods, which represents a large data gap in our ability to quantify the Chemicals of Interest in blended produced water or other environmental media, including soil and food crops. Additionally, most of these 86 Chemicals of Interest are the same chemicals identified in Task 1 as lacking sufficient data to make toxicological hazard evaluations.

The evaluations presented in this section is one of the lines of evidence used to determine whether crops irrigated with blended produced water are expected to accumulate higher levels of the Chemicals of Interest. It also provides a point of reference for the interpretation of the water quality data as it relates to the crop monitoring data. For example, if we saw large discrepancies between concentrations of chemicals in blended produced water and in conventional irrigation water we would want to see if such differences existed in crops irrigated with blended produced water and conventional irrigation water. Similarly, if we saw significant difference in concentrations of chemicals reported in the literature for specific crops and concentrations in the same crops irrigated with blended produced water, we would want to make note of that finding and be sure to check the concentrations seen in crops irrigated with conventional irrigation water as part of this study.

6.0 INORGANIC CHEMICALS OF INTEREST: FATE, TRANSPORT, AND PLANT UPTAKE

The Chemicals of Interest selected in Task 1 include 37 inorganic chemicals, not including six radionuclides addressed in Section 7. One of the key questions addressed in Task 2 is whether any of these chemicals, when present in produced water used for irrigation, could move into and accumulate in the edible portion of irrigated crops. As discussed below, a large body of science is available on general mechanisms of plant uptake of inorganic chemicals from soil and water and on distribution of chemicals into different parts of the plant. Similarly, there is a large body of information on the effect of various soil properties and water chemistry on the movement of inorganic chemicals in soil and on the absorption of inorganic chemicals into roots from soil. The general principles affecting the uptake of inorganic chemicals into irrigated crops are briefly summarized below (Section 6.1). A summary of more chemical-specific factors affecting the potential migration of each of the 37 inorganic Chemicals of Interest list from irrigation water into the edible portion of irrigated crops is also presented below (Section 6.2). Finally, a short summary and discussion of the findings are presented in Section 6.3. While the state of the science does not currently support the ability to predict whether an inorganic chemical in produced water will accumulate in the edible part of an irrigated crop or to estimate the degree to which it will accumulate, there are some useful patterns of metal migration in soil and plant uptake that can help guide future evaluation and management of the use of produced water for irrigating food crops.

6.1 General Principles Affecting Movement of Inorganic Chemicals in Soil and Phytoavailability

A number of soil properties can affect the fate and transport of inorganic chemicals in agricultural soils including, soil redox potential, pH, humic/fulvic acid content, and soil clay content. In particular, the phytoavailability of inorganic chemicals in soils depends, to a large extent, on their distribution between the solid and solution phases. This distribution is, in turn, dependent on the soil characteristics, such as cation exchange capability, specific adsorption, precipitation, and complexing with other ligands (Rieuwerts et al., 1998). Redox potential and pH are generally acknowledged to be the most important factors influencing mobility and phytoavailability of inorganic chemicals in soils (Bourg and Loch, 1995). Redox potential affects the retention of inorganic compounds by controlling its precipitation out of solution (Bourg and Loch, 1995). Solubility is affected by pH; as soil becomes more alkaline, metals are generally less soluble and are absorbed to a greater extent in soil (Bradl, 2004). Organic materials in soil are also an important factor as they can complex with metals, making them less mobile and less available for uptake by plants (Balasoiu et al., 2001). Naturally occurring ligands, such as humic and fulvic acid, can complex with metals and potentially make the metals more available for plant uptake (Evangelou et al., 2004). In addition to being naturally occurring components of soil, humic and fulvic acid are oil field additives. Humic and fulvic acid act as chelators, much like disodium ethylenediaminetetraacetate (EDTA), which is another declared additive. Studies have been performed on the use of EDTA and other similar chelators to enhance phytoremediation of heavy metals by increasing phytoavailability. However, results of these studies have not shown that chelators consistently enhance plant uptake in soils similar to those found in agricultural settings (Liphadzi and Kirkham, 2006; Evangelou et al., 2007; Shariq, 2019). Colloidal clays in soil can also increase metal mobility because they can create colloid-metal complexes that are mobile in the soil solution (Bradl, 2004). However, for the metal to be available for plant uptake, the colloid must release the metal from the surface. Release of the metals by the colloid is dependent on cation exchange, which in turn can be dependent on the soil and mineral types (Evans, 1989; Rieuwerts et al., 1998).

Most agricultural food crops generally grow best in aerobic soils rich in organic matter that are slightly acidic with pH of 6.0 to 7.5 (Brady and Weil, 2004; Osman, 2013; USEPA, 2012a). Ideal soils for growing most plants have 50% solid material and 50% pore space with half of the pore space containing water (Brady and Weil, 2004; USEPA, 2012a). This would mean that most agricultural soils are highly oxidized with moderate moisture content. Additionally, ideal soils for growing have relatively stable redox and pH conditions, as fluctuations can result in nutrient deficiency and potential increased toxicity due to increased mobility of aluminum, iron, and other heavy metals (Husson, 2013). Soil management practices can affect pH and redox conditions, but these practices are typically balanced to create more optimal growing conditions, as those described above (Husson, 2013). Because agricultural soils are generally managed to maintain the optimal growing conditions mentioned above, metals are generally present in soils in a predominate oxidation state due to the relatively stable pH and redox conditions.

Once in the soil-water solution, inorganic chemicals move from the soil through the root and into the plant by three main pathways – the apoplastic, symplastic, and transcellular pathways (Chaumont and Tyerman, 2014). In the apoplastic pathway, water and some inorganic chemicals move by diffusion into the apoplast – the space between the plant cell wall and the plasma membrane – and from there into xylem in the plant root (Gomes et al., 2009). In the symplastic pathway, water and inorganic chemicals move by osmosis along concentration gradients. In the roots, the symplastic pathway facilitates the movement of dissolved inorganic chemicals from soil to the root epidermal cells and into the root endodermis, and eventually into the xylem. Transcellular transport involves water channels known as aquaporins or aquaglyceroporins; these channels–or pores–are formed by membrane proteins, which facilitate the uptake of water and solutes into the root (Gomes et al., 2009). Inorganic chemicals can also be taken up into the plant by active processes which require ATP. In active uptake, inorganic chemicals are mobilized and taken up by root cells from soil, bound by the cell wall, and then transported across the plasma membrane, driven by ATP-dependent proton pumps that catalyze H+ extrusion across the membrane (Singh et al., 2010). Along with cationic nutrients (positively charged ions, i.e., Cu2+), plant transporters (e.g., phosphate transporters) are also involved in shuttling potentially toxic cations (i.e., As3+) across plant membranes (Singh et al., 2010).

The tolerance of plants to increasing levels of potentially toxic inorganic chemicals can result from the sequestration of specific metals (Singh et al., 2010). The major mechanism of acquired tolerance appears to be the compartmentalization of metal ions, i.e., sequestration in the vacuolar compartment. This compartmentalization reduces the levels of specific metals at cellular sites where processes such as cell division and respiration occur, thus serving as a protective mechanism for normal cell function (Singh et al., 2010). These mechanisms of transport and tolerance can affect levels of these metals in certain parts of a food crop. Depending on where the metals concentrate (i.e., root, stem, leaves, fruit), the extent to which the vacuoles in the cells of the edible portion of the food crops can compartmentalize and accumulate metals that may be toxic to humans can directly affect hazards that may be created by consumption of the food crops.

6.2 Chemical-Specific Factors Affecting Movement of Inorganic Chemicals in Soil and Phytoavailability

6.2.1 Antimony

Antimony (Sb) has ten known oxidation states (−3, −2, −1, 0, +1, +2, +3, +4, +5, +6). The pentavalent form (Sb^{5+}) is the most stable form in aerobic environments and more likely to be found in soil and ambient water (Tschan et al., 2009; Mitsunobu et al., 2006). While its trivalent form (Sb^{3+}) can sorb to clay minerals, or to oxides and hydroxides in the soil (Wilson et al., 2010; Johnson et al., 2005), most of the dissolved Sb in natural waters is in the pentavalent oxidation state [Sb^{5+}] under aerobic conditions (Filella et al., 2002). This suggests that there would be minimal attenuation of Sb by sorption onto clay or other minerals in agricultural soils.

The mechanisms of cellular uptake of Sb by plants depends on its oxidation state. Sb^{3+} dissolved in soil pore water may cross cell membranes passively with water through aquaporins, water channel proteins that are expressed in various membrane compartments of plant cells, including the plasma and vacuolar membranes. Such transport appears to be consistent with the observed uptake of Sb^{3+} by plants in amounts that are proportional to the amount of Sb^{3+} in soil (Tschan et al. 2009). Feng et al., (2013) report that As^{3+} and Sb^{3+} may be taken up by similar mechanisms in plants because the uptake of As^{3+} was also found to be facilitated by aquaporins in yeast and in rice. Passive uptake of Sb^{5+} by aquaporins does not occur, and cellular uptake of Sb^{5+} would require mediation by transporters (Tschan et al., 2009). Although most of the available evidence suggests that Sb is translocated within plants primarily along the apoplastic pathway through the xylem, this does not exclude the possibility that some symplastic transport may also occur (Tschan et al., 2009). Together, this suggests Sb is not taken up into plants in appreciable amounts because it normally occurs as Sb^{5+} in aerobic soils.

Studies that have examined the distribution of Sb in plant tissues are generally consistent in their findings that Sb tends to be concentrated in the leaves and shoots of plants, with lower concentrations present in seeds, fruits, and storage organs. For example, Hammel et al. (2000) reported that low concentrations of Sb were detected in carrot root when compared to the carrot leaves, low concentrations were observed in potato tubers, and none was detected in tomato fruits. In comparison, leafy crops like endive, spinach, and kale had levels that approached ten-times higher than those in fruiting/root/grain crops (Hammel et al., 2000). Pierart et al. (2015) reported that accumulation in different parts of food crops is specific to the plant, with potential for orders of magnitude difference between the same plant part.

6.2.2 Arsenic

Arsenic (As) has nine known oxidation states (-3, -2, -1, 0, +1, +2, 3+, +4, 5+). As^{3+} (arsenite) and As^{5+} (arsenate) are most the most predominant form found in soils. As^{5+} predominates in aerobic soils while As^{3+} predominates in slightly reducing soils (ATSDR, 2007a). Many arsenic (As) compounds partition out of solution and into soil under oxidizing conditions (Moore et al., 1988; Pantsar-Kallio and Manninen, 1997; Welch et al.

1988). Arsenic is largely immobile in agricultural soils and tends to concentrate and remain in upper soil layers indefinitely (ATSDR, 2007a). One study that examined the effect of soil characteristics (pH, organic matter content, clay content, iron oxide content, aluminum oxide content, and cation exchange capacity) on As found that increased iron content was the most important parameter in increasing the absorption of arsenic in soils (Janssen et al. 1997). Arsenic may be adsorbed from water onto sediments or soils, especially clays, iron oxides, aluminum hydroxides, manganese compounds, and organic material (Welch et al. 1988). While As can be soluble in water, its solubility depends on its oxidation state and counter ion, which in aerobic agricultural soils is likely to favor the more immobile form.

Both As^{3+} and As^{5+} are taken up by plants, albeit by somewhat different mechanisms. The uptake mechanism for As^{5+} is thought to occur primarily through high-affinity phosphate transporters; as a result, the uptake of As^{5+} can be influenced to some extent by phosphate application to the soil (Gomes et al., 2009). As^{3+} uptake is thought to occur via glycerol transporters, a particular type of aquaporin (Gomes et al., 2009). Arsenic can readily transform between As^{5+} and As^{3+} if aerobic soils become waterlogged, which creates a reducing environment (Raab et al., 2007). Trace amounts of monomethylated arsenic and demethylated arsenic may be present in soils from pesticide or herbicide application, or by biotic methylation (Li et al., 2016). The uptake mechanisms for mono– and demethylated As species, either via the root system or via the shoot system, are as yet not known, but it is known that inorganic and methylated-As species are taken up via both root and shoot (Raab et al., 2007).

The dominant form of As in plant tissue is As^{3+}, reflecting the fact that in general, plants efficiently reduce As^{5+} to As^{3+} (Abbas et al., 2018; Pickering et al., 2000). For example, As^{3+} accounted for 96-100% of the As in the roots and shoots of *Brassica juncea*, 97-100% in the leaves of *A. thaliana* and 92-99% in the roots of tomato and rice (Pickering et al., 2000). Once As has been taken up by the roots, its translocation to the stems and leaves appears limited (Abbas et al., 2018). Although the basis of arsenics' limited mobility is not well-characterized, it has been hypothesized that As^{5+} is rapidly reduced to As^{3+} in the roots, followed by the formation of sulfur-based complexes and the sequestration of these complexes within intracellular vacuoles (Abbas et al., 2018).

Arsenic has been studied in some crops similar to those that are irrigated with produced water in the Central Valley. Helgesen and Larsen (1998) grew carrots in experimental soil plots containing As at concentrations of 6.5 to 338 µg/g. Harvested carrots showed a gradually increasing depression of growth with increasing levels of As. As^{3+} was the dominant form of As in carrots grown in soils with 6.5 to 30.0 µg/g As. In soils with higher As levels, the amounts of As^{3+} and As^{5+} were similar. For root vegetables such as carrots and potatoes, studies indicate that As accumulates in peels rather than root cores (Helgesen and Larsen, 1998; Samoe-Petersen, et al. 2002; Codling et al., 2015; Codling et al. 2016). For fruit (tomatoes), As was measured at significantly lower levels in the tomato fruit, compared to roots, stems, and leaves of the plants; As levels were highest in roots (Barrachina et al. 1995).

6.2.3 Barium

Barium (Ba) has three known oxidation states (0, +1, +2). It almost always exists as Ba^{2+} (ATSDR, 2007b). Barium and its salts are poorly soluble, with most precipitating out of solution as Ba sulfate or Ba carbonate (ATSDR, 2007b), especially in the presence of other sources of sulfate or carbonate. Ba is not very mobile in most soil systems because its salts are insoluble and also because it forms complexes with fulvic and humic acids (Choudhury et al., 2001). Soil properties that influence the transportation of Ba through the vadose zone include cation exchange capacity, calcium carbonate content, and pH. In soil with a high cation exchange capacity, Ba mobility will be limited by adsorption (ATSDR, 2007b). Ba is more mobile and is more likely to be leached from soils in the presence of chloride due to the high solubility of Ba chloride (Bates, 1988). Ba may become more mobile in soils under acid conditions as Ba water-insoluble salts, such as Ba sulfate and carbonate, becomes more soluble in acid environments (Choudhury et al., 2001).

Only a small amount of Ba in soil is typically taken up by plants (ATSDR, 2007b). Some food crops, however, have been known to accumulate Ba; these include tomatoes, soybeans, legumes and brazil nuts (IPCS, 1991; WHO, 2001). Bioconcentration factors for tomatoes and soybeans range between 2 to 20 (WHO, 2001).

6.2.4 Beryllium

Beryllium (Be) has three known oxidation states (0, +1, +2); it only exhibits the Be^{2+} oxidation state in water. Beryllium (Be) is more soluble in alkaline environment and forms complexes with soil fulvic acid in alkaline soils. (Esteves Da Silva et al. 1996). It also forms colloids with clay minerals more strongly than with organic matter. Beryllium clay colloids preferentially form with aluminosilicate clays over iron oxides (ATSDR, 2002). Unlike most metals, Be is mobile in both alkaline and acidic conditions (Cotton & Wilkinson, 1980; Kram et al., 1998), where it will form $Be(OH)_4]^{2-}$ and Be^{2+}, respectively. However, Be should be less mobile in agricultural soils that are not significantly alkaline or acidic, as conditions would favor the formation of beryllium hydroxide, which has low solubility (Hayes & Traina, 1998; ATSDR, 2002).

Literature on the uptake of Be in food crops is limited. Beryllium, however, must be in a soluble form for plant uptake to occur, and most Be is immobile in agricultural soils that have pH between 6.0 and 7.5 (ATSDR, 2002). Therefore, it is not expected that much would be taken up into plants. Some research has shown modest uptake of Be into barley, sunflowers, and tomatoes, but over 95% was found in the roots with little in leaves and fruit (Romney and Childress, 1965).

6.2.5 Boron

Boron (B) has six known oxidation states (-5, -1, 0, +1, +2, +3), but exists exclusively in the B^{3+} oxidation state in the environment. Boron does not exist on its own but forms borates. Boric acid is the main B species that plants uptake (Poschenrieder et al., 2019). It is quite soluble and hydrolyzes in water (ATSDR, 2010). Boron may absorb to minerals under alkaline conditions with pH 7.5-9 (Keren et al., 1981). Agricultural soils have generally lower pH, which rules out this mechanism for sequestration. Unlike other metals, the organic content of water or soils is unlikely to produce significant B complexes or adsorption that would reduce the bioavailability of B in agricultural soils (Mezuman and Keren, 1981).

Boron is an essential element for plant growth but is also toxic when levels get too high. It is taken up passively by plants when a sufficient concentration is available in water and soil for normal growth (Brdar-Jokanović, 2020). Plants are also capable of actively transporting borate to enhance uptake when levels in soil and water are low, and to exclude or compartmentalize borate when levels become toxic (Brdar-Jokanović, 2020).

6.2.6 Cadmium

Cadmium (Cd) has four known oxidation states (-2, 0, +1, 2) and is typically present in soils as Cd^{2+}. It is more mobile in water than most heavy metals (USEPA, 1979). In most natural surface waters, Cd has a preferential affinity to complex with ligands, and follows the order: humic acids > carbonate > hydroxide > chloride >sulfate (USEPA, 1979). In unpolluted natural waters, most Cd will be in the dissolved state as the hydrated ion Cd^{2+}. Minor amounts of Cd are transported with the coarse particulates, and only a small fraction is transported with colloids (ATSDR, 2012c). Adsorption is the main fate and transport mechanism for Cd at low concentrations in soils (Bradl, 2004), with most studies having found that the adsorption behavior of Cd in soils can be explained by its reaction with hydrous iron oxide (Christensen, 1984).

Cd^{2+} is the dominant form of Cd in plant tissues, which is also the dominant form in aerobic soils (Girling & Peterson, 1981). Like many other divalent metal ions, Cd moves into the plant through apoplastic adsorption and then symplastic uptake (Hart et al., 2002). Because Cd^{2+} uptake into plant cells occurs via transmembrane proteins that are also responsible for the uptake of other divalent metal ions, Cd^{2+} uptake can be inhibited by the presence of other metal ions (Gallegos et al., 2012). Only a fraction of Cd taken up by the roots passes to the xylem because it can be bound to peptides in the root, which acts as a barrier to transport of Cd to the shoots (Shentu et al., 2008). Cd accumulation is also greatly affected by the concentrations of organic acids in the rhizosphere, which can facilitate transport through chelation (Cieśliński et al., 1998).

There is large variation in the relative concentration of Cd in different plant tissues among different vegetables. The basis for this variability appears to reflect two different phenomena: (1) the uptake of Cd by the plant increases proportionally to increasing soil Cd, when soil contains substantial concentration of Cd^{2+} salts (Smolders et al, 2001), and (2) leaves and roots have higher Cd concentrations than fruits and seeds (Yang et al., 2009). Yang et al. (2009) observed that the roots of carrots accumulated more Cd than radishes and appeared to be relatively high accumulators of Cd. Samsoe-Petersen et al. (2002) report that mean Cd concentrations were higher in unpeeled root vegetables (carrots and potatoes) than peeled, though the difference was not statistically significant. In a study by Intawongse & Dean (2006), the Cd content in the leaves of both radish and carrots was significantly higher than in their roots, however this trend was apparent only in soils with added Cd. Smolders et al. (2001) reported that Cd concentrations (based on dry weight) are typically higher in the plant leaves than in fruits or storage organs; this is consistent with both Yang et al. (2009) and Intawongse & Dean (2006). Singh et al. (2010) measured Cd in the roots and shoots of tomato plants, and found that in uncontaminated soil, Cd concentrations were similar between tomato roots and shoots. In Cd-enriched soil, Cd concentrations were slightly higher in tomato shoots than roots. In another study, they found that Cd concentrations in the tomato fruit were substantially lower than in other tomato plant parts. For example, Cd levels in the fruit were one order of magnitude lower than in the whole shoot. They report that lower fruit Cd accumulation in tomato are possibly a result of reduced root-to-shoot transfer of Cd at flowering stage and enhanced shoot-to-root retranslocation of Cd (Shentu et al. 2008), which are similar to findings by Chan & Hale (2004). Shentu et al. (2008) also found that Cd concentrations in the shoot of the radish were higher than in the root, in contrast to what has been observed in tomatoes. It suggests that the relative enhancement of Cd concentrations in the root and shoots does not necessarily follow a specific pattern. The lack of a consistent pattern suggests that crops should be carefully selected when soils and/or irrigation water may have higher levels of Cd–especially so for root crops.

6.2.7 Chromium

Chromium (Cr) has ten known oxidation states (−4, −2, −1, 0, +1, +2, +3, +4, +5, +6). Based on the hazard analysis from Task 1 that identified the Chemicals of Interest, hexavalent chromium (Cr^{6+}) is the species of greatest interest because of its toxicity. Most Cr in soil is Cr^{3+}, which has low solubility (Jardine et al., 1999). Adsorption of Cr in soils is controlled by the redox potential of the soil, oxidation state, pH, soil minerals, competing ions, and complexing agents (Bradl, 2004). Cr^{3+} is rapidly adsorbed by iron oxides, manganese oxides, and other clay minerals. About 90% of Cr^{3+} added to soil is adsorbed within 24 hours (Bradl, 2004). In comparison, Cr^{6+} is relatively soluble and mobile. There is the potential that Cr^{3+} can oxidize to Cr^{6+}. However, in a study looking at natural waters, Cr^{3+} did not oxidize to the Cr^{6+} to a significant degree and the reduction of Cr^{6+} to Cr^{3+} was ten-times faster than the re-oxidation rate (Saleh et al., 1989). In soils, the oxidation from Cr^{3+} to Cr^{6+} is facilitated by organic substances, oxygen, manganese dioxide, moisture, and high temperature (e.g., from a brush fire) (ATSDR, 2012a). Due to its immobility in soil, the oxidation of Cr^{3+} to Cr^{6+} is inhibited, as it requires soluble Cr^{3+} (James et al., 1997).

Cr^{3+} is taken up passively by plants while Cr^{6+} is taken up actively (Ertani et al., 2017; Sharma et al., 2020). There is some evidence that when Cr^{6+} is taken up by plants; it is reduced to Cr^{3+} (Cervantes et al., 2001; Hayat et al., 2013). In their review of chromium in agricultural soils and crops, Ertani et al. (2017) report that concentrations of chromium in the different parts of the plant follow a hierarchy with the highest concentrations in roots, followed by the shoots, leaves, and then fruit.

6.2.8 Cobalt

Cobalt (Co) has eight known oxidization states (−3, −1, 0, +1, +2, +3, +4, +5). Cobalt's main oxidation states are Co^{2+} and Co^{3+}, but Co^{2+} is most likely to be found in aqueous environments due to the insolubility of Co^{3+} (Collin and Kinsela, 2010). Cobalt in water may settle in sediments or sorb onto particles (ATSDR, 2004d). The adsorption of cobalt to soil occurs within 1 to 2 hours, as mineral oxides such as iron and manganese oxide, aluminosilicate, goethite, and organic substances can retain cobalt (WHO, 2006). The sorption of Co to sediments or particulates in water may be reduced, as it can complex with dissolved organic substances (Albrecht, 2003).

Environmental conditions can also affect the uptake of Co by plants, by both increasing and decreasing uptake. In highly acidic conditions ($pH < 5.0$), plant uptake can be enhanced an order of magnitude (ATSDR, 2004d). And while increasing solubility and mobility water and soil, cobalt complexed with ethylenediaminetetraacetic acid (EDTA) may decrease cobalt uptake in plants (ATSDR, 2004d).

Plants can take up Co from soil, but most of the Co remains in the roots (WHO, 2006). Insignificant amounts of Co were found in above ground parts of carrots and beets (ATSDR, 2004d). Researchers investigating the uptake of Co in grain crops reported a lack of cobalt in the seeds (Mermut et al., 1996; Smith and Carson 1981). The plant uptake factor for cobalt is between 0.01-0.3 for some grain crops and forage (ATSDR, 2004d).

6.2.9 Copper

Copper (Cu) has six known oxidation states (−2, 0, +1, +2, +3, +4). In soils it may occur in several forms that partition between the solution and solid phases (McGrath et al., 1988). Its two common environmental oxidation states are Cu^{1+} and Cu^{2+}, but Cu^{1+} is found in aerobic conditions (ATSDR, 2004a). The partitioning of Cu within soil is mostly influenced by the presence of soil organic matter, and manganese oxides and iron oxides. Cu shows a strong affinity for soil organic matter so that the organic fraction of Cu is high compared to the that for other metals (McGrath et al., 1988). Copper in soil solution exists primarily in a form complexed mostly with humic materials (Bloomfield and Sanders, 1977). Acidic soils are more likely to mobilize copper in solution (ATSDR, 2004a).

Plants can take up copper into all parts of the plant and may be affected by a number of factors, including its toxicity to plants (ATSDR, 2004a, Fu et al., 2015). The uptake of copper is dependent on bioavailability and concentration (ATSDR, 2004a). Soil pH, however, does not appear to be an important predictor of Cu uptake in plants (Gupta, 1979). Cu accumulation in plants begins with apoplastic transport with root absorption, radial transportation, xylem loading and transportation from the root to the shoot (Fu et al., 2015). As a potentially toxic metal to plants, Cu is compartmentalized or immobilized in proteins and metabolites (Lange et al., 2017). Many copper tolerant plants are excluders, which suggests that the likelihood of hyperaccumulation of copper in crops is low (Lange et al., 2017). Copper tends to accumulate in the roots and shows highest concentration in the epidermis (Kopittke et al., 2011).

The literature related to the uptake of copper in food crops is focused on the response of crops grown in contaminated soils, i.e., soils with artificially high levels of copper due to human activities. There is some evidence to suggest accumulation of Cu in grape leaves (Miotto et al., 2014). Accumulation of copper has also been reported in the roots of cucumber plants with little copper transferred to aerial portions of the plant (Alaoui et al., 2003).

6.2.10 Fluoride

Fluoride is a monatomic anion found in produced water that results from the use of hydrofluoric acid. In water, fluoride complexes with aluminum to form AlF_3, AlF_2^+, and AlF^{2+} (ATSDR, 2003b). Its concentration in water and soil is dependent on aluminum concentration and pH. As water and soils become more basic, complexes with aluminum hydroxide dominate over aluminum-fluoride, thereby increasing fluoride levels (ATSDR, 2003b).

Plants can take up fluoride from both roots and stoma. This means that in addition to uptake through roots, uptake through leaves from aerial application of fluoride containing water can contribute to fluoride in food crops (ATSDR, 2003b). The uptake of fluoride is variable with some crops showing hyperaccumulation, while others show more modest accumulation. In tea, fluoride can accumulate in the leaves to more than 1000 times the concentration of available fluoride in soil (Fung et al., 1999). A study investigating the uptake of fluoride in grain crops reported mixed findings with some crops showing no difference to control samples and some showing concentrations up to 65 times higher than the control sample (Stanley and Schmitt, 1980).

6.2.11 Iodine

Iodine has eight known oxidation states (-1, 0, +1, +3, +4, +5, +6, +7). Iodine (I) in water exists as iodide and iodate (IO_3^-). Microbial action can convert iodide into methyl iodate, which will volatilize from surface waters (ATSDR, 2004b) and reduces availability for plant uptake. Iodine, binds to humic material in sediments like many metallic elements (Rädlinger and Heumann, 2000). It can also bind to inorganic materials in alkaline sediments (Kaplan et al., 2000).

Literature reporting on the uptake of iodine focuses on the biofortification of vegetables by using iodine containing fertilizers. Studies investigating application of these fertilizers to bok choi, carrots, celery, Chinese cabbage, lettuce, onion, tomatoes, spinach, and water spinach, all report increases in iodine in the edible portion of the crops (Dai et al., 2004; Hong et al., 2008; Kiferle et al., 2013). All of these studies reported an increase in iodine concentration in the edible portions of the crops, with leafy vegetables showing the highest uptake followed by carrots and the lowest uptake by tomatoes.

6.2.12 Lead

Lead (Pb) has eight known oxidation states (−4, −2, −1, 0, +1, +2, +3, +4), but will be found as Pb^{2+} in most aerobic environments (ATSDR, 2019c). The amount of lead (Pb) in water depends upon the pH and the ionic strength of the water. The concentration of Pb is likely to be higher in waters with low calcium (Ca) and magnesium (Mg) concentration. Sulfate ions [SO_4^{2-}] also limit Pb in solution through the formation of $PbSO_4$ (ATSDR, 2019c). The formation of Pb carbonates also limit the amount of soluble Pb; Pb carbonate formation is dependent upon the partial pressure of carbon dioxide, pH, and temperature (ATSDR, 2019c). Because Pb forms metal complexes, it would be expected that much of the Pb present in water would be undissolved as colloidal particles or larger undissolved particles (ATSDR, 2019c). Various soil factors also affect both the solubility of Pb in soil and its absorption. These factors include the composition of the soil solution, organic matter content, clay mineral content, pH, and microbial activity (USEPA, 2006). It has been reported that soil pH is the most important factor affecting Pb's solubility, mobility, and availability to plants (USEPA, 2014a).

Lead can be taken up into plants through the root system. In the soil solution it is adsorbed onto the roots, and then becomes bound to either carboxyl groups of mucilage uronic acid, or directly to the polysaccharides of the outermost cells of the root (Seregin and Ivanov, 2001). Lead adsorption onto roots has been documented to occur in several plant species including grasses, legumes, and lettuce (Pourrut et al., 2011). Once adsorbed onto the cells of the root surface, Pb may enter the roots passively and follow translocated water through the plant. However, Pb absorption is not uniform along plant roots, as a Pb concentration gradient has been observed. Indeed, the highest Pb concentrations have been found in root apices, where root cells are young and have thin cell walls that facilitate the uptake of water. Moreover, the root apex is the area of the root where root cell pH is the lowest, a phenomenon which increases the solubility of Pb in solution (Pourrut et al., 2011).

Once Pb has penetrated into the root system, it may accumulate there or may be translocated to aerial plant parts. For most plant species, the majority of absorbed Pb (approximately 95% or more) is accumulated in the roots, and only a small fraction is translocated to above-ground plant parts (Pourrut et al., 2011). There are several reasons the transport of Pb from roots to aerial parts is limited. These reasons include immobilization by negatively charged pectins within the cell wall, precipitation of insoluble Pb salts in intercellular spaces, accumulation in plasma membranes, or sequestration in the vacuoles of root rihizodermal and cortical cells. However, these reasons are not sufficient to fully explain the low rate of Pb translocation from root to shoot. The root endoderm, which acts as a physical barrier, plays an important role in this phenomenon. Apoplastic transport blocks Pb in the root endodermis by the Casparian strip, which must follow symplastic transport. In endodermis cells, the major part of Pb is sequestered or excreted by plant detoxification systems (Pourrut et al., 2011).

There are a number of studies reporting on the uptake of Pb in food crops. Lead was reported to be present at significantly higher concentrations in unpeeled samples of carrots and potatoes than in peeled samples (Samsoe-Peterson et al., 2002). Other studies, however, report that carrots have higher concentration of Pb in the pulp than in the peel (McBride, 2013; Codling et al., 2015). Results from one study showed that concentrations of Pb in the pulp compared to the peel were statistically different in an ANOVA analysis at the 95% confidence level (McBride, 2013). The author speculated that the discrepancy between these findings and others reporting higher concentrations in peel may be a result of the crop having been grown on historically contaminated orchard soil (McBride, 2013). Similarly, Codling et al. (2015) reported that concentrations of Pb in carrot pulp were higher than the peel when grown in lead-arsenate contaminated soils. They also reported opposite patterns in As concentrations where observed concentrations suggested that the peel had higher concentrations than the pulp, but these differences were not statistically assessed (Codling et al., 2015).

Separately, high concentrations of Pb in the root, but not the shoot, of tomato plants was found by Singh et al. (2010). In a UK study looking at urban agricultural sites, they report that on average Pb concentrations in plants exhibited a concentration gradient in the edible portion of the plant. The concentration gradient – from highest to lowest – is roots, shrubs, greens, herbs, tubers, and tree fruit (Singh et al., 2010). In this research, they reported the median concentrations for each of these types of crops range between approximately 0.02 – 0.015 mg/kg [fresh weight] (Entwistle et al. 2019). Other studies indicate that Pb uptake from contaminated soils into root crops, such as carrots, is greater than that into fruits and sometimes comparable to, or higher than, into leafy greens (Preer et al., 1980; Alexander et al., 2006).

6.2.13 Lithium

Lithium (Li) has two known oxidation states (0, 1+); but it does not exist in nature in metallic form. It only exists in nature as a compound, usually in its ionic state. Lithium is unlikely to undergo oxidation-reduction reactions in the environment; as such, it will only be found as Li^{1+} in compounds or dissolved in water (HSDB, 2019). It may undergo precipitation, sorption, or ligand exchange reactions in the environment. Adsorption of Li to suspended solids and sediments is not an important process for Li in the environment (HSDB, 2019). This suggests Li is likely to be mobile in agricultural environments.

The plant uptake of Li is not well-described; but it interferes with the uptake of calcium (Ca), which suggests it moves through plants in a similar way (White and Broadley, 2003). Calcium is taken up passively through Ca^{2+} ion channels, and after being taken up into the plant, a number of active processes take place that appear to reduce the likelihood of cytoxicity of Ca, which is toxic to plants at high concentrations (White and Broadley, 2003). It is posited that a similar process takes place with Li, which is known to be toxic to plants at high concentrations (Anderson, 1990). Evidence suggests that Li is primarily transported in the xylem and has only limited mobility in the phloem (Evangelou et al., 2016).

There are a few studies that report on the uptake of Li in food crops. Robinson et al. (2018) report that the highest concentrations of Li are found in the leaves and that low concentrations are found in fruit and seeds. Concentrations of lithium in a number of crops were reported by Anderson (1990). Results in the material presented by Anderson (1990) corroborate conclusions by Evangelou et al. (2016) and Robinson et al. (2018) that fruit has lower concentrations of Li than other parts of the plant. Beets, however, appear to hyperaccumulate Li in the roots. In soil with 35 mg/kg Li, harvested beets had an average Li concentration of 3500 mg/kg (Anderson, 1990).

6.2.14 Manganese

Manganese has eleven known oxidation states (−3, −2, −1, 0, +1, +2, +3, +4, +5, +6, +7), but Mn^{2+} is most common in aerobic waters with pH between 4 and 7. It can get further oxidized to Mn^{4+} in waters with pH > 8 (ATSDR, 2012d). The interaction of manganese (Mn) with water and soil is complex, as Mn can exist in a variety of oxidation states and form a number of different physical structures. Manganese oxide reacts with both acids and bases and interacts with both cations and anions. Redox reactions involving Mn are affected by various physical, chemical, and biological processes (Bradl, 2004). The solubility of Mn is affected by the solubility of the Mn-compound present, which depends on pH, oxidation-reduction potential, and the characteristics of other anions (ATSDR, 2012d). The processes that affect the adsorption of Mn in soil are more complicated than those of many other metals (ATSDR, 2012d). However, in general, cation exchange reactions with Mn ions and soil particles form manganese oxides, hydroxides, and oxyhydroxides, which in turn form adsorption sites for other metals. It can also be adsorbed to other oxides, hydroxides, and oxyhydroxides through ligand exchange reactions (ATSDR, 2012d). Manganese minerals can precipitate into a new mineral phase that other substances can adsorb to when soils become saturated (Evans, 1989). Oxides of Mn can remove Cu, Pb, Ni, Co and Cr from aerobic waters and wet soil by absorbing them and by reacting with them to create a precipitate, but this can be reversed in reducing conditions (Matagi et al., 1998). The soil absorption of Mn in is highly variable due to the multitude of factors affecting the behavior of Mn in soil. As a result, Mn mobility in soil is highly variable. Baes and Sharp (1983) report that the soil adsorption constant for Mn ranges from 0.2 to 10,000 mL/g and depends heavily on ion exchange capacity and organic content of the soil.

Manganese is an essential trace element for plant metabolism and growth and is taken up into food crops (Socha and Guerinot, 2014); but as Mn^{2+}, it is toxic to plants. To counteract its toxic effects at high levels, Mn^{2+} accumulates in the apoplast where it is oxidized to Mn^{3+} (Fecht-Christoffers et al., 2003; Socha and Guerinot, 2014). Mn^{3+}, however, is also toxic to plants as it oxidizes proteins and lipids (Fecht-Christoffers et al., 2003). To reduce its toxic effect, plants can compartmentalize Mn^{3+} through active symplastic transport. (Socha and Guerinot, 2014).

There is no apparent research reporting on the uptake efficiency of Mn in food crops under typical agricultural conditions.

6.2.15 Mercury

Mercury (Hg) has four known oxidation states (-2, 0, +1, +2). It can occur in soils and water in both inorganic and organic forms (ATSDR, 1999). In soil and water, inorganic Hg exists as Hg^{1+} and Hg^{2+}, and in its organic form, it most commonly occurs as methylmercury (ATSDR, 1999). Inorganic mercury can be converted to methylmercury through biotic and abiotic pathways (ATSDR, 1999). The conversion of inorganic mercury to methylmercury occurs more readily in anoxic-reducing conditions in saturated organic soils (Porvari and Verta, 1995; ATSDR, 1999), which are not common for agricultural soils. The transport and partitioning of mercury in surface waters and soils is influenced by the particular form of the compound (ATSDR, 1999). Metallic mercury is volatile, and along with other volatile organic mercury compounds, is expected to evaporate to the atmosphere. Solid forms of Hg are likely to partition to particulates in the soil or water column and end up in sediments (Hurley et al., 1991). Mercury strongly adsorbed to humic materials in soils with pH higher than 4 (Blume and Brummer, 1991). It also has a high adsorption affinity for soils that are high in iron and aluminum (ATSDR, 1999). Inorganic Hg adsorbed to particulate material is not readily desorbed (Meili, 1991). The availability of Hg for plant uptake appears to be limited. These findings suggest that most Hg in soils will be in the inorganic form and sorbed to inorganic and organic constituents of in aerobic agricultural soils.

The uptake of Hg through the roots of plants has been reported in the literature, but data on food crops is focused on contaminated soils, like those found near mines, refineries, power plants, in areas of sewage release, and other heavy anthropogenic sources. There is some research reporting on factors affecting the uptake of mercury by plants in typical agricultural conditions. Two different studies report that selenium, as both selenite and selenite, reduced the uptake of Hg in both radish and tomato (Shanker et al., 1996a; Shanker et al., 1996b). A few studies have also reported that most mercury resides in the roots and little is translocated to aerial tissue (Beauford et al., 1977; Cavallini et al., 1999).

6.2.16 Molybdenum

Molybdenum (Mo) has ten known oxidation states (−4, −2, −1, 0, +1, +2, +3, +4, +5, +6). Mo^{6+} (or molybdate ion) is the most common form found in aqueous environments and agricultural soils (ATSDR, 2017b). There are competing fate and transport factors that complicate the mobility and availability of Mo in agricultural systems. Molybdenum can be more available for plant uptake as it desorbs from some soils under neutral pH conditions (Goldberg et al., 2002). This bioavailability, however, may be balanced by deposition of Mo to iron oxyhydroxides in perennially aerobic soils (IMOA, 2015).

It is not fully understood how plants access molybdate from soil solution or later redistribute it once it has been taken up by the plant. There is some evidence that plant uptake of Mo occurs via the phosphate pathway like As^{5+}, as deficiencies in soil phosphate enhance Mo uptake in tomatoes (Heuwinkel et al. 1992).

Molybdenum is taken up into plants, but while there is some evidence that it tends to reside in lower portions (root and stem) there are other examples in the literature where this is not the case. Studies of tomatoes by Stout et al. (1951), of alfalfa by Reisenauer (1956), and of soybeans by Singh and Kumar (1979) have shown that leaf tissues contain considerably higher amounts of Mo than stems. Similarly, Gupta (1991) found that among vegetable crops, the lower half of each plant contains more Mo than the upper half. Such differences are greater in plants with higher Mo concentrations. Molybdenum cation has been found to be readily mobile when applied to the leaves of beans; Gupta (1997) reported that most of the Mo is translocated down the plant to the stem and roots. The movement of Mo towards the roots may at least partially explain the higher Mo concentrations in the lower halves of plants, as reported by Gupta (1991). Likewise, Boswell (1980) reported that seeds from the lower third of soybean plant contained more Mo than seeds from the top third or middle third of the plant. The interveinal areas of leaves have also been found to preferentially accumulate Mo (Stout and Meagher, 1948). In the case of cereal crops grown on low-Mo soils, the Mo concentration in the grain was generally lower than that in the straw; however, when Mo was applied at rates of 0.5 ppm or higher, the Mo concentration in the grain was considerably lower than that in the reproductive stage tissues (Gupta, 1971). With increasing maturity, the Mo content in leaves and stems was found to decrease in soybeans (Singh and Kumar 1979); it was also noted that the grain contained higher quantities of Mo than did the leaves, stems, or pod husks. In solution-culture studies of the common bean, the roots were found to contain higher quantities of Mo than the stems and leaves (Wallace and Romney 1977). These responses are congruent with active transport of Mo similar to transport of phosphate (Schactman et al., 1998). Overall, these studies suggest that accumulation of Mo in different parts of a plant is specific to the species, but Mo can preferentially be found in the roots or lower part of the plant.

6.2.17 Nickel

Nickel (Ni) has seven known oxidations states (-2, -1, 0, +1, +2, +3, +4). The most common form found in aerobic waters with pH < 9 is Ni^{+2} (ATSDR, 2005a; Yusuf et al., 2011). In addition to redox potential, pH is an important factor for the mobility and phytoavailability of nickel (Ni) (Peijnenburg et al., 1999). One of the main mechanisms for the removal of Ni from water is adsorption to particulates followed by their settling out of the water column (ATSDR, 2005a). The absorption of Ni onto particulate matter is one of several processes that compete with the complexing of Ni with organic compounds like humic and fulvic acid (Martino et al., 2003). Nickel more strongly adsorbs to organic material in soil than to clay, iron oxide, and manganese oxide in soils (ATSDR, 2005a; Weng et al., 2004). This affinity for organic material can significantly limit (attenuate) its bioavailability for plant uptake (Weng et al., 2004).

The uptake of Ni by plants is carried out through the root system by both passive diffusion and active transport. The relative importance of active and passive processes varies with the plant species, oxidative state of Ni, and concentration in the soil solution. Uptake of Ni by plants also depends on the concentration of Ni^{2+}, plant metabolism, the acidity of soil or solution, the presence of other metals, and the composition of organic matter (Yusef et al., 2011). The uptake of Ni by plants usually declines at higher pH due to the formation of less soluble complexes. Moreover, Ni^{2+} may also compete with other metal ions when it is absorbed by the roots of plants (Yusef et al., 2011). The path of Ni transport in plants is from root to shoot, with elimination occurring through transpiration via xylem (Yusef et al., 2011). Organic acids and amino acids have been reported to be potential Ni chelators, which may facilitate the translocation of these Ni complexes through xylem. Without chelation, the movement of Ni^{2+} from root to shoot is expected to be limited, as xylem cell walls have a high cation exchange capability (Yusef et al., 2011). This suggests that concentration of nickel in the roots will be higher than in other parts of the plant.

There is limited research that compares the uptake of Ni into different parts of the plant. Samoe-Petersen et al. (2002) reported that an increase in the concentration of Ni in vegetable, fruit, and root crops was related to increases in soil Ni concentrations. For example, they reported a linear relationship between soil Ni and potato Ni concentrations. However, there does not appear to be a significant relationship between Ni concentrations in peeled versus unpeeled root crops (Samoe-Petersen et al., 2002). Singh et al. (2010) measured Ni in the roots and shoots of tomato plants, but not edible fruit. In uncontaminated soil, Ni concentrations were similar between tomato roots and shoots. In contaminated soil, Ni concentrations were slightly higher in tomato roots than shoots (Singh et al., 2010).

6.2.18 Nitrite

The nitrogen of nitrite is in the +3 oxidation state, unlike its more common environmental counterpart nitrate, where nitrogen exists in the +5 oxidation state (ATSDR, 2017c). Nitrite is very soluble in water. In aerobic soils, nitrite is oxidized to nitrate and taken up by algae and plants (WHO, 2011). In anerobic soils, nitrite is reduced to gaseous nitrogen (Nolan, 1997).

The literature describing the uptake of nitrite in plants is limited, unlike the more robust literature for nitrate. Some journal articles have reported on the uptake and utilization of nitrite as a source of essential nitrogen, over the more common nitrate (Yoneyama et al., 1980; Breteler & Luczak, 1982; Ibarlucea et al., 1983). However, the uptake pathways have not been described as they have been for nitrate (Agüera et al., 1990).

While less common in agricultural soil, nitrite can be used as a source of essential nitrogen for plants (Yoneyama et al., 1980; Breteler & Luczak, 1982; Ibarlucea et al., 1983., Agüera et al., 1990). Nitrite likely poses no additional health risks to humans from the consumption of crops as nitrite is reduced to ammonia in plants like nitrate (Yoneyama et al., 1980).

6.2.19 Selenium

Selenium (Se) has eight known oxidation states (−2, −1, +1, +2, +3, +4, +5, +6). It is commonly found in water as selenites [Se^{4+}] and selenates [Se^{6+}] and presents as soluble inorganic alkali (Weast, 1988). It is expected to be found in surface water; with the selenic salts and selenious acids present in soil water. The soluble selenate salts of this acid are expected to occur in alkaline waters (ATSDR, 2003a). Elemental Se and Se^{-2} in selenides are not particularly soluble (ATSDR, 2003a). In acidic soils (like those that can be found in agricultural settings) and under high moisture conditions, Se exists as selenite and is bound to colloids as iron hydroxide selenium complexes. These complexes are insoluble and generally are not available to plants (Galgan & Frank, 1995). Inorganic Se can also be methylated by microorganisms in soil that causes it to be volatilized to the atmosphere (Doran, 1982). Plants are also able to release volatile dimethyl selenide to the atmosphere (Wiesner-Reinhold et al., 2017).

Selenium is actively taken up by plants through the roots and then transported through the xylem into the rest of the plant; some of which is converged to organic compounds (Woodbury et al., 1999). As Se^{6+}, and to a lesser extent as Se^{4+}, it is taken up by plants and can be converted to selenomethionine, selenocysteine, dimethyl selenide, and dimethyl diselenide (ATSDR, 2003a; Woodbury et al., 1999).

Selenium is taken up by all plants and is distributed to all organs within the plant (ATSDR, 2003a), but this uptake varies among species (Woodbury et al., 1999). The concentration in plants is usually correlated with the phytoavailability and concentration of Se in soil and water (Banuelos, 1996; White, 2016). This finding, however, does not hold for all crops. It was reported that Se concentrations in rutabaga did not correlated with Se concentration in soil in a study looking at the uptake of Se by various brassica vegetables (Arthur et al., 1992). Selenium concentration differences within different parts of a plant generally follow the hierarchy: seeds > flowers > leaves > roots > stems (Terry et al., 2000; Quinn et al., 2011; Wiesner-Reinhold et al., 2017).

6.2.20 Silver

Silver (Ag) has seven known oxidation states (−2, −1, 0, +1, +2, +3, +4), but is usually found as Ag^0 and Ag^{1+} (ATSDR, 1990a). In aerobic soil and fresh water, Ag is present as compounds of bromide, chloride, and iodide. Sorption is the main process that affects the fate and transport of Ag in water and soils. Silver may leach from soils into groundwater, with the leaching rate increasing with decreasing pH and increasing drainage (ATSDR, 1990a). Silver can move into sediments through adsorption and precipitation (USEPA, 1980). It adsorbs to manganese dioxide, ferric compounds, and clay minerals in addition to precipitating as Ag-halides; this tends to higher concentrations in sediments than in the water column (USEPA, 1980).

The uptake of Ag from soil by plants is low. This is reported in studies where Ag was added through the application of sewer sludge, or in plants grown on mine tailings (WHO, 2002). Pettersson (1976) also reported that cucumbers grown with water containing a mixture of heavy metals, including Ag^{1+}, did not show appreciable translocation of Ag from root to shoot.

6.2.21 Strontium

Strontium has three known oxidation states (0, +1, +2). It is typically found in ambient environments as Sr^{2+} (ATSDR, 2004e). Strontium's mobility in soil and water is dependent on a number of factors, which include pH, ionic strength, solution speciation, mineral composition, organic matter, biological organisms, and temperature; it can also sorb onto metal oxides and clay minerals (Hayes and Traina, 1998). In the presence of organic matter and humic acid, Sr can precipitate out of solution as an organic matter Sr^{2+} complex (Helal et al, 1998a). The formation of these complexes, however, can be inhibited by the application of nitrate fertilizers, thereby increasing Sr^{2+} mobility (Helal et al., 1998b).

Plants appear to absorb Sr^{2+} in proportion to their relative concentrations in soil solution, which is similar to Ca^{2+} (Isermann, 1981). Accordingly, plants like herbs or legumes that absorb more Ca^{2+} than gramineous plants (e.g., corn) will also absorb more Sr^{2+}. The uptake of Sr^{2+} by plants is mainly a passive one, although active processes can also be involved. While terrestrial plants normally do not discriminate between absorption of Ca and Sr, the Sr/Ca ratio may vary between different parts of the plant owing to differences in transport of the two cations inside the plant. The differential transport of Sr^{2+} and Ca^{2+} has been proposed to result from a series of exchange reactions in the xylem where Sr^{2+} is more strongly retained than Ca^{2+}, particularly in the roots and stems. As a consequence, the Sr/Ca ratio in leaves, flowers, and seeds may be lower than in stems and roots (Isermann, 1981).

There does not appear to be a clear pattern as to where strontium will preferentially reside once taken up into plants. The preferential retention of Sr in the roots relative to the shoots has been observed in tomato plants (Bowen and Dymond, 1956); however, no information is available on Sr concentrations in tomato fruit. The opposite pattern has been observed when Sr is chelated within the plant. Smith (1971) found that the Brazil nut tree preferentially accumulated Sr^{2+} in the endosperm with up to 20-fold higher Sr/Ca ratios compared with concentrations in roots or in stem tissues.

6.2.22 Tin

Tin (Sn) has nine known oxidation states (-4, -3, -2, -1, 0, +1, +2, +3, +4). Sn^{2+}, is common in oxygen-poor environments and tends to precipitate out of water as tin sulfide, while Sn^{4+} hydrolyzes (ATSDR, 2005b). Sn^{4+} is the species that is expected to be found in conditions like those in agricultural soils, where it partitions to both water and soil (ATSDR, 2005b). Organotin compounds are thought to be generally immobile in the environment (WHO, 1990), while inorganic compounds tend to be adsorbed to soils (WHO, 1980).

Tin can be taken up by plants through the roots. A study by Muller et al. (2016) reported detectable levels of Sn in spinach when grown using waters with Sn concentrations of 2 and 20 mg/L. They report that seven times more Sn was found in the roots than the shoots (Muller et al., 2016). In another study, Sn was shown to be taken up by a variety of crops including various herbs, radish, and spinach, with reported plant uptake factors ranging from 6.8 to 8.9 for the edible portions of the plants grown in soils having an average soil Sn concentration of 50.9 µg/kg (Ghasemidehkordi et al., 2017).

6.2.23 Vanadium

Vanadium (V) has eight known oxidation states (-3, -1, 0, +1, +2, +3, +4, +5). It is most commonly found as V^{5+} in aerobic surface waters (Crans et al., 1998). Of the three oxidation states found in the environment (+3, +4, +5), V^{5+} is more available to plants because it is the most soluble and more easily leached from soils (ATSDR, 2012e). There are a number of factors that may play a role in the phytoavailability of V for plant uptake. Vanadium can bind to minerals and organic materials in soil by adsorption and complexing (Wehrli and Stumm, 1989). Unlike many metals, V is more mobile in neutral to alkali conditions and becomes more immobile as soil acidity increases (ATSDR, 2012e).

Vanadium can be taken up by plants, where it generally accumulates in the roots (Byerrum et al., 1974). In a review article by Aihemaiti et al. (2019), the authors report on a large variety of food crops and the concentration of vanadium in roots and shoots. They report similar findings to Beyrrum et al. (1974) with V concentration in the roots higher than in the shoots for all food crops, which include leafy vegetables, legumes, tomatoes, watermelon, rice, other grains, and onions (Aihemaiti et al., 2019).

6.2.24 Zinc

Zinc (Zn) has four known oxidation states (-2, 0, +1, +2). In aerobic waters and soils, it occurs in the Zn^{2+} state (ATSDR, 2005c). Zinc can adsorb onto manganese oxide, hydrous iron, clay minerals, and organic material. In waters that do not have high concentrations of Zn, it is adsorbed and transported by suspended solids. In acidic soils, Zn dissolves and is available in the ionic form (Zn^{+2}) where cation exchange can impact its fate. In alkali soils, zinc is more impacted by its interaction with organic ligands (ATSDR, 2005c). More than 90% of Zn in soil is insoluble and unavailable for plant uptake (Broadley et al., 2007).

Zinc is an essential nutrient for plants and is taken up from soil solution (Broadley et al., 2007). It is actively transported within the plant from the roots to aerial parts through both apoplastic and symplastic pathways and is compartmentalized in apoplasts when levels of Zn in soil solution become toxic to the plant (White et al., 2002; Broadley et al., 2007). When taken up by some food crops, Zn does not appear to accumulate preferentially in different parts of the plant that are edible. Schuhmacher et al. (1993) reported that the uptake of zinc from 16 different species of edible crops did not vary substantially. These included roots, tubers, bulbs, leaves, cabbages, and fruits. Another study reporting on the Zn uptake in Chinese cabbage, bok choy, and celery report plant uptake factors of <1 for all crops for root and shoot tissue (Islam et al., 2007).

6.3 Discussion of Inorganic Chemicals of Interest: Fate, Transport, and Plant Uptake

Metals and other inorganic chemicals are potentially the more mobile components of soil, but their behavior is complex and governed by a number of factors that can affect their mobility, availability for uptake by plants, and distribution within a plant. All of the inorganic Chemicals of Interest are also found in soil naturally and many are components of fertilizers, components of other soil amendments, and are present in conventional irrigation water.

As discussed above, there are many factors in agricultural soils affecting the mobility and phytoavailability of metals. The most important of these are pH, redox conditions, and adsorptive potential (Bourg and Loch, 1995; Rieuwerts et al., 1998; Balasoiu et al., 2001, Bradl, 2004). Other factors that may play a role in metal mobility are the adsorption to inorganic colloid-forming minerals like clay that make them more mobile and phytoavailable under favorable cation exchange conditions (Bradl, 2004); and the formation of soluble metal-ligand complexes with humic or fulvic acids, which can also increase metal phytoavailability (Evangelou et al., 2004; Liphadzi and Kirkham, 2006; Shariq, 2019).

Because agricultural soils tend to be managed to optimize crop production, most agricultural soils share many similarities (Husson, 2013). Even so, the soil at various farms, fields, and crops can be expected to be managed with differences that could have a significant effect on the concentration and movement of metals in the soil. Differences in soil management (e.g., application of soil amendments, tillage practices, irrigation practices) and soil conditions (e.g., mineral content, pH, Eh) can affect the concentration of chemicals in soil, in the soil conditions affecting metal mobility, and in the phytoavailability of metals.

While the state of the science is not sufficient to support the development of models to predict concentrations of metals in the edible portions of plants based on levels in soil or irrigation water, the literature on the uptake of metals from soil and their distribution within a plant does point to some predictable patterns. For example, the literature suggests that As, Cr, Pb, Li, Hg, and Ag have little to no tendency to be partitioned to fruit when grown in typical agricultural soils (Byerrum et al., 1974; Pettersson, 1976; Beauford et al., 1977; Barrachina et al. 1995; Cavallini et al., 1999; Hammel et al., 2000; Singh et al., 2010; Ertani et al., 2017; Robinson et al., 2018). The literature also indicates a pattern in which the highest concentrations of As, Be, Cr, Co, Pb, Hg, Mo, Ag, Sr, Sn, and V tend to be found in the roots, rather than other parts of the plant (Pettersson, 1976; Beauford et al., 1977; Preer et al., 1980; Helgesen and Larsen, 1998; Cavallini et al., 1999; Samoe-Petersen, et al. 2002; WHO, 2002; ATSDR, 2004d; Alexander et al., 2006; WHO, 2006; Singh et al., 2010; Codling et al., 2015; Muller et al., 2015; Codling et al. 2016; Ertani et al., 2017; Aihemaiti et al., 2019). There is also some evidence that metal concentrations in the skins of tuber/storage vegetables may be higher than in the core of the root. This pattern appears to be true for As (Helgesen and Larsen, 1998; Samoe-Petersen, et al. 2002; Codling et al., 2015; Codling et al. 2016), Cd (Samoe-Petersen et al., 2002), Pb

(Samoe-Petersen et al., 2002, Codling et al., 2015), and Ni (Samoe-Petersen et al., 2002).

Even with the substantial amount of research that has been devoted to understanding the fate and transport of metals in soil and how they are taken up by plants and subsequently translocated to various parts of a plant, the state of the science is not to a point where we can model the level of chemicals in edible plant parts from levels in soil or irrigation water. However, the available information can be useful in the interpretation of existing sampling data from crops irrigated with produced water. That is, it can help us determine if we might expect to see a particularly high or low level of any specific metal in a crop sample. It could also be valuable in the decision to collect any additional data or in the design of any future sampling plans.

The available information does not suggest that any specific metal or Chemical of Interest poses a particular concern for crop accumulation, nor does it indicate that any can be completely eliminated from concern because they will not be taken up into plants. Nitrite is the only inorganic Chemical of Interest that could be eliminated from any further evaluation because it is converted to an important nutrient for food crops and it is at levels likely to be encountered in many agricultural settings.

7.0 RADIONUCLIDE CHEMICALS OF INTEREST: FATE, TRANSPORT, AND PLANT UPTAKE

The Chemicals of Interest selected in Task 1 include six radionuclide isotopes, including radium-226 (Ra-226), radium-228 (Ra-228), thorium-232 (Th-232), uranium-238 (U-238), krypton-85 (Kr-85), xenon-133 (Xe-133). As in the previous section (Section 6: Inorganic Chemicals of Interest: Fate, Transport, and Plant Uptake), this section addresses the question of whether and to what degree these radionuclides could accumulate in the edible portion of food crops, if present in produced water used for irrigation. Four of the radionuclides are metals that are affected by the same chemical and physical properties that affect the fate and transport of other inorganic compounds including, soil redox potential, pH, complexation processes on inorganic and organic constituents, and biological fixation and transformation (Koch-Steindl and Prohl, 2001). The other two radionuclides (Kr-85 and Xe-133) are gases at ambient temperatures, which affects their movement in the environment and their propensity for plant uptake. A general discussion of the factors affecting the fate, transport, and plant uptake of inorganic chemicals was presented in Section 6.0.

Building on the general discussion of factors affecting the movement of inorganic chemicals in the environment, a summary of chemical-specific factors affecting the potential migration of the radionuclide Chemicals of Interest from irrigation water into the edible portion of irrigated crops is presented below. This summary includes soil-plant uptake factors for the four metal radionuclides, including some uptake factors applicable to crops currently being irrigated with blended produced water in the San Joaquin Valley. While empirical soil-plant uptake factors are available for some plants and plant parts, we found no information of the biochemical mechanisms of plant uptake for the radionuclides.

The fate of radionuclides, unlike stable isotopes, is also affected by radioactive decay. Many radionuclide daughter products are also radioactively unstable and continue to follow a radioactive decay chain, transforming into other elements. For example, Ra-226 is a daughter product of U-238, and R-228 is a daughter product of Th-232. These naturally occurring radionuclides will continue to decay over many years until they become stable isotopes of lead, Pb-206 and Pb-208, respectively. The fate and transport of lead is discussed in Section 6. Xenon-133 and Kr-85 decay to stable isotopes of cesium (Cs) and rubidium (Rb). Elemental Cs is relatively non-toxic, and there is little indication of adverse health effects from chronic exposure (ATSDR, 2004c). Only at high concentrations can cesium cause reversable acute hypokalemia, as it displaces potassium in some biochemical reactions (Melnikov & Zanoni, 2010). Rubidium (Rb) does not appear to cause adverse effects even when exposure is relatively high, i.e., 18 grams or more (USEPA, 2016b). Given that Cs and Rb do not display overt chronic oral toxicity, they were not evaluated further.

7.1 Radium

Radium exists as a divalent ion in water, Ra^{2+}. The solubility of radium increases with increasing alkalinity (ATSDR, 1990b), which is counter to the behavior of most metals in water. Like many metals, it adsorbs to organic materials and forms complexes with humic acid, which increases the rate at which Ra can absorb to organic materials, such as coconut fiber (Laili et al., 2010). Ra also adsorbs to iron hydroxide, silicon dioxide (Benes et al., 1984) and aluminum silicate minerals in clay (Benes et al., 1985). It has the potential to irreversibly bind to these mineral surfaces (Benes et al., 1984; Benes & Strejc, 1986) making it unavailable for plant uptake, especially in acidic soils.

Vandenhove et al., (2009) reported that the average fresh-weight soil transfer factors for radium in vegetable-fruit crops, roots, and fruit are 0.26, 1.9, and 0.027, respectively. Mitchell et al. (2013) has also reported that the roots of a plant more often have a higher concentration of radium than its other parts. There was no relevant data describing the mechanisms of uptake of Ra in plants. A review article reported that there are a number of studies that report on the empirical uptake of Ra in plants, but the mechanisms are not well understood (Mitchell et al., 2013).

7.2 Thorium

Thorium has four oxidation states (+1, +2, +3, +4); and it is only known to have one stable oxidation state in aqueous solution, Th^{4+} (Wickleder et al., 2010). Thorium concentrations in ambient water are generally low (ATSDR, 2019d). Thorium will absorb onto particles, making it relatively immobile, as well as unavailable for plant uptake (Hunter et al., 1988; ATSDR, 2019b). Phosphate fertilizers will reduce the phytoavailability of thorium through the formation of phosphate salts that have low solubility (Guo et al 2010). It may also form complexes with humic acid, which may increase its solubility and availability for uptake in some soils (ATSDR, 2019d).

Vandenhove et al., (2009) reported that the average fresh-weight soil transfer factors for thorium in vegetable-fruit crops, roots, and fruit are 0.0034, 0.0093, and 0.0062, respectively. Estimated soil transfer factors for thorium in almonds and pistachios are 0.005 and 0.001, respectively (Napier, 2013). Mitchell et al. (2013) has also reported that the roots of a plant more often have a higher concentration of thorium than its other parts. There was no relevant data describing the mechanisms of uptake of Th in plants. A review article reported that there are a number of studies that report on the empirical uptake of Th in plants, but the mechanisms are not well understood (Mitchell et al., 2013).

7.3 Uranium

Uranium (U) has four oxidation states in water (+3, +4, +5, +6). It is most soluble in solution as U^{6+} in UO_2^{2+} ion (Grenthe et al., 2006; LANL, 2013), but can also exist as U^{4+} in the environment (Greger, 2004). Uranium is known to concentrate in sediments and suspended solids in water (ATSDR, 2013). It behaves like many metals in that it is more mobile in acidic soils (Herczeg et al., 1988). Uranium will adsorb onto iron and manganese oxides in soil particles (Ames et al., 1982). The mobility of uranium in soil is sensitive to changes in soil properties, with mobility associated with changes in pH, redox-potential, available complexing ions, soil texture, and the amount of available water (ATSDR, 2013). Uranium forms organic complexes that are easily soluble and mobile (Greger, 2004).

Vandenhove et al., (2009) reported that the average fresh-weight soil transfer factors for uranium in vegetable-fruit crops, roots, and fruit are 0.0036, 0.0036, and 0.0057, respectively. In a study by Al-Kharouf et al. (2008), they report U-238 transfer factors for zucchini and watermelon of 0.0105 and 0.0045, respectively. Estimated soil transfer factor for uranium in almonds is 0.004 (Napier, 2013). Napier et al., (2013) was unable to estimate the soil transfer factor for uranium in pistachios because there was insufficient data above the detection limit. Mitchell et al. (2013) has also reported that the roots of a plant more often have a higher concentration of uranium than its other parts. There was no relevant data describing the mechanisms of uptake of U in plants. A review article reported that there are a number of studies that report on the empirical uptake of U in plants, but the mechanisms are not well understood (Mitchell et al., 2013).

7.4 Noble Gases: Krypton and Xenon

The additive radionuclides (Kr-85, Xe-133) are noble gases and, as such, are chemically unreactive. Accordingly, they are not expected to be affected by environmental conditions such as redox potential, pH, or organic content. Krypton and xenon are both soluble in water and, like many other gases, have decreased solubility in water with increased water temperature (Yeh and Peterson, 1964). Because of their volatility, we would expect loss of these radionuclides from water prior to any contact with the roots or foliage of irrigated crops and further loss from soil prior to contact with roots.

Very little published information is available on the plant uptake of krypton and xenon, or noble gases more generally. A small amount of information is available on radon, another radioactive noble gas (ATSDR, 2012g). Even though radon is not a Chemical of Interest for this study, information on radon is expected to be instructive for understanding the chemically similar Chemicals of Interest, Kr-85 and Xe-133. Lewis and MacDonnel (1990) postulate that a major mechanism for radon uptake by plants is through water as it helps to explain their findings about the pattern of transpired radon by plants throughout the day. They reported that the release of radon to the atmosphere by plants is directly proportional to the leaf area index (Lewis and MacDonnel, 1990). These observations on the movement of radon gas may be indicative of the movement of Kr-85 and Xe-133, but we did not find any studies specifically on the uptake or movement of these two radionuclides through plants.

7.5 Discussion of Radionuclide Chemicals of Interest: Fate, Transport, and Plant Uptake

As discussed above, the metallic radionuclides generally have low mobility in soil and a low propensity for plant uptake. Accordingly, only a small quantity of the metallic radionuclides in irrigation water or soil is expected to be taken up by food crops irrigated with blended produced water. The behavior of the metallic radionuclides is similar to other metals in that pH, redox conditions, soil characteristics, and binding capacity to organic and inorganic soil constituents tend to affect their phytoavailability in water and soil. The soil transfer factors suggest that the uptake of uranium and thorium is very low (Vandenhove et al., 2009; Napier, 2013). The fresh-weight soil transfer factors for radium are also low, with only the transfer factor for radium into roots being above 1 (i.e., 1.9). Thus, radium in root crops could be up to 1.9-times that of the concentration in soil, and the concentrations of radium in other plant parts would be less than the concentrations in soil. The concentrations of the other metallic radionuclides in crops would be much lower than the levels in soil.

Less information is available about the potential for the noble gases, Kr-85 and Xe-133, to be taken up into irrigated crops. There is some evidence to suggest, however, that a fraction of the radionuclide taken up by plants will be lost through transpiration, as they are gases (Lewis and MacDonnel, 1990). Because of their volatility, however, we would also expect loss of these gases from water and soil prior to irrigation water coming into contact with the roots of irrigated plants.

As was true for other inorganic chemicals, there is some understanding of factors affecting the fate and transport of metallic and gaseous radionuclides and their propensity to accumulate in irrigated crops. Empirical data is also available for some crops, indicating that radionuclides tend not to accumulate or concentrate in food. As was true for other inorganic chemicals, however, the state of science on this topic does not support the ability to model concentrations of radionuclides in irrigated crops based on concentrations in irrigation water.

While we cannot make a quantitative link between the levels of radionuclides in irrigation water and irrigated crops, the available information suggests radionuclides tend to be poorly absorbed from soil and do not bioaccumulate in crops. In addition, available monitoring data for blended produced water used to irrigate food crops in the San Joaquin Valley has found levels of radionuclides in the blended produced water are low. The statement that radionuclide levels are “low” is based on comparison of monitoring data for radionuclides in blended produced water to drinking water standards. The drinking water standards for radium, uranium, and gross alpha radiation for thorium are 5 pCi/L, 20 pCi/L, and 15 pCi/L, respectively. In blended produced water, water monitoring data (Table 8) suggest there is no systematic exceedance of MCLs for radionuclides. MCLs were only exceeded infrequently: 1 of 32 samples exceeded the gross alpha radiation MCL of 15 pCi/L, with a concentration of 20 pCi/L; 1 of 33 samples exceeded the Ra-226 + Ra-228 MCL of 5 pCi/L, with a concentration of 9.4 pCi/L; and there were no exceedances of the MCL for uranium. The fact that radionuclide levels in blended produced water are low and that radionuclides do not have a propensity to accumulate into crops from soil suggests that radionuclides are not a class of chemicals for which we expect to see significant health risks in irrigated crops.

8.0 ORGANIC CHEMICALS OF INTEREST: FATE, TRANSPORT, AND PLANT UPTAKE

The Chemicals of Interest selected in Task 1 include 101 organic chemicals. One of the key questions addressed in Task 2 is whether any of these chemicals, when present in produced water used for irrigation, could move into and accumulate in the edible portion of irrigated crops. As discussed below, a large body of science is available on general mechanisms of plant uptake of organic chemicals from soil and water and on distribution of chemicals into different parts of the plant. Similarly, there is a large body of information on the effect of various soil properties and water chemistry on the movement of organic chemicals in soil and the on the absorption of organic chemicals into roots from soil. The general principles affecting the uptake of organic chemicals into irrigated crops are briefly summarized below (Section 8.1). Chemical-specific evaluations of the movement of chemicals in soil and plant uptake are presented in Sections 8.2 and 8.3. Unlike the larger body of information describing the factors that affect the general movement of chemicals in water, through soil, and into plants, data for specific chemicals is less available. A summary of the available literature describing the chemical-specific factors affecting the potential migration of the organic Chemicals of Interest from irrigation water into the edible portion of irrigated crops is also presented in Section 8.2. The limited available literature describes, for example, how some organic chemicals are not likely to be phytoavailable because they are poorly soluble in water and absorb to organic matter in soil. In Section 8.3, another chemical-specific evaluation of movement in soil and plant uptake is presented, but the evaluation in Section 8.3 is based on chemical properties and models presented in the database of the EPI Suite software (USEPA, 2012b). Because of a lack of data, neither evaluation presented in Section 8.2 or 8.3 addressed all 101 of the organic Chemicals of Interest. We present an overall summary and discussion of the findings in Section 8.4.

8.1 General Principles Affecting Movement of Organic Chemicals in Soil and Phytoavailability

A number of factors can affect the behavior and ultimate fate of organic chemicals in irrigation water and agricultural environments; these factors include solubility, volatility, sorption to organic matter, biodegradability, other processes that can degrade and transform organic chemicals, and plant uptake (Mackay and Betts, 1991). The solubility of each of the Chemicals of Interest directly affects its potential to impact crops irrigated with produced water, since chemicals with low solubility are less likely to be present in irrigation water in the first place. The volatilization of chemicals can be an important factor in affecting losses of chemicals from water and is related to its vapor pressure (Mackay and Betts, 1991). The potential for organic chemicals to adsorb to organic matter is due to the natural partitioning between polar and non-polar phases; it is often described by the organic carbon portioning coefficient (Biggar, 1987; Mackay and Betts, 1991). Soil type, organic matter content, and the presence of clay mineral can all affect the relative importance of adsorption of organic compounds to the various soil components (Mackay and Betts, 1991). Biodegradability is another important factor in the availability of the organic Chemicals of Interest for uptake by plants. We initially screened the Chemicals of Interest for biodegradability based on OECD water testing ("Ready biodegradability tests") criteria, in Task 1. These testing results, however, may not fully describe the potential for these chemicals to also degrade in soil.

Organic chemicals may also degrade or transform in the environment before they are taken up by plants. Degradation and transformation of the Chemicals of Interest in produced water can potentially happen at the surface—in soils and water—and downhole within the formation. At the surface, chemicals may undergo photolysis or other biological and chemical reactions that alter their structure. The importance of photolysis is limited by the structure of the chemical, sufficient solar radiation, and the presence of co-reactant chemicals (Mackay and Betts, 1999). Downhole, degradation and transformation are limited to biological and chemical processes.

There is some reported interest in the literature with regard to the processes that may transform or degrade chemicals in produced water, due to the known complexity of the produced water solution (Butkovskyi et al., 2017; Neff et al., 2011; USEPA, 2016a). Although there are few studies on the degradation and transformation of chemicals from conventional oil and gas development and extraction, many of the same chemicals are used in hydraulic fracturing operations (Stringfellow et al., 2017); and there are many more studies on the degradation and transformation of chemicals used in hydraulic fracturing operations. Accordingly, the studies summarized below include studies performed at hydraulic fracturing operations, even though none of the produced water evaluated in this study comes from hydraulic fracturing.

The hydraulic fracturing literature focuses on the degradation of two main classes of chemical additives, surfactants and biocides; but the transformation and degradation of a few other chemicals are also reported. Surfactants are used in many stages of oil and gas extraction including drilling, fracturing, acidization, demulsification, and corrosion inhibition. Surfactant chemicals used in oil and gas production include polypropylene glycols, ethoxylated alkylphenols, and polyethylene glycols. Biocides are used to control the growth of bacteria, which cause the creation of hydrogen sulfide gas, growth of bioslimes, oxidation of iron, and degradation of polymers. Biocides include chemicals like glutaraldehyde, quaternary ammonium compounds, and benzyl ammonium chloride. We discuss the literature describing the degradation and transformation of surfactants, biocide, and some other hydraulic fracturing related chemicals similar to the Chemicals of Interest in Section 8.2.

We know that additive chemicals used in oil and gas development are not always recovered, suggesting their possible degradation and/or transformation (Carter et al., 2013; Kahrilas et al., 2016; Lester et al., 2015; Orem et al. 2014). Carter et al. (2013) showed that some of the organic chemical additives that were injected into wells during hydraulic fracturing operations were not recovered, leading the authors to conclude that degradation or sorption of these chemicals had occurred underground. Similar observations have been made by others (Kahrilas et al., 2016; Lester et al., 2015; Orem et al. 2014). While biodegradation is a well-known and documented transformative processes for chemicals used in the oil and gas industry, the chemical transformation of these chemicals in-situ is an ongoing area of research (Kahrilas et al., 2016).

The variety of conditions within a petroleum formation create significant uncertainty about how chemicals may ultimately degrade or transform. Elevated temperatures and inorganic mineral content encountered during production, especially with the high temperature and pressures of hydraulic fracturing, can affect the stability of organic chemicals in solution (Seewald, 2001; Seewald, 2003; Borch et al, 2010). As temperature and pressures increase underground, the chemical equilibrium will shift to maintain lower temperatures and lower pressures (Le Chatelier’s principle). This means that reactions may shift to favor endothermic products, and products with smaller volume. High downhole pressures and temperatures may not only lead to unexpected chemical reactions or degradation but may also alter the potential for biodegradation of organics (including biocides) underground (Kahrilas et al, 2016). One of the complications in extrapolating the potential for chemical degradation between hydraulic fracturing and conventional oil and gas production is that hydraulic fracturing utilizes extremely high pressures, while conventional production pressures are lower. These extreme pressures may work together with elevated temperatures to produce chemical reactions that are not expected under surface conditions (Seewald, 2001; Siskin et al, 2001; Seewald et al., 2006; Shipp et al., 2013).

Organic chemicals may enter a plant by either root or foliar uptake (Simonich and Hites 1995; Trapp and Legind, 2011). In root uptake, chemicals partition from soils to the plant roots followed by translocation via the xylem and transpiration. Organic chemicals may also be taken up through the stomata of leaves from gas-phase and particle-phase deposition of organic compounds (Simonish and Hites, 1995). Chemical translocation of organic compounds to the roots and other plant tissues could occur via the phloem, which transports photosynthates. The uptake pathways utilized by plants are a function of the: (1) chemical and physical properties of the chemical (e.g., lipophilicity, water solubility, vapor pressure, and Henry’s law constant); (2) environmental conditions (e.g., ambient temperature, organic content of soil); and (3) plant species (Simonich and Hites 1995).

Foliar uptake is the dominant uptake pathway for lipophilic organic chemicals. The accumulation of organic compounds within leaves following air-to-leaf uptake is dependent upon vapor-particle partitioning in the atmosphere, the octanol-air partition coefficient (K_{OA}) of the plant, the plant species, and leaf lipid concentration and surface area (Simonich and Hites 1995). Generally, gas-phase pollutants with a large K_{OA} preferentially accumulate in leaves. The partitioning of lipophilic chemicals from the outer leaf to the inner leaf is slow (Simonich and Hites 1995). At low ambient temperatures (autumn and winter), polycyclic aromatic hydrocarbons (PAH) partition to vegetation, and at high ambient temperatures (summer), some PAHs volatilize back to the atmosphere. While PAHs in vegetation can result from particle-phase deposition, the predominant pathway is gas-phase deposition (Simonich and Hites 1995).

The accumulation of organic chemicals within plants from root uptake depends upon the compound's water solubility, Henry's law constant, and octanol-water partition coefficient (K_{OW}) (Simonich and Hites 1995). Additionally, the lipid composition of the plant roots is likely to influence root uptake behavior with roots having higher lipid content potentially facilitating more uptake of organic compounds (Collins et al. 2006). Uptake of anthropogenic organic chemicals by plant roots have been shown to be a passive, diffusive process, except for a few hormone-like chemicals such as phenoxy acid herbicides (Collins et al. 2006). The accumulation of non-ionized chemicals by roots is ascribed to two processes: (1) partitioning of chemicals to lipophilic root solids and (2) uptake into the aqueous phase in roots contained in the free space and within the root cells (Briggs et al. 1982). The partitioning process dominates for lipophilic compounds. Highly lipophilic compounds (i.e., K_{OW} >104, such as PAHs) generally partition to the epidermis of the root or to soil particles, and aside from some exceptions, are not drawn into the inner root or xylem for translocation (Simonich and Hites 1995). The xylem transports water and solutes upward from the root into other plant parts, relying upon a flux created from the water potential gradient during transpiration (Collins et al. 2006). The second process, uptake by the aqueous phase in the root, occurs most preferentially for polar compounds (Briggs et al. 1982). Generally, hydrophilic organic compounds (i.e., compounds with high water solubilities, low Henry law's constants, and low K_{OW} values) can be taken up from soil through plant's roots, translocated within the plant via the xylem, and significantly metabolized (Simonich and Hites 1995). Under normal soil conditions, organic contaminants except those that are polar and non-volatile will preferentially be taken up from air. Soil concentration will not have much impact on the concentration in leaves, unless it is far above chemical equilibrium (Trapp and Legind, 2011).

8.2 Environmental Fate and Transport and Phytoavailability of Chemicals of Interest: Literature Review

Section 8.2.1 through 8.2.8 describe the results of the literature review of the factors affecting the movement of the organic Chemicals of Interest in the environment and into plants. The literature review was focused on identifying data and other information that could help us understand how these chemicals might behave in agricultural environments. Information on chemical-specific factors affecting the movement of chemicals in soil was not available for the organic Chemicals of Interest; and among the chemicals for which information was the available, the amount of information available varied widely. The relevant information for acrylamide, aromatic amines, PAHs[1], biocides, and some other petroleum production related chemicals is summarized below.

8.2.1 Acrylamide

As previously discussed, acrylamide was evaluated in Task 1 and removed from consideration as a Chemical of Interest because it was readily biodegradable in water. We identified research, however, that suggested a further consideration of acrylamide was warranted because it was identified as a chemical that can be a degradation product of polymers that were identified as Chemicals of Interest.

Currently available scientific literature does not address the pathways for plant uptake of acrylamide; however, Briggs et al. (1982) reports that acrylamide is highly soluble in water and could be taken up through the roots of plants. Some studies report the potential for acrylamide monomer to be present in polyacrylamide soil amendments that include polymers on the list of Chemicals of Interest (Bologna et al., 1999; Mroczek et al., 2014). One of these studies reports that residual acrylamide in a polyacrylamide flocculent was taken up by hydroponically grown lettuce (Mroczek et al., 2014). Lettuce was exposed to two water-soluble polyacrylamide flocculants which were dissolved in water with other nutrients. The two types of flocculent had residual acrylamide concentrations of 176 and 763 mg/kg. Exposure to acrylamide stunted growth of the lettuce and reduced their average weight and number of leaves. Resulting acrylamide concentrations in the two exposure groups were not statistically different; reported average acrylamide concentrations in lettuce were 0.01 and 0.03 mg/kg (Mroczek et al., 2014).

8.2.2 Aromatic Amines

Aromatic amines are a broad class of compounds that have an aromatic ring attached to an amine group. Generally, aromatic amines may form strong chemical bonds with the humic acid present in soil, which decreases the mobility of the aromatic amines in water (USEPA, 2012b). Humic acid is also one of the additives potentially present in produced water. As a result, when aromatic amines and humic acid co-occur, aromatic amines may be less available for plant uptake.

In the list of declared additive chemicals used by oil producers, one of the chemicals was declared as “Aromatic amines” without a more specific reference. To further review the environmental fate and transport of aromatic amines in produced water reused for agricultural irrigation, the specific aromatic amine used by the oil producers would be required.

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[1] In the list of the Chemicals of Interest, there are 11 PAHs; these include acenaphthene, anthracene, benzo(a)anthracene, benzo(a)pyrene, benzo(b)fluoranthene, chrysene, dibenzo(a,h)anthracene, fluoranthene, indenopyrene, phenanthrene, and pyrene.

8.2.3 Chlorobenzene

Chlorobenzene has environmental fate and transport characteristics that will attenuate its concentration in blended produced water. Chlorobenzene is highly volatile and has been observed to nearly entirely evaporate from water within 72 hours (Garrison and Hill, 1972; Baduru et al. 2008). It was found to rapidly biodegrade in aerobic waters, with up to 100% biodegradation after microbial adaptation (Tabak et al., 1981). Chlorobenzene was also found to fully biodegrade in a few weeks in soil, where Tabak et al. (1981) reported that microbial adaptation was rapid. Other studies have also found that natural microbial colonies are able to adapt and biodegrade chlorobenzene in soil (Feidieker et al., 1995; Van der Meer et al., 1998).

Little is understood about the pathways and factors that affect the uptake of chlorinated solvents by plants, although the uptake and metabolism of these solvents is known to occur in some plant species (Trapp and Legind, 2011). Chlorinated solvents can be metabolized by some crops, with a study showing that metabolites of TCE have been detected in apples and peaches (Chard et al., 2006). While not described in the experimental or monitoring literature, Trapp and Legind (2011) hypothesized that chlorinated solvents could accumulate in root crops and potatoes.

8.2.4 1,4 Dioxane

Dioxane has the potential to be present in blended produced water if present in produced water. It is soluble in water and environmentally persistent. 1,4-dioxane is relatively resistant to biodegradation in water and soils (ATSDR, 2012b). It binds only weakly to soils and can move readily into groundwater (ATSDR, 2012b). Even in an inoculated natural sediment sample incubated under ambient conditions, there was no biodegradation of 1,4-dioxane, even in the presence of tetrahydrofuran, which is postulated to be co-metabolized with 1,4-dioxane (Zenker et al., 2000). 1,4-dioxane is only slightly volatilized from surface water and soil due to its high water solubility (USEPA, 2015a).

There is little available literature describing the uptake to 1,4-dioxane. One study reported on the uptake of 1,4-dioxane by poplar trees and reported that ~19% of added dioxane in the soil remained after 15 days and that it was likely taken up by the roots and transpired and lost to the atmosphere through the leaves (Aitchison et al., 2000).

8.2.5 Polycyclic Aromatic Hydrocarbons (PAHs)

Because PAHs are generally poorly soluble in water, sorb to organic materials, and are susceptible to photolysis, they are unlikely to be found in blended produced water. PAHs with more aromatic rings are, in general, less soluble than PAHs with fewer aromatic rings. Those with two-ring compounds, such as naphthalene, are soluble to approximately 30 mg/L and compounds with three or more benzene rings having solubilities less than 1 mg/L in water (Baek et al., 1991). Nearly all of the PAHs on the list of Chemicals of Interest have three or more benzene rings, with the exception of acenaphthene, which has a solubility of 2.53 mg/L (USEPA, 2012b). As the molecular weight of PAHs increase, there is also an increasing tendency to sorb onto surfaces or form solids (Baek et al., 1991). PAHs having two to three aromatic rings (acenaphthene, anthracene, phenanthrene) are volatile and can partition to air (Baek et al., 1991; Jones et al., 1989). Those with four aromatic rings (fluoranthene, pyrene, chrysene, benz[a]anthracene) are less volatile, but exist both in the vapor and solid phase. Those having five or more aromatic rings (benzo[a]pyrene, benzo(b)fluoranthene, indenopyrene, dibenzo(a,h)anthracene) exist primarily in the solid phase (Baek et al., 1991; Jones et al., 1989). Low molecular-weight PAHs with Henry's Law constant >1 x 10^{-4} also have a greater tendency for preferential degradation in soil and volatilization into air (Tao et al. 2009, Kipopoulou et al. 1999).

PAHs in aquatic systems are primarily found absorbed to organic particles in the water column or in sediments because of their low solubility and high affinity for organic carbon (HSDB, 2019). Estimates show that two-thirds of PAHs in aquatic systems are associated with particles and only about one-third are present in the dissolved form (Eisler, 1987). Unless high temperature conditions exist in shallow waters, even small PAHs (low molecular weight with few aromatic rings) will not be efficiently volatized from water (Southworth et al., 1978). These properties indicate that PAHs could be transported in open water systems while adsorbed onto organic particulate materials, with little likelihood of being available for uptake by plants.

PAHs can also be degraded by sunlight. Direct photooxidation of PAHs takes place over relatively short time periods with a half-life of 2.2 minutes to 71 hours (Kochany & Maguire, 1994). Fasnacht and Blough (2002) report similar findings with estimated half-lives for 12 PAHs between 2.4 minutes and 94 hours; included in those 12 PAHs are those on the list of Chemicals of Interest. They also report that the photodegradation of PAHs does not appear to be markedly affected by pH, salinity, or the presence of fulvic acid. There is some indication that minor fractions of anthracene can be converted to anthraquinone during photoirradiation (Bertilsson & Widenfalk, 2002). Anthraquinone will bind to organic material in soil and thus be unavailable for plant uptake, as indicated by an estimated K_{OC} between 2,755 and 17,416 (HSDB, 2019).

PAHs are present in soils and plants worldwide due to atmospheric deposition processes – particularly by particle deposition (Wild and Jones 1992). One of the main factors affecting the uptake of PAHs by plants is their molecular weight, i.e., PAHs with more aromatic rings are going to be less phytoavailable. PAHs with high molecular weight (e.g., 5-6 ring PAHs) tend to associate strongly with soil, and consequently have less opportunity for volatilization or root adsorption (Tao et al. 2009, Wild and Jones 1992, Fismes et al. 2002). In contrast, low molecular-weight PAHs (e.g. 2-3 ring PAHs) are more bioavailable in soil and more likely to adsorb onto root tissue (Kipopoulou et al. 1999, Tao et al. 2009). Several studies have documented the foliar uptake and accumulation of PAHs from the atmosphere as a result of deposition of particle-bound compounds, as well as the retention of vapor-phase PAHs on the waxy leaf cuticle (Gao et al. 2004). Historically, PAHs detected in above-ground plant tissues have been attributed to foliar uptake (Wild and Jones 1992). More recent studies, however, suggest the possibility of translocation of PAHs from roots to shoots, in addition to translocation from to leaf to shoots (Gao et al. 2004, Fismes et al. 2002).

Several studies have measured PAHs in vegetables grown in contaminated soil or near industrial sources (Kipopoulou et al. 1999, Wild and Jones 1992). Carrots have high lipid content and oil channels in the root, which have been reported to yield a greater potential for the uptake of non-polar compounds (Kipopoulou et al. 1999). Kipopoulou et al. (1999) found significant seasonal variation in PAH levels in soil, but not in vegetables; they report that this was possibly due to washing of produce. Studies have found that concentrations of PAH in carrots were higher in peels than in cores, with lower-molecular weight PAHs dominating the concentrations in both portions of the carrot (Wilde and Jones 1992, Kipopoulou et al. 1999). PAH concentrations in carrot cores were directly related to the PAH content in the soil (Fismes et al. 2002). As storage organs, potatoes receive chemical compounds from leaves via the phloem vessels (Fismes et al. 2002). Phloem transport from leaves to potato pulp is water-based, resulting in minimal transport of organic lipophilic compounds, such as PAHs. Studies have found that potato peels, rich in lipids, have higher concentrations of PAHs than potato pulp (Fismes et al. 2002). Potato peel PAHs primarily consisted of high molecular weight PAHs, which were adsorbed from soil; while potato pulp PAHs consisted primarily of low molecular weight PAHs assimilated from foliar uptake (Fismes et al. 2002).

8.2.6 Surfactants

Ethoxylated alkylphenols are the main group of surfactants on which the literature focuses. Both abiotic and biotic (microbial) degradation pathways have been identified for the ethoxylated alkylphenols (van Ginkel, 1996; Franska et al, 2003; Sparham et al, 2008). Ethoxylated phenols are common surfactants used in both hydraulic fracturing and conventional oil and gas production. Degradation products of the ethoxylated alkylphenols include nonylphenol and octylphenol (Orem et al., 2014), both of which are suspected endocrine disruptors (Ying et al., 2002). There is the potential that the concentrations of nonylphenol and octylphenol may be attenuated though the action of other bacterial degradation pathways that yield unidentified metabolites (Kohler et al, 2008). These metabolites may pose some additional risks depending on their structure (Kohler et al., 2008). Others have observed that alkyl ethothoxylates, nonylphenol ethoxylates, and polypropylene glycols biodegrade under anerobic conditions with the ultimate formation of alcohols and carboxylic acids (Heyob et al., 2017). Heyob et al. (2017) discuss the potential hazards associated with the partial degradation products of these surfactants, which include ketones, aldehydes, and alkylphenol compounds. McAdams et al., (2019) documented polyethylene glycols as microbial degradation products of alkyl ethoxylated phenols downhole. However, in other research, the polyethylene glycols were fully mineralized in agricultural topsoil over a period of 41 to 71 days (McLaughlin et al., 2016).

8.2.7 Biocides

The degradation and transformation of biocides have also been described in the literature. Of the biocides used in hydraulic fracturing, some are also on the list of chemicals initially evaluated in Task 1. These compounds include glutaraldehyde, quaternary ammonium compounds, benzyl ammonium chloride, alkyl dimethyl benzyl ammonium chloride, hypochlorite, methylchloroisothiazolinone, and tetrakis (hydroxymethyl) phosphonium sulfate. Glutaraldehyde, a common biocide used in the oil and gas industry, was observed to cross-link (i.e., to form chemical bonds) with polyacrylamide (McLaughlin et al., 2016). The same researchers also observed that free glutaraldehyde was completely biodegraded in agricultural soils within 57 days. In aerobic conditions, glutaraldehyde is expected to completely biodegrade, with the intermediate formation of glutaric acid prior to full mineralization (Kahrilas et la., 2015). Under anaerobic conditions at high temperature glutaraldehyde is expected to polymerize into 1,5-pentanediol and 3-formyl-6-hydroxy-2-cyclohexene-1-propanal (Kahrilas et al., 2015); it can also form dimers with itself, or otherwise auto-polymerize (Kahrilas et la., 2016). Kahrilas et al. (2015) report known toxicities associated with degradation products of some biocides. For example, formaldehyde is a degradation product of tetrakis (hydroxymethyl) phosphonium sulfate (Kahrilas et al., 2015). Formaldehyde, however, was assessed in Task 1 and found to be readily biodegradable in water and of limited concern in agricultural environments. Hypochlorite is a possible source of trihalomethanes [known carcinogens] and have been reported in hydraulic fracturing flowback waters (Kahrilas et al., 2015; Hoelzer et al., 2016)

8.2.8 Other Hydraulic Fracturing Chemicals Related to Chemicals of Interest

Samples taken of produced water and flowback water have reported the presence of chemicals not otherwise associated with additives or formation waters. Acetone, acetate, halogenated methane compounds, and pyridine were reported to be potential transformation products of other organic compounds (Hayes, 2009; Lester et al., 2015; Hoelzer et al., 2016). The halogenated methane compounds, as discussed above in section *8.2.7*, may be a product of chemical reactions that involve hypochlorite. The general mechanisms of degradation (i.e., microbial vs. abiotic) were not identified in the literature. The other three compounds are biodegradable or of limited health concern: acetone is biodegradable in water (ECHA, Acetone), acetate is an anion found in food additives and fruit, and pyridine is biodegradable in soil (Sims et al., 1989).

In the case of some chemicals, there has been clear identification of a chemical and the pathway responsible for its formation. For example, benzyl alcohol has been identified as a reaction product of benzyl chloride by way of the unimolecular nucleophilic substitution reaction [SN1] (Elsner and Hoelzer, 2016; USEPA, 2016a; Rogers et al., 2015). Benzyl chloride is one of the additives reviewed in Task 1. The transformation of organic compounds in hydraulic fracturing fluid has also been predicted to form halogenated organic compounds as there are high chloride and bromide levels in hydraulic fracturing fluid (Maguire-Boyle and Barron, 2014). Only a few other degradation products have been identified in flowback and produced water, namely, several halogenated aliphatic compounds (Hayes, 2009; Maguire-Boyle and Barron, 2014).

8.3 Environmental Fate and Transport of Organic Chemicals of Interest: Phytoavailability Screening Analysis Using the EPI Suite Database

In this section, we present a phytoavailability screening evaluation based on a review of solubility, volatility, absorptive potential, and biodegradability data from the EPI Suite software (USEPA, 2012b). The screening evaluation has the goal of determining how a chemical's combination of environmental fate and transport factor attributes may affect its phytoavailability. For example, an organic chemical may be highly soluble in water, which by itself would imply that it could be highly phytoavailable. However, if this chemical also had a high potential to sorb to organic material in soil, the chemical's phytoavailability would be greatly reduced. This discussion is limited to 45 of the organic Chemicals of Interest for which the previously mentioned fate and transport factor data were available in the EPI Suite database. Our aim was to identify those chemicals with the greatest phytoavailability potential in agricultural environments.

EPI Suite contains multiple sub-programs (modules) that can describe and report on the physical properties of over 40,000 chemicals. From the EPI Suite software, we collated estimates of water solubility [mg/L], Henry's Law Constants [atm-m^3], estimated Log K_{OC}, and selected BioWIN estimates of biodegradability for available organic Chemicals of Interest. Table 12 reports interpretation guidance for the collated parameter estimates, which are presented in Table 13. These interpretation guidelines are reported in the EPI Suite v4.11 technical documentation (USEPA, 2012b). We used estimated solubility to identify chemicals that may be more likely to be present in produced water. We used estimates of Henry's Law Constants to identify chemicals that may volatilize into air from water. We used estimates of Log K_{OC} to identify those chemicals that are likely to remain partitioned to the aqueous phase. A subset of BioWIN aerobic biodegradation estimates were used to identify potentially non-biodegradable organic Chemicals of Interest.

The USEPA provides limited guidance as to which of the seven BioWIN biodegradability estimates are likely to give results with the least uncertainty. The European Union (EU) Technical Guidance Document on Risk Assessment (EU, 2003) provides some guidance on which of the parameters and models will be most informative in aquatic environments. They suggest that parameters from BIOWIN 2 (non-linear model), BIOWIN 3 (ultimate biodegradation timeframe), and BIOWIN 6 (non-linear Japanese Ministry of International Trade and Industry [MITI] model) should be used when experimental or real-world data are not available (EU, 2003). The three models estimate biodegradability under aerobic conditions in water. BioWIN estimates are reported in Table 12 and classified according to reported guidelines in Table 13. Consensus among the three BioWIN estimates was considered stronger evidence of biodegradability than if there was no consensus among the estimates. We also made attempts during the review to identify literature that reported other experimental biodegradation data for the 45 organic Chemicals of Interest in an agricultural or similar setting. However, no such literature was found, except for 1,4-dioxane which is not biodegradable (ATSDR, 2012b).

In addition to the fate and transport parameters reported in Table 13, the last column of this table reports a phytoavailability score that we developed for this screening evaluation. In the absence of a published method to evaluate the phytoavailability of a large variety of organic chemicals, we developed a semi-quantitative approach to systematically evaluate the organic Chemicals of Interest, where data were available. The phytoavailability score used in the screening evaluation aims to identify chemicals having a combination of characteristics that increase the likelihood that it could reach food crops if present in blended produced water. It is the sum of a simple scoring system applied to each of the EPI Suite fate and transport parameters reported in Table 13. Scores were assigned to table entries representing solubility classification, volatility in water classification, sorptive classification, and an aggregated biodegradation classification. Each of these columns had three potential classes, and a value was assigned to each that correlated with their likelihood to promote phytoavailability. Each class could take a value of 0, 1, or 2. A value of zero represented the class value that is least associated with phytoavailability, i.e., chemicals being non-soluble, very volatile, strongly sorptive to organic matter, and a higher likelihood of biodegradability based on a consensus of the three BioWIN models. Conversely, a value of two represented the class that most promoted phytoavailability, i.e., soluble, non-volatile, mobile (i.e., not sorptive to organic matter), and non-biodegradability based on a consensus of the three BioWIN models. Values of one were assigned to represent the middle class between those assigned zero or two. The phytoavailability score could take a value between zero and eight.

Using the phytoavailability score, we identified three of the Chemicals of Interest that have the least likelihood of being phytoavailable in blended produced water and eleven chemicals with the greatest potential to be present and phytoavailable in blended produced water. Reported values of the phytoavailability scores in Table 13 ranged from two to seven. Lower values of the phytoavailability score report the potential for lower concentrations, more removal from water through volatilization, more sorption to organic material, and more biodegradation. The converse is true for higher values. Chemicals of Interest with the least likelihood of being phytoavailable, having scores of two, include diester of sulfosuccinic acid sodium salt, hydrogenated tallow amine acetone, and stoddard solvents. The highest phytoavailability scores were calculated for the following eleven organic Chemicals of Interest: 1H, 3H-Pyrano (4,3-b)(1)benzopyran-9-carboxylic acid; 4,10-dihydro-3,7,8 trihydroxy-3-methyl-10-oxo (fulvic acid); 2-methyl-3-Butyn-2-ol; Alkanolamine phosphate; Bis (2-chloroethyl) ether; Hydroxyethylidenediphosphonic acid; Oxyalkylated polyamine; Polydimethyl diallyl ammonium chloride; Polyglycol ether; Polyoxyethylene nonyl phenyl ether phosphate; Tetrasodium ethylenediaminetetraacetate; and 1,4 Dioxane. These chemicals all have similar characteristics in that they are likely to persist for longer periods of time in irrigation water and in agricultural environments. Those Chemicals of Interest with phytoavailability scores from three to six, i.e., those in the middle, need to be addressed more individually, as they may have certain characteristics that will substantially attenuate their potential for reaching food crops during irrigation.

In further evaluating the chemicals with phytoavailability scores between three and six, we identified chemicals that did not have the extreme fate and transport factor attributes that would attenuate their phytoavailability, i.e., those that were not “non-soluble,” “strongly sorbtive,” “very volatile,” or have a consensus on biodegradability. From this evaluation, we identified the following five chemicals that had moderate or increasing potential to be phytoavailable: ethoxylated 4–nonylphenol; nonylphenol polyethylene glycol ether; chlorobenzene; isoquinoline; and light aromatic petroleum solvent naphtha. The remaining chemicals have characteristics that will likely keep their concentrations in irrigation water low due to volatility or solubility, make their phytoavailability low due to sorption to organic material in soil and water, or they will likely biodegrade.

8.4 Discussion of Organic Chemicals of Interest: Fate, Transport, and Plant Uptake

This review of the fate, transport, and plant uptake of the organic Chemicals of Interest illustrates the complexity of factors that affect the phytoavailability of organic chemicals to be taken up by food crops. The main fate and transport characteristics that affect the uptake of organic compounds are solubility, volatility, sorption to organic matter, lipophilicity, and biodegradation; however, other degradation and transformation factors may also affect the phytoavailability of the organic Chemicals of Interest. Plant uptake of organic compounds is dependent on solubility, volatility, and lipophilicity (Briggs et al. 1982; Simonich and Hites 1995; Collins et al. 2006), where water soluble compounds are being taken up through the roots and volatile lipophilic compounds taken up through the leaves (Simonish and Hites, 1995). The fact that lipophilic organic compounds like PAHs can be taken up through the leaves highlights the question of how irrigation practices, i.e., drip irrigation vs. aerial/spray irrigation, may affect the ultimate concentration of organic chemicals in the edible portion of food crops. The available literature, however, does not address this question.

Most of the available literature and data were focused on the factors affecting the environmental fate and transport of the organic Chemicals of Interest, not their uptake by plants. The available literature suggests that chlorobenzene, PAHs, and biocides may be affected by fate and transport factors that will attenuate their phytoavailability in agricultural soils. Based on the screening evaluation, we also identified other chemicals that are likely to be of low priority due to environmental fate and transport factors that attenuate their phytoavailability. These chemicals include the diester of sulfosuccinic acid sodium salt, hydrogenated tallow amine acetone, and stoddard solvent. We also identified a small number of organic Chemicals of Interest that may be persistent and phytoavailable in agricultural environments, including fulvic acid; 2-methyl-3-Butyn-2-ol; alkanolamine phosphate; bis (2-chloroethyl) ether; hydroxyethylidenediphosphonic acid; oxyalkylated polyamine; polydimethyl diallyl ammonium chloride; polyglycol ether; polyoxyethylene nonyl phenyl ether phosphate; tetrasodium ethylenediaminetetraacetate; and 1,4 dioxane. Articles identified in the hydraulic fracturing literature indicate that degradation and transformation of petroleum-related chemicals, outside of biodegradation, may be an important factor in assessing the potential hazards associated with the organic Chemicals of Interest. For example, ethoxylated alkylphenols may degrade into chemicals that are suspected endocrine disruptors while biocides are unlikely to pose additional health hazards. Biocides were reported to completely biodegrade or degrade into chemicals reviewed and deemed to be of low concern based on Task 1 screening evaluation criteria. While fate and transport data were available for nearly half of the organic Chemicals of Interest, plant uptake data were only available for PAHs, acrylamide, and chlorobenzene.

A substantial amount of research has been devoted to understanding the fate and transport of organic chemicals in soil, but the state of the science is not to a point where we can predict the level of chemicals in edible plant parts from levels in soil or irrigation water or make general conclusions about the impact that organic Chemicals of Interest could have on food crops, if present in irrigation water. The available data is only informative for interpreting the environmental fate and transport of some of the organic Chemicals of Interest. We were able to determine that environmental transformation and transport processes may attenuate the phytoavailability for a small subset of the 45 organic Chemicals of Interest, with others being potentially persistent in agricultural environments. However, a large data gap exists because more than half (56 of 101) of the organic Chemicals of Interest do not have specific environmental fate and transport data, and most of the organic Chemicals of Interest don’t have any relevant plant uptake data.

9.0 SUPPLEMENTAL EVALUATION OF THE TOXICITY OF THE CHEMICALS OF INTEREST

As part of Task 1 of this project, toxicity information was collected and used to screen a list of 399 chemicals down to a more manageable, but still long, list of 143 Chemicals of Interest for further evaluation in Task 2. As noted in the Task 1 report, the primary purpose of using toxicity in that initial screening effort was to ensure that the most toxic chemicals were carried forward in the evaluation. In Task 2, the chemicals carried forward were looked at in greater depth with the goal of developing information that supported interpretation of the findings of the crop sampling performed under Task 3. Information collected under Task 2 was intended to support a more definitive evaluation of health risks posed by the shorter list of chemicals, to identify data gaps and uncertainties in the evaluation, and to provide information that may be used for any future evaluations.

Evaluation of the toxicity of the chemicals reviewed in Task 1 was focused on identifying chemicals with the greatest potential to pose a health risk because of high chronic toxicity. In Task 2, more specific information on toxicity was sought to support the more in-depth evaluation of the shorter list of Chemicals of Interest. Accordingly, we report additional toxicity information for the Chemicals of Interest for which toxicity data is available, including chemicals for which agency-derived toxicity factors were available, and chemicals for which project-specific toxicity factors were developed. For chemicals lacking chronic oral toxicity data per the Task 1 screening effort, we searched for additional toxicity data. This included further searches for Safety Data Sheets, consideration of Quantitative Structure-Activity Relationship (QSAR) modeling, and assessing the potential for additional read-across toxicity assessments. As the project progressed, questions about the toxicity of polymers and chemical mixtures arose. These topics are addressed below, as well.

9.1 Chronic Oral Toxicity of Chemicals of Interest with Agency Derived Toxicity Values

In accordance with the scope of work for this project and to provide additional information for future evaluations of blended produced water, in Table 14 we provided more detailed reporting of the chronic oral toxicity associated with the Chemicals of Interest with agency derived toxicity values. Table 14 reports summaries of the most sensitive health outcomes associated with chronic oral exposure for each of the chemicals with agency derived toxicity values. These data may be useful in future studies to understand how exposures to the Chemicals of Interest in food crops irrigated with blended produced water may increase health risks.

Of the 143 Chemicals of Interest, 53 of the Chemicals had agency derived toxicity values. Of the 53 chemicals, 10 are associated with cancer outcomes, 6 are associated with adverse developmental or reproductive outcomes, and 37 are associated with non-cancer systemic health outcomes.

9.2 Chemicals without Chronic Toxicity Data: Update to Task 1 Toxicity Review

As a focused update to the toxicity hazard assessment (i.e., search for chronic toxicity factors) conducted in Task 1, we conducted a supplemental review of potential sources of data in search of additional chronic toxicity factors. More specifically, we searched for additional Safety Data Sheets, and we looked at the potential for developing additional chronic toxicity factors using read-across toxicity evaluations and QSAR modeling. As discussed below, we found additional toxicity information for some chemicals in Safety Data Sheets, but this data was of limited use for evaluating those chemicals. In addition, we were not able to derive useful toxicity factors from read-across toxicity evaluations or QSAR. The Chemicals of Interest for which we could not find or derive a chronic oral toxicity factor are listed in Table 15.

9.2.1 Review of Safety Data Sheets

Safety Data Sheets (SDSs) were identified for 12 of the chemicals identified in Task 1 as having no available chronic oral toxicity data. We reviewed the SDSs for subchronic and chronic toxicity information. There was some data available in three of the SDSs: 2-(Dimethylamino) ethyl acrylate and methyl chloride (44992-01-0), polyquaternary amine (42751-79-1), and lignite (129521-66-0). While the SDS sheets suggested that these chemicals did not pose a risk for cancer, a thorough review of these chemicals' potential carcinogenicity has not been undertaken by any authoritative body. No additional subchronic or chronic toxicity information was obtained from the SDSs. An additional SDS was located for a chemical mixture containing the chemical formaldehyde polymer with 2-methyloxirane, 4-nonylphenol and oxirane (63428-92-2) at a range of 10-20% within the mixture (MSDS Penetone1005D, 2011). However, due to inherent difficulty in accurately applying the findings of an SDS for a mixture to the chronic toxicity evaluation of a single constituent within the mixture at an unknown concentration, the SDS for the mixture was not utilized for the individual chemical.

9.2.2 Supplemental Read-Across Assessment for Chemicals Without Chronic Toxicity Data

No additional read-across assessments could be performed based on chemicals having similar biologically active functional groups or based on chemicals with structurally similar forms.

9.2.3 Feasibility of Quantitative Structure-Activity Relationship Modeling

QSAR modeling was investigated as a possible approach to evaluating the toxicity of the chemicals without chronic toxicity information. We were ultimately unable to apply these methods to the chemicals without chronic oral toxicity data.

QSAR is a is computation modeling approach used to predict specific physicochemical properties, acute toxicity, and chronic toxicity. The QSAR modeling approach utilized machine learning, mathematical models, and data mining, which all require robust supporting datasets. The supplemental read-across assessment of chemicals without chronic toxicity (Section 9.2.2, above) reported a lack of data on chemicals having similar biologically active functional groups or based on chemicals with structurally similar form. Additionally, QSAR modeling has some limitations that preclude its use for evaluating the toxicity of polymers (Boethling & Nabholz, 1996). Because QSAR could not be applied to polymers and because of a lack of data for other chemicals, we were not able to use QSAR to develop toxicity factors for any of the chemicals in Table 15.

9.3 Supplemental Toxicokinetic and Toxicodynamic Information for Selected Chemicals of Interest

As discussed in the previous section some of the toxicity factors developed for the screening evaluation performed in Task 1 had a relatively high degree of uncertainty (e.g., the toxicity factors were not based on exposure limits developed by regulatory agencies). As a result, we searched for additional toxicity information to use as the basis of toxicity factors for the more focused evaluations performed under Task 2. While some additional toxicity information was developed as part of the effort described above, we still had several toxicity factors that had been used for screening for which we wanted to decrease the degree of uncertainty. For that purpose, we looked for toxicokinetic and toxicodynamic information to support the evaluations of chemicals that had been identified in Task 1 as having a relatively high degree of uncertainty, including chemicals with incomplete or inconclusive toxicity data and chemicals for which we developed project-specific surrogate toxicity values. As discussed in the Task 1 report, we applied methods used by regulatory agencies to derive the project-specific screening values used in Task 1 (USEPA, 2002; OEHHA, 2008; described in detail in the Task 1 Report); but fewer toxicity studies were available for most of these chemicals than typically provide the basis for regulatory exposure limits, for example. The primary purpose of collecting and evaluating the toxicokinetic and toxicodynamic information was to see if the additional information tended to confirm or contradict the validity of the screening-level toxicity factors we developed and to reduce the uncertainty associated with the screening-level toxicity factors used in this project. The toxicokinetic or toxicodynamic data found as part of this evaluation is summarized in Table 16; and, as discussed below, none of the information contradicted the screening values developed in Task 1.

Toxicokinetics is used to describe how a chemical is absorbed, distributed, metabolized, and excreted by the body (Ashauer and Escher, 2010): it is how the body processes a chemical. In contrast, toxicodynamics is the study of the interaction between a chemical and the site-of-action that results in the adverse effect (Ashauer and Escher, 2010). Generally, toxicokinetic data is useful for extrapolating results from animal studies to humans, and toxicodynamic data describes how chemicals cause adverse health effects (Bachman et al., 1996). While information about these processes is not a substitute for having more toxicity studies, it may tell us if a chemical is not absorbed from the gut following ingestion, for example. It may also tell us if a laboratory test species responds completely differently from humans, for example, and that we should not extrapolate results from laboratory test species to humans.

The toxicokinetic and toxicodynamic data for the Chemicals of Interest with project-specific surrogate toxicity values, and those that had incomplete or inconclusive toxicity data for deriving toxicity values, are reported in Table 16. This information was only available for some of the Chemicals of Interest reported in Table 16 and includes a mixture of information on the specific Chemicals of Interest and, for some chemicals, their related congeners. Table 16 also includes summaries of the studies used to estimate the project-specific surrogate toxicity values and additional information on toxicity for those chemicals with inconclusive toxicity data for deriving toxicity values.

As shown in the table, chemical-specific information was available for 2-mercaptoethanol, hydroxyethylidene-diphosphonic acid, fulvic acid, phenanthrene, and quinaldine. We found toxicokinetic and/or toxicodynamic data for the following chemical congeners: gossypol for cottonseed flour, trimethylammonium bromide and alkyldimethylbenzyl-ammonium chloride for quaternary ammonium compound (CASRN: 61790-41-8), monosodium ethylenediaminetetraacetate for the disodium and trisodium variants, and sorbitan monostearate for an ambiguous sorbitan ester. We also present a short general discussion on aromatic amines because a CASRN or unique chemical name was not provided by the petroleum producers in their declared list of chemical additives.

The available toxicokinetic and toxicodynamic information provides mechanistic support for the outcomes identified in studies that were used to estimate some of the project specific surrogate toxicity values. Toxicokinetic and toxicodynamic information for 2-mercaptoethanol and hydroxyethylidenediphosphonic acid provided support for the respective project-specific surrogate toxicity values that were ultimately derived. For mercaptoethanol, the subchronic rat study that we used to inform the toxicity value reported fatty liver, decreased cholesterol, and decreased triglycerides (ECHA, 2-mercaptoethanol); the toxicodynamic data reported fatty liver and increases in free fatty acid mobilization (Sabourault et al., 1997). Both findings are in support of related hepatotoxicity, likely due to 2-mercaptoacetate, which forms through the oxidation of 2-mercaptoethanol (Sabourault et al., 1997). In the chronic rat study investigating the effects of hydroxyethylidenediphosphonic acid, anemia and retarded bone marrow development were reported (ECHA, Etridronic acid). The available toxicodynamic data offer mechanistic support for these finding with a measurable decrease in the affinity of hemoglobin for oxygen (Koltsova et al., 1979)—a disfunction of the red blood cells, which are formed in the bone marrow. Toxicodynamic data for gossypol (the potentially toxic component of cottonseed flour) did not provide any additional support for, or contradict, its identification as a male reproductive toxicant. There is evidence to suggest that gossypol has potential chemotherapeutic effects for leukemia (Balakrishnan et al., 2008; Huang et al., 2006; Sahin et al., 2010). While toxicokinetic or toxicodynamic information provided additional support for the basis of some project specific surrogate toxicity values, this kind of data was not available for many of the chemicals.

Some toxicokinetic information was available for Chemicals of Interest with incomplete or inconclusive chronic oral toxicity data that are helpful in understanding the degree to which oral exposures could reach systemic sites in the body. There is evidence that fulvic acid, phenanthrene, and sorbitan esters (as sorbitan monostearate) are absorbed through the gastrointestinal tract, making them potential systemic exposures (Cavret et al., 2003; Gosselin et al., 1976; Islam et al., 2005; Kang et al., 2007). There appears to be limited potential for systemic exposures with the consumption of sodium ethylenediamine-tetraacetate (DrugBank, 2020). While there are some reports that quinaldine is poorly absorbed in the gut (Komiya, 1965), other evidence suggests that it may partially absorbed. In a study that investigated the excretion of quinoline, which is structurally similar to quinaldine and only lacks a methyl group, 6.7-11% of quinoline was absorbed by rabbits after oral exposure (Smith and Williams, 1954).

Aromatic amines represent a large class of potentially carcinogenic chemicals (IARC, 2010); one of the Chemicals of Interest was ambiguously identified as an "aromatic amine" additive by petroleum producers. Both monocyclic and polycyclic aromatic amines are potentially carcinogenic aromatic amines (IARC, 2010), but not all aromatic amines are carcinogenic (Benigni and Passerini, 2002). Several aromatic amines have been identified as carcinogenic by EPA, IARC, and NTP (EPA, IRIS; IARC, 2010; NTP, 2016). More specific evaluation of "aromatic amines" would require more specific identification of the aromatic amine compounds used for oil production.

9.4 Evaluation of Polymers Without Chronic Oral Toxicity Data

There are 32 polymers without chronic oral toxicity data in the group of chemicals listed in Table 14. Due to several factors specific to polymers, evaluating their toxicity is more complex than for non-polymers. Factors we reviewed that are important for evaluating polymer toxicity include the quantity of unreacted monomer present in the polymer, the molecular weight of the polymer, percentage of low molecular weight oligomers, and structural features of the polymer (Boethling & Sabholz, 1996). We also review a computer modeling approach that is applicable to polymer toxicity. Federal and intergovernmental organizations have various criteria for classifying whether a polymer may potentially be a health concern. The USEPA, the Australian Department of Health, and the OECD Expert Group Meeting on Polymer Toxicity Evaluation have evaluated polymer toxicity based on its potential to cause human health effects and effects on the environment (NICNAS, 2019; OECD, 2009; USEPA, 1997). We reviewed federal and intergovernmental agency criteria for evaluating potential hazards of polymers for the 32 polymers. Available polymer guidance incorporates both inhalation and oral routes of exposure for polymer human health hazard assessment (OECD, 2009). Because this project is focused on food consumption, only guidance relevant to ingestion of polymers was reviewed.

9.4.1 Monomer Toxicity Data for Evaluating Polymers

One possible approach to assessing the toxicity of polymers with limited toxicity data is to conduct a read-across assessment using the polymer's respective monomer (Lithner et al., 2011; USEPA, 2013). Based on the availability of monomer toxicity data for polymers without chronic toxicity information, this approach could be applied to six chemicals: "cationic acrylamide copolymer" (69418-26-4), "copolymer of acrylamide and sodium acrylate" (25987-30-8), "polydimethyl diallyl ammonium chloride" (26062-79-3), "triethanolamine homopolymer" (64114-46-1), "poly triethanolamine methylene chloride quaternized" (68938-70-5), and an "amine salt" (67924-33-8).

Lithner et al. (2011) applied read-across assessment methods using the monomer to evaluate the risk associated with the production, use, and degradation of polymers for prioritization. The authors noted that a polymer's monomer could be used for toxicity evaluation because there is potential for unreacted monomer to remain in the polymer, and the polymer may degrade to the monomer during disposal. Lithner et al. (2011) stated the purpose of their approach was to prioritize polymers for additional hazard evaluation and alternatives assessments, rather than to evaluate toxicity alone. It can be concluded from Lithner et al. (2011) that this approach, by itself, is not sufficient for evaluating the oral chronic toxicity of a polymer. They also noted "It should be emphasized that a polymer ranked as hazardous is not the same as the polymer being hazardous. The ranking means that the polymer is made from hazardous substances (the greatest part being transformed during polymerization)" (Lithner et al., 2011). When monomers are polymerized to form a polymer, the physicochemical properties and toxicity can be altered considerably (OECD, 2009). Polymerization can greatly increase molecular weight relative to the monomer, which can reduce absorption when ingested (Lipinski et al., 1997). Additionally, polymerization generally results in the formation of a polymer that is more stable and less reactive than its associated monomer (OECD, 2009). For most polymers, this results in considerably reduced toxicity relative to their respective monomers (IARC, 2019). For instance, vinyl chloride is classified by IARC as a group 1 carcinogen, while its corresponding polymer, polyvinyl chloride, is not classified as carcinogenic (IARC, 2019). Similarly, acrylamide is a known neurotoxin that is classified as a carcinogen by OEHHA and a probable human carcinogen by IARC. However, the acrylamide polymer, polyacrylamide, is non-toxic, and is not classified as carcinogenic (IARC, 2019). Furthermore, the USEPA recommends polymer toxicity assessment based on the monomer when the residual monomer constitutes a significant portion of the polymer (>10%) (USEPA, 2013). Residual monomer content, however, is likely low since it can affect the performance and stability of the polymer (Gleadall et al., 2014).

To address the prioritization of polymers, as suggested by Lithner et al. (2011), we report on monomer toxicity of five polymers, which had available toxicity data. Three monomer units with toxicity data were identified for the six polymers mentioned above: acrylamide for cationic acrylamide copolymer" (69418-26-4) and "copolymer of acrylamide and sodium acrylate" (25987-30-8); dimethyl diallyl ammonium chloride for "polydimethyl diallyl ammonium chloride" (26062-79-3); and triethanolamine for "triethanolamine homopolymer" (64114-46-1), "poly triethanolamine methylene chloride quaternized" (68938-70-5) and an "amine salt" (67924-33-8).

As briefly discussed above, acrylamide is carcinogenic and is a neurotoxin (USEPA, IRIS), which was evaluated in Task 1. In this literature review—discussed in Section 8—we identified a study that reported acrylamide was taken up by lettuce as a result of the use of polyacrylamide soil conditioner that are similar to the polyacrylamide polymers on the list of Chemicals of Interest (Mroczek et al., 2014). Acrylamide was not added to the list of Chemicals of Interest in Task 1, however, because it is biodegradable in water. Given its biodegradability and the reduced toxicity of its polymers, using the monomer to assess toxicity would likely overestimate the hazard of the two acrylamide polymers. Acrylamide has not been detected in any of the water quality samples (see Section 5).

Diallyldimethylammonium chloride is the monomer of polydimethyl diallyl ammonium chloride" (26062-79-3) and likely of low health concern. It is poorly absorbed through the gastrointestinal tract with studies showing the majority is excreted in feces (ECHA, Diallyldimethylammonium chloride). It does not display reproductive or genotoxic effects. In a 28-day rat study, no health effects were observed at any of the dosage levels, up to 500 mg/kg/day. A 13-week dog study reported reduced body weight in the 800 mg/kg/d diallyl ammonium chloride exposure group (NOAEL = 200 mg/kg/d), but no other reportable systemic effects. Additionally, diallyl ammonium chloride was reported to partially degrade in the OECD 301A DOC die away test with a 40-50% degradation after 28-day (ECHA, Diallyldimethylammonium chloride). Due to minor observed health effects only observed at dose levels above 500 mg/kg/day and the potential for at least partial biodegradation, diallyldimethylammonium chloride is unlikely to pose a significant health hazard.

"Triethanolamine homopolymer" (64114-46-1), "poly triethanolamine methylene chloride quaternized" (68938-70-5), and an "amine salt" (67924-33-8) are polymers based on triethanolamine and are unlikely to a pose significant health hazard. Triethanolamine has low chronic toxicity, and effects are expected to arise from acute exposure due to its alkalinity (Bingham et al., 2001).

Residual monomer content of polymers does not appear to pose significant health hazards, given the available data, as long as residual monomer content is low. Data gaps exist with regard to the toxicities for many of the monomer units and the quantity of residual monomer.

9.4.2 Polymer Size for Evaluating Toxicity

The size of a polymer is important for evaluating polymer toxicity. The OECD Expert Group Meeting on Polymer Toxicity identified molecular number (M_N) as a primary driver of polymer toxicity. Polymers with lower M_N have a higher likelihood of toxicity (OECD, 2009); in other words, larger polymers have lower toxicities. Most chemical formulations of polymers, however, are not uniform and have a distribution of molecular sizes (USEPA, 2015b).

The most commonly accepted molecular weight for a polymer to be considered of low health concern is >1,000 Daltons (OECD, 2009). Additionally, most polymers with a molecular weight > 10,000 Daltons are poorly absorbed when ingested and are only a human health concern via inhalation (Lipinski et al., 1997; Boethling & Nabholz, 1996). Toxicity related to polymer size extends to oligomer content, where the OECD Expert Group Meeting on Polymer Toxicity identified the fraction of oligomers present as a primary driver of toxicity for any specific polymer (OECD, 2009). For a polymer >1,000 Da to be considered low concern for toxicity by the USEPA (2003), oligomers <1,000 Da must comprise <25% of the polymer content, and the oligomers <500 Da must comprise <10% of the content. For a polymer with a molecular weight >10,000 Da to be considered low concern for toxicity, there must be <5% content of <1,000 Da oligomers and <2% content of <500 Da oligomers (OECD, 2009).

While much of the evidence suggests that polymers are unlikely to be a significant health hazard, data about polymer size and oligomer content was not provided by petroleum producers when they declared the list of chemical additives they use during petroleum development, extraction, and treatment.

9.4.3 Polymer Structure for Evaluating Polymer Toxicity

Another possible approach for evaluating polymers without toxicity data is to identify structural aspects of the polymer associated with toxicity. These structural aspects are termed reactive functional groups (RFGs). Examples of RFGs include acrylates, epoxides, isocyanates, methacrylates, phenols, and sulphonates (OECD, 2009). RFGs can then be utilized by grouping polymers with the same RFGs into various classes such as polyesters, polyolefins, polyacrylates, polyethers, polyurethanes, polyamides, polyimides, polysaccharides, polyvinyl, siloxanes, and epoxy resin (USEPA, 1997).

The OECD Expert Group Meeting on Polymer Toxicity found polymers with RFGs are more likely to be considered polymers of potential concern, but polymers with RFG are not necessarily toxic (OECD, 2009). Additionally, while the OECD Expert Group Meeting on Polymer Toxicity investigated the incorporation of RFGs for polymer evaluation, the consideration of RFGs is not universally utilized to determine whether a polymer may be a health concern (OECD, 2009). The value of considering RFGs to evaluate the toxicity of polymers appears to be limited given that RFGs are not a specific indicator of toxicity. Such an approach, however, may be valuable for categorizing polymers into "low concern" and "potential concern," but without additional information on the polymers, the presence or absence of RFGs alone is not sufficient to assess the hazard of polymers.

9.4.4 Predictive Modeling for Evaluating Polymer Toxicity

Predictive modeling is a possible method to evaluate polymer toxicity. The USEPA Sustainable Futures Program has developed a software program to evaluate polymer toxicity called Oncologic. (USEPA, 2013). Oncologic was developed to predict the carcinogenic potential of chemicals and requires physiochemical, toxicokinetic, and toxicodynamic data about the chemical of interest as input data. The required input data to estimate carcinogenic potential in polymers includes average molecule weight, whether the polymer is comprised of covalently linked repeating units, the percent residual monomer, the percent of polymer with molecular weight <500 Daltons, polymer solubility, whether the polymer is expected to be inflammatory, whether the polymer is expected to accumulate in soft tissues, what reactive functional groups are present in the polymer, whether certain metals are present in the polymer, and what route of exposure is expected with the polymer of interest (USEPA, 2013). Data describing the majority of these required input parameters are not available for the polymers without chronic oral toxicity data. As such, we were unable to implement this modeling approach. If the required polymer input data were made available, however, Oncologic could be used as a screening tool to prioritize polymers for potential health hazards associated with chronic oral toxicity.

9.5 Toxicity of Chemical Mixtures and Uncharacterized Chemicals in Produced Water

Produced water is a complex aqueous solution that may contain organic chemicals, inorganic chemicals, and radionuclides. This section addresses ways that could be used to fill the following data gaps: our inability to assess the toxicity of chemicals that cannot be monitored in produced water, our lack of knowledge regarding specific toxicities associated with all possible individual chemicals in produced water, and our lack of knowledge of how mixtures of these chemicals may affect the toxicity of produced water.

Produced water consists of a complex mixture whose composition may vary based on the degradation or transformation of parent compounds, local geochemistry, the use of additives, and other factors. One of the uncertainties associated with produced water sampling is whether the full range of chemicals, including degradation or transformation products from oil field chemicals, were identified and measured in produced water samples. As discussed in Section 8.4, the identity of all of the potential degradation or transformation products is not known. Additionally, organic chemicals not on the list of Chemicals of Interest were detected in food crop samples (reported in the Task 3 Report). While the likely sources of these chemicals were identified, the possibility remains that some of the detected chemicals were degradation or transformation products of oil field additives and other chemicals in produced water.

A common approach to assessing the toxicity of a mixture is to identify individual components, evaluate the toxicity of each, and then sum the toxicity of all components as a way of estimating the overall toxicity of the mixture (European Commission, 2011). A chemical mixture, however, may have toxicity that is both distinct from its individual component chemicals and is not represented by a simple sum of its component toxicities (European Commission, 2011). It is documented that assessing the toxicity of mixtures of known composition is challenging; and addressing the toxicity of mixtures of unknown and uncharacterized chemical components is much more difficult (Cassee et al., 1998; Feron et al., 1995; Suk et al., 2002; Monosson, 2005; Simmons et al., 2004).

Whole Effluent Toxicity (WET) is a whole-water testing framework, under the National Pollutant Discharge Elimination System (NPDES) that could be applied to assess health hazards associated with the reuse of produced water for agricultural irrigation of food crops. WET testing characterizes the toxic effects of exposure to ambient mixtures present in the effluent without identifying individual pollutants. Freshwater, marine, and estuarine organisms are the target receptors of WET testing. There is no requirement under the NPDES, however, to test for toxicity to humans with WET testing. A similar strategy could be used to evaluate the toxicity of produced water if tests could be adapted so that the results were relevant to mammalian species.

Our search for test methods to be applied to mixtures turned up many examples of studies that tested impacts of chemical mixtures to aquatic species, but very few examples investigated how mixtures of chemicals in produced water mixtures might affect human or mammalian receptors. We report the results of the literature review that was conducted to identify methods and studies that have investigated whole water testing relevant to mammalian or human health outcomes. Toxicity methods reported here include *in vivo, in vitro,* and high throughput *in vitro* methods.

9.5.1 In Vivo Methods for Assessing Toxicity of Whole Produced Water

There are a few examples in the literature of *in vivo* methods being used to assess the toxicity of produced water, but these were conducted in the context of hydraulic fracturing. The use of experimental animals in toxicity testing dates back to the 1920's (Parasuraman, 2011) and has been typically used as the basis for developing toxicity values, such as RfDs and cancer slope factors.

A study by Balise et al. (2019) reported decreased activity among adult female mice exposed during early life to a mixture of hydraulic fracturing chemicals in water at levels that might be expected in flowback and produced water. Kassotis et al. (2015) exposed mice to hydraulic fracturing chemicals in water and observed adverse developmental and reproductive effects.

While the results of the Balise et al. (2019) and Kassotis et al. (2015) studies suggest that mixtures of chemicals in raw produced water pose potential health hazards, the resource costs for conducting chronic oral toxicity animal studies are substantial in both money and time. For example, conducting a single rodent study to investigate the effects of chronic exposure to a single chemical may cost approximately $1.75 million dollars and takes over two years to complete (USEPA, 2018a). With a variable and ever-changing effluent stream from oil and gas production, the time and cost requirements of using *in vivo* animal studies to characterize the toxicity of produced water mixtures do not appear to represent a realistic strategy. The trend towards the use of other screening approaches, including *in vitro* and *in silico* (computational) methods for toxicity testing (USEPA, 2019b; Krewski et al., 2010), may be due in part to the substantial resource costs of *in vivo* testing.

9.5.2 In Vitro Methods for Assessing Toxicity of Whole Produced Water

In vitro testing for chemical toxicity is of growing interest in the United States. The USEPA, the National Toxicology Program (NTP), and the National Institutes of Health (NIH) have developed "Toxicology in the 21st Century" (Tox21) with the goal of developing and validating methods to rapidly test chemicals for potential toxicity (USEPA, 2019b). The Tox 21 program is currently using *in vitro* methods to screen thousands of chemicals over a range of concentrations, to understand the ability of chemicals and chemical mixtures to impact various biological pathways that could ultimately cause toxicity. There is no data reported from the Tox21 program that related to produced water. Research in the peer reviewed literature has reported on the use of *in vitro* methods for assessing whole effluent toxicity of produced water (Crosby et al., 2018; Hull et al., 2018; Kassotis et al., 2014; Kassotis et al., 2018; Payne et al., 2015); similarly to research reporting on *in vivo* toxicity testing of produced water, most of the available test results are testing of produced water from hydraulic fracturing and could not be extrapolated to produced water from conventional oil production.

In vitro research reporting on the whole water toxicity of produced water suggests that produced water from hydraulic fracturing may be cytotoxic (Crosby et al., 2018; Hull et al., 2018; Payne et al., 2015) and endocrine disrupting (Kassotis et al., 2014; Kassotis et al., 2018). A study by Hull et al., (2018) looked at flowback and produced water from hydraulic fracturing, using the BioLuminescence Inhibition Assay (BLIA), Ames II mutagenicity assay (AMES), and Yeast Estrogen Screen (YES). These assays measure cell toxicity, mutagenicity, and estrogenicity (endocrine disrupting), respectively. Hull et. al (2018) tested raw flowback and produced water as received from hydraulically fractured well. Overall, their results suggested negligible toxicity, although some cytotoxicity was observed with the BLIA test (Hull et al., 2018). Kassotis et al. (2014) collected surface and groundwater samples in an area impacted by hydraulic fracturing in Colorado. They used the HepG2 human cell assay to assess endocrine disrupting activity of the mixture of chemicals in the water. Solid phase-extraction was used to concentrate the samples before being diluted to 4x and 40x the original concentration. Kassotis et al. (2014) reported that samples collected from the impacted sites showed estrogenic, anti-estrogenic, and/or anti-androgenic responses compared to control samples (Kassotis et al., 2014). In a similarly designed study to Kassotis et al. (2014), and using similar sampling locations, Kassotis et al., (2018) reported that chemicals in produced water at concentrations at or below environmental levels, elicited a response in peroxisome proliferator-activated receptor gamma (PPAR-γ) in the GeneBlazer™ PPARγ assay. PPAR-γ is a type II nuclear receptor in humans that regulates the expression of genes involved in lipogenesis (the synthesis of fat). In a study assessing the toxicity of produced water from both conventional and hydraulically fractured wells in the Marcellus Shale formation, Crosby et al. (2018) used a liver (HepG2 hepatocellular carcinoma) and kidney (HK-2) cell assay to assess the toxicity of diluted produced water (Crosby et al., 2018). They reported adverse effects to cell growth from both sources of water that may be applicable to humans. In another study, hydraulic fracturing chemicals were reported to be cytotoxic based on tests that expose human colon epithelial cells in the Caco-2 cell assay (Payne et al., 2015).

The zebrafish embryo model is a commonly used assay model for assessing potential human health impacts of chemicals on immune function, organ systems (kidney, heart, liver, blood cells generation), and genetic effects (Bambino and Chu, 2017). Zebrafish and humans share many similarities between molecular signaling and developmental pathways that lead to disease (Padilla et al., 2012), and they have been identified as a potential model organism for assessing the toxicity of mixtures (Sukardi et al., 2010; Bambino et al., 2018; Michiels et al., 2017; Shi et al., 2019; Mentor et al., 2020). There are examples of the zebrafish embryo model having been used to screen for potential health effects from produced water.

Carlsson et al. (2014) used a zebrafish embryo toxicity assay to screen produced water and reported potentially adverse developmental effects to the embryos. Folkerts et al., (2017) reported that exposure to produced water was associated with a decreased metabolic rate in the developing zebrafish embryo, as well as with changes to genes that control cardiac development.

We also identified a review article that summarized examples of *in vitro* assay systems that can be used to test recycled water to determine its suitability for various kinds of reuse. Many of the assay methods identified in Leusch and Snyder (2015) are applicable to assessing potential toxicity in humans. The material from Leusch and Snyder (2015) is reproduced in Table 16[1]. As many of the methods are applicable to understanding potential toxicity to humans, this list of assay systems is valuable for identifying potential strategies to assess the toxicity profile of produced water used for irrigation. However, further assessment of these methods is needed prior to developing a testing plan for produced water used for agricultural irrigation.

Overall, the examples in the literature suggest that *in vitro* methods may be a viable tool for screening potential health hazards associated with chemicals in produced water; but

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[1] References originally included as part of Table 1 in Leusch and Snyder (2015) have not be reproduced in Table 16. Please refer back to the original article for these references.

the test results that are available to date cannot be directly applied to the evaluation of the reuse of produced water for agricultural irrigation.

9.5.3 High-throughput In Vitro Testing of Mixtures of Whole Water

In the US, consistent with the federal agency initiatives, high-throughput methods have been identified as potentially useful for screening chemicals present in produced water (Colborn et al., 2011; Kahrilis et al., 2015; Wattenberg et al., 2015; Kassotis et al., 2016; Yost et al., 2016; Elliot et al., 2017). High-throughput toxicity testing utilize existing testing methods, such as the AMES, BLIA, or zebrafish embryo assay and extends its utility by integrating automation that allows for testing many samples at one time. There are many assays amendable to the use of high throughput testing that are relevant to human health (Schoonen et al., 2009); many of these methods are reported in Table 17.

Using the zebrafish embryo model as an example of high throughput methods for assessing toxicity, Reif et al. (2016) reported the development and implementation of a high-throughput system that used embryonic zebrafish to identify teratogenic effects. They reported the ability to identify multiple teratogenic outcomes that represent impacts to multiple organ systems. While this research investigated exposures to chemicals at concentrations that might be expected in ambient water or in produced water, it only investigated single chemical exposures. Truong et al. (2014) reported on the use of high-throughput methods with zebrafish to assess 1,060 unique chemicals and 18 unique endpoints. As with many assay methods, however, there are limitations because it may be difficult to extrapolate results to humans due to differences in the response of enzyme functions to chemical exposures (Saad et al., 2016). Additionally, extrapolating results from assay to humans is further complicated when the chemicals causing the response are not known, and the respective response pathway cannot be identified.

As discussed briefly above, high-throughput methods can be used to rapidly conduct toxicity assessments of chemicals or chemical mixtures. Our literature review did not identify any publications that described the use of high-throughput methods to assess the toxicity of produced water. There is some research that reports on the use of high throughput methods for assessing human health hazards to individual chemicals in water. More research is still needed to validate these methods for chemical mixtures.

9.6 Discussion of Supplemental Review of Toxicity of the Chemicals of Interest

The information provided above included supplemental information and toxicity evaluations of the Chemicals of Interest beyond the work conducted as part of Task 1. This supplemental review had four main goals: (1) to update and expand the literature review presented in Task 1 for chronic toxicity information on the Chemicals of Interest for which chronic oral toxicity data was not found as part of Task 1; (2) to research and evaluate supplemental toxicity information (i.e., toxicokinetic and toxicodynamic information) to supplement the often limited information on the chronic toxicity of chemicals without agency-derived toxicity factors addressed in this project; (3) to review of the toxicity of polymeric Chemicals of Interest using procedures for evaluating polymers developed by regulatory agencies; and (4) to review of methods that may be appropriate for assessing the toxicity of uncharacterized chemicals and chemical mixtures.

The search for additional chronic toxicity data and additional toxicity support information (i.e., toxicokinetic and toxicodynamic information) reduced the uncertainty associated with selection of the Chemicals of Interest to a modest degree. Many of the Chemicals of Interest were still lacking chronic toxicity data that could be used to evaluate health risks associated with the presence of the chemicals in blended produced water or produce. We evaluated the possibility of using alternative approaches, such as read-across toxicology evaluations or Quantitative Structure Activity Relationship modeling, to develop chronic toxicity factors for the chemicals still lacking chronic toxicity factors. The data needed to support these alternative approaches for the remaining Chemicals of Interest were not sufficient, however.

Identification of the specific “aromatic amine” used in oil production would help focus the evaluation of toxicity of this substance and would help the evaluation of any health risks it may pose. (Evaluation of the fate and transport of the compound could also be performed along with a determination of whether the amine is present in other irrigation water.)

Another toxicity issue that arose as part of this project was the toxicity associated with polymers. Because polymers are used widely in commercial and domestic settings and have specific uses in water treatment, their toxicity and presence in water has been the subject of substantial attention by regulatory agencies and other organizations. Our review of the factors associated with polymer toxicity did not reveal any specific reasons for concern, but the data on the specific polymers used in oil production was not sufficient to support a more definitive conclusion. Because of their widespread use, it would be important to understand the concentration of polymers (and associated degradation products) in other sources of irrigation water if an evaluation of differences in blended produced water and other irrigation water is to be performed.

Finally, the toxicity of mixtures and the possible presence of unidentified chemicals, such as degradation products, was raised as a topic to be addressed. One key issue associated with testing blended produced water is the variability in the composition of the water because of variability in the composition of the treated produced water, variability in the composition of the irrigation water with which it is blended, and variability in the ratio of treated produced water and other irrigation water comprising blended produced water. Largely due to cost, testing mammals would not be practical; and there are several aquatic toxicity assays or in vitro assays that could be applied to help understand if blended produced water had different toxicity characteristics than other irrigation water. However, the utility of using these whole water tests to identify health hazards associated with irrigating crops with blended produced water is unclear as the composition of blended produced water is variable and there are uncertainties in extrapolating such tests to humans.

10.0 DISCUSSION AND CONCLUSIONS

The literature review performed under Task 2 was focused on collecting and evaluating information related to the reuse of produced water for agricultural irrigation and on summarizing general fate and transport principles relevant to chemicals in agricultural settings. It also focused on collecting chemical-specific fate and transport properties of the Chemicals of Interest to further support an evaluation of the practice of using produced water for irrigation on the crops addressed in Task 3. As we did not expect to find sufficient information to support a comprehensive risk assessment for the chemicals in produced water, the research conducted in Task 2 included an evaluation of multiple sources of information and several different evaluations focused on developing a better understanding of the potential for chemicals in blended produced water to accumulate in irrigated crops.

Task 2 focused on the 143 Chemicals of Interest that were selected from the 399 chemicals identified in Task 1 as potentially being present in produced water from the San Joaquin Valley. The list of 399 chemicals were winnowed down to the 143 Chemicals of Interest by eliminating from further consideration chemicals that were not likely to accumulate in crops at levels that would pose a health risk by virtue of having low toxicity or of being sufficiently rapidly biodegraded in water that they could not be expected to accumulate in crops. Using this criterion, some chemicals were carried forward as Chemicals of Interest because they were relatively more likely to pose a risk to human health; but other chemicals were carried into Task 2 because there was insufficient information to support eliminating them from further evaluation.

To help us understand the range of sources of the Chemicals of Interest that may impact the chemical content of food crops irrigated with blended produced water, we performed a search for sources of Chemicals of Interest that could impact blended produced water, including petroleum production, as well as other domestic, industrial, and agricultural uses. Most of the Chemicals of Interest have catalogued uses outside of petroleum production; and many of them are also known to be used in agriculture or are naturally occurring metals ubiquitous in soil and irrigation water.

Several evaluations were performed in Task 2 as independent evaluations of factors that could be expected to enhance the accumulation of irrigation water chemicals in crops. We looked for consistency of the results of these findings with the results of Task 3 that levels of chemicals in crops irrigated with blended produced water were essentially the same as levels seen in crops irrigated with conventional irrigation water. As is discussed earlier in this report, these evaluations included a search for chemicals that might be present at elevated levels in blended produced water and a comparison of the levels of chemicals in blended produced water to levels in other water suitable for irrigation. We also searched the literature for information on the fate and transport of Chemicals of Interest in water and soil, plant uptake tendency, and chemical movement patterns within plants. In addition, we compared the levels of chemicals detected in crops irrigated with blended produced water to the levels detected in crops grown in other geographic areas.

When we looked at the available monitoring data for blended produced water for evidence of any elevated levels of Chemicals of Interest, we found that (with the exception of arsenic) Chemicals of Interest were present in blended in irrigation water at levels that were safe to drink. We also found that concentrations of Chemicals of Interest in blended produced water were essentially the same as concentrations in other water suitable for irrigation, including for arsenic. Phenanthrene, however, was found to be at higher levels in blended produced water than in other water suitable for irrigation in Kern County. While phenanthrene appeared to be present in blended produced water at levels higher than in other water suitable for irrigation, it is expected to bind to soil and not be available for plant uptake from irrigation water. We acknowledged that many of the Chemicals of Interest are not included in routine monitoring of both blended produced water and other sources of water due to a lack of analytic methods; and we observed that target analytes, detection limits, and analytic methods were not identical for the testing performed for blended produced water and other irrigation water.

The information on the Chemicals of Interest regarding their fate and transport in the soil, plant uptake, and translocation within a plant does not point to the suggestion that we should have seen a particularly high degree of accumulation of any of them in the Task 3 crop studies. Similarly, the information collected on fate and transport and plant uptake did not suggest any of the results from Task 3 are inconsistent with available information on fate and transport and plant uptake. While a great deal of research has been conducted on the fate and transport of chemicals in water and soil, as well as on plant uptake of chemicals and the transport of chemicals to various plant parts, the current state of science does not support the ability to predict concentrations in the edible portions of plants based on concentrations of chemicals in irrigation water. Accordingly, the current state of science does not support the ability to set chemical-specific concentration limits for irrigation water designed to limit chemical concentrations in the edible portions of crops.

As part of Task 2, we also searched the literature for reports—from other geographic areas—of the level of chemicals detected in the types of crops tested under Task 3. Comparable data was available in the literature for most of the types of crops and chemicals detected in Task 3. While there were some data gaps, the available data supported the conclusion that the levels seen in crops irrigated with produced water were consistent with levels of individual chemicals seen in similar crops grown in other geographic areas. Reports of concentrations measured in crops grown in other areas or available in the market was not available for all crop types; and there may have been differences in plant varieties tested, sample preparation, or other aspects of testing of the crops grown in other geographic areas that could have affected test results.

The several evaluations mentioned above and performed under Task 2 are consistent with the conclusions of the crop sampling analysis performed under Task 3. The fundamental finding of the crop testing was that there were no significant differences in the concentrations of chemicals measure in the crops irrigated blended produced water or conventional irrigation water. While each evaluation had data gaps and associated uncertainties, the result of each evaluation was consistent with the finding of no difference between the two water sources. The fact that all evaluations were consistent with the finding of no difference in the chemical concentrations measured in crops irrigated with blended produced water and conventional irrigation provides an additional degree of confidence to the finding.

Our ability to evaluate the hazards associated with the reuse of produce water is limited by a lack of chemical analytic methods and toxicity information for many of the Chemicals of Interest, and by uncertainties surrounding the toxicity of mixtures of unidentifiable chemicals in produced water. We recognize that new information on the levels of chemicals in water or other environmental media or new information on the toxicity of any of the Chemicals of Interest could affect the conclusions from this project. It is also worth noting that the evaluations performed in Task 2 were based on the evaluation of individual Chemicals of Interest. The approach of evaluating mixtures of chemicals in the environment by examining individual chemicals in the mixture is the most common approach applied to mixtures of chemicals, but it does not address the possibility of effects due to unidentified components of the mixture, interactions between constituents of mixtures, or the presence of degradation products (e.g., degradation of polymers or surfactants). Research identified in this report suggests that toxicity testing of whole effluent samples may be of value in addressing these issues.

It is recognized that the evaluation performed under Task 2 is based on a subset of the 399 chemicals identified as potentially present in produced water. This approach includes uncertainties associated with the fact that exposure and toxicity information is not available for all 399 chemicals and recognizes that all 399 chemicals were not necessarily present in the produced water used for irrigation of the crops studied under Task 3. Of necessity, the primary focus of the evaluation performed under Task 2 is biased toward chemicals that historically have been studied and evaluated. Reliance on such indicator chemicals as the basis for environmental risk assessments is a typical, if not the most common, way in which health risks of mixtures of chemicals in the environment are evaluated. Occasional updated reviews of the published literature for new information on the toxicity and fate and transport properties of these chemicals would be a way to address and reduce the uncertainty associated with the reliance on a subset of chemicals. Similarly, updated reviews of ongoing water quality monitoring data from the produced water my help confirm the presence or absence of chemicals identified as potentially present in produced water in produced water reused locally for irrigation.

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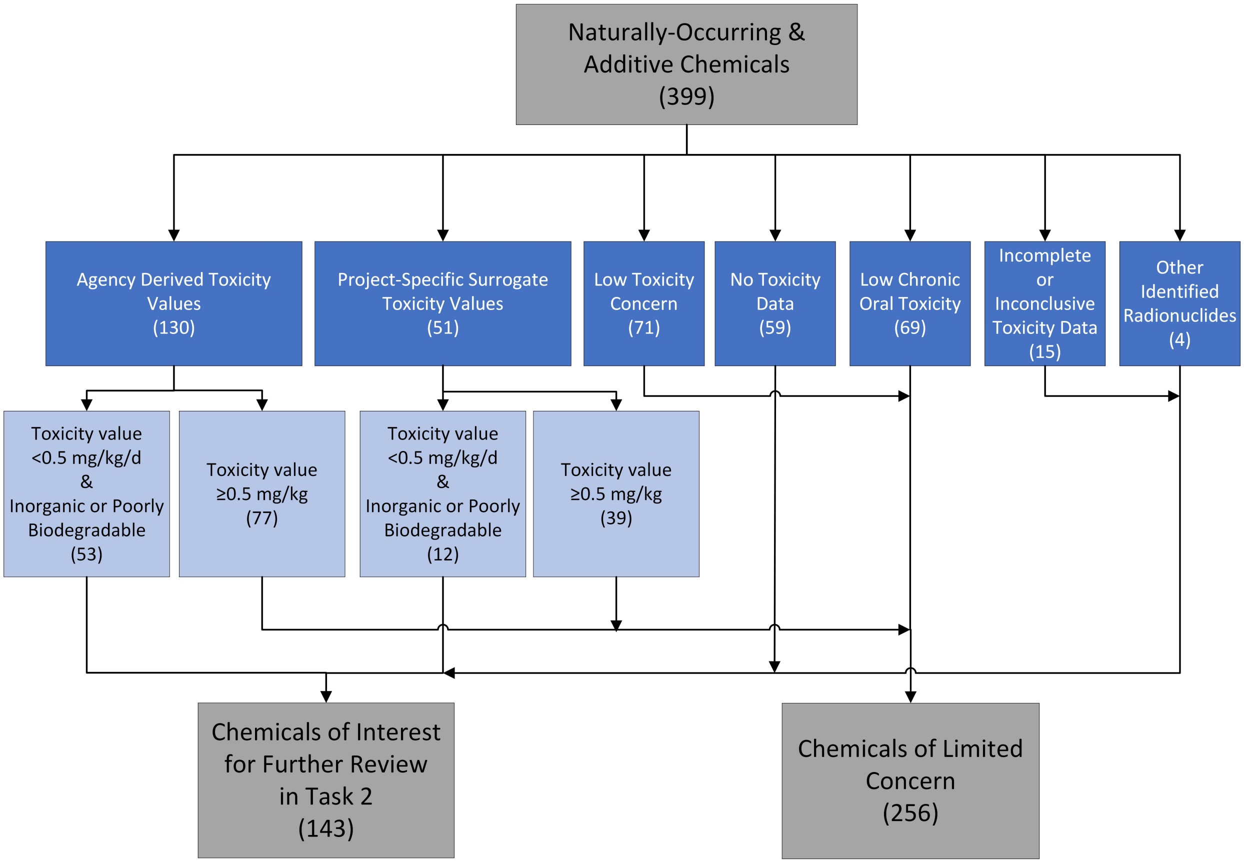

Figure 1: Flowchart presenting overview of risk-based hazard assessment of produced water related chemicals in the context of agricultural irrigation of food crops

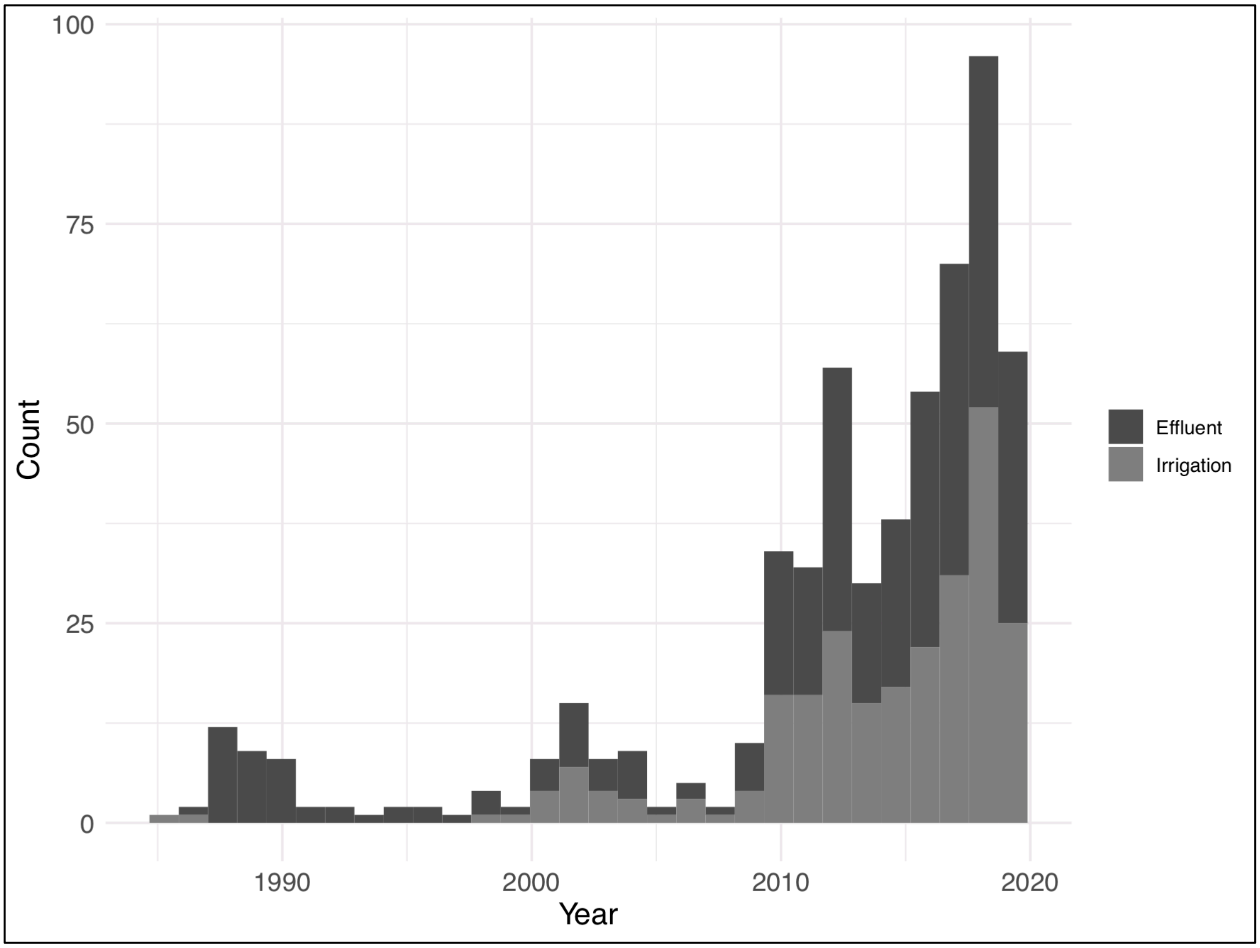

Figure 2: Histogram of water quality sampling events for both treated effluent and blended produced water

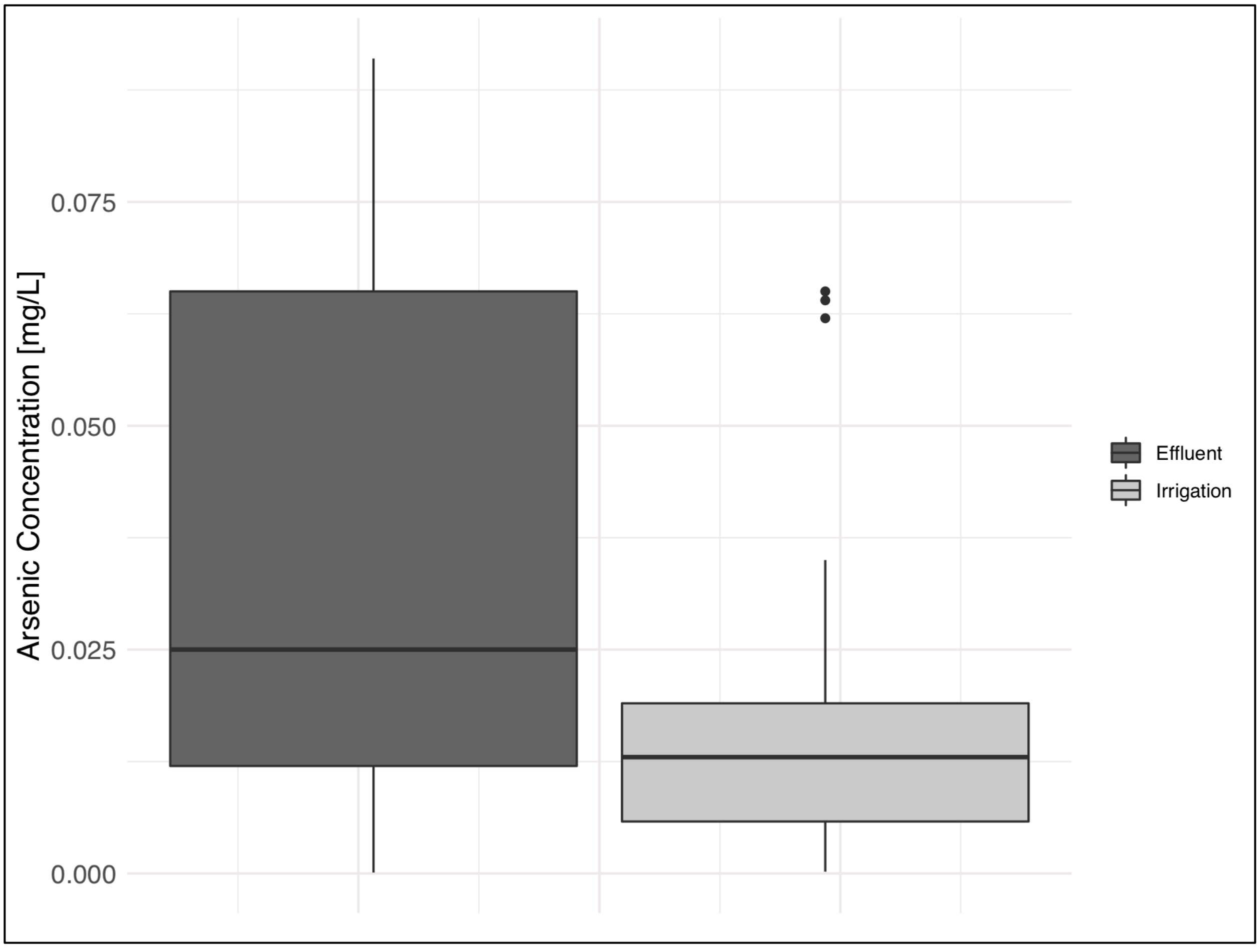

Figure 3: Boxplots of detected arsenic in samples of treated effluent and blended produced water

Table 1: Inclusion/exclusion guidance criteria used to identify relevant literature for the review

Evaluation Factor	Description
Date	• Year 2000 to present for literature focused on produced water • No restrictions for other literature
Method/Sources of Petroleum Extraction	• On-shore oil and gas production • Focus on conventional production methods o Specific results from hydraulic fracturing literature may be reviewed (on a case-by-case basis)
Location	• Focus on North America
Language	• English
Sources of Publications	• Peer Reviewed Literature • Government Publications • Scientific Letters • Industry Reports

Table 2: Identified uses of chemicals additives from the list of Chemicals of Interest

CASRN	Chemical Name	Organic / Inorganic / Radionuclide	Conventional Oil & Gas
1309-64-4	Antimony trioxide	Inorganic	Specific use could not be identified
7727-43-7	Barite	Inorganic	Weighting mud in oil-drilling (PubChem); drilling fluids (80% of world production). Weighing agent to add weight to drilling fluid
7440-39-3	Barium	Inorganic	It is unclear whether elemental additives were declared as they are “ingredients” and not necessarily present or used in their elemental form
7440-41-7	Beryllium	Inorganic	It is unclear whether elemental additives were declared as they are “ingredients” and not necessarily present or used in their elemental form
7440-43-9	Cadmium	Inorganic	It is unclear whether elemental additives were declared as they are “ingredients” and not necessarily present or used in their elemental form
7440-47-3	Chromium	Inorganic	It is unclear whether elemental additives were declared as they are “ingredients” and not necessarily present or used in their elemental form
7440-50-8	Copper	Inorganic	Petroleum isomerization/cracking catalyst (PubChem); bactericide (Identified by GSI expert)
7758-99-8	Copper sulfate pentahydrate	Inorganic	Gel breaker (Identified by GSI expert)
7664-39-3	Hydrofluoric acid	Inorganic	Used in acid treatment (Schlumberger, 2020)
7553-56-2	Iodine	Inorganic	It is unclear whether elemental additives were declared as they are “ingredients” and not necessarily present or used in their elemental form
7439-92-1	Lead	Inorganic	It is unclear whether elemental additives were declared as they are “ingredients” and not necessarily present or used in their elemental form

CASRN	Chemical Name	Organic / Inorganic / Radionuclide	Conventional Oil & Gas
554-13-2	Lithium carbonate	Inorganic	Cement setting accelerator (Fink, 2015)
13453-71-9	Lithium chlorate	Inorganic	Specific use could not be identified
7447-41-8	Lithium chloride	Inorganic	Specific use could not be identified
1310-65-2	Lithium hydroxide	Inorganic	Emulsifier, thickening agent (Identified by GSI Expert)
13840-33-0	Lithium hypochlorite	Inorganic	Biocide (Identified by GSI expert)
7439-97-6	Mercury	Inorganic	It is unclear whether elemental additives were declared as they are “ingredients” and not necessarily present or used in their elemental form; biocide (Identified by GSI Expert)
7440-02-0	Nickel	Inorganic	It is unclear whether elemental additives were declared as they are “ingredients” and not necessarily present or used in their elemental form; possibly oxygen scavenger (Identified by GSI expert)
7786-81-4	Nickel sulfate	Inorganic	Oxygen scavenger (Identified by GSI expert)
65996-69-2	Steel mill slag	Inorganic	Light weight cement (Fink, 2015)
7446-09-5	Sulfur dioxide	Inorganic	Non-emulsifier/breaker (Identified by GSI expert)
7440-66-6	Zinc	Inorganic	It is unclear whether elemental additives were declared as they are “ingredients” and not necessarily present or used in their elemental form; anti-corrosion (Identified by GSI expert)
7646-85-7	Zinc chloride	Inorganic	Anti-sludge (Identified by GSI expert)
123-91-1	1,4 Dioxane	Organic	Cement, degreasing agents, coatings (USEPA, 2017a)
479-66-3	1H, 3H-Pyrano (4,3-b)(1)benzopyran-9-carboxylic acid, 4,10-dihydro-3,7,8 trihydroxy-3-methyl-10-oxo	Organic	Extraction and solubilization of crude oil and volatile petroleum hydrocarbons by purified humic and fulvic acids and sodium dodecylbenzenesulfonate (Eljack & Hussam, 2014)

CASRN	Chemical Name	Organic / Inorganic / Radionuclide	Conventional Oil & Gas
60-24-2	2-mercaptoethanol	Organic	Ingredient in system integrity fluid; corrosion control (Chevron, 2018)
115-19-5	2-methyl-3-Butyn-2-ol	Organic	Corrosion inhibitor (Parchem, 2020a)
27646-80-6	2-Methylamino-2-methyl-1-propanol	Organic	Corrosion inhibitor, gas absorbent (Fink, 2015)
67990-40-3	2-Propen-1-aminium, N,N-dimethyl-N-2-propenyl-, chloride, polymer with 2-hydroxypropyl 2-propenoate and 2-propenoic acid	Organic	Specific use could not be identified
145417-45-4	2-Propenoic acid, 2-methyl-, polymer with methyl 2-methyl-2-propenoate, octadecyl 2-methyl 2 propenoate and 2propenoic acid, sodium salt	Organic	Ingredient used for drilling (SapuraOMV, 2020); Surfactant, biocide (Identified by GSI expert)
9033-79-8	2-propenoic acid, polymer with sodium 2-propenoate	Organic	Water softeners, scale inhibitor, friction reducer; surfactant (Identified by GSI expert)
130800-24-7	2-Propenoic acid, telomer with 2-methyl-2-(1-oxo-2-propenyl)-1-propanesulfonic acid, sodium salt	Organic	Corrosion inhibitor, biocide, scale inhibitor (Identified by GSI expert)
100-73-2	Acrolein dimer	Organic	Ingredient in system integrity fluid (Chevron, 2018)
29868-05-1	Alkanolamine phosphate	Organic	Corrosion inhibitor (Identified by GSI expert)
68439-70-3	Alkyl amine	Organic	Oil and gas drilling (PubChem)
300-92-5	Aluminum distearate	Organic	Defoamer (Schlumberger, 2020)
No CASRN	Amide surfactant acid salt	Organic	Emulsifiers, surfactant (Schlumberger, 2020), corrosion and scale inhibitors (Identified by GSI Expert)
No CASRN	Amides, Non Ionics	Organic	Emulsifiers, surfactant (Schlumberger, 2020), corrosion and scale inhibitors (Identified by GSI Expert)

CASRN	Chemical Name	Organic / Inorganic / Radionuclide	Conventional Oil & Gas
61791-24-0	Amine derivative	Organic	Surfactant, emulsifiers, oil wetting agents (Schlumberger, 2020)
67924-33-8	Amine salt	Organic	Specific use could not be identified
NP-U2856	Amine salt	Organic	Specific use could not be identified
64346-44-7	Amine sulfate	Organic	Breaker, oxygen scavenger (Identified by GSI expert)
No CASRN	Aromatic Amine	Organic	Corrosion inhibitor (Identified by GSI expert)
68239-30-5	Bis (HDMA) EPI Copolymer hydrochloride	Organic	Emulsifier, oil wetting agent (Identified by GSI expert)
69418-26-4	Cationic acrylamide copolymer	Organic	Friction reducer, sludge dewatering, water treatment (Identified by GSI expert)
44992-01-0	Cationic acrylamide monomer	Organic	Used in water treatment as flocculant and coagulant polymers (Parchem, 2020b); friction reducer, antifoaming agents, coagulating agents, dispersion agents, emulsifiers, flotation agents, foaming agents, viscosity adjustors (Identified by GSI expert)
54076-97-0	Cationic polymer	Organic	Gelling agent (Identified by GSI expert)
681331-04-4	Causticized Lignite	Organic	Drilling mud thinner, clay deflocculant, emulsifying agent, surfactant (Chatterjee, 2002); used for rheology and filtration controls in water base muds and maintaining constant pH; used for stabilizing, thinning, and filtration control purpose in water base muds (Global Drilling Fluids & Chemicals, 2008)
64743-05-1	Coke (petroleum), calcined	Organic	Used in cement (Fink, 2015; Chevron, 2018)
25987-30-8	Copolymer of acrylamide and sodium acrylate	Organic	Friction reducer, scale inhibitor (Schlumberger, 2020)
68308-87-2	Cottonseed, flour	Organic	Absorber (Identified by GSI expert)

CASRN	Chemical Name	Organic / Inorganic / Radionuclide	Conventional Oil & Gas
129828-31-5	Crosslinked polyol ester	Organic	Unknown use, but similar structure to other formaldehyde-nonylphenol-oxirane polymers the list of chemicals of interest used as corrosion inhibitors (Identified by GSI expert)
2673-22-5	Diester of sulfosuccinic acid sodium salt	Organic	Surfactant (Ash, 1997)
38011-25-5	Disodium ethylenediaminetetraacetate	Organic	Scale inhibitor, breaker (Identified by GSI expert)
64742-53-6	Distillates, hydrotreated light naphthenic	Organic	Non-emulsifier, friction reducer, crosslinker, gelling agent (Identified by GSI expert)
No CASRN	Drilling paper	Organic	Specific use could not be identified
126-97-6	Ethanolamine thioglycolate	Organic	Corrosion inhibitors and anti-scaling agent (PubChem)
26027-38-3	Ethoxylated 4- nonphenol	Organic	Corrosion inhibitor, surfactant, emulsifier (Identified by GSI expert)
61791-26-2	Ethoxylated amine	Organic	Surfactants, emulsifiers, degreaser (Identified by GSI expert)
9081-83-8	Ethoxylated octylphenol	Organic	Surfactant, friction reducer, emulsifier, detergent (Identified by GSI expert)
5877-42-9	Ethyl octynol	Organic	Industrial acid corrosion inhibitor and anti-scaling agent (PubChem)
63428-92-2	Formaldehyde, polymer with 2-methyloxirane, 4-nonylphenol and oxirane	Organic	Corrosion inhibitor (Identified by GSI expert)
30704-64-4	Formaldehyde, polymer with 4-(1,1-dimethylethyl)phenol, 2-methyloxirane and oxirane	Organic	Identified use in hydraulic fracturing fluid, no specific use identified (ACToR); likely non-emulsifier (Identified by GSI Expert)

CASRN	Chemical Name	Organic / Inorganic / Radionuclide	Conventional Oil & Gas
30846-35-6	Formaldehyde, polymer with 4-nonylphenol and oxirane	Organic	Identified use in hydraulic fracturing fluid, no specific use identified (ACToR); likely corrosion inhibitor (Identified by GSI expert)
No CASRN	Heavy catalytic reformed naptha	Organic	Friction reducer, paraffin inhibitor, emulsifier, viscocifier (Identified by GSI expert)
1415-93-6	Humic acids	Organic	Drilling mud, viscosity modifier, fluid loss agent, emulsifier; reduces viscosity and gel strength, controls rheology and acts as a dispersant (Parchem, 2020c)
61790-59-8	Hydrogenated tallow amine acetone	Organic	Scale inhibitor, corrosion inhibitor, flotation agent (Identified by GSI expert)
2809-21-4	Hydroxyethylidenediphosphonic acid	Organic	Scale inhibitor (salts of the acid) (Identified by GSI expert)
119-65-3	Isoquinoline	Organic	Corrosion inhibitor and anti-scaling agent (PubChem)
68648-89-5	Kraton G1702H	Organic	Used as Ingredient in workover fluid (Chevron, 2018)
129521-66-0	Lignite	Organic	Drilling mud (see causticized lignite); fluid control (Parchem, 2020d)
PE-M2464	Methyl oxirane polymer	Organic	Specific use could not be identified
No CASRN	Nonylphenol ethoxylates	Organic	Activator, emulsifier, wetting agent (Identified by GSI expert)
127087-87-0	Nonylphenol polyethylene glycol ether	Organic	Non-ionic surfactant, non-emulsifier (Identified by GSI expert)
No CASRN	Organic acid ethoxylated alcohols	Organic	Surfactants (Identified by GSI expert)
68412-54-4	Oxyalkylated alkylphenol	Organic	Non-ionic surfactant (Solvay, 2020)
68171-44-8	Oxyalkylated alkylphenolic resin	Organic	Ingredient in system integrity fluid (Chevron, 2018)
67939-72-4	Oxyalkylated polyamine	Organic	Demulsifiers, cross-link agent, friction modifier, surfactant (Identified by GSI expert)

CASRN	Chemical Name	Organic / Inorganic / Radionuclide	Conventional Oil & Gas
68910-19-0	Oxyalkylated polyamine	Organic	Demulsifiers, cross-link agent, friction modifier, surfactant (Identified by GSI expert)
68123-18-2	Phenol, 4,4'-(1-methylethylidene) bis-, polymer with 2-(chloromethyl)oxirane, 2-methyloxirane and oxirane	Organic	Corrosion inhibitor (Identified by GSI expert)
68425-75-2	Phosphate ester salt	Organic	Scale inhibitor, surfactant (Identified by GSI expert)
9005-70-3	POE (20) Sorbitan Trioleate	Organic	Used in slurry and spacer system (Chevron, 2018)
68938-70-5	Poly (triethanolamine.mce)	Organic	Reverse emulsion breaker (Golder Associates, 2018)
68955-69-1	Polyamine salts	Organic	Corrosion inhibitors, drilling mud lubricants, clay stabilizers (Identified by GSI expert)
19019-43-3	Polycarboxlate salt [Trisodium ethylenediaminetetraacetate]	Organic	Scale inhibitor (Identified by GSI expert)
26062-79-3	Polydimethyl diallyl ammonium chloride	Organic	Clay stabilizer, water treating, flocculant (Henan Go Biotech, 2019)
74-84-0	Polyethylene	Organic	Specific use could not be identified
68036-92-0	Polyglycol diepoxide	Organic	Surfactant (Identified by GSI expert)
68036-95-3	Polyglycol diepoxide	Organic	Specific use could not be identified
9038-95-3	Polyglycol ether	Organic	Emulsifier, friction reducer, acid stabilizer (Identified by GSI expert)
64741-71-5	Polymers (petroleum) viscous	Organic	Drilling fluid additive (Drilling Specialties Company, 2017)
36484-54-5	Polyoxyalkylene glycol	Organic	Specific use could not be identified
61790-86-1	Polyoxyalkylenes	Organic	Corrosion inhibitor (Identified by GSI expert)

CASRN	Chemical Name	Organic / Inorganic / Radionuclide	Conventional Oil & Gas
9014-93-1	Polyoxyethylene dinonylphenol	Organic	Used in crude oil production as lubricant demulsifier component (Parchem, 2020e); surfactant, emulsifier, lubricant (Identified by GSI expert)
12068-19-8	Polyoxyethylene nonyl phenyl ether phosphate	Organic	Specific use could not be identified
70142-34-6	Polyoxyl 15 hydroxystearate	Organic	Specific use could not be identified
42751-79-1	Polyquaternary amine	Organic	Quaternary amines (class): oil-wetting agents, corrosion and shale inhibitors and bactericides (Schlumberger, 2020)
61790-41-8	Quaternary ammonium compound	Organic	Corrosion inhibitor, biocide (eliminates bacteria in drilling fluid water that produce corrosive by-products (Identified by GSI expert)
68609-18-7	Quaternized condensed alkanolamines	Organic	Antibacterial, corrosion inhibitors (Identified by GSI expert)
91-63-4	Quinaldine	Organic	Corrosion inhibitor (Identified by GSI expert)
12179-04-3	Sodium tetraborate pentahydrate	Organic	Cross-linker to add viscosity (Identified by GSI expert)
64742-95-6	Solvent naphtha, petroleum, light arom.	Organic	Ingredient in system integrity fluid (Chevron, 2018)
NP-SMO3_U1240	Sorbitan ester	Organic	Nonionic surfactants used as emulsifiers (Identified by GSI expert)
8052-41-3	Stoddard Solvents	Organic	Flocculent, gelling agent (Identified by GSI expert)
68140-11-4	Tall oil, DETA/ midazoline acetates	Organic	Corrosion inhibitors and anti-scaling agents (PubChem)
72480-70-7	Tar bases, quinoline derivatives, quaternized benzyl chloride	Organic	Acid corrosion inhibitor (Identified by GSI expert)
64-02-8	Tetrasodium ethylenediaminetetraacetate	Organic	Chelant (Golder Associates, 2018), flocculant, gelling agent (Identified by GSI expert)

CASRN	Chemical Name	Organic / Inorganic / Radionuclide	Conventional Oil & Gas
68527-49-1	Thiourea, polymer with formaldehyde and 1-phenylethanone	Organic	Corrosion inhibitor (along with polyoxyalkylenes)
64114-46-1	Triethanolamine homopolymer	Organic	Surfactant compatible acid corrosion inhibitor; used in the recovery of hydrogen sulfide from sour natural gases and sour crude petroleum (PubChem); crosslinker, breaker activator (Identified by GSI expert)
13983-27-2	Krypton-85	Radionuclide	Used during drilling to indicate drill bit wear or failure (Fries, 1974)
14932-42-4	Xenon-133	Radionuclide	Tracer used by the oil and gas industry because they are easily identified and measured (IAEA, 2003)

Table 3: Agricultural and other general uses of the Chemicals of Interest

CASRN	Chemical Name	Organic / Inorganic / Radionuclide	Agricultural Use or Link	Other General Uses	Is Additive?	Is Naturally Occurring?
7440-36-0	Antimony	Inorganic	present in soil (USEPA, 2000)	alloys, bullets and bearing metal, fireworks, coatings, flame retardants, former medication (PubChem)	N	Y
1309-64-4	Antimony trioxide	Inorganic	present in biosolids-amended fertilizer (USEPA, 2014b)	tartar emetic, paint pigments, stains for iron and copper, enamels, ceramics, glasses, mordants plastic stabilizers, phosphors, flame-retardants for canvas, textiles, and plastics (PubChem); industrial air streams (USEPA 2014b)	Y	N
7440-38-2	Arsenic	Inorganic	historically registered as CA pesticide ingredient (CDPR, 2019); present in fertilizer (CDFA, 2004); formerly use as herbicide, pesticide (PubChem);	alloy, wood preservative, catalyst, electronics, pharmaceuticals, explosives (PubChem)	N	Y
7727-43-7	Barite	Inorganic	historically registered as CA pesticide ingredient (CDPR, 2019); approved as Inert ingredients used pre-harvest pesticide (carrier), food and non-food use (USEPA, 2019c), agricultural applications related to growing crops and livestock (PubChem)	adhesives, dyes, construction, electronics, industrial chemicals, colorants, lubricants, oxidizing/reducing agents, processing aids, plating agents (PubChem)	Y	N
7440-39-3	Barium	Inorganic	micronutrient in fertilizer (Krueger, 2018)	alloy, deoxidizer, lubricant, heat stabilizer for plastics, fluorescent lamp cathodes, drying agent for inks, etc. (PubChem)	Y	Y
7440-41-7	Beryllium	Inorganic	present in fertilizer (ATSDR, 2002)	alloys and ceramics; components in automotive, electronics, industrial components, medical devices, nuclear, etc. (PubChem)	Y	Y

CASRN	Chemical Name	Organic / Inorganic / Radionuclide	Agricultural Use or Link	Other General Uses	Is Additive?	Is Naturally Occurring?
7440-42-8	Boron	Inorganic	formerly used in pesticide (PubChem); micronutrient in fertilizer (Krueger, 2018)	catalyst, alloy (PubChem)	N	Y
7440-43-9	Cadmium	Inorganic	historically registered as CA pesticide ingredient (CDPR, 2019); present in fertilizer (CDFA, 2004); fungicide, agricultural applications related to growing crops and livestock (PubChem)	alloys, electronics/batteries, pigments, photosensitive chems, plating agents, etc. (PubChem)	Y	Y
7440-47-3	Chromium	Inorganic	micronutrient in fertilizer (Mansfield, 2017); naturally occurring in soil (ATSDR, 2012c)	alloys (PubChem)	Y	Y
7440-48-4	Cobalt	Inorganic	present as trace element in fertilizer (CDFA, 2004; PubChem); naturally occuring in soil (ATSDR, 2004a)	catalyst in petrochemical and plastics, electroplating, colorants, alloy (PubChem)	N	Y
7440-50-8	Copper	Inorganic	actively registered as CA pesticide ingredient (CDPR, 2019); present in fertilizer (CDFA, 2004); microbiocide; formerly used as pesticide (PubChem); naturally occuring in soil (ATSDR, 2004b)	electronics/electrical wiring, electroplating, alloys, ammunition, antimicrobial (PubChem)	Y	Y
7758-99-8	Copper sulfate pentahydrate	Inorganic	actively registered as CA agricultural pesticide ingredient (CDPR, 2019); algicide, fungicide (PubChem); approved as inert ingredient in pesticide, food and non-food use (USEPA, 2019c)	antimicrobial, disinfectant, drug, manufacturing, paint, water treatment (PubChem)	Y	N
16984-48-8	Fluoride	Inorganic	result of sulfuryl fluoride (pesticide, fumigant) decay (OEHHA, 2020)	drugs, food, personal care, gas extraction (PubChem); industrial streams (Choudhary et al, 2019)	N	Y

CASRN	Chemical Name	Organic / Inorganic / Radionuclide	Agricultural Use or Link	Other General Uses	Is Additive?	Is Naturally Occurring?
7664-39-3	Hydrofluoric acid	Inorganic	no agricultural uses found	household products; process regulators; plating agent; alkylation catalyst (PubChem); precursor to almost all fluorine compounds; used in etching/polishing glass, aluminum production, uranium processing, stainless steel pickling, fluorocarbon production used in aerosol sprays and refrigerants (Speight, 2017)	Y	N
7553-56-2	Iodine	Inorganic	actively registered as CA agricultural pesticide ingredient, various agricultural, commercial, industrial applications, not including food crops (CDPR, 2019); pesticide and fertilizer amendment (Ajay-SQM); inert ingredient in pesticide, food and non-food use, for food use limited to 25 ppm titratable iodine (USEPA, 2019c)	microbiocide, anti-infective agent, catalyst in alkylation, manufacturing of organic and inorganic chemicals (PubChem)	Y	N
7439-92-1	Lead	Inorganic	historically registered as CA pesticide ingredient (CDPR, 2019); present in fertilizer (CDFA, 2004)	batteries, pigments, rolled/extruded products, alloys, shot ammunition, cable sheathing, gasoline additive (PubChem)	Y	Y
7439-93-2	Lithium	Inorganic	lithium salts of the herbicide 2,4-dichlorophenoxyacetic acid (PubChem)	batteries, Al alloy component, metal ingot and foil manufacturing, manufacturing of greases, ceramics, aircraft fuel, and organic chems; drugs for bipolar depression (PubChem)	N	Y
554-13-2	Lithium carbonate	Inorganic	historically registered as CA pesticide ingredient (CDPR, 2019); lithium grease (wiki lithium soap); approved as inert pesticide ingredient, non-food use (USEPA, 2019c)	adhesive, drugs, catalyst, electronics, lubricant, manufacturing, oxidizing/reducing agents, building/construction (PubChem)	Y	N

CASRN	Chemical Name	Organic / Inorganic / Radionuclide	Agricultural Use or Link	Other General Uses	Is Additive?	Is Naturally Occurring?
13453-71-9	Lithium chlorate	Inorganic	inert pesticide ingredient, non-food use (PubChem, USEPA, 2019c)	oxidizing agent; used in air conditioning and propellants (Chemical Book, 2017)	Y	N
7447-41-8	Lithium chloride	Inorganic	historically registered as CA pesticide ingredient (CDPR, 2019); pesticide, inert ingredient in pesticide, acaricide, non-food use (PubChem; USEPA, 2019c)	desiccant and humectant; air conditioning; batteries; adhesive; drug; chemical intermediate; used in soldering; dry batteries; mineral waters; catalyst for low temperature reactions between epoxides and carboxyl groups to yield polyester product (PubChem)	Y	N
1310-65-2	Lithium hydroxide	Inorganic	historically registered as CA pesticide ingredient (CDPR, 2019); lithium grease for agricultural machinery/engines (Mowitz, 2013)	adsorbents, dyes, lubricants (PubChem); used in the production of lithium greases like lithium stearate; used in electric car batteries; chemical intermediates; oxidizing/reducing agents (MarketWatch, 2019)	Y	N
13840-33-0	Lithium hypochlorite	Inorganic	historically registered as CA pesticide ingredient (CDPR, 2019); algicide, disinfectant, fungicide, and food contact surface sanitizer (PubChem, USEPA 1993)	bleaching agent, microbiocide (PubChem)	Y	N
7439-96-5	Manganese	Inorganic	micronutrient in fertilizer (Krueger, 2018); naturally occuring in soil (ATSDR, 2012a)	manufacturing, automotive, electronics, etc. (PubChem)	N	Y
7439-97-6	Mercury	Inorganic	present in fertilizer (CDFA, 2004); discontinued use in pesticide (PubChem)	lighting, processing aids (PubChem)	Y	Y
7439-98-7	Molybdenum	Inorganic	historically registered as CA pesticide ingredient (CDPR, 2019); present in fertilizer (CDFA, 2004)	alloy, electronics, lubricants (PubChem)	N	Y
7440-02-0	Nickel	Inorganic	historically registered as CA pesticide ingredient (CDPR, 2019); present in fertilizer (CDFA, 2004)	alloys, catalyst, electroplating, batteries (PubChem)	Y	Y

CASRN	Chemical Name	Organic / Inorganic / Radionuclide	Agricultural Use or Link	Other General Uses	Is Additive?	Is Naturally Occurring?
7786-81-4	Nickel sulfate	Inorganic	pesticide (PubChem)	plating agent, catalyst, drug, electronics, manufacturing, paints, process regulator, water treatment, etc. (PubChem)	Y	N
14797-65-0	Nitrite	Inorganic	naturally occurring; nitrogen-containing fertilizer (ATSDR, 2017b)	automotive, industrial manufacturing (PubChem)	N	Y
7782-49-2	Selenium	Inorganic	present in fertilizer (CDFA, 2004); dietary supplement for livestock and fertilizer additive (PubChem)	photographic toning baths, pigments, glass mfr, electronics, catalyst, rubber tires, construction, food packaging (PubChem)	N	Y
7440-22-4	Silver	Inorganic	actively registered as CA pesticide ingredient (CDPR, 2019); biosolids-amended fertilizer from silver nanoparticles (Jesmer et al, 2017); microbiocide; formerly used as pesticide (PubChem)	electroplating; batteries, electronics (PubChem)	N	Y
65996-69-2	Steel mill slag	Inorganic	no agricultural uses found	asphalt concrete aggregate, granular base, embankment, fill (USDOT, 2016);	Y	N
7440-24-6	Strontium	Inorganic	naturally occurring in water and soils (ATSDR, 2004e); no agricultural uses found	large variety of uses in consumer products, cosmetics, and industrial applications (PubChem)	N	Y
7446-09-5	Sulfur dioxide	Inorganic	actively registered as CA agricultural pesticide ingredient, food crop applications (CDPR, 2019); pesticide (PubChem), approved as inert pesticide ingredient, non-food use (USEPA, 2019c)	food preservative, bleaching agent, disinfectant, solvent and reagent in organic synthesis, reducing agent, oxygen scavenger and extractive solvent in oil refining (PubChem)	Y	N
7440-31-5	Tin	Inorganic	lawn and garden care products (PubChem)	fuel additive, alloy, electronics, chemical intermediate, tubes, etc. (PubChem)	N	Y
7440-62-2	Vanadium	Inorganic	plant micronutrient (Krueger, 2018)	alloy, fuel additive (PubChem)	N	Y

CASRN	Chemical Name	Organic / Inorganic / Radionuclide	Agricultural Use or Link	Other General Uses	Is Additive?	Is Naturally Occurring?
7440-66-6	Zinc	Inorganic	actively registered as CA pesticide ingredient, marine applications (CDPR, 2019); present in fertilizer (CDFA, 2004); fungicide (PubChem); approved as inert pesticide ingredient, non-food use as metallic zinc (USEPA, 2019c); naturally occuring in soil (ATSDR, 2005c)	alloy, electroplating, stabilizing (PubChem)	Y	Y
7646-85-7	Zinc chloride	Inorganic	historically registered as CA pesticide ingredient (CDPR, 2019); pesticide (PubChem), approved as inert pesticide ingredient, non-food use (USEPA, 2019c)	adhesive/sealant, wood preservatives, metallurgical fluxes, batteries, antiseptic, plating agent, solvent, etc. (PubChem)	Y	N
123-91-1	1,4 Dioxane	Organic	historically registered as CA pesticide ingredient (CDPR, 2019); pesticides (USEPA 2017b, PubChem)	cement, degreasing agents, coatings (USEPA, 2017a); adhesive, solvent, historical use as stabilizer in chlorinated solvents (PubChem); by-product in paint strippers, dyes, antifreeze and aircraft deicing fluids, and in consumer products (e.g. deodorant, shampoos, cosmetics); used as a purifying agent in pharmaceutical manufacturing and produced as a byproduct of polyethylene terephthalate (PET) plastic manufacturing (USEPA, 2017b)	Y	N
479-66-3	1H, 3H-Pyrano (4,3-b)(1)benzopyran-9-carboxylic acid, 4,10-dihydro-3,7,8 trihydroxy-3-methyl-10-oxo	Organic	naturally found in soils, sediment, and aquatic envs (Winkler and Ghosh, 2018)	dietary supplement (Winkler and Ghosh, 2018)	Y	N

CASRN	Chemical Name	Organic / Inorganic / Radionuclide	Agricultural Use or Link	Other General Uses	Is Additive?	Is Naturally Occurring?
60-24-2	2-mercaptoethanol	Organic	insecticides; agricultural chemicals; naturally occurring in swine manure and marine algae/plants (HSDB, 2019)	adhesives, plastics manufacturing, process regulators, corrosion inhibitors and anti-scaling, process regulators, oil & gas drilling, water treatment (PubChem); used to reduce disulfide bonds, can act as a biological antioxidant to scavenge hydroxyl radicals (ThermoFisher, n.d.)	Y	N
115-19-5	2-methyl-3-Butyn-2-ol	Organic	historically registered as CA pesticide ingredient (CDPR, 2019); pesticide (PubChem); approved as inert pesticide ingredient, non-food use (USEPA, 2019c)	solvent, manufacturing, consumer, surface treatment, intermediates, etc. (PubChem)	Y	N
27646-80-6	2-Methylamino-2-methyl-1-propanol	Organic	no agricultural uses found	buffer or pH regulating agent; used in paint and manufacturing (PubChem); corrosion inhibitor (Angus Chemical Company, 2017); used in synthesis of surface-active agents, vulcanization accelerators, pharmaceuticals; absorbent for acid gases; emulsifying agent for cosmetic creams and lotions, mineral oil & paraffin wax emulsions, leather dressings, textile specialties, polishes, cleaning compounds (Spectrum, 2019)	Y	N
67990-40-3	2-Propen-1-aminium, N,N-dimethyl-N-2-propenyl-, chloride, polymer with 2-hydroxypropyl 2-propenoate and 2-propenoic acid	Organic	approved as inert ingredient in pesticide, non-food use (USEPA, 2019c)		Y	N

CASRN	Chemical Name	Organic / Inorganic / Radionuclide	Agricultural Use or Link	Other General Uses	Is Additive?	Is Naturally Occurring?
145417-45-4	2-Propenoic acid, 2-methyl-, polymer with methyl 2-methyl-2-propenoate, octadecyl 2-methyl 2 propenoate and 2propenoic acid, sodium salt	Organic	no agricultural uses found		Y	N
9033-79-8	2-propenoic acid, polymer with sodium 2-propenoate	Organic	approved as inert ingredient in pesticide, non-food use (USEPA, 2019c)		Y	N
130800-24-7	2-Propenoic acid, telomer with 2-methyl-2-(1-oxo-2-propenyl)-1-propanesulfonic acid, sodium salt	Organic	no agricultural uses found		Y	N
83-32-9	Acenaphthene	Organic	historically registered as CA pesticide ingredient (CDPR, 2019); pesticide (PubChem)	dye intermediate, manufacturing plastics, pharmaceuticals, PAHs from gasoline and diesel exhaust (PubChem)	N	Y
100-73-2	Acrolein dimer	Organic	no agricultural uses found	used to make other chemicals, plastics (PubChem)	Y	N
29868-05-1	Alkanolamine phosphate	Organic	no agricultural uses found	alkanoamines, as a class, are used in surfactants, cosmetics, toiletry products, metal working fluids, textile chemicals, gas conditioning chemicals, agricultural chemical intermediates, and cement grinding aids (Davis and Carpenter, 1997)	Y	N
68439-70-3	Alkyl amine	Organic	inert ingredient pesticide (PubChem), approved as inert ingredient in pesticides, non-food use (USEPA, 2019c)	surfactant, solvent, home maintenance, construction, manufacturing (PubChem)	Y	N

CASRN	Chemical Name	Organic / Inorganic / Radionuclide	Agricultural Use or Link	Other General Uses	Is Additive?	Is Naturally Occurring?
300-92-5	Aluminum distearate	Organic	agricultural crop/animal application (PubChem), inert ingredient in pesticide, non-food use (PubChem; USEPA, 2019c)	emulsion stabilizer; opacifying agent; viscosity control agent; thickener in paints, inks, and greases; water repellent; lubricant in plastics and ropes; gasoline gelling agent; used in cement production, used in cosmetic products in preparing clear cosmetic gels and pomades; adhesive and sealant chemicals; fillers; intermediates (PubChem)	Y	N
No CASRN	Amide surfactant acid salt	Organic	no agricultural uses found	surfactant (Negm et al, 2018)	Y	N
No CASRN	Amides, Non Ionics	Organic	no agricultural uses found	surfactant (Negm et al, 2018)	Y	N
61791-24-0	Amine derivative	Organic	historically registered as CA pesticide ingredient (CDPR, 2019); approved as inert ingredients used pre-harvest pesticides (surfactant), food and non-food use (USEPA, 2019c)	emulsifier, surfactant (The Good Scents Company, 2018)	Y	N
67924-33-8	Amine salt	Organic	inert pesticide ingredient (PubChem), though not listed in InertFinder	adhesives, dyes, paper products, fabric/leather, personal care (PubChem)	Y	N
NP-U2856	Amine salt	Organic	no agricultural uses found		Y	N
64346-44-7	Amine sulfate	Organic	no agricultural uses found		Y	N
120-12-7	Anthracene	Organic	insecticide, acaricide, herbicide, rodenticide (PubChem)	dyes, PAHs from exhaust (PubChem)	N	Y
No CASRN	Aromatic Amine	Organic	no agricultural uses found	used in dyes, as antioxidants, and as precursors of pharmaceutical products (Sogorb et al, 2014)	Y	N
56-55-3	Benzo(a)anthracene	Organic	no agricultural uses found	PAHs from fires and diesel & gasoline exhaust; research chemical (PubChem)	N	Y

CASRN	Chemical Name	Organic / Inorganic / Radionuclide	Agricultural Use or Link	Other General Uses	Is Additive?	Is Naturally Occurring?
50-32-8	Benzo(a)pyrene	Organic	no agricultural uses found	PAHs from fires and diesel exhaust; chemical intermediate; fuels and related products (PubChem)	N	Y
205-99-2	Benzo(b)fluoranthene	Organic	no agricultural uses found	PAHs from fires and gasoline exhaust; research chemical; component of coal tar and creosote (PubChem)	N	Y
111-44-4	Bis (2-chloroethyl) ether	Organic	historically registered as CA pesticide ingredient (CDPR, 2019); formerly used in pesticide (PubChem); intermediate ingredient in pesticide; speculated to exist in trace amounts in fungicides (EC, 1993)	chlorination by-product in waste streams w/ethylene or propylene (WHO, 1998)	N	Y
68239-30-5	Bis (HDMA) EPI Copolymer hydrochloride	Organic	no agricultural uses found		Y	N
69418-26-4	Cationic acrylamide copolymer	Organic	Cationic polyacrylamide copolymers (PAMs) are used for sludge dewatering in municipal waste water treatment and might enter the environment by spreading of the sludge on agricultural land (Hennecke et al, 2018).	Polycationic polymers used in the personal care industry: conditioners, shampoo, hair mousse, hair spray, hair dye, personal lubricant, and contact lens solutions (Rajput, 2015). Cationic polyacrylamide copolymers (PAMs) are used extensively in water treatment, enhanced oil recovery and sludge dewatering (Hennecke et al, 2019)	Y	N
44992-01-0	Cationic acrylamide monomer	Organic	no agricultural uses found	antistatic finish for polyester fibers; flocculant and coagulant polymers for water treatment, mineral recovery, ion-exchange resins, adhesives, acid dye receptivity; retention aid for paper manufacturing; food-contact paper paperboard (Parchem, 2020b)	Y	N
54076-97-0	Cationic polymer	Organic	no agricultural uses found		Y	N

CASRN	Chemical Name	Organic / Inorganic / Radionuclide	Agricultural Use or Link	Other General Uses	Is Additive?	Is Naturally Occurring?
681331-04-4	Causticized Lignite	Organic	fertilizer precursor (Chatterjee, 2002)		Y	N
108-90-7	Chlorobenzene	Organic	historically registered as CA pesticide ingredient (CDPR, 2019); pesticide (PubChem); Inert ingredients used pre-harvest, not for use after edible parts of plant begin to form, food and non-food use (USEPA, 2019c)	primary uses of chlorobenzene are as a solvent for pesticide formulations, diisocyanate manufacture, and degreasing automobile parts and for the production of nitrochlorobenzene (PubChem)	N	Y
218-01-9	Chrysene	Organic	no agricultural uses found	PAHs from fires and diesel & gasoline exhaust; research chemical (PubChem)	N	Y
64743-05-1	Coke (petroleum), calcined	Organic	no agricultural uses found	used to make anodes for the aluminum, steel and titanium smelting industry (Oxbow, 2015)	Y	N
25987-30-8	Copolymer of acrylamide and sodium acrylate	Organic	historically registered as CA pesticide ingredient (CDPR, 2019); inert ingredient in pesticide (USEPA, 2004); sodium polyacrylate is added to potted plants and soils for moisture retention (Gilani, 2017)	sodium polyacrylate absorbs water molecules, making it ideal for use in diapers and female hygiene products; added to gas containers; applied to conductor/shielding of power cables; used in industrial processes to dissolve soaps by absorbing water molecules (Gilani, 2017)	Y	N
68308-87-2	Cottonseed, flour	Organic	no agricultural uses found	cosmetic ingredient for skin conditioner (The Good Scents Company, 2018)	Y	N
129828-31-5	Crosslinked polyol ester	Organic	no agricultural uses found		Y	N
53-70-3	Dibenzo(a,h)anthracene	Organic	no agricultural uses found	PAHs from fires and gasoline exhaust; research chemical (PubChem)	N	Y
2673-22-5	Diester of sulfosuccinic acid sodium salt	Organic	historically registered as CA pesticide ingredient (CDPR, 2019); approved as inert pesticide ingredient, non-food use (USEPA, 2019c)	fluid property modulator, lubricant, solvent, mfg, paint (PubChem)	Y	N

CASRN	Chemical Name	Organic / Inorganic / Radionuclide	Agricultural Use or Link	Other General Uses	Is Additive?	Is Naturally Occurring?
38011-25-5	Disodium ethylenediaminetetraacetate	Organic	no agricultural uses found	EDTA: Added to food as preservative, stabilizer, sequestrant (PubChem)	Y	N
64742-53-6	Distillates, hydrotreated light naphthenic	Organic	mineral base oil in agricultural spray oils (Beattie, 2002)	lubricants and greases, adhesives and sealants, polishes and waxes, anti-freeze products and coating products (ECHA, 2020)	Y	N
No CASRN	Drilling paper	Organic	no agricultural uses found		Y	N
126-97-6	Ethanolamine thioglycolate	Organic	no agricultural uses found	fuel, personal care, process regulator (PubChem); reducing agent; depilatories; hair straightening and waving agents (The Good Scents Company, 2018)	Y	N
26027-38-3	Ethoxylated 4- nonphenol	Organic	actively registered as CA agricultural pesticide ingredient (CDPR, 2019); formerly used in pesticide (PubChem); approved as inert ingredients used pre- and post-harvest pesticide (surfactant), food and non-food use (USEPA, 2019c)	surfactant, adhesive/sealant, lubricant, processing aid, solvent, automotive products, cleaning products (PubChem); nonoxynols, as a class, are used as detergents, emulsifiers, wetting agents, defoaming agents, etc. (NLM, 2020)	Y	N
61791-26-2	Ethoxylated amine	Organic	actively registered as CA adjuvant pesticide ingredient (CDPR, 2019); approved as inert ingredients used pre-harvest pesticides (surfactant), food and non-food use (USEPA, 2019c)	non-ionic surfactants; used in textile industry as emulsifiers, dispersants, lubricants, and antistats; used in toilet bowl cleaners and hard surface cleaners; used in detergents; antistats in conditioners and shampoo (Gunstone et al, 2001).	Y	N
9081-83-8	Ethoxylated octylphenol	Organic	no agricultural uses found	non-ionic surfactant used in wide array of products like latex paints, adhesives, paper coatings, and textile applications (DeWolf, 2019).	Y	N

CASRN	Chemical Name	Organic / Inorganic / Radionuclide	Agricultural Use or Link	Other General Uses	Is Additive?	Is Naturally Occurring?
5877-42-9	Ethyl octynol	Organic	no agricultural uses found	industrial acid corrosion inhibitor and anti-scaling agent (PubChem)	Y	N
206-44-0	Fluoranthene	Organic	pesticide (PubChem)	adhesive and sealants, PAHs from exhaust (PubChem)	N	Y
63428-92-2	Formaldehyde, polymer with 2-methyloxirane, 4-nonylphenol and oxirane	Organic	no agricultural uses found		Y	N
30704-64-4	Formaldehyde, polymer with 4-(1,1-dimethylethyl)phenol, 2-methyloxirane and oxirane	Organic	historical inert pesticide ingredient (USEPA, 2004)		Y	N
30846-35-6	Formaldehyde, polymer with 4-nonylphenol and oxirane	Organic	historically registered as CA pesticide ingredient (CDPR, 2019); approved as inert pesticide ingredient, non-food use (USEPA, 2019cs)		Y	N
No CASRN	Heavy catalytic reformed naptha	Organic	no agricultural uses found	used in fuels, air care products, anti-freeze products, coating products, lubricants and greases, washing/cleaning products, and welding/soldering products (ECHA, Naphtha (petroleum), heavy catalytic reformed)	Y	N
1415-93-6	Humic acids	Organic	actively registered as CA pesticide ingredient (CDPR, 2019); naturally occurring in soil (Weber et al, 2018)		Y	N
61790-59-8	Hydrogenated tallow amine acetone	Organic	approved as inert ingredients used pre- and post-harvest pesticides (surfactant), food and non-food use (USEPA, 2019c)	flotation agent; bactericide; emulsifier; anticaking agent; soil stabilizer; flocculant; corrosion inhibitor; industrial detergent (Ash, 2004)	Y	N

CASRN	Chemical Name	Organic / Inorganic / Radionuclide	Agricultural Use or Link	Other General Uses	Is Additive?	Is Naturally Occurring?
2809-21-4	Hydroxyethylidenediphosphonic acid	Organic	historically registered as CA pesticide ingredient (CDPR, 2019); animal medication, agricultural application (PubChem), approved as inert ingredients used pre- and post-harvest in pesticide, food and non-food use (USEPA, 2019c)	water treatment, detergent, lubricant & greases, corrosion inhibitor & anti-scaling agent, finishing agent, plating agent, solvents, surface active agent, automotive, construction, cleaning, metal, drugs, etc. (PubChem)	Y	N
193-39-5	Indenopyrene	Organic	no agricultural uses found	PAHs from fires and diesel & gasoline exhaust; research chemical (PubChem)	N	Y
119-65-3	Isoquinoline	Organic	used in pesticides (Xu et al. 2014); approved as inert ingredient in pesticides, fragrance use (USEPA, 2019c); naturally occurring – produced by fungi (Everts 2016)	adhesive, drug, food additives, fluid property modulator (PubChem); used as solvents for extraction of terpenes and resins; used in production of paints and dyes (World of Chemicals, 2020)	Y	N
68648-89-5	Kraton G1702H	Organic	approved as inert pesticide ingredient, non-food use (USEPA, 2019c)	lubricant and greases (PubChem)	Y	N
129521-66-0	Lignite	Organic	no agricultural uses found	coal	Y	N
PE-M2464	Methyl oxirane polymer	Organic	no agricultural uses found		Y	N
No CASRN	Nonylphenol ethoxylates	Organic	historically used as an active ingredient in pesticide (PubChem); lawn care products (USEPA, 2016c)	surfactant; additive to metal cleaners as dispersing agent (PubChem)non-ionic surfactants; industrial processes; consumer laundry detergent, personal hygiene, automotive, latex paints (USEPA, 2016c)	Y	N
127087-87-0	Nonylphenol polyethylene glycol ether	Organic	actively registered as CA agricultural pesticide ingredient, use otherwise not specified (CDPR, 2019); fungicide (PubChem); approved as inert ingredients used pre- and post-harvest pesticide(surfactant), food and non-food use (USEPA, 2019c)	surface-active agent (PubChem)	Y	N

CASRN	Chemical Name	Organic / Inorganic / Radionuclide	Agricultural Use or Link	Other General Uses	Is Additive?	Is Naturally Occurring?
No CASRN	Organic acid ethoxylated alcohols	Organic	alcohol ethoxylates, as a class, are used as non-ionic surfactants in agrochemicals (HERA, 2009)	alcohol ethoxylates, as a class, are non-ionic surfactants used in detergents, household/industrial cleaners, cosmetics, textile, paper, oil and other process industries (HERA, 2009)	Y	N
68412-54-4	Oxyalkylated alkylphenol	Organic	formerly used as pesticide (PubChem); approved as inert ingredients used pre- and post-harvest pesticides (surfactant, fragrance), food, and non-food use (USEPA, 2019c)	adhesives, surfactant, lubricants and greases, solvents, cleaning, automotive (PubChem); alkylphenols, as a class, are used in detergent, fuel and lubricant, polymers, phenolic resin, fragrances, antioxidants, oil field chemicals, and fire retardants (Zhu and Zuo, 2013)	Y	N
68171-44-8	Oxyalkylated alkylphenolic resin	Organic	no agricultural uses found		Y	N
67939-72-4	Oxyalkylated polyamine	Organic	no agricultural uses found	alkyl polyamines, as a class, occur naturally, but synthetic polyamines are often used for therapeutic purposes (Woster, 2006)	Y	N
68910-19-0	Oxyalkylated polyamine	Organic	no agricultural uses found	alkyl polyamines, as a class, occur naturally, but synthetic polyamines are often used for therapeutic purposes (Woster, 2006)	Y	N
85-01-8	Phenanthrene	Organic	no agricultural uses found	dyestuffs, explosives, synthesis of drugs, biochemical research, adhesives and seals; byproduct of petroleum combustion (PubChem)	N	Y
68123-18-2	Phenol, 4,4'-(1-methylethylidene) bis-, polymer with 2-(chloromethyl)oxirane, 2-methyloxirane and oxirane	Organic	no agricultural uses found		Y	N

CASRN	Chemical Name	Organic / Inorganic / Radionuclide	Agricultural Use or Link	Other General Uses	Is Additive?	Is Naturally Occurring?
68425-75-2	Phosphate ester salt	Organic	inert ingredient (surfactant) in pesticide formulation (CASRN residue specified under 40 CFR § 180.910)		Y	N
9005-70-3	POE (20) Sorbitan Trioleate	Organic	actively registered as CA adjuvant agricultural pesticide ingredient (CDPR, 2019); approved as inert ingredients used pre- and post-harvest pesticides (surfactant), food, and non-food use (USEPA, 2019c)	polysorbates are a class of emulsifiers used in pharmaceuticals, cosmetics, and food preparation (Venus Ethoxyethers, 2020).	Y	N
68938-70-5	Poly (triethanolamine.mce)	Organic	no agricultural uses found		Y	N
68955-69-1	Polyamine salts	Organic	no agricultural uses found		Y	N
19019-43-3	Polycarboxlate salt [Trisodium ethylenediaminetetraacetate]	Organic	no agricultural uses found	EDTA trisodium salt: food additive (PubChem)	Y	N
26062-79-3	Polydimethyl diallyl ammonium chloride	Organic	historically registered as CA pesticide ingredient (CDPR, 2019); approved for use as inert pesticide ingredient (food-contact surface sanitizing solutions, food and non-food use (USEPA, 2019c)	disinfectant; cleaning product; solids separation agents; water treatment; used in the synthesis of water soluble polymers; used in cosmetics and personal care products (PubChem)	Y	N
74-84-0	Polyethylene	Organic	no agricultural uses found	ethane used as feedstock for chemical manufacturing (PubChem)	Y	N
68036-92-0	Polyglycol diepoxide	Organic	no agricultural uses found		Y	N
68036-95-3	Polyglycol diepoxide	Organic	no agricultural uses found		Y	N
9038-95-3	Polyglycol ether	Organic	historically registered as CA pesticide ingredient (CDPR, 2019); approved for use as inert pesticide ingredient, food and non-food use (USEPA, 2019c)	lubricant and grease, household products (PubChem)	Y	N

CASRN	Chemical Name	Organic / Inorganic / Radionuclide	Agricultural Use or Link	Other General Uses	Is Additive?	Is Naturally Occurring?
No CASRN	Polyhydroxyalkanoates (PHA)	Organic	naturally-occurring, produced by microorganisms (Ten et al, 2015)	biodegradable matrix for natural fiber-reinforced biocomposites; used in packaging materials, disposable items, automotive parts, and medical devices (Ten et al, 2015)	N	Y
64741-71-5	Polymers (petroleum) viscous	Organic	no agricultural uses found		Y	N
36484-54-5	Polyoxyalkylene glycol	Organic	no agricultural uses found	epoxy resin used in adhesives, paints, and electricity; used in molding and casting of fiber-reinforced plastic (New Japan Chemical Co., RIKARESIN)	Y	N
61790-86-1	Polyoxyalkylenes	Organic	historically registered as CA pesticide ingredient (CDPR, 2019); approved as inert ingredients used pre- and post-harvest pesticides (surfactant), food and non-food use (USEPA, 2019c)		Y	N
9014-93-1	Polyoxyethylene dinonylphenol	Organic	historically registered as CA pesticide ingredient (CDPR, 2019); approved as inert ingredient in pesticide, food and non-food use, for food use required to be produced by condensation of 1 mole of dinonylphenol (nonyl group is a propylene trimer isomer) with an average of 140-160 moles of ethylene oxide (USEPA, 2019c)	surfactant, emulsifier, lubricant (Parchem, 2020e); used in cosmetics (The Good Scents Company, 2018)	Y	N
12068-19-8	Polyoxyethylene nonyl phenyl ether phosphate	Organic	no agricultural uses found		Y	N
70142-34-6	Polyoxyl 15 hydroxystearate	Organic	approved as inert ingredient in pesticide with minimum number average molecular weight (in amu), 3,690, food and non-food use (USEPA, 2019c)	USEPA Safer Chemical Class: green circle classification, which means the chemical has been verified to be of low concern (PubChem)	Y	N

CASRN	Chemical Name	Organic / Inorganic / Radionuclide	Agricultural Use or Link	Other General Uses	Is Additive?	Is Naturally Occurring?
42751-79-1	Polyquaternary amine	Organic	no agricultural uses found	household product in landscape/yard; clarifier (PubChem); generally, quaternary ammonium salts used as disinfectants, surfactants, fabric softeners, and as antistatic agents (e.g. shampoos) (CAMEO Chemicals, nd)	Y	N
129-00-0	Pyrene	Organic	no agricultural uses found	adhesive and sealants, PAHs from exhaust (PubChem)	N	Y
61790-41-8	Quaternary ammonium compound	Organic	approved as inert ingredients used pre-harvest (surfactant) in pesticide, food and non-food use (USEPA, 2019c)	cosmetics & personal care, formulation (ECHA); anti-microbial, disinfectant, cleaning products (Gerba, 2015)	Y	N
68609-18-7	Quaternized condensed alkanolamines	Organic	no agricultural uses found		Y	N
91-63-4	Quinaldine	Organic	no agricultural uses found	used to make dyes, pharmaceuticals, and other chemicals; used as corrosion inhibitors and anti-scaling agents (PubChem)	Y	N
12179-04-3	Sodium tetraborate pentahydrate	Organic	actively registered as CA pesticide ingredient (CDPR, 2019); fungicide, pesticide, herbicide (PubChem)	preservative, antiseptic; manufacturing; cleaning products; soldering additive to fiberglass, weatherproofing wood and fireproofing fabrics (PubChem)	Y	N
64742-95-6	Solvent naphtha, petroleum, light arom.	Organic	historically registered as CA pesticide ingredient (CDPR, 2019); approved as inert ingredients used pre- and post-harvest pesticides (solvent and coating agent), food and non-food use (USEPA, 2019c)	solvent used in industrial applications such as fuel additives, paints and coatings, pesticides, industrial cleaning, mastics and sealants, and process fluids (The Good Scent Company, 2018)	Y	N

CASRN	Chemical Name	Organic / Inorganic / Radionuclide	Agricultural Use or Link	Other General Uses	Is Additive?	Is Naturally Occurring?
NP-SMO3_U1240	Sorbitan ester	Organic	no agricultural uses found	sorbitan esters (aka Spans) are nonionic surfactants used as emulsifying agents in the preparation of emulsions, creams, and ointments for pharmaceutical and cosmetic use; also used as emulsifiers and stabilizers in food (Ankit Polymers Industries, Sorbitan Esters)	Y	N
No CASRN	Steranes or cyclopentanoperhydrophenanthrene	Organic	naturally occurring (Summons Lab, nd)	biomarkers; core structure of steroids (Summons Lab, nd)	N	Y
8052-41-3	Stoddard Solvents	Organic	no agricultural uses found	used as paint thinner; in toners, inks, and adhesives; dry cleaning solvent; general cleaner and degreaser (ATSDR, 1995b); anti-freeze and de-icing products; lubricant and greases; water treatment products (PubChem)	Y	N
68140-11-4	Tall oil, DETA/ midazoline acetates	Organic	no agricultural uses found		Y	N
72480-70-7	Tar bases, quinoline derivatives, quaternized benzyl chloride	Organic	no agricultural uses found		Y	N
64-02-8	Tetrasodium ethylenediaminetetraacetate	Organic	actively registered as CA pesticide ingredient (CDPR, 2019)	tetrasodium EDTA: general purpose chelating agent; sanitizer; stabilizer; sequestrant (PubChem)	Y	N
68527-49-1	Thiourea, polymer with formaldehyde and 1-phenylethanone	Organic	no agricultural uses found		Y	N
64114-46-1	Triethanolamine homopolymer	Organic	former use as inert pesticide ingredient (PubChem)	chelating agent, intermediate, personal care products, adhesives, medication, flame retardant finish, etc. (PubChem)	Y	N
13983-27-2	Krypton-85	Radionuclide	no agricultural uses found	used in arc discharge lamps (Harvey et al., 2010); for the assessment of cerebral blood flow (Raichle, 1998)	Y	N

CASRN	Chemical Name	Organic / Inorganic / Radionuclide	Agricultural Use or Link	Other General Uses	Is Additive?	Is Naturally Occurring?
7440-14-4	Radium-226	Radionuclide	no agricultural uses found	used as a radiation source for various processes (PubChem)	N	Y
15262-20-1	Radium-228	Radionuclide	no agricultural uses found		N	Y
7440-29-1	Thorium-232	Radionuclide	no agricultural uses found	used in ceramic and welding electrodes (PubChem)	N	Y
7440-61-1	Uranium	Radionuclide	present in soil (ATSDR, 2013)	commercial nuclear power, ceramic fuel pellets; depleted U used in armor-piercing military ammunition, inertial guidance devices, x-ray targets (ATSDR, 2013)	N	Y
14932-42-4	Xenon-133	Radionuclide	no agricultural uses found	used for the evaluation of pulmonary function, for imaging the lungs, and applied to assessment of cerebral flow (PubChem)	Y	N

Table 4: Produced water suppliers, water discharge requirements, and identified beneficial uses of those waters

Entity/Order No.	Beneficial Uses
Chevron USA, Inc., and Cawelo Water District/WDRs Order R5-2012-0058	Municipal and domestic supply (MUN), AGR, industrial process supply (PRO), and industrial service supply (IND)
California Resources Production Corporation and Cawelo Water District/WDRs Order R5-2012-0058	MUN, AGR, PRO, IND
Hathaway, LLC; Kern-Tulare Water District; and Jasmin Ranchos Mutual Water Company/WDRs Order R5-2019-0043	MUN, AGR, PRO, IND, and water contact recreation (REC-1)
California Resources Production Corporation and North Kern Water Storage District/WDRs Order R5-2015-0127	MUN, AGR, PRO, IND

Table 5: Water quality objectives (WQOs) of the Chemicals of Interest that were monitored in treated produced water and blended produced water

CASRN	Chemical Analyte	Organic / Inorganic / Radionuclide	Screening Value	Units	Screening Value Type[1]
7440-36-0	Antimony	Inorganic	0.006	mg/L	MCL
7440-38-2	Arsenic	Inorganic	0.01	mg/L	MCL
7440-39-3	Barium	Inorganic	1	mg/L	MCL
7440-41-7	Beryllium	Inorganic	0.004	mg/L	MCL
7440-42-8	Boron	Inorganic	---	---	NA
7440-42-8	Boron [annual average]	Inorganic	1	mg/L	WQO
7440-43-9	Cadmium	Inorganic	0.005	mg/L	MCL
7440-47-3	Chromium (total)	Inorganic	0.05	mg/L	MCL
18540-29-9	Chromium (VI)	Inorganic	0.01	mg/L	MCL
7440-48-4	Cobalt	Inorganic	0.012	mg/L	Toxicity
7440-50-8	Copper	Inorganic	1.3	mg/L	MCL
16984-48-8	Fluoride	Inorganic	2	mg/L	MCL
20461-54-5	Iodide	Inorganic	0.38	mg/L	Toxicity
7439-92-1	Lead	Inorganic	0.015	mg/L	MCL
7439-93-2	Lithium	Inorganic	0.077	mg/L	Toxicity
7439-96-5	Manganese	Inorganic	3.8	mg/L	Toxicity
7439-97-6	Mercury (total, including organic compounds)	Inorganic	0.002	mg/L	MCL
7439-98-7	Molybdenum	Inorganic	0.19	mg/L	Toxicity
7440-02-0	Nickel	Inorganic	0.1	mg/L	MCL
14797-65-0	Nitrite	Inorganic	1	mg/L	MCL
7782-49-2	Selenium	Inorganic	0.05	mg/L	MCL
7440-22-4	Silver	Inorganic	0.19	mg/L	Toxicity
7440-24-6	Strontium	Inorganic	23.1	mg/L	Toxicity
7440-31-5	Tin	Inorganic	11.5	mg/L	Toxicity
7440-62-2	Vanadium	Inorganic	0.38	mg/L	Toxicity
7440-66-6	Zinc	Inorganic	11.5	mg/L	Toxicity
123-91-1	1,4-Dioxane	Organic	0.0055	mg/L	Toxicity
134-32-7	2-Naphthylamine	Organic	0.00031	mg/L	Toxicity
83-32-9	Acenaphthene	Organic	2.3	mg/L	Toxicity
79-06-1	Acrylamide	Organic	0.00011	mg/L	Toxicity
62-53-3	Aniline	Organic	---	---	NA
120-12-7	Anthracene	Organic	11.5	mg/L	Toxicity
56-55-3	Benz(a)anthracene	Organic	0.00044	mg/L	Toxicity
50-32-8	Benzo(a)pyrene	Organic	0.2	mg/L	MCL
205-99-2	Benzo(b)fluoranthene	Organic	0.00044	mg/L	Toxicity
111-44-4	Bis(2-chloroethyl) ether	Organic	0.00022	mg/L	Toxicity
108-90-7	Chlorobenzene	Organic	0.07	mg/L	MCL
218-01-9	Chrysene	Organic	0.0044	mg/L	Toxicity
53-70-3	Dibenz(a,h)anthracene	Organic	0.00011	mg/L	Toxicity
206-44-0	Fluoranthene	Organic	1.5	mg/L	Toxicity

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[1] MCL – Maximum Contaminant Level; Toxicity – Screening value estimated from toxicity value identified in Task 1 report; WQO – Water Quality Objective; NA – Screening value was not available

CASRN	**Chemical Analyte**	**Organic / Inorganic / Radionuclide**	**Screening Value**	**Units**	**Screening Value Type[1]**
193-39-5	Indeno(1,2,3-c,d)pyrene	Organic	0.00044	mg/L	Toxicity
85-01-8	Phenanthrene	Organic	---	---	NA
129-00-0	Pyrene	Organic	1.2	mg/L	Toxicity
8052-41-3	Stoddard Solvent	Organic	---	---	NA
13983-27-2	Krypton 85	Radionuclide	---	---	NA
---	Radioactivity, Gross Alpha	Radionuclide	15	pCi/L	MCL
---	Radioactivity, Gross Beta	Radionuclide	50	pCi/L	MCL
7440-14-4	Radium-226	Radionuclide	---	---	NA
7440-14-4	Radium-226 plus Radium-228	Radionuclide	5	pCi/L	MCL
15262-20-1	Radium-228	Radionuclide	---	---	NA
7440-61-1	Uranium	Radionuclide	20	pCi/L	MCL

Table 6: Sampling locations of treated produced water and blended produced water used for agricultural irrigation in the Central Valley of California

Water Type	Sample Location
Treated Produced Water	27/26 4L
Treated Produced Water	28/26 4H
Treated Produced Water	Beardsley Canal
Treated Produced Water	Carrier Canal
Treated Produced Water	Kern Front No. 2 Treatment Facility
Treated Produced Water	Kern River Station 36 Facility
Treated Produced Water	Quinn Treatment Facility
Treated Produced Water	Section 23 Treatment Facility
Treated Produced Water	Discharge to Poso Creek
Blended Irrigation Water	26/26 27L2
Blended Irrigation Water	Jasmin Ranchos Mutual Water Company Reservoir
Blended Irrigation Water	Lerdo Canal
Blended Irrigation Water	Kern Tulare Water District Big Four Reservoir
Blended Irrigation Water	Outfall from Reservoir B
Blended Irrigation Water	Jasmin Ranchos Mutual Water Company Reservoir
Blended Irrigation Water	Kern-Tulare Water District Big Four Reservoir

Table 7: Water quality data for treated produced water and frequency of samples exceeding Water Quality Objectives

CASRN	Chemical Analyte	Screening Value Type	Total Number of Samples	Frequency of Detection	Minimum of Detected [mg/L]	Mean of Detected [mg/L]	Maximum of Detected [mg/L]	Fraction of Samples Exceeding Water Quality Objective Concentration Limit
7440-36-0	Antimony	MCL	61	0.44	0.00011	0.0027	0.006	0
7440-38-2	Arsenic	MCL	159	0.89	0.0001	0.037	0.091	0.75
7440-39-3	Barium	MCL	79	0.67	0.0021	0.053	0.12	0
7440-41-7	Beryllium	MCL	71	0.03	0.000081	0.000087	0.000092	0
7440-42-8	Boron [individual samples]	WQO	337	1	0.032	0.84	2.2	0.16
7440-42-8	Boron [annual average]	WQO	66	1	0.1	0.86	2.2	0.24
7440-43-9	Cadmium	MCL	72	0	ND	ND	ND	ND
18540-29-9	Chromium (VI)	MCL	37	0.19	0.000034	0.0016	0.0086	0
7440-48-4	Cobalt	NA	60	0.05	0.00011	0.00013	0.00017	NA
7440-50-8	Copper	MCL	63	0.4	0.00011	0.0016	0.0045	0
16984-48-8	Fluoride	MCL	38	0.79	0.41	1	2.4	0.03
20461-54-5	Iodide	NA	7	0.14	0.21	0.21	0.21	NA
7439-92-1	Lead	MCL	74	0.05	0.000073	0.00021	0.00054	0
7439-93-2	Lithium	NA	55	0.67	0.015	0.05	0.074	NA
7439-96-5	Manganese	NA	107	0.88	0.0026	1.9	87	NA
7439-97-6	Mercury (total, including organic compounds)	MCL	63	0.3	0.0000007	0.00016	0.00033	0
7439-98-7	Molybdenum	NA	63	0.65	0.00028	0.0069	0.015	NA
7440-02-0	Nickel	MCL	74	0.46	0.0003	0.00091	0.0026	0
14797-65-0	Nitrite	MCL	6	0.17	1	1	1	0
7782-49-2	Selenium	MCL	67	0.31	0.0003	0.00089	0.0028	0
7440-22-4	Silver	NA	66	0	ND	ND	ND	NA

CASRN	Chemical Analyte	Screening Value Type	Total Number of Samples	Frequency of Detection	Minimum of Detected [mg/L]	Mean of Detected [mg/L]	Maximum of Detected [mg/L]	Fraction of Samples Exceeding Water Quality Objective Concentration Limit
7440-24-6	Strontium	NA	66	0.85	0.079	0.18	0.91	NA
7440-31-5	Tin	NA	11	0	ND	ND	ND	NA
7440-62-2	Vanadium	NA	53	0.06	0.0011	0.002	0.0027	NA
7440-66-6	Zinc	NA	67	0.48	0.0018	0.0097	0.036	NA
123-91-1	1,4-Dioxane	NA	11	0.55	0.00058	0.0013	0.004	NA
134-32-7	2-Naphthylamine	NA	12	0	ND	ND	ND	NA
83-32-9	Acenaphthene	NA	80	0.35	0.000031	0.00058	0.00091	NA
79-06-1	Acrylamide	NA	7	0	ND	ND	ND	NA
62-53-3	Aniline	NA	23	0	ND	ND	ND	NA
120-12-7	Anthracene	NA	78	0.03	0.00004	0.00012	0.00019	NA
56-55-3	Benz(a)anthracene	NA	78	0.01	0.000031	0.000031	0.000031	NA
50-32-8	Benzo(a)pyrene	MCL	78	0	ND	ND	ND	ND
205-99-2	Benzo(b)fluoranthene	NA	78	0.04	0.000032	0.000056	0.00008	NA
111-44-4	Bis(2-chloroethyl) ether	NA	29	0	ND	ND	ND	NA
108-90-7	Chlorobenzene	MCL	90	0	ND	ND	ND	ND
218-01-9	Chrysene	NA	79	0.1	0.000032	0.0001	0.00021	NA
53-70-3	Dibenz(a,h)anthracene	NA	74	0	ND	ND	ND	NA
206-44-0	Fluoranthene	NA	78	0.05	0.00003	0.00006	0.00008	NA
193-39-5	Indeno(1,2,3-c,d)pyrene	NA	78	0	ND	ND	ND	NA
85-01-8	Phenanthrene	NA	76	0.33	0.000038	0.00053	0.0012	NA
129-00-0	Pyrene	NA	78	0.1	0.000037	0.00012	0.0002	NA
8052-41-3	Stoddard Solvent	NA	1	1	0.06	0.06	0.06	NA

CASRN	Chemical Analyte	Screening Value Type	Total Number of Samples	Frequency of Detection	Minimum of Detected [mg/L]	Mean of Detected [mg/L]	Maximum of Detected [mg/L]	Fraction of Samples Exceeding Water Quality Objective Concentration Limit
13983-27-2	Krypton 85[1]	NA	7	0	ND	ND	ND	NA
---	Radioactivity, Gross Alpha	MCL	36	0.62	0.12	3.2	12	0
---	Radioactivity, Gross Beta	MCL	19	0.84	3.1	4.8	7.3	0
---	Radium-226 plus Radium-228 (calculated by lab)	MCL	7	0.86	0.43	1.4	2.4	0
---	Radium-226 plus Radium-228 (calculated from individual measurements)	MCL	38	0.92	0.23	1.6	9.6	0.03
7440-14-4	Radium-226	NA	36	0.72	0.09	0.66	1.6	NA
15262-20-1	Radium-228	NA	37	0.7	0.007	1.4	9	NA
7440-61-1	Uranium	MCL	44	0.11	0.41	2.7	6.9	0

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[1] Radionuclides reported in units of pCi/L

Table 8: Water quality data for blended produced water and frequency of samples exceeding the Water Quality Objectives

CASRN	Chemical Analyte	Screening Value Type	Total Number of Samples	Frequency of Detection	Minimum of Detected [mg/L]	Mean of Detected [mg/L]	Maximum of Detected [mg/L]	Fraction of Samples Exceeding Water Quality Objective Concentration Limit
7440-36-0	Antimony	MCL	54	0.44	0.0001	0.0014	0.011	0.019
7440-38-2	Arsenic	MCL	132	0.86	0.0002	0.014	0.065	0.53
7440-39-3	Barium	MCL	61	0.87	0.0043	0.031	0.2	0
7440-41-7	Beryllium	MCL	53	0.04	0.00028	0.003	0.0056	0.019
7440-42-8	Boron [individual samples]	WQO	252	0.97	0.02	0.48	2.2	0.012
7440-42-8	Boron [annual average]	WQO	50	1	0.11	0.55	2.2	0.04
7440-43-9	Cadmium	MCL	54	0.02	0.004	0.004	0.004	0
18540-29-9	Chromium (VI)	MCL	24	0.12	0.000035	0.000055	0.000072	0
7440-48-4	Cobalt	Toxicity	53	0.3	0.000092	0.0013	0.01	0
7440-50-8	Copper	MCL	54	0.74	0.00064	0.0089	0.087	0
16984-48-8	Fluoride	MCL	13	0.69	0.17	0.45	0.91	0
20461-54-5	Iodide	Toxicity	4	0	ND	ND	ND	ND
7439-92-1	Lead	MCL	53	0.47	0.000096	0.00086	0.0044	0
7439-93-2	Lithium	Toxicity	49	0.61	0.0068	0.022	0.053	0
7439-96-5	Manganese	Toxicity	95	0.86	0.003	0.046	0.61	0
7439-97-6	Mercury (total, including organic compounds)	MCL	52	0.13	0.000001	0.000042	0.000095	0
7439-98-7	Molybdenum	Toxicity	54	0.76	0.00038	0.0032	0.012	0
7440-02-0	Nickel	MCL	54	0.67	0.00036	0.002	0.02	0
14797-65-0	Nitrite	MCL	5	0.4	0.8	9.9	19	0.2
7782-49-2	Selenium	MCL	55	0.38	0.00019	0.0011	0.0075	0
7440-22-4	Silver	Toxicity	54	0	ND	ND	ND	ND

CASRN	Chemical Analyte	Screening Value Type	Total Number of Samples	Frequency of Detection	Minimum of Detected [mg/L]	Mean of Detected [mg/L]	Maximum of Detected [mg/L]	Fraction of Samples Exceeding Water Quality Objective Concentration Limit
7440-24-6	Strontium	Toxicity	52	0.87	0.018	0.13	0.46	0
7440-31-5	Tin	Toxicity	1	0	ND	ND	ND	ND
7440-62-2	Vanadium	Toxicity	52	0.46	0.00099	0.0032	0.01	0
7440-66-6	Zinc	Toxicity	55	0.62	0.0018	0.013	0.1	0
123-91-1	1,4-Dioxane	Toxicity	9	0.22	0.00052	0.00075	0.00098	0
134-32-7	2-Naphthylamine	Toxicity	0	NA	NA	NA	NA	NA
83-32-9	Acenaphthene	Toxicity	61	0.15	0.00003	0.00015	0.00061	0
79-06-1	Acrylamide	Toxicity	4	0	ND	ND	ND	ND
62-53-3	Aniline	NA	10	0	ND	ND	ND	NA
120-12-7	Anthracene	Toxicity	60	0	ND	ND	ND	ND
56-55-3	Benz(a)anthracene	Toxicity	60	0.02	0.00003	0.00003	0.00003	0
50-32-8	Benzo(a)pyrene	MCL	60	0	ND	ND	ND	ND
205-99-2	Benzo(b)fluoranthene	Toxicity	60	0.02	0.00011	0.00011	0.00011	0
111-44-4	Bis(2-chloroethyl) ether	Toxicity	12	0	ND	ND	ND	ND
108-90-7	Chlorobenzene	MCL	69	0	ND	ND	ND	ND
218-01-9	Chrysene	Toxicity	60	0.03	0.000039	0.000041	0.000042	0
53-70-3	Dibenz(a,h)anthracene	Toxicity	59	0	ND	ND	ND	ND
206-44-0	Fluoranthene	Toxicity	74	0	ND	ND	ND	ND
193-39-5	Indeno(1,2,3-c,d)pyrene	Toxicity	61	0.02	0.000091	0.000091	0.000091	0
85-01-8	Phenanthrene	NA	60	0.18	0.000029	0.00011	0.00029	NA
129-00-0	Pyrene	Toxicity	60	0.02	0.00004	0.00004	0.00004	0
8052-41-3	Stoddard Solvent	NA	1	1	0.025	0.025	0.025	NA

CASRN	Chemical Analyte	Screening Value Type	Total Number of Samples	Frequency of Detection	Minimum of Detected [mg/L]	Mean of Detected [mg/L]	Maximum of Detected [mg/L]	Fraction of Samples Exceeding Water Quality Objective Concentration Limit
13983-27-2	Krypton 85[1]	NA	4	0	ND	ND	ND	NA
---	Radioactivity, Gross Alpha	MCL	32	0.69	0.2	3.3	20	0.031
---	Radioactivity, Gross Beta	MCL	11	0.91	0.89	3.3	7.3	0
---	Radium-226 plus Radium-228 (calculated by lab)	MCL	3	1	0.63	1.1	1.5	0
---	Radium-226 plus Radium-228 (calculated from individual measurements)	MCL	30	0.83	0.32	1.8	9.4	0.033
7440-14-4	Radium-2261	NA	30	0.73	0.12	1.2	9.2	NA
15262-20-1	Radium-2281	NA	30	0.63	0.12	1	4.7	NA
7440-61-1	Uranium1	MCL	41	0.54	0.0001	0.64	8.6	0

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[1] Radionuclides reported in units of pCi/L

Table 9: Comparison of blended produced water and treated produced water

CASRN	Chemical Analyte	Organic / Inorganic / Radionuclide	Frequency of Detection -Treated Produced Water	Frequency of Detection -Blended Produced Water	Frequency of Detection Ratio (Treated Produced / Conventional)[1]	Mean of Detected Concentration [mg/L] - Treated Produced Water[2]	Mean of Detected Concentrations [mg/L] - Blended Produced Water[28]	Mean Detected Concentrations Ratio (Treated Produced Water/ Blended Produced Water)
7440-36-0	Antimony	Inorganic	0.44	0.44	1.00	2.66E-03	1.36E-03	1.96
7440-38-2	Arsenic	Inorganic	0.89	0.86	1.03	3.69E-02	1.39E-02	2.67
7440-39-3	Barium	Inorganic	0.67	0.87	0.77	5.32E-02	3.12E-02	1.70
7440-41-7	Beryllium	Inorganic	0.03	0.04	0.75	8.65E-05	2.94E-03	0.03
7440-42-8	Boron [individual samples]	Inorganic	1	0.97	1.03	8.44E-01	4.79E-01	1.76
7440-42-8	Boron [annual average]	Inorganic	1	1	1.00	8.64E-01	5.47E-01	1.58
7440-43-9	Cadmium	Inorganic	0	0.02	0.00	ND	4.00E-03	ND in TPW
18540-29-9	Chromium (VI)	Inorganic	0.19	0.12	1.58	1.58E-03	5.50E-05	28.64
7440-48-4	Cobalt	Inorganic	0.05	0.3	0.17	1.33E-04	1.26E-03	0.11
7440-50-8	Copper	Inorganic	0.4	0.74	0.54	1.61E-03	8.93E-03	0.18
16984-48-8	Fluoride	Inorganic	0.79	0.69	1.14	1.02E+00	4.52E-01	2.25
20461-54-5	Iodide	Inorganic	0.14	0	ND in BIW	2.10E-01	ND	ND in BIW
7439-92-1	Lead	Inorganic	0.05	0.47	0.11	2.13E-04	8.62E-04	0.25
7439-93-2	Lithium	Inorganic	0.67	0.61	1.10	4.98E-02	2.17E-02	2.29
7439-96-5	Manganese	Inorganic	0.88	0.86	1.02	1.92E+00	4.58E-02	41.84
7439-97-6	Mercury (total, including organic compounds)	Inorganic	0.3	0.13	2.31	1.62E-04	4.19E-05	3.87
7439-98-7	Molybdenum	Inorganic	0.65	0.76	0.86	6.91E-03	3.24E-03	2.13

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[1] ND – Non-detect; ND in BIW – Non-detect in blended produced water; ND in TPW – Non-detect in treated produced water

[2] Radionuclides reported in units of pCi/L

CASRN	Chemical Analyte	Organic / Inorganic / Radionuclide	Frequency of Detection -Treated Produced Water	Frequency of Detection -Blended Produced Water	Frequency of Detection Ratio (Treated Produced / Conventional)[1]	Mean of Detected Concentration [mg/L] - Treated Produced Water[2]	Mean of Detected Concentrations [mg/L] - Blended Produced Water[28]	Mean Detected Concentrations Ratio (Treated Produced Water/ Blended Produced Water)
7440-02-0	Nickel	Inorganic	0.46	0.67	0.69	9.07E-04	2.07E-03	0.44
14797-65-0	Nitrite	Inorganic	0.17	0.4	0.43	1.00E+00	9.90E+00	0.10
7782-49-2	Selenium	Inorganic	0.31	0.38	0.82	8.94E-04	1.11E-03	0.81
7440-22-4	Silver	Inorganic	0	0	ND	ND	ND	ND
7440-31-5	Tin	Inorganic	0	0	ND	ND	ND	ND
7440-62-2	Vanadium	Inorganic	0.06	0.46	0.13	1.97E-03	3.25E-03	0.61
7440-66-6	Zinc	Inorganic	0.48	0.62	0.77	9.68E-03	1.34E-02	0.72
123-91-1	1,4-Dioxane	Organic	0.55	0.22	2.50	1.30E-03	7.50E-04	1.73
134-32-7	2-Naphthylamine	Organic	0	NA	ND in TPW	ND	not measured	ND in TPW
83-32-9	Acenaphthene	Organic	0.35	0.15	2.33	5.79E-04	1.49E-04	3.89
79-06-1	Acrylamide	Organic	0	0	ND	ND	ND	ND
62-53-3	Aniline	Organic	0	0	ND	ND	ND	ND
120-12-7	Anthracene	Organic	0.03	0	ND in BIW	1.15E-04	ND	ND in BIW
56-55-3	Benz(a)anthracene	Organic	0.01	0.02	0.50	3.10E-05	3.00E-05	1.03
50-32-8	Benzo(a)pyrene	Organic	0	0	ND	ND	ND	ND
205-99-2	Benzo(b)fluoranthene	Organic	0.04	0.02	2.00	5.63E-05	1.10E-04	0.51
111-44-4	Bis(2-chloroethyl) ether	Organic	0	0	ND	ND	ND	ND
108-90-7	Chlorobenzene	Organic	0	0	ND	ND	ND	ND
218-01-9	Chrysene	Organic	0.1	0.03	3.33	1.07E-04	4.05E-05	2.65
53-70-3	Dibenz(a,h)anthracene	Organic	0	0	ND	ND	ND	ND

CASRN	**Chemical Analyte**	**Organic / Inorganic / Radionuclide**	**Frequency of Detection -Treated Produced Water**	**Frequency of Detection -Blended Produced Water**	**Frequency of Detection Ratio (Treated Produced / Conventional)[1]**	**Mean of Detected Concentration [mg/L] - Treated Produced Water[2]**	**Mean of Detected Concentrations [mg/L] - Blended Produced Water[28]**	**Mean Detected Concentrations Ratio (Treated Produced Water/ Blended Produced Water)**
206-44-0	Fluoranthene	Organic	0.05	0	ND in BIW	6.03E-05	ND	ND in BIW
193-39-5	Indeno(1,2,3-c,d)pyrene	Organic	0	0.02	ND in TPW	ND	9.10E-05	ND in TPW
85-01-8	Phenanthrene	Organic	0.33	0.18	1.83	5.34E-04	1.06E-04	5.02
129-00-0	Pyrene	Organic	0.1	0.02	5.00	1.17E-04	4.00E-05	2.93
8052-41-3	Stoddard Solvent	Organic	1	1	1.00	6.00E-02	2.50E-02	2.40
13983-27-2	Krypton 85	Radionuclide	0	0	ND	ND	ND	ND
---	Radioactivity, Gross Alpha	Radionuclide	0.62	0.69	0.90	3.20E+00	3.30E+00	0.97
---	Radioactivity, Gross Beta	Radionuclide	0.84	0.91	0.92	4.80E+00	3.31E+00	1.45
---	Radium-226 plus Radium-228 (calculated by lab)	Radionuclide	0.86	1	0.86	1.42E+00	1.09E+00	1.30
---	Radium-226 plus Radium-228 (calculated from individual measurements)	Radionuclide	0.92	0.83	1.11	1.57E+00	1.75E+00	0.90
7440-14-4	Radium-226	Radionuclide	0.72	0.73	0.99	6.60E-01	1.20E+00	0.55
15262-20-1	Radium-228	Radionuclide	0.7	0.63	1.11	1.40E+00	1.00E+00	1.40
7440-61-1	Uranium	Radionuclide	0.11	0.54	0.20	2.70E+00	6.38E-01	4.23

Table 10: Concentrations of Chemicals of Interest in soil, air, water and crops

CASRN	Chemical name	Organic / Inorganic / Radionuclide	Soil	Air	Water	Blended Produced Water Quality [Central Valley California]	In Food	Task 3 Food Crop Results (only samples irrigated with blended produced water)
7440-36-0	Antimony	Inorganic	Kern County sample range: 0.45-1.40 mg/kg in benchmark soils (Bradford et al, 1996); US: Sb concentrations ranged <1-8.8 mg/kg (ATSDR, 2019a).	Bakersfield: 2010-2017 annual avg of 2.1 ng/m3 (CARB, 2019); Background levels of Sb in ambient air are ~1 ng/m3, but can be higher in urban areas (ATSDR, 2019a).	Surface Water: Only 70 of 1077 water samples from the USGS Resource Division (1960-1988) detected dissolved Sb above the detection limit of 5 ppb. The geometric mean (standard deviation) of the 70 detected samples was 12 (sd:1.93) ppb (HSDB, 2019).	Reported frequency of detection: 0.44; Mean: 1.36; Range: 0.1 - 11 [µg/L]	Concentration of antimony in food are reported to be <1.0 mg/kg dry weight (ATSDR, 2019a); in the French Total Diet Study nut, fruit, vegetables range 0.0005 - 0.025 mg/kg (Millour et al., 2011); range of mean concentrations of detected Sb in a variety of fruits and vegetables was 0.00005 - 0.0042 mg/kg (Oakes and Shank, 1997)	Detected in garlic and almonds; concentration in treated samples, mean: 0.85 [mg/kg] (range: 0.52 - 1.8)
1309-64-4	Antimony trioxide	Inorganic	na	na	na	see Antimony	na	na
7440-38-2	Arsenic	Inorganic	Kern County sample range: 4.0-6.7 mg/kg in benchmark soils (Bradford et al, 1996).	Bakersfield: 2010-2017 annual avg of 0.99 ng/m3 (CARB, 2019); US: avg ambient air levels range <1-3 ng/m3 in remote areas and 20-30 ng/m3 in urban areas (ATSDR, 2007a).	Surface water: As detected in 1,298/3,342 surface water samples in 2004 USEPA STORET database, with detected samples ranging 0.138-1,700 µg/L (ATSDR, 2007a). In Kaweah and Tule Rivers, reported frequency of detection: 0.84; detected dissolved concentrations of mean: 2.09; range: 0.15 - 29 [µg/L] (CEDEN, 2020). In Kern County municipal groundwater, reported frequency of detection: 1; Mean: 18.02; Range: 0.03 - 278 [µg/L] (GAMA, USGS)	Reported frequency of detection: 0.86; Mean: 13.85; Range: 0.2 - 65 [µg/L]	In a wide variety of foods in the US marketplace. avg. 0.024 mg/kg (range: ND-10.4 mg/kg) (FDA, 2007); arsenic was detected in cucumbers at concentration of 0.0064 mg/kg (Oakes and Shank, 1997)	Detected at trace levels in carrots (both treated and control samples); concentration in treated samples, mean: 0.11 [mg/kg] (range: 0.093 - 0.12)
7727-43-7	Barite	Inorganic	na	na	na	see Barium	na	na

CASRN	Chemical name	Organic / Inorganic / Radionuclide	Soil	Air	Water	Blended Produced Water Quality [Central Valley California]	In Food	Task 3 Food Crop Results (only samples irrigated with blended produced water)
7440-39-3	Barium	Inorganic	Kern County sample range: 493-556 mg/kg in benchmark soils (Bradford et al, 1996).	Bakersfield: 1995-2002 annual avg of 51.0 ng/m3 (CARB, 2019); US: ambient Ba ranged 1.5-950 µg/m3 (ATSDR, 20007).	Occurs naturally in almost all surface water examined, in concentrations of 2-340 µg/L, with an avg of 43 µg/L (HSDB, 2019). In Kern County municipal groundwater, reported frequency of detection: 1; Mean: 48.34; Range: 1.61 - 147 [µg/L] (GAMA, USGS)	Reported frequency of detection: 0.87; Mean: 31.21; Range: 4.3 - 200 [µg/L]	concentration barium in vegetables: avg. 0.43 µg/kg (range: 0.048-2.3 µg/kg) (ATSDR, 2007b); range of mean concentrations of detected Ba in a variety of fruits and vegetables was 0.024 - 1.4 mg/kg (Oakes and Shank, 1997)	Detected in Navel oranges, carrots, Valencia oranges, Mandarin oranges, almond, garlic, pistachios; concentration in treated samples, mean: 1.23 [mg/kg] (range: 0.5 - 4.6)
7440-41-7	Beryllium	Inorganic	Kern County sample range: 0.77-1.75 mg/kg in benchmark soils (Bradford, et al, 1996); avg. US conc. 0.6 mg/kg (Eckel and Langley, 1988)	Bakersfield: 2015-2017 annual avg of 0.15 ng/m3 (CARB, 2019); US: avg daily Be concentrations <0.5 ng/m3 (ATSDR, 2002).	Surface water: ATSDR (2002) reports on a number of studies: generally detected in less than 20% of samples with reported means of 1.9 µg/L, 1.1 µg/L, 20.8 µg/L, 4.4 µg/L; In Kern County municipal groundwater, reported frequency of detection: 0.11; Mean: 0.03; Range: 0.004 - 0.06 [µg/L] (GAMA, USGS)	Reported frequency of detection: 0.04; Mean: 2.94; Range: 0.28 - 5.6 [µg/L]	concentration in food: avg. 0.22 µg/kg (range: <0.1-2200 µg/kg). 2200 µg/kg reported for kidney beans (ATSDR, 2002).	na

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7440-42-8	Boron	Inorganic	Kern County sample range: 19-74 mg/kg in benchmark soils (Bradford et al, 1996); US: geometric mean of 26 mg/kg with a max of 300 mg/kg (ATSDR, 2010).	Air concentrations range <0.5 – 80 ng/m3, with an avg of 20 ng/m3. In general, B does not appear to be present in ambient air at significant concentrations (HSDB, 2019).	Surface water: avg concentrations in surface waters collected composite water from Merced River and Salt Slough, CA in 1988 were 1,520 µg/L (filtered) and 1,730 µg/L (unfiltered) (HSDB, 2019). Avg for US surface water was 0.1 mg/L (ATSDR, 2010). In Kaweah and Tule Rivers, reported frequency of detection: 0.91; detected dissolved concentrations of mean: 0.05; range: 0.0018 - 0.34 [µg/L] (CEDEN, 2020). In Kern County municipal groundwater, reported frequency of detection: 0.97; Mean: 402.66; Range: 8 - 1790 [µg/L] (GAMA, USGS)	Reported frequency of detection: 0.97; Mean: 478.74; Range: 20 - 2200 [µg/L]	concentration in food: range: 46-1222 mg/kg in fresh fruits and vegetables). 2200 µg/kg reported in raisin (ATSDR, 2010).	na

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7440-43-9	Cadmium	Inorganic	Kern County sample range: 0.14-1.70 mg/kg in benchmark soils (Bradford et al, 1996); Cd levels not contaminated by anthropogenic sources range 0.01-2.7 mg/kg (ATSDR, 2012d).	Bakersfield: 2009-2017 annual avg of 0.77 ng/m3 (CARB, 2019); Cd levels in ambient air generally range 0.1-5 ng/m3 in rural areas (ATSDR, 2012d).	Surface water: most unpolluted surface water has Cd <1 ng/g. However, near Cd-bearing minerals, levels may exceed 10 ng/L. Cd levels in normal stream, river, and lake waters ranged <0.01-5.0 µg/L with avg of 0.3 µg/L. Streams and rivers near Cd deposits ranged <0.01 – 1000 µg/L (HSDB, 2019). In Kaweah and Tule Rivers, reported frequency of detection: 0.04; detected dissolved concentrations of mean: 0.23; range: 0.006 - 1.1 [µg/L] (CEDEN, 2020). In Kern County municipal groundwater, reported frequency of detection: 0.46; Mean: 0.06; Range: 0.015 - 0.23 [µg/L] (GAMA, USGS).	Reported frequency of detection: 0.02; Mean: 4; Range: 4 - 4 [µg/L]	In a wide variety of foods in the US marketplace. avg. 0.010 mg/kg (range: ND-0.657 mg/kg) (FDA, 2007); range of mean concentrations of detected Cd in a variety of fruits and vegetables was 0.0000028 - 0.0052 mg/kg (Oakes and Shank, 1997)	Detected in cherries (both treated and controls, at similar concentrations) and only at trace levels in carrots; concentration in treated samples, mean: 0.123 [mg/kg] (range: 0.048 - 0.26)
7440-47-3	Chromium	Inorganic	Kern County sample range: 38-50 mg/kg in benchmark soils (Bradford et al, 1996); US: Cr concentrations range 1-2,000 mg/kg, with a geometric mean of 37 mg/kg (ATSDR, 2012c).	Bakersfield: 2007-2017 annual avg of 4.5 ng/m3 (CARB, 2019); US: total Cr in urban and nonurban areas from 1977-1984 ranged 5-525 ng/m3 (ATSDR, 2012c).	Surface water: US river water usually range <1-30 µg/L, with a median of 10 µg/L. Lake water generally contained <5 µg/L (ATSDR, 2012c). Drinking water typically has less 10 µg/L of Cr (VI) (ATSDR, 2012c). In Kern County municipal groundwater [total chromium], reported frequency of detection: 0.57; Mean: 3.41; Range: 0.41 - 13 [µg/L] (GAMA, USGS)	Cr(VI), reported frequency of detection: 0.12; Mean: 0.06; Range: 0.035 - 0.072 [µg/L]	ranges from 0.020-0.14 mg/kg in fresh fruits and vegetables (ATSDR, 2012c); range of mean concentrations of detected Cr in a variety of fruits and vegetables was 0.0.013 - 0.099 mg/kg (Oakes and Shank, 1997)	Detected at trace levels in carrots (both treated and control samples); concentration in treated samples, mean: 0.265 [mg/kg] (range: 0.22 - 0.31)

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7440-48-4	Cobalt	Inorganic	Kern County sample range: 8-9 mg/kg in benchmark soils (Bradford et al, 1996); Various US soils ranged 3.5– 7.0 mg/kg dry-weight (HSDB, 2019).	Bakersfield: 2007-2017 annual avg of 0.94 ng/m3 (CARB, 2019); Avg Co in unpolluted sites generally <1-2 ng/m3 (ATSDR, 2004a).	Drinking water: low levels of Co, usually between 0.1-5 µg/L (HSDB, 2019); Surface water: observed only in trace amounts. Most waters have no detectable Co; values >10 µg/L are rare. Maximum recorded value in any of several broad studies was 99 µg/L (HSDB, 2019). In Kern County municipal groundwater, reported frequency of detection: 0.77; Mean: 0.14; Range: 0.02 - 0.523 [µg/L] (GAMA, USGS).	Reported frequency of detection: 0.3; Mean: 1.26; Range: 0.092 - 10 [µg/L]	ranges from 2.4-35.7 µg/kg in fresh fruits and vegetables (ATSDR, 2004a). Detected in carrots up to 0.15 mg/kg (Thomas et al., 1974)	Detected in carrots; at trace levels in 1 of 2 samples; concentration in treated samples, mean: 0.089 [mg/kg] (range: 0.058 - 0.12)
7440-50-8	Copper	Inorganic	Kern County sample range: 11.8-22.3 mg/kg in benchmark soils (Bradford et al, 1996); US: Cu ranges 1-300 mg/kg dry-weight, with avg values 14-41 mg/kg as a function of soil type (ATSDR, 2004b).	Bakersfield: 2015-2017 annual avg of 55 ng/m3 (CARB, 2019); US: remote and rural areas have Cu ranges of 0.029-12 and 3-280 ng/m3, respectively (ATSDR, 2004b).	Surface water: US rivers have concentration ranges of 0.83-105 µg/L (median 5.3) (HSDB, 2019). In Kaweah and Tule Rivers, reported frequency of detection: 0.81; detected dissolved concentrations of mean: 1.4; range: 0.078 - 8.1 [µg/L] (CEDEN, 2020). In Kern County municipal groundwater, reported frequency of detection: 0.23; Mean: 2.9; Range: 1.8 - 5.3 [µg/L] (GAMA, USGS)	Reported frequency of detection: 0.74; Mean: 8.93; Range: 0.64 - 87 [µg/L]	In a wide variety of foods in the US marketplace. avg. 1.3 mg/kg (range: ND-335 mg/kg) (FDA, 2007)	Detected in Navel oranges, cherries, carrots, garlic, Valencia oranges, lemons, Mandarin oranges, almonds, apple, potato, grapes, pistachios, tomato; concentration in treated samples, mean: 3.4 [mg/kg] (range: 0.5 - 12)
16984-48-8	Fluoride	Inorganic	US: range <10-3,700 ppm with avg of 430 ppm (ATSDR, 2003a).	Gaseous fluoride varied from 0.01-1.65 µg/m3 in Canada and US, approx. 75% of which exists as hydrogen fluoride (ATSDR, 2003a).	Surface water: fluoride levels in rivers range <1-6,500 µg/L, with avg ~200 µg/L (ATSDR, 2003a). In Kern County municipal groundwater, reported frequency of detection: 1; Mean: 616.25; Range: 40 - 2100 [µg/L] (GAMA, USGS)	Reported frequency of detection: 0.69; Mean: 452.22; Range: 170 - 910 [µg/L]	vegetables grown on uncontaminated land were reported to have concentration ranging from 0.63-11.3 ppm (ATSDR, 2003a)	na

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7664-39-3	Hydrofluoric acid	Inorganic	na	Southern CA: avg hydrogen fluoride (gas) concentrations of 0.13-0.22 μg/m3 at San Nicolas Island and onshore at Rubidoux, CA in 1986 (HSDB, 2019); US: ambient levels of hydrogen fluoride ranged 1.0-7.5 μg/m3 in 1985 (ATSDR, 2003a).	na	see Fluoride	na	na
7553-56-2	Iodine	Inorganic	Kern County sample range: 0.23 – 0.60 mg/kg in benchmark soils (Bradford et al, 1996); US: avg I was 1.2 mg/kg (ATSDR, 2004c).	San Francisco, CA (urban): I content ranged 4.7-10 ng/m3 in 1970; Global: avg concentrations range 10-20 ng/m3 with gaseous I usually exceeding particulate I by 2-6x (ATSDR, 2004c).	Surface water: avg ranged 0.1-18 μg/L in river water (ATSDR, 2004c). In Kern County municipal groundwater, reported frequency of detection: 0.58; Mean: 11.28; Range: 1 - 71 [μg/L] (GAMA, USGS)	Non-detect	In a wide variety of foods in the US marketplace. avg. 0.106 mg/kg (range: ND-6.88 mg/kg) (FDA, 2007)	na
7439-92-1	Lead	Inorganic	Kern County sample range: 14.6-22.4 mg/kg in benchmark soils (Bradford et al, 1996).	Bakersfield: 2010-2017 annual avg of ~3.5 ng/m3 (CARB, 2019).	Surface Water: 2005 USEPA STORET detected Pb in 3/224 surface water samples in UT and IA; detected samples ranged 7.8-142 μg/L (ATSDR, 2019b). In Kaweah and Tule Rivers, reported frequency of detection: 0.19; detected dissolved concentrations of mean: 0.31; range: 0.032 - 2.1 [μg/L] (CEDEN, 2020). In Kern County municipal groundwater, reported frequency of detection: 0.26; Mean: 1.09; Range: 0.68 - 2.26 [μg/L] (GAMA, USGS)	Reported frequency of detection: 0.47; Mean: 0.86; Range: 0.096 - 4.4 [μg/L]	In a wide variety of foods in the US marketplace. avg. 0.003 mg/kg (range: ND-0.210 mg/kg) (FDA, 2007)	Detected at trace levels in carrots (both treated and control samples); concentration in treated samples, mean: 0.073 [mg/kg] (range: 0.056 - 0.09)

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7439-93-2	Lithium	Inorganic	Kern County sample range: 7-51 mg/kg in benchmark soils (Bradford, et al, 1996).	na	Surface Water: 1994 avg concentrations of 0.86-1.9 µg/L in Alamosa River, CO and 20 µg/L in Big Arsenic Springs, NM (HSDB, 2019). In Kern County municipal groundwater, reported frequency of detection: 1; Mean: 39.7; Range: 0.8 - 179 [µg/L] (GAMA, USGS)	Reported frequency of detection: 0.61; Mean: 21.72; Range: 6.8 - 53 [µg/L]	lithium in fruit can range from 383–6707 µg/kg (Caballero et al., 2003a)	na
554-13-2	Lithium carbonate	Inorganic	na	na	na	see Lithium	na	na
13453-71-9	Lithium chlorate	Inorganic	na	na	na	see Lithium	na	na
7447-41-8	Lithium chloride	Inorganic	na	na	na	see Lithium	na	na
1310-65-2	Lithium hydroxide	Inorganic	na	na	na	see Lithium	na	na
13840-33-0	Lithium hypochlorite	Inorganic	na	na	na	see Lithium	na	na
7439-96-5	Manganese	Inorganic	Kern County sample range: 259-682 mg/kg in benchmark soils (Bradford et al, 1996).	Bakersfield: 2007-2017 annual avg of 34 ng/m3 (CARB, 2019); Annual avgs of Mn in urban and rural areas w/o significant Mn pollution range 10-70 ng/m3 (ATSDR, 2012a).	Surface water: Dissolved Mn was detected in 51% of US surface water samples, at an avg of 59 µg/L (ATSDR, 2012a). Avg concentration of Mn in drainage basins was 2.8 µg/L in the Southeastern US, Pacific Northwest US, and CA (HSDB, 2019). In Kaweah and Tule Rivers, reported frequency of detection: 0.97; detected dissolved concentrations of mean: 3.73; range: 0.22 - 160 [µg/L] (CEDEN, 2020). In Kern County municipal groundwater, reported frequency of detection: 0.74; Mean: 128.95; Range: 0.2 - 2250 [µg/L] (GAMA, USGS)	Reported frequency of detection: 0.86; Mean: 45.79; Range: 3 - 610 [µg/L]	In a wide variety of foods in the US marketplace. avg. 2.5 mg/kg (range: ND-44.4 mg/kg) (FDA, 2007)	na

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7439-97-6	Mercury	Inorganic	Kern County sample range: 0.10-0.40 mg/kg in benchmark soils (Bradford et al, 1996); Globally, avg Hg content of virgin and uncultivated surface soils range 0.020-0.625 mg/kg (ATSDR, 1999).	Bakersfield: 1995-2002 annual avg of 1.65 ng/m3 (CARB, 2019); Ambient air levels of Hg have been reported to avg ~10-20 ng/m3 (ATSDR, 1999).	Surface water (aerobic): In California, Hg ranges from 0.0005 to 0.104 µg/L (Gill and Bruland, 1990). In Kaweah and Tule Rivers, reported frequency of detection: 0.39; detected dissolved concentrations of mean: 0.12; range: 0.035 - 0.31 [µg/L] (CEDEN, 2020). In Kern County municipal groundwater, reported frequency of detection: 0.07; detected in 1 of 15 samples with concentration 0.02 [µg/L] (GAMA, USGS).	Reported frequency of detection: 0.13; Mean: 0.04; Range: 0.001 - 0.095 [µg/L]; Virtually any mercurial compound may be microbially converted to methylmercury upon entering an aqueous system (HSDB, 2019).	In a wide variety of foods in the US marketplace. avg. 0.005 mg/kg (range: ND-0.332 mg/kg) (FDA, 2007)	na
7439-98-7	Molybdenum	Inorganic	Kern County sample range: 3.7-9.6 mg/kg in benchmark soils (Bradford et al, 1996).	Bakersfield: 2007-2017 annual avg of 0.81 ng/m3 (CARB, 2019)	Surface water: 62 agricultural drainage and evaporation ponds in San Joaquin Valley, CA ranged 0.138-23.7 mg/L (HSDB, 2019). In Kaweah and Tule Rivers, reported frequency of detection: 0.95; detected dissolved concentrations of mean: 1.69; range: 0.00083 - 9.7 [µg/L] (CEDEN, 2020). In Kern County municipal groundwater, reported frequency of detection: 1; Mean: 23.03; Range: 0.451 - 157 [µg/L] (GAMA, USGS)	Reported frequency of detection: 0.76; Mean: 3.24; Range: 0.38 - 12 [µg/L]	typical range in plants 1-2 ppm (ATSDR, 2017a)	Detected in carrots, almonds, garlic; concentration in treated samples, mean: 0.32 [mg/kg] (range: 0.055 - 0.61)

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7440-02-0	Nickel	Inorganic	Kern County sample range: 21 – 27 mg/kg in benchmark soils (Bradford et al, 1996); US: Ni content ranges 4-80 ppm (ATSDR, 2005a).	Bakersfield: 2007-2017 annual avg of 5.8 ng/m3 (CARB, 2019); US: Ni in particulate matter ranged 0.01-60 and 0.6-78 ng/m3 in remote and rural areas, respectively (ATSDR, 2005a).	Surface water: avg between 15-20 µg/L (ATSDR, 2005a). In Kaweah and Tule Rivers, reported frequency of detection: 0.78; detected dissolved concentrations of mean: 0.36; range: 0.037 - 2.2 [µg/L] (CEDEN, 2020). In Kern County municipal groundwater, reported frequency of detection: 0.59; Mean: 1.39; Range: 0.36 - 3.19 [µg/L] (GAMA, USGS)	Reported frequency of detection: 0.67; Mean: 2.07; Range: 0.36 - 20 [µg/L]	In a wide variety of foods in the US marketplace. avg. 0.133 mg/kg (range: ND-4.69 mg/kg) (FDA, 2007)	Detected in carrots, almonds, pistachios; concentration in treated samples, mean: 0.89 [mg/kg] (range: 0.24 - 1.6)
7786-81-4	Nickel sulfate	Inorganic	na	na	na	see Nickel	na	na
14797-65-0	Nitrite	Inorganic	na	na	Surface water: detected in 23% of US public water system surface water sources with a median of 0.02 mg nitrite-nitrogen/L and max of 8.68 mg nitrite-nitrogen/L (USEPA 1990a). In Kern County municipal groundwater, total nitrate-nitrite as nitrogen reported frequency of detection: 0.92; Mean: 3551.08; Range: 70 - 12100 [µg/L] (GAMA, USGS)	Reported frequency of detection: 0.4; Mean: 9900; Range: 800 - 19000 [µg/L]	Nitrite levels in food are low, except when subject to microbial degradation; usually less than 2 mg/kg (Caballero et al., 2003b)	na

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7782-49-2	Selenium	Inorganic	Kern County sample range: 0.015-0.018 mg/kg in benchmark soils (Bradford et al, 1996); US: most seleniferous soils contained <2 mg/kg, with a max of 100 mg/kg (ATSDR, 2003b).	Bakersfield: 2007-2017 annual avg of 1.2 ng/m3 (CARB, 2019); Avg Se levels generally <10 ng/m3 (ATSDR, 2003b).	Surface water: Colorado River delta concentrations ranged 0.005-0.019 mg/L with a median of 0.011 mg/L for samples collected Oct 1996-Mar 1997 (HSDB, 2019). In Kaweah and Tule Rivers, reported frequency of detection: 0.25; detected dissolved concentrations of mean: 1.62; range: 0.17 - 12 [µg/L] (CEDEN, 2020). In Kern County municipal groundwater, reported frequency of detection: 0.82; Mean: 0.86; Range: 0.05 - 3.2 [µg/L] (GAMA, USGS)	Reported frequency of detection: 0.38; Mean: 1.11; Range: 0.19 - 7.5 [µg/L]	In a wide variety of foods in the US marketplace. avg. 0.076 mg/kg (range: ND-1.8 mg/kg) (FDA, 2007)	Detected only at trace levels in carrots; concentration in treated samples, mean: 0.053 [mg/kg] (range: 0.053 - 0.053)
7440-22-4	Silver	Inorganic	Kern County sample range: 0.28-0.39 mg/kg in benchmark soils (Bradford et al, 1996).	Air concentrations ranged 0.05-4.3 ng/m3, with no appreciable/apparent differences between rural and urban areas (HSDB, 2019); US: background Ag in national parks were <1 ng/m3 (ATSDR, 1990b).	Public drinking water supplies and river waters have a median concentration between 0.09-0.23 µg/L (HSDB, 2019). In Kern County municipal groundwater, reported frequency of detection: 0.03; Mean: 0.01; Range: 0.012 - 0.012 [µg/L] (GAMA, USGS)	Non-detect	fruit: <0.050 mg/kg; leafy vegetables: avg. 0.007 (range ND-0.039 mg/kg) (ATSDR, 1990b)	na
7775-09-9	Sodium Chlorate	Inorganic	na	na	na	na	na	na
12179-04-3	Sodium tetraborate pentahydrate	Inorganic	na	na	na	na	na	na
65996-69-2	Steel mill slag	Inorganic	na	na	na	na	na	na
7440-24-6	Strontium	Inorganic	Kern County sample range: 176-299 mg/kg in benchmark soils (Bradford et al, 1996)..	Bakersfield: 1994-2017 annual avg. range from 10.4 – 18.3 ng/m3 (CARB, 2019)	In Kern County municipal groundwater, reported frequency of detection: 1; Mean: 729.64; Range: 7.7 - 2790 [µg/L] (GAMA, USGS)	Reported frequency of detection: 0.87; Mean: 130; Range: 18 - 460 [µg/L]	In a wide variety of fruits and vegetables, avg. concentrations range from 3.1 – 64 mg/kg (ATSDR, 2004e)	Detected in all crops; concentration in treated samples, mean: 2.2 [mg/kg] (range: 0.51 – 9.5)

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7446-09-5	Sulfur dioxide	Inorganic	na	Bakersfield: 2008-2011 annual avg S concentration was 734 ng/m3 (CARB, 2019); Avg 8-hr max SO2 conc was 4.6 ppb in high traffic area in Los Angeles County 1999-2000. Avg SO2 level of 2.6 ppbw reported for a relatively pristine region in W. Maryland that was >50km downwind of power plants in OH, PA, and W. Va 2006-2014 (HSDB, 2019).	na	na	na	na
7440-31-5	Tin	Inorganic	Kern County sample range: 1.07-1.91 mg/kg in benchmark soils (Bradford et al, 1996); US: avg background of 0.89 mg/kg (ATSDR, 2005b).	Bakersfield: 2009-2017 annual avg of 1.8 ng/m3 (CARB, 2019); US: avg air levels are generally <0.1 µg/m3, with higher concentrations near industrial sources (ATSDR, 2005b).	Surface water: 56/59 water samples from 15 rivers in US & Canada did not detect Tin. Detected samples ranged 1.3-2.1 µg/L (HSDB, 2019).	Non-detect	fruits and vegetables not packaged in metal cans typically contain <2 mg/kg (ATSDR, 2005b)	na
7440-62-2	Vanadium	Inorganic	Kern County sample range: 58-77 mg/kg in benchmark soils (Bradford et al, 1996); US: avg 200 mg/kg (ATSDR, 2012b).	Background concentrations in unpolluted air range 0.02-2.0 ng/m3. Rural sites may have V levels as high as 65 ng/m3 (avg range <1-40 ng/m3) while industrialized urban centers w/high levels of residual fuel oil will range 500-2000 ng/m3 (HSDB, 2019).	San Joaquin Valley, CA: agricultural drainage and evaporation ponds ranged 0.004-0.544 mg/L, with an avg of 0.087 mg/L (HSDB, 2019); Surface water: US levels range 0.04-200 µg/L (ATSDR, 2012b). In Kern County municipal groundwater, reported frequency of detection: 0.88; Mean: 10.06; Range: 0.1 - 41.5 [µg/L] (GAMA, USGS)	Reported frequency of detection: 0.46; Mean: 3.25; Range: 0.99 - 10 [µg/L]	fresh fruit and vegetables have concentrations that can range ND – 0.72 µg/kg with mean of 0.6 µg/kg (ATSDR, 2012b)	Detected at trace levels in carrots (both treated and control samples); concentration in treated samples, mean: 0.545 [mg/kg] (range: 0.42 - 0.67)

CASRN	Chemical name	Organic / Inorganic / Radionuclide	Soil	Air	Water	Blended Produced Water Quality [Central Valley California]	In Food	Task 3 Food Crop Results (only samples irrigated with blended produced water)
7440-66-6	Zinc	Inorganic	Kern County sample range: 152 – 180 mg/kg in benchmark soils (Bradford et al, 1996).	Bakersfield: 2015-2017 annual avg of 70.7 ng/m3 (CARB, 2019).	Zn background in surface waters is generally <50 µg/L, but can range between 0.002-50 mg/L in surface and groundwater (ATSDR, 2005c). In Kaweah and Tule Rivers, reported frequency of detection: 0.89; detected dissolved concentrations of mean: 2.5; range: 0.067 - 87 [µg/L] (CEDEN, 2020). In Kern County municipal groundwater, reported frequency of detection: 0.37; Mean: 12.08; Range: 4.9 - 27.5 [µg/L] (GAMA, USGS)	Reported frequency of detection: 0.62; Mean: 13.44; Range: 1.8 - 101 [µg/L]	In a wide variety of foods in the US marketplace. avg. 9.4 mg/kg (range:ND-261.0 mg/kg) (FDA, 2007)	Detected in carrots, garlic, almonds, pistachios; concentration in treated samples, mean: 17.5 [mg/kg] (range: 2.7 - 39)
7646-85-7	Zinc chloride	Inorganic	na	na	na	see Zinc	na	na
123-91-1	1,4 Dioxane	Organic	na – expected to volatilize (HSDB, 2019).	US: average levels of 1,4-dioxane in outdoor air samples in the mid-1980s was ~0.4 µg/m3 (HSDB, 2019).	Drinking water: 1970s municipal US water supplies reported to contain 1 µg/L, but frequency of this level was not provided. 1,4-dioxane levels are expected to have declined due to decreased use (ATSDR, 2012f). Not detected in Kern County Municipal groundwater (GAMA, USGS)	Reported frequency of detection: 0.22; Mean: 0.75; Range: 0.52 - 0.98 [µg/L]	Dioxane has been identified to be present in food, but unquantified (ATSDR, 2012f)	na
479-66-3	1H, 3H-Pyrano (4,3-b)(1)benzopyran-9-carboxylic acid, 4,10-dihydro-3,7,8 trihydroxy-3-methyl-10-oxo (fulvic acid)	Organic	na	na	na	na	na	na
60-24-2	2-mercaptoethanol	Organic	na	na	na	na	na	na
115-19-5	2-methyl-3-Butyn-2-ol	Organic	na	na	na	na	na	na
27646-80-6	2-Methylamino-2-methyl-1-propanol	Organic	na	na	na	na	na	na
67990-40-3	2-Propen-1-aminium, N,N-dimethyl-N-2-propenyl-, chloride, polymer with 2-hydroxypropyl 2-propenoate and 2-propenoic acid	Organic	na	na	na	na	na	na

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145417-45-4	2-Propenoic acid, 2-methyl-, polymer with methyl 2-methyl-2-propenoate, octadecyl 2-methyl 2 propenoate and 2propenoic acid, sodium salt	Organic	na	na	na	na	na	na
9033-79-8	2-propenoic acid, polymer with sodium 2-propenoate	Organic	na	na	na	na	na	na
130800-24-7	2-Propenoic acid, telomer with 2-methyl-2-(1-oxo-2-propenyl)-1-propanesulfonic acid, sodium salt	Organic	na	na	na	na	na	na
83-32-9	Acenaphthene	Organic	Rural soil: 1.7 µg/kg; Agricultural soil: 6 µg/kg (ATSDR, 1995a).	Glendora, CA: avg conc of 5 ng/m3 for day and 25 ng/m3 for night in 1981. Tampa, FL: range of 0.07-0.45 ng/m3, avg of 0.20 ng/m3 in 2002 (HSDB, 2019).	Surface water: STORET median of US ambient water from 1980-1982 was <10µg/L (ATSDR, 1995a).	Reported frequency of detection: 0.15; Mean: 0.15; Range: 0.03 - 0.61 [µg/L]	PAHs in most foods are less than 2 ppb. Those foods that are smoked, like smoked salmon can contain upwards of 86.6 ppb (ATSDR, 1995a)	na
100-73-2	Acrolein dimer	Organic	na	na	na	na	na	na
29868-05-1	Alkanolamine phosphate	Organic	na	na	na	na	na	na
68439-70-3	Alkyl amine	Organic	na	na	na	na	na	na
300-92-5	Aluminum distearate	Organic	na	na	na	na	na	na
No CASRN	Amide surfactant acid salt	Organic	na	na	na	na	na	na
No CASRN	Amides, Non Ionics	Organic	na	na	na	na	na	na
61791-24-0	Amine derivative	Organic	na	na	na	na	na	na
67924-33-8	Amine salt	Organic	na	na	na	na	na	na
NP-U2856	Amine salt	Organic	na	na	na	na	na	na
64346-44-7	Amine sulfate	Organic	na	na	na	na	na	na
120-12-7	Anthracene	Organic	MA and RI: 54/62 soil samples detected with a range of 0.029-5.70 mg/kg in July 1992 (HSDB, 2019); Agricultural soil: 11-13 µg/kg (ATSDR, 1995a).	Los Angeles: ambient particle-phase avg 0.54 ng/m3 (ATSDR, 1995a); Great Lakes area: range of 0.1-1.0 ng/m3 with an avg of 0.6 ng/m3 (HSDB, 2019).	Great Lakes: 14-430 pg/L. (HSDB, 2019). STORET median of US ambient water from 1980-1982 was <10µg/L (ATSDR, 1995a).	Not detected in blended produced water	PAHs in most foods are less than 2 ppb. Those foods that are smoked, like smoked salmon can contain upwards of 86.6 ppb (ATSDR, 1995a)	na
No CASRN	Aromatic Amine	Organic	na	na	na	Aniline was not detected in irrigation water, 2-Napthylamine was not measured; Aniline and 2-Naphthylamine was not detected in effluent	na	na

CASRN	Chemical name	Organic / Inorganic / Radionuclide	Soil	Air	Water	Blended Produced Water Quality [Central Valley California]	In Food	Task 3 Food Crop Results (only samples irrigated with blended produced water)
56-55-3	Benzo(a)anthracene	Organic	Rural soil: 5-20 µg/kg; Agricultural soil: 56-110 µg/kg (ATSDR, 1995a).	US avg 1965 urban levels ~4 ng/m3, with an avg range of 0.18-4.6 ng/cu3. Detroit, MI ranged 0.4-21.6 ng/m3, New York City ranged 0.1-16 ng/m3; Cleveland, OH had a max value of 140 ng/m3 (HSDB, 2019); Atascadero and Lompoc (rural CA): vapor-phase 6-25 pg/m3 (Eiguren-Fernandez et al, 2010); Los Angeles: ambient particle-phase avg 0.48 ng/m3 (ATSDR, 1995a).	Surface water: detected at 4-5 ppt in the Mississippi River near Cairo, IL and Memphis, TN (HSDB, 2019). STORET median of US ambient water from 1980-1982 was <10µg/L (ATSDR, 1995a).	Reported frequency of detection: 0.02; Mean: 0.03; Range: 0.03 - 0.03 [µg/L]	PAHs in most foods are less than 2 ppb. Those foods that are smoked, like smoked salmon can contain upwards of 86.6 ppb (ATSDR, 1995a)	na
50-32-8	Benzo(a)pyrene	Organic	Rural soil: 2-1,300 µg/kg; Agricultural soil: 4.6-900 µg/kg (ATSDR, 1995a).	Bakersfield: 1995-2004 annual avg of 0.2 ng/m3 (CARB, 2019); avg PM2.5 BAP of ~0.5 ng/m3 from CARB 2010 monitoring site (Noth et al, 2016); Atascadero and Lompoc (rural CA): vapor-phase 9-88 pg/m3 (Eiguren-Fernandez et al, 2010); NJ (rural): geo. mean ranged 0.04-0.06 ng/m3 in summer and 0.17-0.32 in winter (ATSDR, 1995a).	Drinking water: detected in 87% of samples from 15 US cities; range of 0.1 to 2.1 ppt with an avg of 0.55 ppt (HSDB, 2019); Surface water: detected in 9.4% of samples from 139 streams in 30 states (1999-2000); max of 0.24 µg/L and median concentration of 0.04 µg/L (HSDB, 2019). STORET median of US ambient water from 1980-1982 was <10µg/L (ATSDR, 1995a).	Non-detect	PAHs in most foods are less than 2 ppb. Those foods that are smoked, like smoked salmon can contain upwards of 86.6 ppb (ATSDR, 1995a)	na
205-99-2	Benzo(b)fluoranthene	Organic	Rural soil: 20-30 µg/kg; Agricultural soil: 58-220 µg/kg (ATSDR, 1995a)	Bakersfield: particles collected Dec 2000-Jan 2001 (day/night) measured 6.5/43 PM0.1, 37/306 PM0.18, 439/2120 PM1.8 pg/m3 (HSDB, 2019); Atascadero and Lompoc (rural CA): vapor-phase 12-65 pg/m3 (Eiguren-Fernandez et al, 2010).	Surface water: STORET median of US ambient water from 1980-1982 was <10µg/L (ATSDR, 1995a).	Reported frequency of detection: 0.02; Mean: 0.11; Range: 0.11 - 0.11 [µg/L]	PAHs in most foods are less than 2 ppb. Those foods that are smoked, like smoked salmon can contain upwards of 86.6 ppb (ATSDR, 1995a)	na

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111-44-4	Bis (2-chloroethyl) ether	Organic	na	na	Drinking water: detected in 13/113 samples with reporting limit of 0.005 µg/L; detected samples ranged 0.01-0.36 µg/L with avg of 0.1 µg/L (ATSDR, 2017c); Surface water: USEPA STORET database, with an unspecified portion pertaining to surface water, showed 3/808 water samples detected bis(2-chloroethyl) ether residues. Median: <10 µg/L (HSDB, 2019).	Non-detect	No studies were located regarding the occurrence of BCEE in food or other media. (ATSDR, 2017c)	na
68239-30-5	Bis (HDMA) EPI Copolymer hydrochloride	Organic	na	na	na	na	na	na
69418-26-4	Cationic acrylamide copolymer	Organic	na	na	na	na	na	na
44992-01-0	Cationic acrylamide monomer	Organic	na	na	Drinking water in West Virginia: acrylamide detected 0.024–0.041 µg/L (ATSDR, 2012g)	Acrylamide was not detected in irrigation water	acrylamide is typically found in food cooked with dry heat, i.e., potato chips, baked goods, coffee. Mean reported concentration range from 36-1312 µg/kg with max. concentrations as high as 3500 µg/kg (ATSDR, 2012g)	na
54076-97-0	Cationic polymer	Organic	na	na	na	na	na	na
681331-04-4	Causticized Lignite	Organic	na	na	na	na	na	na
108-90-7	Chlorobenzene	Organic	na	Bakersfield: 1992-1993 annual avg of 0.07 ppb (CARB, 2019); US: avg of 0.66 ppb in urban and suburban areas; not detected in rural and remote areas (ATSDR, 2019d).	Surface water: has been detected in US rivers up to and >10 ppb, though frequency was not given (ATSDR, 2019d).	Non-detect	Chlorobenzene is not common in food. Not reported in US setting. (ATSDR, 2019d)	na

CASRN	Chemical name	Organic / Inorganic / Radionuclide	Soil	Air	Water	Blended Produced Water Quality [Central Valley California]	In Food	Task 3 Food Crop Results (only samples irrigated with blended produced water)
218-01-9	Chrysene	Organic	Rural soil: 38.3 µg/kg; Agricultural soil: 78-120 µg/kg (ATSDR, 1995a).	Bakersfield: particles collected Dec 2000-Jan 2001, daytime/night concentration of $PM_{0.1}$ was 0.95/11.6 pg/m3, daytime/night concentration of $PM_{0.18}$ was 7.4/129 pg/m3, daytime/night concentration of $PM_{1.8}$ was 178/902 pg/m3 (HSDB, 2019); Atascadero and Lompoc (rural CA): 8-22 pg/m3 (Eiguren-Fernandez et al, 2010).	Surface water: detected in water samples from the Mississippi River at 7, 12, and 10 ng/L for samples collected near the inflow of the Ohio River, 20 miles below Memphis, TN, and in New Orleans, LA, respectively (HSDB, 2019). STORET median of US ambient water from 1980-1982 was <10µg/L (ATSDR, 1995a).	Reported frequency of detection: 0.03; Mean: 0.04; Range: 0.039 - 0.042 [µg/L]	PAHs in most foods are less than 2 ppb. Those foods that are smoked, like smoked salmon can contain upwards of 86.6 ppb (ATSDR, 1995a)	na
64743-05-1	Coke (petroleum), calcined	Organic	na	na	na	na	na	na
25987-30-8	Copolymer of acrylamide and sodium acrylate	Organic	na	na	na	na	na	na
53-70-3	Dibenzo(a,h)anthracene	Organic	MA & RI: 32/62 soil samples detected with a range of 0.02-2.90 mg/kg in July 1992 (HSDB, 2019).	Bakersfield 1995-2005 annual avg: 0.035 ng/m3 (CARB, 2019); Atascadero and Lompoc (rural CA): vapor-phase 2-11 pg/m3 (Eiguren-Fernandez et al, 2004).	na	Non-detect	PAHs in most foods are less than 2 ppb. Those foods that are smoked, like smoked salmon can contain upwards of 86.6 ppb (ATSDR, 1995a)	na
2673-22-5	Diester of sulfosuccinic acid sodium salt	Organic	na	na	na	na	na	na
38011-25-5	Disodium ethylenediaminetetraacetate	Organic	na	na	na	na	na	na
64742-53-6	Distillates, hydrotreated light naphthenic	Organic	na	na	na	na	na	na
No CASRN	Drilling paper	Organic	na	na	na	na	na	na
126-97-6	Ethanolamine thioglycolate	Organic	na	na	na	na	na	na
26027-38-3	Ethoxylated 4– nonphenol	Organic	na	na	Surface water: Iowa streams ranged <1 µg/L to 2.5 µg/L in 2001 (HSDB, 2019).	na	na	na
61791-26-2	Ethoxylated amine	Organic	na	na	na	na	na	na
9081-83-8	Ethoxylated octylphenol	Organic	na	na	na	na	na	na
5877-42-9	Ethyl octynol	Organic	na	na	na	na	na	na

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206-44-0	Fluoranthene	Organic	3 Northeastern US cities: avg concentration of 3.05 mg/kg (HSDB, 2019); Rural soil: 0.3-40 µg/kg; Agricultural soil: 120-210 µg/kg (ATSDR, 1995a).	ambient air at 8 locations of US in 2016 averaged 0.44-1.86 ng/m3 (HSDB, 2019); Los Angeles: ambient particle-phase avg 0.94 ng/m3 (ATSDR, 1995a).	Surface water: STORET median of US ambient water from 1980-1982 was <10µg/L (ATSDR, 1995a). San Joaquin River, CA: <1.0 to 3.0 ng/L (HSDB, 2019).	Non-detect	PAHs in most foods are less than 2 ppb. Those foods that are smoked, like smoked salmon can contain upwards of 86.6 ppb (ATSDR, 1995a)	na
63428-92-2	Formaldehyde, polymer with 2-methyloxirane, 4-nonylphenol and oxirane	Organic	na	na	na	na	na	na
30704-64-4	Formaldehyde, polymer with 4-(1,1-dimethylethyl)phenol, 2-methyloxirane and oxirane	Organic	na	na	na	na	na	na
30846-35-6	Formaldehyde, polymer with 4-nonylphenol and oxirane	Organic	na	na	na	na	na	na
No CASRN	Heavy catalytic reformed naptha	Organic	na	na	na	na	na	na
No CASRN	Heavy catalytic reformed naptha	Organic	na	na	na	na	na	na
1415-93-6	Humic acids	Organic	na	na	na	na	na	na
61790-59-8	Hydrogenated tallow amine acetone	Organic	na	na	na	na	na	na
2809-21-4	Hydroxyethylidenediphosphonic acid	Organic	na	na	na	na	na	na
193-39-5	Indenopyrene	Organic	Rural soil: 10-15 µg/kg; Agricultural soil: 63-100 µg/kg (ATSDR, 1995a).	Bakersfield: particles collected Dec 2000-Jan 2001 Bakersfield (day/night) measured 0.0/37 PM0.1, 61/478 PM0.18, 1120/4540 PM1.8 pg/m3 (HSDB, 2019). Avg PM2.5 IDP ~0.4 ng/m3 from 2010 CARB monitoring site (Noth et al, 2016).	Surface water: detected in water samples from the Mississippi River at 2-8 ng/L in samples collected near the inflow of the Ohio River and 20 miles below Memphis, TN, respectively (HSDB, 2019). STORET median of US ambient water from 1980-1982 was <10µg/L (ATSDR, 1995a).	Reported frequency of detection: 0.02; Mean: 0.09; Range: 0.091 - 0.091 [µg/L]	PAHs in most foods are less than 2 ppb. Those foods that are smoked, like smoked salmon can contain upwards of 86.6 ppb (ATSDR, 1995a)	na
119-65-3	Isoquinoline	Organic	na	na	Rainwater: 3 samples Los Angeles rainwater (collected 1981-1982) contained concentrations of quinoline plus isoquinoline and their substituted compounds 0.7-2 µg/L, 1.6 µg/L avg, respectively (HSDB, 2019).	na	na	na

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68648-89-5	Kraton G1702H	Organic	na	na	na	na	na	na
129521-66-0	Lignite	Organic	na	na	na	na	na	na
PE-M2464	Methyl oxirane polymer	Organic	na	na	na	na	na	na
No CASRN	Nonylphenol ethoxylates	Organic	na	na	na	na	na	na
No CASRN	Nonylphenol ethoxylates	Organic	na	na	na	na	na	na
127087-87-0	Nonylphenol polyethylene glycol ether	Organic	na	na	na	na	na	na
No CASRN	Organic acid ethoxylated alcohols	Organic	na	na	na	na	na	na
68412-54-4	Oxyalkylated alkylphenol	Organic	na	na	Surface water: total nonylphenols detected 1.6-14.9 in several rivers in US (HSDB, 2019).	na	na	na
68171-44-8	Oxyalkylated alkylphenolic resin	Organic	na	na	na	na	na	na
67939-72-4	Oxyalkylated polyamine	Organic	na	na	na	na	na	na
68910-19-0	Oxyalkylated polyamine	Organic	na	na	na	na	na	na
85-01-8	Phenanthrene	Organic	combined phenanthrene/anthracene residues in CA soils ranged 7.0-9.5 ppb (HSDB, 2019); Rural soil: 30 µg/kg; Agricultural soil: 48-140 µg/kg (ATSDR, 1995a).	Savannah, GA: 6->14 ng/m3; Great Lakes: 0.1-1.0 ng/m3 with avg of 0.6 ng/m3 (HSDB, 2019); Denver, CO: ambient conc (combined particle– and vapor-phase) avg 39 ng/m3 (ATSDR, 1995a).	Raw surface water from various US sites ranged 0.006-0.020 µg/L (HSDB, 2019).	Reported frequency of detection: 0.18; Mean: 0.11; Range: 0.029 - 0.29 [µg/L]	PAHs in most foods are less than 2 ppb. Those foods that are smoked, like smoked salmon can contain upwards of 86.6 ppb (ATSDR, 1995a)	na
68123-18-2	Phenol, 4,4'-(1-methylethylidene) bis-, polymer with 2-(chloromethyl)oxirane, 2-methyloxirane and oxirane	Organic	na	na	na	na	na	na
68425-75-2	Phosphate ester salt	Organic	na	na	na	na	na	na
9005-70-3	POE (20) Sorbitan Trioleate	Organic	na	na	na	na	na	na
68938-70-5	Poly (triethanolamine.mce)	Organic	na	na	na	na	na	na
68955-69-1	Polyamine salts	Organic	na	na	na	na	na	na
19019-43-3	Polycarboxlate salt [Trisodium ethylenediaminetetraacetate]	Organic	na	na	na	na	na	na
26062-79-3	Polydimethyl diallyl ammonium chloride	Organic	na	na	na	na	na	na

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74-84-0	Polyethylene [CASRN indicates ethane]	Organic	na	Huntington Park, CA: ground-level concentrations of ethane ranged 79-406 ppb (HSDB, 2019).	Surface water: ethane detected in 3/7 surface water samples from Gulf of Mexico; range of <1 – 90nL/L; avg 35 nL/L (HSDB, 2019).	na	na	na
68036-92-0	Polyglycol diepoxide	Organic	na	na	na	na	na	na
68036-95-3	Polyglycol diepoxide	Organic	na	na	na	na	na	na
9038-95-3	Polyglycol ether	Organic	na	na	na	na	na	na
No CASRN	Polyhydroxyalkanoates (PHA)	Organic	na	na	na	na	na	na
64741-71-5	Polymers (petroleum) viscous	Organic	na	na	na	na	na	na
36484-54-5	Polyoxyalkylene glycol	Organic	na	na	na	na	na	na
61790-86-1	Polyoxyalkylenes	Organic	na	na	na	na	na	na
9014-93-1	Polyoxyethylene dinonylphenol	Organic	na	na	na	na	na	na
12068-19-8	Polyoxyethylene nonyl phenyl ether phosphate	Organic	na	na	na	na	na	na
70142-34-6	Polyoxyl 15 hydroxystearate	Organic	na	na	na	na	na	na
42751-79-1	Polyquaternary amine	Organic	na	na	na	na	na	na
129-00-0	Pyrene	Organic	3 Northeastern US cities: average concentration of 2.4 mg/kg (HSDB, 2019); Rural soil: 1019.7 µg/kg; Agricultural soil: 99-150 µg/kg (ATSDR, 1995a).	CA: outdoor air concentrations for West Los Angeles (0.12 ng/m3), Downtown LA (0.26 ng/m3), Pasadena (0.17 ng/m3), and Rabidoux (0.14 ng/m3) (HSDB, 2019); Los Angeles: ambient particle-phase avg 1.62 ng/m3 (ATSDR, 1995a).	Surface water: detected at 1-15 ng/L in Mississippi River in 1984; avg conc of 0.28 ng/L in Lake Superior (HSDB, 2019). STORET median of US ambient water from 1980-1982 was <10µg/L (ATSDR, 1995a).	Reported frequency of detection: 0.02; Mean: 0.04; Range: 0.04 - 0.04 [µg/L]	PAHs in most foods are less than 2 ppb. Those foods that are smoked, like smoked salmon can contain upwards of 86.6 ppb (ATSDR, 1995a)	na
61790-41-8	Quaternary ammonium compound	Organic	na	na	na	na	na	na
68609-18-7	Quaternized condensed alkanolamines	Organic	na	na	na	na	na	na
91-63-4	Quinaldine	Organic	na	na	na	na	na	na
2893-78-9	Sodium dichloroisocyanurate	Organic	na	na	na	na	na	na
64742-95-6	Solvent naphtha, petroleum, light arom.	Organic	na	na	na	na	na	na
NP-SMO3_ U1240	Sorbitan ester	Organic	na	na	na	na	na	na

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No CASRN	Steranes or cyclopentanoperhydrophenanthrene	Organic	na	na	na	na	na	na
8052-41-3	Stoddard Solvents	Organic	na	Not monitored in air; volatile components are more likely to be detected as individual compounds in air (ATSDR, 1995b).	na	Detected in one sample at 25 µg/L	na	na
68140-11-4	Tall oil, DETA/ midazoline acetates	Organic	na	na	na	na	na	na
72480-70-7	Tar bases, quinoline derivatives, quaternized benzyl chloride	Organic	na	na	na	na	na	na
64-02-8	Tetrasodium ethylenediaminetetraacetate	Organic	na	na	na	na	na	na
68527-49-1	Thiourea, polymer with formaldehyde and 1-phenylethanone	Organic	na	na	na	na	na	na
64114-46-1	Triethanolamine homopolymer	Organic	na	na	na	na	na	na
13983-27-2	Krypton 85	Radionuclide	na	NV Test Site: 16 pCi/m3 in 1972 to 25 pCi/m3 in 1983 -increase due to worldwide use of nuclear technology, not nuclear testing activities at site (Grossman and Holloway, 1985); Northern hemisphere: mean 85-Kr surface air activity increased from ~20 dpm/mmol Kr in 1950 to ~750 dpm/mmol Kr in 1977 (Różański, 1979).	na	Reported frequency of detection: 0 of 4	na	na

CASRN	Chemical name	Organic / Inorganic / Radionuclide	Soil	Air	Water	Blended Produced Water Quality [Central Valley California]	In Food	Task 3 Food Crop Results (only samples irrigated with blended produced water)
7440-14-4	Radium 226	Radionuclide	33 US states: avg soil contained 1.1 pCi/g (HSDB, 2019). Ra-226 is naturally-occurring and fairly ubiquitous at low concentrations in water and rock-forming minerals (ATSDR, 1990a).	New York City, NY: dust samples contained Ra-226 at 8E-5 pCi/m3 (ATSDR, 1990a).	Surface water: generally, range 0.1-0.5 pCi/L (HSDB, 2019). Drinking water sources from ground water have population-weighted average concentrations of 0.91 pCi/L (Ra-226) and 1.41 pCi/L (Ra-228). In 200 US public drinking water supplies with high levels of Radium, mean levels were about 10 pCi/L (ATSDR, 1990a). In Kern County untreated municipal groundwater wells, Ra-226 + Ra-228 reported frequency of detection: 1; Mean: 2.26; Range: 0.023 - 31.0 [pCi/L], 6% exceeded MCL of 5 pCi/L (GAMA, CDPH)	Reported frequency of detection: 0.97; Mean: 0.86; Range: 0 - 9.2 [pCi/L]	mean content of Ra-226 in whole diets estimated be 0.52 – 0.73 pCi/kg (ATSDR, 1990a); range of mean concentrations of Ra-226 in a variety of fruits and vegetables 3.1 - 21 pCi/kg (Oakes and Shank, 1997)	na
15262-20-1	Radium 228	Radionuclide	Ra-228 is naturally-occurring but rarer than Ra-226 (ATSDR, 1990a).	New York City, NY: dust samples contained Ra-228 at 1.5E-4 pCi/m3 (ATSDR, 1990a).	Ra is naturally-occurring and fairly ubiquitous at low concentrations in water and rock-forming minerals (ATSDR, 1990a). In Kern County municipal groundwater, reported frequency of detection: 1; Mean: 0.32; Range: 0.03 - 0.69 [pCi/L] (GAMA, USGS)	Reported frequency of detection: 0.97; Mean: 0.61; Range: 0 - 4.7 [pCi/L]	na	na
7440-29-1	Thorium	Radionuclide	typical mean concentration in soil is 6 mg/kg (range: 2 - 12) (ATSDR, 2019c)	atmospheric concentration in US is 0.3 ng/m3 (range: 0.2 - 1.0) (ATSDR, 2019c)	community water supplies from surface and groundwater, <0.01 and <0.04 pCi/L, respectively (ATSDR, 2019c)	na	from samples taken in New York City, concentration in samples of fruits, vegetables, and other foods <0.01 pCi/g; estimated daily intake of Th-232 is 0.1 pCi/d (Fisenne et al., 1987); range of mean concentrations of Th-232 in a variety of fruits and vegetables 2.3 - 12 pCi/kg (Oakes and Shank, 1997)	na

CASRN	Chemical name	Organic / Inorganic / Radionuclide	Soil	Air	Water	Blended Produced Water Quality [Central Valley California]	In Food	Task 3 Food Crop Results (only samples irrigated with blended produced water)
7440-61-1	Uranium	Radionuclide	Kern County sample range: 5.6-21.3 mg/kg in benchmark soils (Bradford et al, 1996); Avg total U in rocks and soils ~1.2 pCi/g (ATSDR, 2013).	Bakersfield: 1995-2002 annual avg of 1.2 ng/m3 (CARB, 2019); US: 2007 RadNet samples of 234-U, 235-U, and 238-U were low, in the attocurie/m3 range (ATSDR, 2013).	Surface water: agricultural irrigation evaporation pond in S. San Joaquin Valley, CA contained U as high as 250-360 µg/L (HSDB, 2019).; USEPA NURE surface water samples avg 1.1 pCi/L for U (ATSDR, 2013). In Kern County municipal groundwater, reported frequency of detection: 1; Mean: 5; Range: 0.0622 - 30.5 [µg/L] (GAMA, USGS)	Reported frequency of detection: 0.54; Mean: 0.64; Range: 0.002 - 8.6 [pCi/L]	fresh fruit and vegetables have concentrations that can range 0.52 – 1.29 µg/kg (ATSDR, 2013); from samples of fruits, vegetables, and other foods taken in New York City, estimated daily intake of uranium is 0.4 pCi/d (Fisenne et al., 1987)	na
14932-42-4	Xenon radionuclide	Radionuclide	na	Pennsylvania: avg 133-Xe concentrations ranged 1-3 mBq/m3 (Bowyer et al, 1997).	na	na	na	na

Table 11: Review of potential chemical analytical methods for the Chemicals of Interest not analyzed in previous water quality sampling

CASRN	Chemical Name	EPA Method 624 or 8216 VOAs	EPA Method 625 or 8270 VOAs	EPA Method 8015 – Total carbon containing compounds" or "TPH", as total extractable and analyzed by GC	EPA Method 415.1, as total organic carbon (water)	EPA Method 350.2: Total Kieldahl Nitrogen, total nitrogen (water)	Total Sulfur (water)	Total Phosphorus (water)	EPA Method 6010B - Total or Extractable Metals	Other Methods
479-66-3	1H, 3H-Pyrano (4,3-b)(1)benzopyran-9-carboxylic acid, 4,10-dihydro-3,7,8 trihydroxy-3-methyl-10-oxo				X					
60-24-2	2-mercaptoethanol thioglycol				X		X			
115-19-5	2-methyl-3-Butyn-2-ol	X (not current target, could be analyzed)	X (not current target, could be analyzed)	X	X					
27646-80-6	2-Methylamino-2-methyl-1-propanol				X	X				
67990-40-3	2-Propen-1-aminium, N,N-dimethyl-N-2-propenyl-, chloride, polymer (CASRN 26062-79-3) with 2-hydroxypropyl 2-propenoate and 2-propenoic acid				X	X				
145417-45-4	2-Propenoic acid, 2-methyl-, polymer with methyl 2-methyl-2-propenoate, octadecyl 2-methyl 2 propenoate and 2propenoic acid, sodium salt				X				X	
9033-79-8	2-propenoic acid, polymer with sodium 2-propenoate				X				X	
130800-24-7	2-Propenoic acid, telomer with 2-methyl-2-(1-oxo-2-propenyl)-1-propanesulfonic acid, sodium salt				X		X		X	
100-73-2	Acrolein dimer. 3,4-Dihydro-2H-pyran-2-carbaldehyde				X					
29868-05-1	Alkanolamine phosphate				X	X		X		
68439-70-3	Alkyl amine				X	X				
300-92-5	Aluminum distearate								X	
No CASRN	Amide surfactant acid salt				X	X				
No CASRN	Amides, Non Ionics				X	X				
61791-24-0	Amine derivative				X	X				
67924-33-8	Amine salt				X	X				
NP-U2856	Amine salt					X				
64346-44-7	Amine sulfate				X	X	X			
No CASRN	Aromatic Amine				X	X				
68239-30-5	Bis (HDMA) EPI Copolymer hydrochloride				X	X				
69418-26-4	Cationic acrylamide copolymer, Ethanaminium, N,N,N trimethyl2-[(1-oxo-2-propenyl)oxy]-, chloride, polymer with 2-propenamide				X	X				
44992-01-0	Cationic acrylamide monomer				X	X				
54076-97-0	Cationic polymer				X	X				
681331-04-4	Causticized Lignite									

CASRN	Chemical Name	EPA Method 624 or 8216 VOAs	EPA Method 625 or 8270 VOAs	EPA Method 8015 – Total carbon containing compounds" or "TPH", as total extractable and analyzed by GC	EPA Method 415.1, as total organic carbon (water)	EPA Method 350.2: Total Kieldahl Nitrogen, total nitrogen (water)	Total Sulfur (water)	Total Phosphorus (water)	EPA Method 6010B - Total or Extractable Metals	Other Methods
64743-05-1	Coke (petroleum), calcined									
25987-30-8	Copolymer of acrylamide and sodium acrylate				X	X			X	
68308-87-2	Cottonseed, flour									
129828-31-5	Crosslinked polyol ester				X					
2673-22-5	Diester of sulfosuccinic acid sodium salt									
38011-25-5	Disodium ethylenediaminetetraacetate				X				X	
64742-95-6	Distillates, hydrotreated light naphthenic			X	X					
No CASRN	Drilling paper									
126-97-6	Ethanolamine thioglycolate				X	X	X			
26027-38-3	Ethoxylated 4– nonphenol				X					LC/MS or LC/UV[1]
61791-26-2	Ethoxylated amine				X	X				
9081-83-8	Ethoxylated octylphenol				X					
5877-42-9	Ethyl octynol				X					
63428-92-2	Formaldehyde, polymer with 2-methyloxirane, 4-nonylphenol and oxirane				X					
30704-64-4	Formaldehyde, polymer with 4-(1,1-dimethylethyl)phenol, 2-methyloxirane and oxirane									
30846-35-6	Formaldehyde, polymer with 4-nonylphenol and oxirane				X					
64742-94-5	Heavy aromatic naphtha			X	X					
64741-68-0	Heavy catalytic reformed naphtha			X	X					
1415-93-6	Humic acids				X					
61790-59-8	Hydrogenated tallow amine acetone				X	X				
2809-21-4	Hydroxyethylidenediphosphonic acid (Etidronic acid)				X	X		X		
119-65-3	Isoquinoline			X	X	X				
68648-89-5	Kraton G1702H									
129521-66-0	Lignite									
PE-M2464	Methyl oxirane polymer				X					
No CASRN	Nonylphenol ethoxylates				X					LC/MS or LC/UV[29]
127087-87-0	Nonylphenol polyethylene glycol ether				X					LC/MS or LC/UV[29]

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[1] Nonylphenol methods can only report: p-Nonylphenol (Technical mixtures), Nonylphenol Monoethoxylate (Technical mixture), Nonylphenol Diethoxylate (Technical mixture), and Bisphenol-A

CASRN	Chemical Name	EPA Method 624 or 8216 VOAs	EPA Method 625 or 8270 VOAs	EPA Method 8015 – Total carbon containing compounds" or "TPH", as total extractable and analyzed by GC	EPA Method 415.1, as total organic carbon (water)	EPA Method 350.2: Total Kieldahl Nitrogen, total nitrogen (water)	Total Sulfur (water)	Total Phosphorus (water)	EPA Method 6010B - Total or Extractable Metals	Other Methods
No CASRN	Organic acid ethoxylated alcohols				X					
68412-54-4	Oxyalkylated alkylphenol				X					LC/MS or LC/UV[29]
68171-44-8	Oxyalkylated alkylphenolic resin				X					
68910-19-0	Oxyalkylated polyamine				X	X				
67939-72-4	Oxyalkylated polyamine				X	X				
68123-18-2	Phenol, 4,4'-(1-methylethylidene) bis-, polymer with 2-(chloromethyl)oxirane, 2-methyloxirane and oxirane				X					
68425-75-2	Phosphate ester salt				X			X		
9005-70-3	POE (20) Sorbitan Trioleate				X					
68938-70-5	Poly (triethanolamine.mce)				X	X				
68955-69-1	Polyamine salts									
19019-43-3	Polycarboxlate salt [Trisodium ethylenediaminetetraacetate]				X	X				
26062-79-3	Polydimethyl diallyl ammonium chloride				X	X				
74-84-0	Polyethylene				X					
68036-92-0	Polyglycol diepoxide				X					
68036-95-3	Polyglycol diepoxide				X					
9038-95-3	Polyglycol ether				X					
No CASRN	Polyhydroxyalkanoates (PHA)									
64741-71-5	Polymers (petroleum) viscous				X					
36484-54-5	Polyoxyalkylene glycol				X					
61790-86-1	Polyoxyalkylenes				X					
9014-93-1	Polyoxyethylene dinonylphenol				X					
12068-19-8	Polyoxyethylene nonyl phenyl ether phosphate				X			X		
70142-34-6	Polyoxyl 15 hydroxystearate				X					
42751-79-1	Polyquaternary amine				X	X				
61790-41-8	Quaternary ammonium compound				X	X				
68609-18-7	Quaternized condensed alkanolamines				X	X				
91-63-4	Quinaldine				X	X				
12179-04-3	Sodium tetraborate pentahydrate								X	
64742-95-6	Solvent naphtha, petroleum, light arom.			X	X					
NP-SMO3_U1240	Sorbitan ester				X					
65996-69-2	Steel mill slag									

CASRN	**Chemical Name**	**EPA Method 624 or 8216 VOAs**	**EPA Method 625 or 8270 VOAs**	**EPA Method 8015 – Total carbon containing compounds" or "TPH", as total extractable and analyzed by GC**	**EPA Method 415.1, as total organic carbon (water)**	**EPA Method 350.2: Total Kieldahl Nitrogen, total nitrogen (water)**	**Total Sulfur (water)**	**Total Phosphorus (water)**	**EPA Method 6010B - Total or Extractable Metals**	**Other Methods**
No CASRN	Steranes or cyclopentanoperhydrophenanthrene									
8052-41-3	Stoddard Solvents			X	X					
7446-09-5	Sulfur dioxide				X					In air method
68140-11-4	Tall oil, DETA/ midazoline acetates				X	X				
72480-70-7	Tar bases, quinoline derivatives, quaternized benzyl chloride				X	X				
64-02-8	Tetrasodium ethylenediaminetetraacetate				X				X	
68527-49-1	Thiourea, polymer with formaldehyde and 1-phenylethanone				X	X				
64114-46-1	Triethanolamine homopolymer				X	X				
14932-42-4	Xenon-133									Xenon-133 produces beta radiation and stable daughter product

Table 12: Fate and transport parameter classifications related to EPI Suite output

Solubility [mg/L]	BioWIN Biodegradation [biodegradable/not biodegradable]	Log Koc	Henry's Law Constant [atm-m3]
>100 – Soluble	BioWIN 2: >0.5 biodegradable	>3.5 – Strongly Adsorbs to Organic Material	> 0.1 – Very Volatile
>0.1 to < 100 – Slightly Soluble	BioWIN 3: >2.2 biodegradable	>2.5 to 3.5 – Moderately Adsorbs to Organic Material	>0.001 to 0.1 – Slightly Volatile
<0.1 – Negligibly Soluble	BioWIN 6: >0.5 biodegradable	<2.5 – Less Likely to Adsorb to Organic Material	<0.001 – Not Volatile

Table 13: Available fate and transport parameters extracted from EPI Suite for the Chemicals of Interest and estimated phytoavailability score

CASRN	Chemical Name	Estimated Water Sol. (mg/L)	Solubility Classification	Henry's Law Constant (atm-m3)	Volatility in Water Classification	Estimated Log Koc	Sorptive Classification	BIOWIN2 (Non-Linear Model) Probability	BioWIN 2 Classification	BIOWIN3 numerical output	BioWIN 3 Classification	BIOWIN6 (Non-Linear MITI Model) Probability	BioWIN 6 Classification	Aggregated Biodegradation Classification	Phytoavailability Score
2673-22-5	Diester of sulfosuccinic acid sodium salt	0.000000366	Non	8.54E-11	Non	5.56	Strong	1	Biodeg.	3.03	Biodeg.	0.76	Biodeg.	Biodeg.	2
61790-59-8	Hydrogenated tallow amine acetone	0.05	Non	5.89E-13	Non	4.66	Strong	0.54	Biodeg.	2.77	Biodeg.	0.54	Biodeg.	Biodeg.	2
8052-41-3	Stoddard Solvents	1.25	Moderate	5.3	Very Volatile	3.16	Moderate	0.99	Biodeg.	3.48	Biodeg.	0.82	Biodeg.	Biodeg.	2
68439-70-3	Alkyl amine	0.879	Moderate	0.00145	Volatile	4.27	Strong	0.31	Non	2.71	Biodeg.	0.4	Non	No Consensus	3
300-92-5	Aluminum distearate	1.78E-11	Non	0	Non	8.13	Strong	0.12	Non	2.45	Biodeg.	0.28	Non	No Consensus	3
61791-26-2	Ethoxylated amine	0.0815	Non	5.12E-15	Non	4.19	Strong	0	Non	2.57	Biodeg.	0.19	Non	No Consensus	3
9014-93-1	Polyoxyethylene dinonylphenol	0.0000193	Non	1.02E-13	Non	5.45	Strong	0	Non	2.46	Biodeg.	0.17	Non	No Consensus	3
83-32-9	Acenaphthene	2.53	Moderate	0.000282	Non	3.7	Strong	0.88	Biodeg.	2.71	Biodeg.	0.29	Non	No Consensus	4
61791-24-0	Amine derivative	0.128	Moderate	4.5E-15	Non	4.19	Strong	0	Non	2.57	Biodeg.	0.12	Non	No Consensus	4
120-12-7	Anthracene	0.691	Moderate	0.0000513	Non	4.21	Strong	1	Biodeg.	2.22	Biodeg.	0.25	Non	No Consensus	4
56-55-3	Benzo(a)anthracene	0.0291	Non	0.00000501	Non	5.25	Strong	0	Non	1.9	Non	0.13	Non	Non	4
50-32-8	Benzo(a)pyrene	0.0104	Non	0.00000081	Non	5.77	Strong	0	Non	1.84	Non	0.09	Non	Non	4
205-99-2	Benzo(b)fluoranthene	0.0207	Non	0.00000081	Non	5.78	Strong	0	Non	1.84	Non	0.09	Non	Non	4
218-01-9	Chrysene	0.0264	Non	0.00000501	Non	5.26	Strong	0	Non	1.9	Non	0.13	Non	Non	4
53-70-3	Dibenzo(a,h)anthracene	0.0033	Non	0.000000489	Non	6.28	Strong	0	Non	1.78	Non	0.06	Non	Non	4
193-39-5	Indenopyrene	0.00249	Non	0.000000131	Non	6.29	Strong	0	Non	1.79	Non	0.06	Non	Non	4
85-01-8	Phenanthrene	0.677	Moderate	0.0000513	Non	4.22	Strong	1	Biodeg.	2.22	Biodeg.	0.25	Non	No Consensus	4
9005-70-3	POE (20) Sorbitan Trioleate	2.72E-19	Non	3.65E-20	Non	10	Strong	0	Non	2.02	Non	0.12	Non	Non	4
74-84-0	Polyethylene	939	Soluble	0.55	Very Volatile	1.12	Mobile	0.93	Biodeg.	3.13	Biodeg.	0.83	Biodeg.	Biodeg.	4
61790-86-1	Polyoxyalkylenes	0.00307	Non	1.28E-21	Non	2.96	Moderate	0	Non	2.63	Biodeg.	0.23	Non	No Consensus	4
61790-41-8	Quaternary ammonium compound	4.33	Moderate	3.99E-10	Non	5.39	Strong	0.49	Non	2.74	Biodeg.	0.29	Non	No Consensus	4
26027-38-3	Ethoxylated 4– nonphenol	0.827	Moderate	9.61E-15	Non	3.13	Moderate	0	Non	2.52	Biodeg.	0.23	Non	No Consensus	5
206-44-0	Fluoranthene	0.13	Moderate	0.0000083	Non	4.74	Strong	0	Non	1.95	Non	0.18	Non	Non	5
127087-87-0	Nonylphenol polyethylene glycol ether	1.1	Moderate	9.61E-15	Non	3.02	Moderate	0	Non	2.22	Biodeg.	0.09	Non	No Consensus	5
129-00-0	Pyrene	0.225	Moderate	0.0000083	Non	4.74	Strong	0	Non	1.95	Non	0.18	Non	Non	5
60-24-2	2-mercaptoethanol	194000	Soluble	0.000000127	Non	0.28	Mobile	0.95	Biodeg.	3.19	Biodeg.	0.82	Biodeg.	Biodeg.	6
100-73-2	Acrolein dimer	81100	Soluble	0.0000343	Non	0.17	Mobile	0.99	Biodeg.	2.97	Biodeg.	0.63	Biodeg.	Biodeg.	6
44992-01-0	Cationic acrylamide monomer	1000000	Soluble	6.96E-15	Non	1.17	Mobile	0.99	Biodeg.	2.91	Biodeg.	0.63	Biodeg.	Biodeg.	6
108-90-7	Chlorobenzene	401	Soluble	0.00399	Volatile	2.37	Mobile	0.77	Biodeg.	2.77	Biodeg.	0.29	Non	No Consensus	6
126-97-6	Ethanolamine thioglycolate	1000000	Soluble	8.21E-21	Non	0	Mobile	0.88	Biodeg.	3.02	Biodeg.	0.54	Biodeg.	Biodeg.	6
5877-42-9	Ethyl octynol	834	Soluble	0.00000427	Non	2.02	Mobile	0.98	Biodeg.	3.32	Biodeg.	0.63	Biodeg.	Biodeg.	6
119-65-3	Isoquinoline	1550	Soluble	0.000000688	Non	3.19	Moderate	0.76	Biodeg.	2.91	Biodeg.	0.42	Non	No Consensus	6

CASRN	Chemical Name	Estimated Water Sol. (mg/L)	Solubility Classification	Henry's Law Constant (atm-m3)	Volatility in Water Classification	Estimated Log Koc	Sorptive Classification	BIOWIN2 (Non-Linear Model) Probability	BioWIN 2 Classification	BIOWIN3 numerical output	BioWIN 3 Classification	BIOWIN6 (Non-Linear MITI Model) Probability	BioWIN 6 Classification	Aggregated Biodegradation Classification	Phytoavailability Score
19019-43-3	Polycarboxlate salt [Trisodium ethylenediaminetetraacetate]	1000000	Soluble	3.62E-20	Non	1.78	Mobile	0.62	Biodeg.	3.55	Biodeg.	0.95	Biodeg.	Biodeg.	6
64742-95-6	Solvent naphtha, petroleum, light arom.	142	Soluble	0.000526	Non	3.19	Moderate	1	Biodeg.	2.33	Biodeg.	0.43	Non	No Consensus	6
123-91-1	1,4 Dioxane	214000	Soluble	0.00000591	Non	0.42	Mobile	0.01	Non	2.99	Biodeg.	0.55	Biodeg.	No Consensus	7
479-66-3	1H, 3H-Pyrano (4,3-b)(1)benzopyran-9-carboxylic acid, 4,10-dihydro-3,7,8 trihydroxy-3-methyl-10-oxo (fulvic acid)	139000	Soluble	1.36E-22	Non	1	Mobile	0.38	Non	2.42	Biodeg.	0.21	Non	No Consensus	7
115-19-5	2-methyl-3-Butyn-2-ol	240000	Soluble	0.00000104	Non	0.62	Mobile	0.52	Biodeg.	2.8	Biodeg.	0.33	Non	No Consensus	7
29868-05-1	Alkanolamine phosphate	1000000	Soluble	3.21E-27	Non	0	Mobile	0.87	Biodeg.	3.01	Biodeg.	0.46	Non	No Consensus	7
111-44-4	Bis (2-chloroethyl) ether	6440	Soluble	0.000189	Non	1.51	Mobile	0	Non	2.53	Biodeg.	0.21	Non	No Consensus	7
2809-21-4	Hydroxyethylidenediphosphonic acid	134000	Soluble	9.79E-26	Non	0.13	Mobile	0.16	Non	2.53	Biodeg.	0.04	Non	No Consensus	7
68910-19-0	Oxyalkylated polyamine	1000000	Soluble	3.4E-24	Non	1	Mobile	0	Non	2.62	Biodeg.	0.04	Non	No Consensus	7
26062-79-3	Polydimethyl diallyl ammonium chloride	1000000	Soluble	7.2E-12	Non	2.04	Mobile	0.67	Biodeg.	2.84	Biodeg.	0.27	Non	No Consensus	7
9038-95-3	Polyglycol ether	1190	Soluble	5.26E-16	Non	1.75	Mobile	0	Non	2.74	Biodeg.	0.07	Non	No Consensus	7
12068-19-8	Polyoxyethylene nonyl phenyl ether phosphate	844	Soluble	1.36E-22	Non	2.79	Moderate	0	Non	2.07	Non	0.02	Non	Non	7
64-02-8	Tetrasodium ethylenediaminetetraacetate	1000000	Soluble	1.19E-23	Non	2.5	Mobile	0.05	Non	3.5	Biodeg.	0.95	Biodeg.	No Consensus	7

Table 14: Additional toxicity information on the Chemicals of Interest with agency derived toxicity values

CASRN	Chemical Name	Toxicity Value (mg/kg/d)	Toxicity Value Basis Summary	Toxicity Value Drinking Water Equivalent Concentration [mg/L]
53-70-3	Dibenzo(a,h)anthracene	0.000002	Dibenzo(a,h)anthracene toxicity value is based on the OEHHA oral cancer slope factor of 4.1 per mg/kg/day (OEHHA, Chemicals). The oral cancer slope factor is based on chronic oral mouse studies, which identified an increase in pulmonary adenomas, pulmonary carcinomas, mammary carcinomas, and hemangioendotheliomas (Snell & Stewart, 1962; Snell & Stewart, 1963; Biancifiori & Caschera, 1962; Berenblum & Haran, 1955).	0.000077
50-32-8	Benzo(a)pyrene	0.000003	Benzo(a)pyrene toxicity value is based on the OEHHA oral cancer slope factor of 2.9 per mg/kg/day (OEHHA). The Benzo(a)pyrene oral cancer slope factor is based on chronic rat studies which identified an increase in tumors in the forestomach, liver, oral cavity, jejunum or duodenum, and auditory canal (Kroese et al., 2001; Kroese et al., 2002; Beland & Culp, 1998; Neal & Rigdon, 1967; Rigdon & Neal, 1966; Rigdon & Neal, 1969). Oral benzo(a)pyrene exposure is also associated with less sensitive developmental effects such as neurobehavioral and cardiovascular effects. Additionally, benzo(a)pyrene is associated with decreased sperm counts, ovary weight, follicle numbers, immunoglobulin, B cell numbers, and thymus weight (Chen et al., 2011; Xu et al., 2010; De Jong et al., 1999; Kroese et al., 2001; Kroese et al., 2002).	0.00012

CASRN	Chemical Name	Toxicity Value (mg/kg/d)	Toxicity Value Basis Summary	Toxicity Value Drinking Water Equivalent Concentration [mg/L]
119-65-3	Isoquinoline	0.000003	isoquinoline toxicity value is based on U.S. EPA IRIS oral cancer slope factor of 3 per mg/kg/day for quinoline (U.S. EPA, IRIS). The quinoline oral cancer slope factor is based on oral subchronic rodent studies that identified an increase in hepatic hemangioendotheliomas and hemangiosarcomas (Hirao et al., 1976; Hasegawa et al., 1989; Shinohara et al., 1977). At higher quinoline concentrations, oral exposure was also associated with absolute and relative weight increases, fatty liver change, bile duct proliferation, and oval cell infiltration.	0.00012
111-44-4	Bis (2-chloroethyl) ether	0.000004	Bis (2-chloroethyl) ether toxicity value is based on the OEHHA oral cancer slope factor of 2.5 per mg/kg/day (OEHHA, Chemicals). The Bis (2-chloroethyl) ether oral cancer slope factor is based on a 79 week oral mouse study which identified an increase in hepatomas in both male and female mice (Innes et al., 1969). Oral exposure to Bis (2-chloroethyl) ether has also been associated with reduction in mean weight in males and females (Weisburger et al., 1981)	0.00015
7440-38-2	Arsenic	0.000007	Arsenic toxicity value is based on the U.S. EPA IRIS oral cancer slope factor of 1.5 per mg/kg/day (U.S. EPA, IRIS). The arsenic U.S. EPA IRIS oral cancer slope factor is based on human epidemiological studies that identified a significant increase in prevalence of skin cancer (Tseng et al., 1968; Tseng et al., 1977; Sommers & McManus, 1953). Oral arsenic exposure is also associated with hyperpigmentation, keratosis, and vascular complications (Tseng et al., 1968; Tseng et al., 1977).	0.00027

CASRN	Chemical Name	Toxicity Value (mg/kg/d)	Toxicity Value Basis Summary	Toxicity Value Drinking Water Equivalent Concentration [mg/L]
205-99-2	Benzo(b)fluoranthene	0.000008	Benzo(b)fluoranthene toxicity value is based on OEHHA oral cancer slope factor of 1.2 per mg/kg/day (OEHHA, Chemicals). The oral cancer slope factor is based on potency equivalency factor (PEF) that compares the potency of Benzo(b)fluoranthene to Benzo(a)pyrene. Based on two studies on the carcinogenic potential of polycyclic aromatic hydrocarbons, Benzo(b)fluoranthene was assigned a PEF of 0.1 (Habs et al., 1980; Deutsch-Wenzel et al., 1983).	0.00031
193-39-5	Indenopyrene	0.000008	Indenopyrene toxicity value is based on OEHHA oral cancer slope factor of 1.2 per mg/kg/day (OEHHA, Chemicals). The OEHHA oral cancer slope factor is based on a potency equivalency factor (PEF) that compares the potency of indenopyrene to Benzo(a)pyrene. Based on three studies on the carcinogenic potential of polycyclic aromatic hydrocarbons, indenopyrene was assigned a PEF of 0.1 (Clement Associates, 1988; Habs et al., 1980; Deutsch-Wenzel et al., 1983).	0.00031
56-55-3	Benzo(a)anthracene	0.000008	Benzo(a)anthracene toxicity value is based on OEHHA oral cancer slope factor of 1.2 per mg/kg/day (OEHHA, Chemicals). The OEHHA oral cancer slope factor is based on a potency equivalency factor (PEF) that compares the potency of Benzo(a)anthracene to Benzo(a)pyrene. Based on two studies on the carcinogenic potential of polycyclic aromatic hydrocarbons, Benzo(a)anthracene was assigned a PEF of 0.1 (Clement Associates, 1988; Bingham & Falk, 1969; Wislocki et al., 1986).	0.00031

CASRN	Chemical Name	Toxicity Value (mg/kg/d)	Toxicity Value Basis Summary	Toxicity Value Drinking Water Equivalent Concentration [mg/L]
218-01-9	Chrysene	0.00008	Chrysene toxicity value is based on OEHHA oral cancer slope factor of 0.12 per mg/kg/day (OEHHA, Chemicals). The OEHHA oral cancer slope factor is based on a potency equivalency factor (PEF) that compares the potency of chrysene to Benzo(a)pyrene. Based on a study on the carcinogenic potential of polycyclic aromatic hydrocarbons in tobacco smoke, chrysene was assigned a PEF of 0.01 (Clement Associates, 1988; Wynder & Hoffman, 1959).	0.0031
123-91-1	1,4 Dioxane	0.0001	1,4-Dioxane toxicity value listed is based on the U.S. EPA IRIS oral cancer slope factor of 0.1 per mg/kg/day (U.S. EPA, IRIS). The oral cancer slope factor is based on 2-year chronic rodent studies, which identified an increase in hepatocellular adenoma and carcinomas (Kano et al., 2009). Additionally, less sensitive effects of chronic 1,4-dioxane exposure include hepatocellular degeneration, liver necrosis, reduced weight gain, and kidney necrosis (Kociba et al., 1974; Kano et al., 2009; Argus et al., 1973).	0.0038
7440-43-9	Cadmium	0.0001	Cadmium toxicity value listed is the oral chronic ATSDR MRL (ATSDR, 2012d). The noncancer oral chronic toxicity value was based on the toxicity value of 0.5 µg/kg-day, which was calculated from the 95% lower confidence limit of the urinary cadmium level that was associated with a 10% increase in risk of proteinuria. Proteinuria was identified from a meta-analysis of a subset of environmental exposure studies (Buchet et al., 1990; Järup et al., 2000; Jin et al., 2004c; Kobayashi et al., 2006; Shimizu et al., 2006; Suwazono et al., 2006; Wu et al., 2001). The Nordberg-kjellstrom pharmacokinetic model was utilized to estimate the intake of cadmium necessary for the identified urine concentration (Kjellstrom & Nordberg, 1978).	0.0056

CASRN	Chemical Name	Toxicity Value (mg/kg/d)	Toxicity Value Basis Summary	Toxicity Value Drinking Water Equivalent Concentration [mg/L]
7439-97-6	Mercury	0.0002	Mercury toxicity value listed is the OEHHA mercury chronic REL (OEHHA, Chemicals). The noncancer oral chronic toxicity value was based on a NOAEL of 0.16 mg/kg/day identified in a chronic rat study conducted by the National Toxicology Program that identified renal toxicity as the most sensitive endpoint (NTP, 1993a). Chronic mercury exposure is also associated with motor skill deficits, mood changes, poor concentration, short-term memory deficits, blurred vision, paresthesia, and impaired nerve conduction.	0.011
7440-48-4	Cobalt	0.0003	Cobalt toxicity value listed is the PPRTV chronic provisional RfD (USEPA, 2008a). The PPRTV chronic provisional RfD was based on an identified LOAEL of 1 mg/kg/day for decreased iodine uptake in humans for a subchronic exposure (Roche & Layrisse, 1956). Less sensitive chronic cobalt exposure endpoints include increased erythrocyte number, increased hemoglobin, and cardiomyopathy (Taylor et al., 1977; Duckham & Lee, 1976; Davis & Fields, 1958; Morin et al., 1971; Alexander, 1969; Alexander, 1972).	0.017
7439-92-1	Lead	0.0003	Lead toxicity value listed is based on U.S. FDA guidance on recommended maximum level of lead in children's candy (USFDA, 2006). U.S. FDA recommends lead levels in children's candy not exceed 0.1ppm (USFDA, 2006). U.S. FDA based recommended maximum level of lead in candy on the Provisional total tolerable intake level (PTTIL) value of 6µg/day for children (USFDA, 2006). The PTTIL is based on developmental and neurological adverse effects.	0.017

CASRN	Chemical Name	Toxicity Value (mg/kg/d)	Toxicity Value Basis Summary	Toxicity Value Drinking Water Equivalent Concentration [mg/L]
7440-36-0	Antimony	0.0004	Antimony toxicity value listed is the RfD derived by U.S. EPA IRIS (USEPA, IRIS). The RfD was based on a chronic rat oral bioassay LOAEL of 0.35 mg/kg/day for reduced longevity, decreased blood glucose, and decreased cholesterol (Schroeder et al., 1970). A case study noted 56 people experienced burning stomach pain, colic, nausea, and vomiting after accidental ingestion of approximately 0.5 mg/kg of antimony (Dunn 1928, Monier-Williams, 1934).	0.022
1309-64-4	Antimony trioxide	0.0004	Antimony trioxide toxicity value is based on U.S. EPA IRIS RfD for antimony (USEPA, IRIS). See antimony.	0.022
7439-93-2	Lithium	0.002	Lithium toxicity value listed is the PPRTV chronic provisional RfD (USEPA, 2008b). As lithium is commonly used as a therapeutic, the RfD was based on a LOAEL of 2.1 mg/kg/day derived from the lower bound of the therapeutic serum concentration range of 0.6 mmol/L. Animal studies provide evidence that lithium causes adverse effects in multiple organs and systems at serum concentrations commonly reached for therapeutic purposes. Less sensitive adverse effects of lithium exposure include renal toxicity such as nephrogenic diabetes insipidus, and impaired renal concentrating ability (Gitlin et al., 1999; Berk & Berk, 2003).	0.11
1310-65-2	Lithium hydroxide	0.002	Lithium hydroxide toxicity value listed is based on U.S. EPA PPRTV RfD for lithium (USEPA, 2008b). See lithium.	0.11
13453-71-9	Lithium chlorate	0.002	Lithium chlorate toxicity value listed is based on U.S. EPA PPRTV RfD for lithium (USEPA, 2008b). See lithium.	0.11
13840-33-0	Lithium hypochlorite	0.002	Lithium hypochlorite toxicity value listed is based on U.S. EPA PPRTV RfD for lithium (USEPA, 2008b). See lithium.	0.11
554-13-2	Lithium carbonate	0.002	Lithium carbonate toxicity value listed is based on U.S. EPA PPRTV RfD for lithium (USEPA, 2008b). See lithium.	0.11

CASRN	Chemical Name	Toxicity Value (mg/kg/d)	Toxicity Value Basis Summary	Toxicity Value Drinking Water Equivalent Concentration [mg/L]
7440-41-7	Beryllium	0.002	Beryllium toxicity value listed is the U.S. EPA IRIS RfD (USEPA, IRIS). The noncancer oral chronic toxicity value was based on the BMD10 of 0.46 mg/kg/day for intestinal lesions observed in a 172-week dog study on oral exposure to beryllium sulfate tetrahydrate (Morgareidge et al., 1976).	0.11
7447-41-8	Lithium chloride	0.002	Lithium chloride toxicity value listed is based on U.S. EPA PPRTV RfD for lithium (USEPA, 2008b). See lithium.	0.11
7440-61-1	Uranium	0.003	Uranium toxicity value listed is the RfD derived by U.S. EPA IRIS for uranium salts (USEPA, IRIS). The noncancer oral chronic toxicity value was based on a LOAEL of 2.8 mg/kg/day for decreased body weight and nephrotoxicity observed in a 30 day oral rabbit bioassay.	0.17
7440-47-3	Chromium	0.003	Chromium toxicity value listed is the RfD derived by U.S. EPA IRIS for chromium (VI) (USEPA, IRIS). The RfD was based on a 1-year rat drinking water study that did not identify a LOAEL, but they report that tissue concentrations of chromium were higher in the hexavalent exposure group when compared to the trivalent group. The NOAEL of 2.5mg/kg/day was identified for chromium (VI) (MacKenzie et al, 1958). Other adverse effects associated with chromium (VI) include developmental toxicity at high concentrations (Junaid et al., 1996; Kanojia et al., 1996).	0.16
7439-98-7	Molybdenum	0.005	Molybdenum toxicity value listed is the RfD derived by U.S. EPA IRIS (USEPA, IRIS). The RfD was based on a LOAEL of 0.14 mg/kg/day for increased uric acid levels observed in an epidemiological study (Koval'skiy et al., 1961). Oral exposure to molybdenum was also associated with increased gout-like illness. Molybdenum also is associated with alterations in copper homeostasis (Arthur, 1965).	0.28

CASRN	Chemical Name	Toxicity Value (mg/kg/d)	Toxicity Value Basis Summary	Toxicity Value Drinking Water Equivalent Concentration [mg/L]
7782-49-2	Selenium	0.005	Selenium toxicity value listed is the RfD derived by U.S. EPA IRIS (USEPA, IRIS). The RfD was based on a NOAEL of 0.015 mg/kg/day for clinical selenosis observed in an epidemiological study (Yang et al., 1983; Yang et al., 1989a; Yang et al., 1989b). Symptoms associated with selenosis include gastrointestinal disorders, hair loss, morphological changes in nails, fatigue, neurological damage, and liver cirrhosis (Nelson et al., 1943; Harr & Muth, 1972).	0.28
7440-22-4	Silver	0.005	Silver toxicity value listed is the RfD derived by U.S. EPA IRIS (USEPA, IRIS). The RfD was based on a LOAEL of 0.014 mg/kg/day for argyria, a permanent discoloration of skin, in a human study (Gaul & Staud et al., 1935). While argyria is considered an adverse effect, the discoloration of skin is not associated with any additional adverse effects.	0.28
7440-50-8	Copper	0.01	Copper toxicity value listed is the intermediate oral MRL derived by ATSDR (ATSDR, 2004b). The noncancer oral intermediate toxicity value for copper was based on a NOAEL of 0.042 mg/kg/day for gastrointestinal effects in humans ingesting copper sulfate for 2 months (Araya et al., 2003). As nausea and vomiting, both acute effects, were the primary adverse effects noted in the study utilized for the MRL calculation, the intermediate oral MRL was utilized as the toxicity value. At considerably higher copper concentrations, copper is also associated with increased rates hepatocellular necrosis (Haywood et al., 1985; Olivares et al., 2001; Pizarro et al., 2001; NTP, 1993b)	0.56

CASRN	Chemical Name	Toxicity Value (mg/kg/d)	Toxicity Value Basis Summary	Toxicity Value Drinking Water Equivalent Concentration [mg/L]
7553-56-2	Iodine	0.01	Iodine toxicity value listed is the chronic oral MRL derived by ATSDR (ATSDR, 2004c) for iodide. Oral exposure to iodine was associated with subclinical hypothyroidism with thyroid gland enlargement in epidemiological studies (Boyages et al., 1989; Mu et al., 1987). Urinary iodide levels were utilized to estimate iodine oral intake levels. Oral overexposure to iodide is primarily associated with altered thyroid function, which can affect other endocrine organs, skin, cardiovascular system, central nervous system, kidneys, gastrointestinal tract, and reproductive systems (Braverman & Utiger, 2000).	0.56
7758-99-8	Copper sulfate pentahydrate	0.01	Copper sulfate pentahydrate toxicity value listed is based on the intermediate oral MRL derived by ATSDR for inorganic copper (ATSDR, 2004b). See copper.	0.56
7440-02-0	Nickel	0.01	Nickel toxicity value listed is the chronic oral REL derived by OEHHA for nickel and nickel compounds (OEHHA, Chemicals). The nickel REL was based on two NOAELs identified for perinatal mortality observed in two developmental rodent studies (NiPERA, 2000a; NiPERA, 2000b). Oral ingestion of nickel is also associated with reduced functional integrity of intestine, increased alkaline phosphatase, and spermatotoxicity (Singla et al., 2006; Kakela et al., 1999).	0.56
7786-81-4	Nickel sulfate	0.01	Nickel sulfate toxicity value listed is based on OEHHA REL for nickel and nickel compounds (OEHHA, Chemicals). See nickel.	0.56

CASRN	Chemical Name	Toxicity Value (mg/kg/d)	Toxicity Value Basis Summary	Toxicity Value Drinking Water Equivalent Concentration [mg/L]
7440-62-2	Vanadium	0.01	Vanadium toxicity value listed is the ATSDR oral intermediate MRL (ATSDR, 2012b). The noncancer oral chronic toxicity value was based on a NOAEL of 0.12 mg/kg/day for hematological alterations and blood pressure observed in a 12 week human study (Fawcett et al., 1997). No adverse effect was noted in the exposed group in the oral chronic study. Because no adverse effect was noted in the human study, no additional uncertainty factor was applied for derivation of a chronic toxicity value. Additionally, the vanadium MRL of 0.01 mg/kg/day is considerably below the National Academies Dietary Reference Intake (DRI) Tolerable Upper Intake Level of 0.025 mg/kg/day for vanadium. However, vanadium oral exposure at higher levels has been associated with alterations in erythrocyte and reticulocyte levels, increased blood pressure, neurodevelopmental toxicity, and developmental toxicity in rodents (Boscolo et al., 1994; Carmignani et al., 1991; Carmignani et al., 1992; Zaporowska et al. 1993; Domingo et al., 1986; Elfant & Keen, 1987).	0.56
108-90-7	Chlorobenzene	0.02	Chlorobenzene toxicity value listed is the U.S. EPA IRIS RfD (USEPA, IRIS). The RfD was based on a NOAEL of 27.25 mg/kg/day for histopathologic changes in the liver observed in a 13 week dog study (Monsanto, 1967a; Knapp et al., 1971). Histopathologic changes in the liver included bile duct proliferation, cytologic alternations, and leukocytic infiltration of the stroma. Less sensitive adverse effects of oral exposure to chlorobenzene included body weight loss, altered clinical chemistry, as well as pathologic changes in the kidney, gastrointestinal mucosa, and hematopoietic tissue (Monsanto, 1967b; Knapp et al., 1971).	1.1

CASRN	Chemical Name	Toxicity Value (mg/kg/d)	Toxicity Value Basis Summary	Toxicity Value Drinking Water Equivalent Concentration [mg/L]
129-00-0	Pyrene	0.03	Pyrene toxicity value listed is the U.S. EPA IRIS RfD (U.S. EPA, IRIS). The RfD was based on a NOAEL of 75 mg/kg/day for renal tubular pathology and decreased kidney weights identified in a mouse subchronic oral study (USEPA, 1989a). Oral exposure to pyrene is also associated with decreased body weight gain (White & White, 1939).	1.7
64742-95-6	Solvent naphtha, petroleum, light arom.	0.03	Solvent naphtha toxicity value listed is the U.S. PPRTV chronic oral RfD (U.S. EPA, PPRTV). The RfD was based on a NOAEL of 125 mg/kg/day for anemia, clotting deficits, and changes in liver chemistry identified in subchronic dog and rat studies (Mobil Oil Corporation, 1994; Bio/Dynamics, 1990a.; Bio/Dynamics, 1990b). Oral exposure to solvent naphtha was also associated with developmental effects such as decreased maternal mean body weight gain, decreased fetal body weight, and increased fetal skeletal variations (Bio/Dynamics, 1990c).	1.7
29868-05-1	Alkanolamine phosphate	0.04	Alkanolamine phosphate toxicity value listed is based on the toxicity value for monoethanolamine. NSF International evaluated the noncancer oral toxicity data for ethanolamine and calculated a reference dose (RfD) of 0.04 mg/kg/day. The RfD was based on a NOAEL of 120 mg/kg/day for maternal toxicity observed in pregnant rats that received ethanolamine via gavage (Hellwig and Liberacki, 1997).	2.2
206-44-0	Fluoranthene	0.04	Fluoranthene toxicity value listed is the U.S. EPA IRIS RfD (USEPA, IRIS). The noncancer oral chronic toxicity value was based on a NOAEL of 125 mg/kg/day for hepatic and urinary toxicity observed in a subchronic oral mouse bioassay (USEPA, 1988). Fluoranthene oral exposure is also associated with increased food consumption and increased body weight (USEPA, 1988).	2.2

CASRN	Chemical Name	Toxicity Value (mg/kg/d)	Toxicity Value Basis Summary	Toxicity Value Drinking Water Equivalent Concentration [mg/L]
16984-48-8	Fluoride	0.05	Fluoride toxicity value listed is the ATSDR MRL listed for fluorides (ATSDR, 2003a). The noncancer oral toxicity value was based on a NOAEL of 0.15 mg/kg/day for increased fracture rate observed in a human study (Li et al., 2001).	2.8
7664-39-3	Hydrofluoric acid	0.05	hydrofluoric acid toxicity value listed is based on ATSDR MRL for fluoride (ATSDR, 2003a). See fluoride.	2.8
83-32-9	Acenaphthene	0.06	Acenaphthene toxicity value listed is the U.S. EPA PPRTV RfD (USEPA, IRIS). The noncancer chronic oral toxicity value was based on a NOAEL of 175 mg/kg/day for hepatotoxicity in a mouse oral subchronic bioassay (USEPA, 1989b). Acenaphthene oral exposure was also associated with increased liver weight.	3.3
14797-65-0	Nitrite	0.1	Nitrite toxicity value listed is the U.S. EPA IRIS RfD (USEPA, IRIS). The noncancer oral chronic toxicity value was based on a NOEL of 1.0 mg/kg/day for methemoglobinemia in infants observed in an epidemiological study (Walton, 1951). Nitrate oral exposure is also associated with hyperglycemia and insulin resistance and reduced body weight in subchronic rat studies (El-Wakf et al., 2015; Al-Gayyar et al., 2015).	5.5
7439-96-5	Manganese	0.1	Manganese toxicity value listed is the ATSDR MRL (USEPA, IRIS). The noncancer oral chronic toxicity value was based on a NOAEL of 0.14 mg/kg/day for central nervous system adverse effects based on multiple chronic human studies on manganese consumption (Freeland-Graves et al., 1987; NRC, 1989; WHO, 1973).	5.5

CASRN	Chemical Name	Toxicity Value (mg/kg/d)	Toxicity Value Basis Summary	Toxicity Value Drinking Water Equivalent Concentration [mg/L]
7446-09-5	Sulfur dioxide	0.1	Sulfur dioxide toxicity value listed is based on the OEHHA MADL of 10 mg/day (OEHHA, Chemicals). There are no studies available for oral exposure to sulfur dioxide. However, OEHHA Developmental and Reproductive Toxicant Identification Committee (DARTIC) determined a need for the determination of an oral MADL due to presence of sulfites in food, which can form sulfur dioxide. Therefore, DARTIC determined a noncancer oral chronic toxicity value. The noncancer oral chronic toxicity value was extrapolated from an inhalation LOEL identified for reduction in fetal weight observed in two inhalation mouse studies (Murray et al., 1977; Murray et al., 1979). The extrapolated NOEL for a 30g mouse was calculated to be 3.864 mg/kg/day.	5.5
7440-42-8	Boron	0.2	Boron toxicity value listed is the U.S. EPA IRIS RfD (USEPA, IRIS). The noncancer oral chronic toxicity value was based on a BMDL05 of 10.3 mg/kg/day for decreased fetal weight observed in two rat studies on gestational oral exposure to boric acid (Price et al., 1996; Heindel et al., 1992). Boron was also associated with decreased relative testes weight, testicular atrophy, and reduced tubular size in a two year rat bioassay (Weir & Fisher, 1972).	11
12179-04-3	Sodium tetraborate pentahydrate	0.2	Sodium tetraborate pentahydrate toxicity value listed is based on USEPA IRIS RfD for boron (U.S. EPA, IRIS). See boron.	11
7440-39-3	Barium	0.2	Barium toxicity value listed is the ATSDR oral chronic MRL (ATSDR, 2007b). The noncancer oral chronic toxicity value was based on a BMDL05 of 61.13 mg/kg/day based on nephropathy in male mice in a two year drinking study (NTP, 1994). Barium oral exposure has also been associated with increased blood pressure.	11
7727-43-7	Barite	0.2	Barite toxicity value listed is based on ATSDR oral chronic MRL for barium (ATSDR, 2007b). See barium.	11

CASRN	Chemical Name	Toxicity Value (mg/kg/d)	Toxicity Value Basis Summary	Toxicity Value Drinking Water Equivalent Concentration [mg/L]
120-12-7	Anthracene	0.3	Anthracene toxicity value listed is the U.S. EPA IRIS RfD (USEPA, IRIS). The noncancer oral chronic toxicity value was based on a NOEL of 1,000 mg/kg/day in a subchronic oral mouse bioassay (USEPA, 1989c). No adverse effect was noted in this study. A 550 day oral rat bioassay found no adverse effects in rats exposed to up to 15 mg/kg/day (Schmahl et al., 1955).	17
7440-31-5	Tin	0.3	Tin toxicity value listed is the ATSDR intermediate oral MRL(ATSDR, 2005b). The noncancer oral intermediate toxicity value was based on a NOEL of 32 mg/kg/day for decreased hemoglobin concentration observed in a 13 week rat study (De Groot et al., 1973). Tin oral exposure was also associated with homogenous cytoplasm and bile duct epithelium proliferation at higher concentrations (De Groot et al., 1973).	17
7440-66-6	Zinc	0.3	Zinc toxicity value listed is the U.S. EPA IRIS RfD for zinc and zinc compounds (USEPA, IRIS). The noncancer oral chronic toxicity value was based on a LOAEL of 0.91 mg/kg/day for decreased erythrocyte Cu, Zn-superoxide dismutase activity (ESOD) identified in multiple human studies (Yadrick et al., 1989; Fischer et al., 1984; Davis et al., 2000; Milne et al., 2001). The human studies were conducted to determine zinc nutritional requirements. The LOAEL was calculated by averaging the LOAELs of the three studies (0.81 mg/kg/day, 0.94 mg/kg/day, 0.99 mg/kg/day) to obtain the LOAEL of 0.91 mg/kg/day.	17
7646-85-7	Zinc chloride	0.3	Zinc chloride toxicity value listed is the U.S. EPA IRIS RfD for zinc and zinc compounds (U.S. EPA, IRIS). See zinc.	17

Table 15: Chemicals of Interest without chronic oral toxicity data

CASRN	Chemical Name	Alternate Chemical Name	Is Polymer?
27646-80-6	2-Methylamino-2-methyl-1-propanol	--	no
67990-40-3	2-Propen-1-aminium, N,N-dimethyl-N-2-propenyl-, chloride, polymer with 2-hydroxypropyl 2-propenoate and 2-propenoic acid	--	yes
145417-45-4	2-Propenoic acid, 2-methyl-, polymer with methyl 2-methyl-2-propenoate, octadecyl 2-methyl 2 propenoate and 2propenoic acid, sodium salt	--	yes
9033-79-8	2-propenoic acid, polymer with sodium 2-propenoate	Sodium Acrylate Copolymer (absorbent polymer)	yes
130800-24-7	2-Propenoic acid, telomer with 2-methyl-2-(1-oxo-2-propenyl)-1-propanesulfonic acid, sodium salt	--	no
300-92-5	Aluminum distearate	--	no
No CASRN	Amide surfactant acid salt	--	no
No CASRN	Amides, Non Ionics	--	no
61791-24-0	Amine derivative	Polyethylene glycol soyamine	no
67924-33-8	Amine salt	Ethanol, 2,2',2''-nitrilotris-, homopolymer, hydrochloride	yes
NP-U2856	Amine salt	--	no
64346-44-7	Amine sulfate	Bis(isopropylammonium) sulphate	no
68239-30-5	Bis (HDMA) EPI Copolymer hydrochloride	--	yes
69418-26-4	Cationic acrylamide copolymer	Polyquaternium-33	yes
44992-01-0	Cationic acrylamide monomer	2-(Dimethylamino)ethyl acrylate methochloride; Ethanaminium, N,N,N-trimethyl-2-[(1-oxo-2-propenyl)oxy]-, chloride	yes
54076-97-0	Cationic polymer	Ethanaminium, N,N,N-trimethyl-2-((1-oxo-2-propenyl)oxy)-, chloride, homopolymer	yes

CASRN	Chemical Name	Alternate Chemical Name	Is Polymer?
681331-04-4	Causticized Lignite	--	no
64743-05-1	Coke (petroleum), calcined	--	no
25987-30-8	Copolymer of acrylamide and sodium acrylate	2-Propenoic acid, polymer with 2-propenamide, sodium salt	yes
129828-31-5	Crosslinked polyol ester	2-Propenoic acid, polymer with 4-(1,1-dimethylethyl)phenol, formaldehyde, 2,5-furandione, 2-methyloxirane, 4-nonylphenol and oxirane	yes
2673-22-5	Diester of sulfosuccinic acid sodium salt	--	no
No CASRN	Drilling paper	--	no
61791-26-2	Ethoxylated amine	PEG-10 Hydrogenated tallow amine	no
9081-83-8	Ethoxylated octylphenol	--	no
5877-42-9	Ethyl octynol	4-Ethyl-3-hydroxy-1-octyne	no
63428-92-2	Formaldehyde, polymer with 2-methyloxirane, 4-nonylphenol and oxirane	p-Nonylphenol, formaldehyde copolymer, ethoxylated and propoxylated	yes
30704-64-4	Formaldehyde, polymer with 4-(1,1-dimethylethyl)phenol, 2-methyloxirane and oxirane	p-tert-Butylphenol-formaldehyde resin, copolymer with ethylene oxide and propylene oxide	yes
30846-35-6	Formaldehyde, polymer with 4-nonylphenol and oxirane	--	yes
No CASRN	Heavy catalytic reformed naptha	--	no
61790-59-8	Hydrogenated tallow amine acetone	--	no
68648-89-5	Kraton G1702H	Benzene, ethenyl-, polymer with 2-methyl-1,3-butadiene, hydrogenated	yes
129521-66-0	Lignite	--	no
PE-M2464	Methyl oxirane polymer	--	yes
No CASRN	Organic acid ethoxylated alcohols	--	no

CASRN	Chemical Name	Alternate Chemical Name	Is Polymer?
68171-44-8	Oxyalkylated alkylphenolic resin	Formaldehyde, polymer with 4-(1,1-dimethylethyl)phenol, 4-nonylphenol and oxirane	yes
67939-72-4	Oxyalkylated polyamine	Triethylenetetramine polymer with oxirane and methyl oxirane	yes
68910-19-0	Oxyalkylated polyamine	Diethylenetriamine, propoxylated, ethoxylated	no
68123-18-2	Phenol, 4,4'-(1-methylethylidene) bis-, polymer with 2-(chloromethyl)oxirane, 2-methyloxirane and oxirane	--	yes
68425-75-2	Phosphate ester salt	Ethanol, 2-amino-, polymer with alpha-tridecyl-omega-hydroxypoly(oxy-1,2-ethanediyl) phosphate	yes
9005-70-3	POE (20) Sorbitan Trioleate	Polysorbate 85. No chronic oral studies are available, dermal studies show minor erythema (Mezei., 1975).	no
68938-70-5	Poly (triethanolamine.mce)	--	yes
68955-69-1	Polyamine salts	Hexanedinitrile, hydrogenated, high-boiling fraction, polymer with epichlorohydrin, acetate (salt)	yes
26062-79-3	Polydimethyl diallyl ammonium chloride	Polyquaternium-6; Quaternium-40	yes
68036-92-0	Polyglycol diepoxide	Oxirane, methyl-, polymer with oxirane, ether with 1,2,3-propanetriol (3:1), ether with (chloromethyl)oxirane polymer with 4,4'-(1-methylethylidene)bis(phenol)	yes
68036-95-3	Polyglycol diepoxide	Oxirane, methyl-, polymer with oxirane, ether with (chloromethyl)oxirane polymer with 4,4'-(1-methylethylidene)bis(phenol)	yes
No CASRN	Polyhydroxyalkanoates (PHA)	--	yes

CASRN	Chemical Name	Alternate Chemical Name	Is Polymer?
64741-71-5	Polymers (petroleum) viscous	TSCA Definition 2018: A complex combination of hydrocarbons obtained from distillation of products from the polymerization of propylene or butylene. It has a carbon number range from C12 upward and a boiling range from approximately 220.degree.C (428.degree.F) upward. The hydrocarbons are predominantly monoolefinic.	yes
36484-54-5	Polyoxyalkylene glycol	--	yes
61790-86-1	Polyoxyalkylenes	Fatty acids, tall-oil, monoesters with sorbitan, ethoxylated	no
9014-93-1	Polyoxyethylene dinonylphenol	Nonyl nonoxynol-10	no
12068-19-8	Polyoxyethylene nonyl phenyl ether phosphate	PEG-6 Nonyl phenyl ether phosphate, sodium salt	no
70142-34-6	Polyoxyl 15 hydroxystearate	--	yes
42751-79-1	Polyquaternary amine	Dimethylamine, polymer with epichlorohydrin and ethylenediamine	yes
68609-18-7	Quaternized condensed alkanolamines	Ethanol, 2,2',2''-nitrilotris-, homopolymer, reaction products with chloromethane	yes
No CASRN	Steranes or cyclopentanoperhydrophenanthrene	--	no
68140-11-4	Tall oil, DETA/ midazoline acetates	--	no
72480-70-7	Tar bases, quinoline derivatives, quaternized benzyl chloride	--	no
68527-49-1	Thiourea, polymer with formaldehyde and 1-phenylethanone	--	yes
64114-46-1	Triethanolamine homopolymer	--	yes

Table 16: Description of toxicity and available relevant toxicokinetic and toxicodynamic data for Chemicals of Interest with project specific surrogate toxicity values and chemicals with insufficient or incomplete data to derive a toxicity value

CASRN	Chemical Name	Toxicity Value (mg/kg/d)	Description of Toxicity	Relevant Toxicokinetic Data	Relevant Toxicodynamic Data
60-24-2	2-mercaptoethanol	0.005	In a sub-chronic rat study, changes in body weight gain and food consumption in addition to (in males) ptyalism, minimal to marked vacuolated hepatocytes accompanied by lower cholesterol and triglyceride levels, paleness and accentuated lobular pattern of the liver were observed. NOAEL = 15 mg/kg/d (ECHA, 2-mercaptoethanol).	In a toxicokinetic study, male rats received intraperitoneal injection of 2-mercaptoethanol (Federici et al., 1976). In this study, sulphate was identified as a major metabolite and isethionic acid was identified as a minor metabolite. In the same study, approximately 99% of the radiolabeled 2-mercaptoethanol was excreted in 48 hours. A separate in vitro study studied toxicokinetics of 2-mercaptoethanol using partly purified rat-liver preparation and alcohol dehydrogenase (Lambe et al., 1965). The study noted that 2-mercaptoethanol was likely oxidized by the liver alcohol dehydrogenase. A third publication on 2-mercaptoethnol toxicokinetics confirmed 2-mercaptoethanol is oxidized by aldehyde dehydrogenase in vivo in rat (Sabourault et al., 1977).	Using isolated rat spleen lymphocytes, Morris et al. observed a reduction in sister chromatid exchange (SCE) frequency when cultured with 20 uM 2-mercaptoethanol (Morris et al., 1990). A separate study by Janjic et al. (1992) noted a notable increase in glutathione levels in two rat insulinoma cell lines cultured with 2-mercaptoethanol. Lastly, a study on the effects of 2-mercaptoethanol on the liver found 2-mercaptoethanol induces fatty liver, and indirectly increases free fatty acid mobilization (Sabourault et al., 1997). These effects are most likely due to 2-mercaptoacetate, which forms through the oxidation of 2-mercaptoethanol.
64742-53-6	Distillates, hydrotreated light naphthenic	0.04	A sub-chronic rat study found hematologic effects. LOAEL = 125 mg/kg/d (ECHA, Distillates (petroleum), hydrotreated light naphthenic).	--	--
126-97-6	Ethanolamine thioglycolate	0.07	A chronic rat study found reproductive effects. NOAEL = 20 mg/kg/d (ECHA, 2-hydroxyethyl)ammonium mercaptoacetate).	--	--
115-19-5	2-methyl-3-Butyn-2-ol	0.2	A sub-chronic rat study found systemic toxicity manifested on kidney, as well as reproductive organs epididymis, testis, and ovary effects. NOAEL = 45 mg/kg/d (ECHA, 2-methylbut-3-yn-2-ol).	--	--
68308-87-2	Cottonseed, flour	0.2	Cottonseed flour contains gossypol, which is a liver, erythrocyte, and male reproductive toxicant; these are related to acute exposure and generally reversible once exposure has ended. Work had been done to test gossypol as a male contraceptive, however this work was stopped because in some cases fertility didn't return once gossypol was no longer being taken (Coutinho, 2002). In the case of male fertility, the contraceptive action of gossypol appears to be reversible at a daily dose of 5 mg/kg/day (Gu et al., 2000). GSI has applied a factor of 10 to account for susceptible populations.	Toxicokinetic data are available for gossypol. Gossypol is easily absorbed from the GI tract. It binds readily to dietary iron and amino acids, particularly lysine. Gossypol is not readily conjugated, metabolized or excreted via urine. It is predominantly eliminated in the feces (Garland, 2019).	Gossypol has been shown to by cytotoxic to human promyelocytic leukemia cell line (HL-60) leukemic cells, with an IC50 of 4.5 uM. Treatment of HL-60 cells with gossypol found a significant decrease in PP2A and hTERT activity (Sahin et al., 2010). In chronic lymphocytic leukemia cells, Gossypol has also been shown to act as a BH3-mimetic, resulting in induction of apoptosis (Balakrishan et al., 2008). Gossypol-induced apoptosis has also been shown to be caused by the downregulation of BCL-2 activation of numerous caspases (Huang et al., 2006).

CASRN	Chemical Name	Toxicity Value (mg/kg/d)	Description of Toxicity	Relevant Toxicokinetic Data	Relevant Toxicodynamic Data
26027-38-3	Ethoxylated 4– nonphenol	0.2	A reproductive rat study that exposed dams to nonoxynol-9 during gestation found developmental effects. NOAEL = 50 mg/kg/d (Meyer et al., 1988). This is a read-across study substituting NP-9 for NP-4	--	--
No CASRN	Nonylphenol ethoxylates	0.2	This is a polyoxyethylene alkylphenols, see Ethoxylated 4-nonphenol	--	--
127087-87-0	Nonylphenol polyethylene glycol ether	0.2	This is a polyoxyethylene alkylphenols, see Ethoxylated 4-nonphenol	--	--
68412-54-4	Oxyalkylated alkylphenol	0.2	This is a polyoxyethylene alkylphenols, see Ethoxylated 4-nonphenol	--	--
2809-21-4	Hydroxyethylidenediphosphonic acid	0.3	A chronic rat study found prolonged anemia in both sexes at the top dose, with a slight retardation of bone marrow development. Severe pallor of the skin of the top dose group animals and slight pallor in the mid dose rats was seen. A pale color was also noted for organs well supplied with blood (spleen and kidneys). These observations are consistent with perturbation of iron homeostasis. The NOAEL takes into consideration the most susceptible juvenile life period . NOAEL = 34 mg/kg/d (ECHA, Etidronic acid).	In an oral-repeated dose study in male Wistar rats, Hydroxyethylidenediphosphonic acid was found to be poorly absorbed (ECHA, Etidronic acid). Outside of the skeleton and liver, very limited Hydroxyethylidenediphosphonic acid was found in the body. Approximately 0.0065% of the overall intake was found in the skeletal tissue.	Hydroxyethylidenediphosphonic acid measurably decreased the affinity of hemoglobin for oxygen (Kol'tsova et al., 1979)
68439-70-3	Alkyl amine	0.4	In a chronic rat study given a diet containing 0, 0.01, 0.1 or 0.2 % test substance ad libitum for 104 weeks. No substance related effect was observed except decreased mean body weight in the highest dose group. NOAEL = 50 mg/kg/d (ECHA,Amines, C12-16-alkyldimethyl).	--	--

CASRN	Chemical Name	Toxicity Value (mg/kg/d)	Description of Toxicity	Relevant Toxicokinetic Data	Relevant Toxicodynamic Data
61790-41-8	Quaternary ammonium compound	0.4	A sub-chronic rat study found clinical signs of toxicity including reduced body weight gain, reduced food efficiency and occurrence of haemosiderine in kidneys of high dose animals. NOAEL = 40 mg/kg/d (ECHA, Quaternary ammonium compounds, trimethylsoya alkyl, chlorides).	Read-across studies provided toxicokinetic information relevant to Quaternary ammonium compounds. C16 TMAB is poorly absorbed in the gastro-intestinal tract (Isomaa et al., 1975). Livers and kidneys showed the highest levels of C16 TMAB. After approximately 4 days, only trace amounts were detected in the liver and kidneys. Greater than 50% of C16 TMAB was detected unchanged in feces. Major identified metabolites were oxidation products of the two decyl side chains. Identified metabolites were more polar than parent compound. Approximately 92% of the administered dose was detected in feces, while only 1% was detected in urine. Another study on quaternary ammonium compounds, C12-C16 ADBAC, found a small amount of an orally administered dose was rapidly absorbed (ECHA, Quaternary ammonium compounds). Residual levels of C12-C16 ADBAC was negligible after single and repeated dosing, which indicates low concern for bioaccumulation. The study found less than 50% of the administered dose was metabolized to side-chain oxidation products.	--
100-73-2	Acrolein dimer	Incomplete or insufficient data for toxicity value assessment	Acrolein dimer is the polymerized version of acrolein; it has a free aldehyde group. There is some evidence that the polymer is less toxic than the monomers with LD50 of 4920mg/kg and 26mg/kg, respectively. Long-term oral exposure to acrolein, at an amount within the range of human unsaturated aldehyde intake, induces a phenotype of dilated cardiomyopathy in the mouse, i.e., 1mg/kg for 48 days. Human exposure to acrolein may have analogous effects and raise consideration of an environmental, aldehyde-mediated basis for heart failure (Ismahil et al., 2011). The literature suggests that the toxicity for most aldehydes are mediated through similar pathways and similar function groups (LoPachin and Gavin, 2014). There is also concern unreacted acrolein may be present within the polymer. However, acrolein was evaluated in Task 1. Given acrolein is readily biodegradable and inherently volatile, concern regarding unreacted acrolein is limited.	--	--
No CASRN	Aromatic Amine	Incomplete or insufficient data for toxicity value assessment	Toxicity of aromatic amines is related to the form. See discussion in text.	--	--

CASRN	Chemical Name	Toxicity Value (mg/kg/d)	Description of Toxicity	Relevant Toxicokinetic Data	Relevant Toxicodynamic Data
38011-25-5	Disodium ethylenediaminetetraacetate	Incomplete or insufficient data for toxicity value assessment	Sodium EDTA has been shown in some studies to be cytotoxic, a reproductive toxicant, and to demineralize teeth, bones and organs in animals. However, for these studies, identifying the mg/kg doses is not possible because exposure groups are categorized by percentage of EDTA in food. Other studies reported in the same EDTA assessment report show no toxicity in rats exposed to 375 mg/kg/day for 721 days; no effects in a multigeneration study where rats were exposed up to 250 mg/kg/day; and in a dog study, no effects were seen in exposures up to 250 mg/kg/day (Lanigan and Yamerick 2002).	EDTA is poorly absorbed from the gastrointestinal tract (DrugBank, 2020). EDTA is primarily excreted unmetabolized (Bingham et al., 2001). When absorbed, it is primarily excreted by the kidney. Approximately 95% of EDTA is excreted within 24 hours (DrugBank, 2020).	EDTA are believed to be due to the formation of EDTA chelation with divalent and trivalent metals (Drugbank, 2020; Oosterlinck et al., 1991; Oosterlinck et al., 1992). It has also been reported that EDTA had a stabilizing effect on unbound hepatic glucocorticoid receptors, possibly due to interaction with endogenous metal ions involved in the glucocorticoid-receptor complex stabilization (Hubbard & Kalimi, 1983).
No CASRN	Heavy catalytic reformed naptha	Incomplete or insufficient data for toxicity value assessment	Heavy catalytic reformed naphtha is a complex combination of hydrocarbons formed through the catalytic reforming process. Heavy catalytic reformed naphtha is a component of full range catalytic reformed naphtha. Full range catalytic reformed naphtha is a broad molecular weight hydrocarbon mixture of various hydrocarbons. There is little evidence of acute toxicity, with an oral LD50 of > 5,000mg/kg in rats (SDS, 0129MAR020). There are no studies looking at chronic oral exposure to heavy catalytic reformed naphtha. The SDS for full range catalytic reformed naphtha lists the mixture as a Category 1A carcinogen (known carcinogen) and a Category 2 reproductive toxicant (suspected reproductive toxicant). However, the full range catalytic reformed naphtha is known to contain benzene, toluene, ethylbenzene, xylene, and naphthalene; chemicals likely absent from heavy catalytic reformed naphtha(SDS, 0129MAR020).	--	--
1415-93-6	Humic acids	Incomplete or insufficient data for toxicity value assessment	There is some evidence that Humic Acid could mechanistically be chronically toxic, as it promotes lipid peroxidation (Ho et al., 2003); damage to vascular endothelial cells (Kihara et al., 2014); and damage to cultured human umbilical endothelial cells (Hseu, 2002). However, there are no studies looking at exposures in humans. Humic acids are naturally occurring and no dosage information is available.	--	--

CASRN	Chemical Name	Toxicity Value (mg/kg/d)	Description of Toxicity	Relevant Toxicokinetic Data	Relevant Toxicodynamic Data
85-01-8	Phenanthrene	Incomplete or insufficient data for toxicity value assessment	There are no reliable human studies assessing chronic oral exposure to phenanthrene. The acute toxicity of phenanthrene has been determined for phenanthrene at 700 mg/kg (Lewis, 2004). It is not assessed under IRIS for oral exposure (US EPA, 1990). It is also not classifiable as to its human carcinogenicity due to a lack of studies (IARC, 2010b). Tests for DNA damage in mammalian cell cultures did not show any effect, however, a test of human lymphoblast TK6 cells incubated with rat liver S9 (Arochlor) and 9 µg/mL phenanthrene yielded a forward mutation (Barfknecht et al., 1981).	Phenanthrene is readily absorbed when ingested. Approximately 86% of orally-dosed phenanthrene was absorbed by pigs in the 24 hours following ingestion (Cavret et al., 2003). An oral repeated-dose study in rats found the highest phenanthrene tissue concentrations in fat, followed by muscle (Kang et al., 2007). The predominant metabolites of phenanthrene include 3-hydroxy phenanthrene, trans-9,10-dihydro-9,10-dihydroxyphenanthrene (Kang et al., 2007; Goodwin, 1976). Nordqvist et al determined approximately 92-96% of the metabolism of phenanthrene using rat microsomes results in the formation of dihydriodiols (Nordqvist et al., 1981).	Phenanthrene has been shown to induce cardiomyocyte hypertrophy rat and H9C2 cells (Huang et al., 2016). In this study, phenanthrene induced atrial natriuretic peptide, b-type natriuretic peptide, and c-myc in H9C2 cells and rats hearts. The authors believe the mechanism of cardiomyocyte hypertrophy may be due to reduction of mIR-133a expression by DNA methylation.
19019-43-3	Polycarboxlate salt [Trisodium ethylenediaminetetraacetate]	Incomplete or insufficient data for toxicity value assessment	See Disodium ethylenediaminetetraacetate	--	--
74-84-0	Polyethylene	Incomplete or insufficient data for toxicity value assessment	For this entry, “Polyethylene” in the list of chemical additives, a query of the CASRN number associated with the entry does not return polyethylene, but instead returns Ethane. Ethane is considered to be physiologically and toxicologically inert. At high concentration, risks are associated with the displacement of oxygen, which results in asphyxiation (Snyder, 1987). It is also possible that the CASRN is incorrect and this should be polyethylene glycol. Polyethylene glycols (PEGs) are acutely toxic, with no known chronic effects. The probably lethal oral dose in adult humans is between 1 oz and 1 pint (Laurence, 1977). However, PEG 3350 is used as a mild laxative in Miralax™, and other similar over-the-counter laxative products, with a dose of 17 g per day.	Negligible data regarding pharmacokinetics of ingested ethane. Based on a rat liver microsome study, metabolism of ethane to ethanol is expected to be limited (Snyder, 1987). The expected half-life of ethane in rats is 0.95 hours (Snyder, 1987).	--
9038-95-3	Polyglycol ether	Incomplete or insufficient data for toxicity value assessment	Comptox references 3 studies as available in COSMOS. COSMOS references 1964 studies by US FDA CFSAN. However, no additional report is available. The studies cannot be found electronically. Findings of the three studies area: Chronic oral "HNEL" in dog of 616 mg/kg-day for 714-day study; Chronic oral "HNEL" in rat of 500 mg/kg-day for 734-day study; Chronic oral "HNEL" in rat of 500 mg/kg-day for 793-day study. (COSMOS, CMS-14254)	--	--

CASRN	Chemical Name	Toxicity Value (mg/kg/d)	Description of Toxicity	Relevant Toxicokinetic Data	Relevant Toxicodynamic Data
91-63-4	Quinaldine	Incomplete or insufficient data for toxicity value assessment	Unable to find studies looking at chronic exposure to quinaldine. LD50 is 1230mg/kg in rats. It has the weakest mutagenicity among methylquinoline, with some indication of mutagenicity in bacterial cultures. Different bacteria studies of genotoxicity report both mutagenic (Dong et al., 1978; Takahashi et al., 1988) and null effects (Bowden et al., 1976). These kinds of bacterial culture studies do not necessarily predict cancer in higher life forms well (Hakura et al., 1999). However, innocuous chemicals rarely give false positives (Priva et al 1991)	When given orally, quinaldine was excreted unchanged (Komiya, 1965). When tested in vitro, quinaldine was metabolized to 2-methylquinoline-5,6-dihydro-5,6-diol (Saeki et al., 1996)	--
NP-SMO3_U1240	Sorbitan ester	Incomplete or insufficient data for toxicity value assessment	There are three main esters of sorbitan (sorbitan monostearate, sorbitan tristearate, and sorbitan monolaurate). Each of these esters of sorbitan are food additives and act as emulsifiers or wetting agents. It is unclear from the entry if the sorbitan used in oil and gas production is the same as that which is used as a food additive. For this reason, it is unclear as to the toxic potential of this oil/gas field additive. A number of 2-year oral repeated-dose rat studies of sodium monostearate were conducted at levels of 2% to 25% in diet. The studies found no adverse effects on survival, growth rate, reproduction, lactation, metabolism, behavior, food efficiency, organ weights or organ histology at 5% (Krantz et al., 1950a; Krantz et al., 1950b; Krantz et al., 1947; Oser & Oser, 1956a; Oser & Oser, 1956b; Fitzhugh et al., 1959). The NOAEL of 5% in the diet was equivalent to 2,500 mg/kg. For context, sorbitan monostearate is practically non-toxic with a probably human-lethal dose greater than 15 g/kg (Gosselin et al., 1976).	Both the fatty acid and polyhydric alcohol moiety of sorbitan monostearate are partially absorbed. The Polyhydric alcohol sorbitan is rapidly excreted in urine (Gosselin et al., 1976). In a study of sorbitan monostearate in drinking water, 16-25% of the administered dose was recovered in urine (Wick & Joseph, 1953).	--
65996-69-2	Steel mill slag	Incomplete or insufficient data for toxicity value assessment	TSCA Definition 2018: The fused substance formed by the action of a flux upon the gangue of the iron-bearing materials charged to a blast furnace and upon the oxidized impurities in the iron produced. Depending upon the particular blast furnace operation, the slag is composed primarily of sulfur and oxides of aluminum, calcium, magnesium, and silicon. Toxicity for steel mill slag will likely be attributable to metals discussed further in other sections of this report. There was no available literature directly assessing toxicity of steel mill slag contamination of waters.	--	--
8052-41-3	Stoddard Solvents	Incomplete or insufficient data for toxicity value assessment	In general, ingestion of most petroleum distillates at doses less than 1,000 mg/kg causes little toxicity (Ellenhorn and Barceloux, 1988)	--	--

CASRN	Chemical Name	Toxicity Value (mg/kg/d)	Description of Toxicity	Relevant Toxicokinetic Data	Relevant Toxicodynamic Data
64-02-8	Tetrasodium ethylenediaminetetraacetate	Incomplete or insufficient data for toxicity value assessment	See Disodium ethylenediaminetetraacetate	--	--
479-66-3	1H, 3H-Pyrano (4,3-b)(1)benzopyran-9-carboxylic acid, 4,10-dihydro-3,7,8 trihydroxy-3-methyl-10-oxo (fulvic acid)	Incomplete or insufficient data for toxicity value assessment	Fulvic acid is an organic acid structurally similar to humic acids. Fulvic acid is associated with Kashin-beck disease (KBD), a chronic osteoarthritic disease endemic to parts of china. Consumption of drinking water containing 211 ppm fulvic acid in conjunction with a low-selenium diet for 49 days resulted in reduced skeletal tissue structural integrity in mice (Yang et al., 1993). There is some evidence that fulvic acid could mechanistically be chronically toxic, as it alters immune response and has been shown to reduce thyroid function (Vucskits et al., 2010).	Fulvic acid is readily soluble in water and due to its low molecular weight, it is readily absorbed from the intestinal tract and eliminated from the body within hours (Islam et al., 2005).	--

Table 17: Reproduction of Table 1 in Leusch and Snyder (2015), "Summary of bioanalytical tools applied to various recycled water scheme (sorted by project and/or publication date)"

Site Location	Assay Test
Dan Region Sewage Reclamation Project, Israel (1960-present)	Mutagenicity (Ames test)
Montebello Forebay Groundwater Recharge Project, California, USA (1962-present)	Mutagenicity (Ames test)
	Carcinogenicity (mammalian cell transformation assay)
Orange County Water Factory 21 (1975–2004) and Groundwater Replenishment System (2004-present), California, USA	Mutagenicity (Ames test)
Potomac Estuary Experimental Water Treatment Plant, Virginia, USA (1980–1982)	Mutagenicity (Ames test)
	Carcinogenicity (mammalian cell transformation assay)
Tampa Water Resource Recovery Project, Florida, USA (1987–1989)	Mutagenicity (Ames test)
	Genotoxicity (sister chromatid exchange test)
San Diego Total Resources Recovery Project, California, USA (1981–1999)	Mutagenicity (Ames test)
	Genotoxicity (micronucleus test, 6-thioguanine resistance assay)
	Carcinogenicity (mammalian cell transformation assay)
Tucson Reclaimed Water System, Arizona, USA (1989-present)	Mutagenicity (Ames test)
Windhoek Direct Potable Reuse Scheme, Namibia (1968-present),	Cytotoxicity to bacteria (bacterial growth test)
	Cytotoxicity to human cells (LDH leakage assay with whole blood cells)
	Mutagenicity (Ames test)
	Neurotoxicity (AChE inhibition)
	Immunotoxicity (cytokine production with whole blood cells)
Landsborough Water Reclamation Plant, Queensland, Australia	Cytotoxicity to bacteria (Microtox)
	Estrogenicity (E-SCREEN, ERBA)
Five water reclamation plants in the USA	Estrogenicity (E-SCREEN, YES)
	Androgenicity (A-SCREEN, YAS)
Perth Groundwater Replenishment Scheme, Western Australia, Australia (2009-present)	Cytotoxicity to bacteria (Microtox)
	Genotoxicity (umuC)

Site Location	Assay Test
	Estrogenicity (E-SCREEN)
	Androgenicity (AR-CALUX)
	Phytotoxicity (I-PAM)
Qld Western Corridor Recycled Water Scheme, Queensland, Australia (2009-present)	Cytotoxicity to bacteria (Microtox)
	Genotoxicity (umuC)
	AhR induction (AhR-CAFLUX)
	Estrogenicity (E-SCREEN)
	Phytotoxicity (I-PAM)
	Neurotoxicity (AChE inhibition)
South Caboolture Water Reclamation Plant, Queensland, Australia	Cytotoxicity to bacteria (Microtox)
	Estrogenicity (E-SCREEN)
	AhR induction (AhR-CAFLUX)
	Neurotoxicity (AChE inhibition)
	Phytotoxicity (I-PAM)
	Genotoxicity (umuC)
Gerringong Water Reclamation Plant, Victoria, Australia	Cytotoxicity to bacteria (Microtox)
	Estrogenicity (E-SCREEN)
Unidentified water reclamation plant in Queensland, Australia	Cytotoxicity to bacteria (ToxScreen3)
	Androgenicity (AR-CALUX)
	Estrogenicity (ER-CALUX)
	Genotoxicity (umuC)
Nine water reclamation plants in various Australian states	Cytotoxicity to human cells (Caco2 NRU, WIL2NS TOX, HepaTOX)
	Mutagenicity (Ames test)
	Genotoxicity (WIL2NS FCMN)
	Endocrine activity (CALUX [ERα, AR, GR, PR and TRβ])
	Neurotoxicity (AChE inhibition)
	Immunotoxicity (cytokine production with THP1 cells)
	MFO induction (HepCYP1A2)

Site Location	Assay Test
	Cytotoxicity (AREc32 cell viability, Caco2 NRU, RTG2 MTT, DART 28 lethality, SK-N-SH cytotoxicity, algae growth inhibition, Microtox, Photobacterium phosphoreum T3)
	Phytotoxicity (I-PAM)
	Endocrine activity (CALUX [ERα, AR, GR, PR and TRβ], GeneBLAzer [ER, AR, GR and PR], yeast screen [estrogen and androgen], E-SCREEN, hER yeast, medER yeast, HELN [ERα, ERβ, AR and TR], FACTORIAL [ERE-cis, ERα-trans, AR-trans, GR-trans, THRα1-trans and RORβ-trans], hERα-HeLa-9903, MCF7 [ERE and ARE], steroidogenesis, DART CYP19A1B aromatase, MDA-kb2 [AR and GR], switchgear-GR, T-SCREEN, P19/A15, hRAR yeast assay)
	Neurotoxicity (AChE inhibition)
	Immunotoxicity (THP1 cytokine production assay)
	Mutagenicity (Ames [TA98, TA100 and TAmix])
	Genotoxicity (umuC, micronucleus assay)
	Protein toxicity (E. coli GSH±)
	Adaptive stress response (FACTORIAL [HSE-cis, HIF-1a-cis, NFκB-cis, Nrf2/ARE-cis and p53-cis], DART HSPB11 induction, switchgear– hypoxia, GeneBLAzer [NFκB and p53], CALUX [NFκB, Nrf2 and p53], Jurkat E6.1 IκB, AREc32, Nrf2-keap)
	Xenobiotic metabolism (FACTORIAL [PXR-cis, PXR-trans, CAR-trans, PPARγ-cis, PPARγ-trans and AhR-cis], HG5LN PXR, CAR-yeast, CALUX [PPARα and PPARγ], MCF7-PPAR, PPARγ-GeneBLAzer, AhR-yeast, AhR-CAFLUX, H4IIEluc, MCF7-DRE, DART CYP1A induction)

Table 18: Cross comparison of chemicals detected in crops with list of Chemicals of Interest and potential sources of chemicals detected in crops

Target Analytes	**Chemical of Interest**	**Additive Chemical**	**Identified in the Literature as Associated with Oil Production**	**Naturally Occurring Chemical**	**Number of Crop Types the Chemical was Detected**
Strontium	X	X	X	X	13
Copper	X	X	X	X	12
Acetone		X	X	X	11
Acrolein		X	X	X	7
Barium	X	X	X	X	7
Ethyl acetate		X	X	X	6
Methanol		X	X	X	5
p-Isopropyltoluene		X	X	X	5
Zinc	X	X	X	X	3
Antimony	X	X	X	X	2
Bis(2-ethylhexyl)phthalate					2
Cadmium	X	X	X	X	2
Molybdenum	X	X	X	X	2
Nickel	X	X	X	X	2
2-Butanone			X	X	1
2-Chloroethyl vinyl ether					1
2-Hexanone				X	1
Arsenic	X		X	X	1
Bromomethane					1
Chloromethane					1
Chromium	X	X	X	X	1
Lead	X	X	X	X	1
Methyl tert-butyl ether (MTBE)					1
sec-Butylbenzene					1