SUPERFUND CHEMICAL DATA MATRIX (SCDM) METHODOLOGY

Prepared for:

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1200 Pennsylvania Avenue, NW (5204P)
Washington, DC 20460

January 2024

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ACRONYMS and ABBREVIATIONS

AALAC	Ambient Aquatic Life Advisory Concentrations
ACF	Area Correction Factor
ACGIH	American Conference of Governmental Industrial Hygienists
ATSDR	Agency for Toxic Substances and Disease Registry
AWQC	Ambient Water Quality Criteria
BCF	Bioconcentration Factor
CAS RN	Chemical Abstracts Survey Registry Number
CCC	Criterion Continuous Concentration
CERCLA	Comprehensive Environmental Response, Compensation, and Liability Act
CFR	Code of Federal Regulations
CMC	Criterion Maximum Concentration
ED	Effective Dose
EPA	United States Environmental Protection Agency
EPI	Estimation Programs Interface
FDAAL	Food and Drug Administration Action Levels
f_s	Sorbent Content (fraction of clays plus organic carbon)
HEAST	Health Effects Assessment Summary Tables
HEDR	Handbook of Environmental Degradation Rates
HESD	U.S. EPA Office of Water Health Effects Support Documents
HLC	Henry's Law Constant
HRS	Hazard Ranking System
HSDB	Hazardous Substances Data Bank
HTF	Human Toxicity Factor
ICRP	International Commission on Radiological Protection
Int	Intermediate
IRIS	Integrated Risk Information System
IUR	Inhalation Unit Risk
K_d	Soil/Water Distribution Coefficient
K_{oc}	Soil Organic/Carbon Partition Coefficient
LC	Lethal Concentration
LD	Lethal Dose
Log K_{ow}	Logarithm of the n-Octanol-Water Partition Coefficient
MCI	Molecular Connectivity Index
MCLs	Maximum Contaminant Levels
MCLGs	Maximum Contaminant Level Goals
MRL	Minimal Risk Level
MW	Molecular Weight
NAAQS	National Ambient Air Quality Standards
NESHAPs	National Emission Standards for Hazardous Air Pollutants
NHL	Non-Hodgkin's Lymphoma
NIOSH	National Institute for Occupational Safety and Health
NPL	National Priorities List
OEHHA	California Environmental Protection Agency Office of Environmental Health Hazard Assessment
OSRTI	Office of Superfund Remediation and Technology Innovation
PAH	Polyaromatic Hydrocarbons
PCB	Polychlorinated Biphenyls
PFAS	Per- and Polyfluoroalkyl Substances

PPRTV	Provisional Peer Reviewed Toxicity Values
PRG	Preliminary Remediation Goals
RBA	Relative Bioavailability Adjustment
REL	Reference Exposure Level
RfC	Reference Concentration
RfD	Reference Dose
RPF	Relative Potency Factor
RME	Reasonable Maximum Exposure
RTECS	Registry of Toxic Effects of Chemical Substances
RTI	Research Triangle Institute
SC	Screening Concentration
SCDM	Superfund Chemical Data Matrix
SF	Slope Factor
SPHEM	Superfund Public Health Evaluation Manual
SRC	Syracuse Research Corporation
SsI	Subsurface Intrusion
STSC	Superfund Health Risk Technical Support Center
TCDD	2,3,7,8-Tetrachlorodibenzo-p-dioxin
TCE	Trichloroethylene
TEF	Toxicity Equivalence Factor
UMTRCA	Uranium Mill Tailings Radiation Control Act
WOE	Weight-of-Evidence

SUPERFUND CHEMICAL DATA MATRIX (SCDM) METHODOLOGY

[January 2024]

1.0 INTRODUCTION

The Superfund Chemical Data Matrix (SCDM) contains factor values and screening concentration benchmarks that can be used when applying the Hazard Ranking System (HRS; 40 CFR Part 300 Appendix A, 55 FR 51532; 82 FR 2760) to evaluate potential National Priorities List (NPL) sites. The HRS assigns factor values including those for toxicity, gas and vapor migration potential, gas and ground water mobility, surface water persistence, subsurface intrusion (SsI) degradation, and bioaccumulation potential. These assignments are based on the physical, chemical, ecological, toxicological, and radiological properties of hazardous substances present at a site. Hazardous substances, as defined for HRS purposes, include both hazardous substances referenced in the Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA) section 101(14), which are substances specifically listed under other federal laws and are known as "CERCLA hazardous substances," and "pollutants or contaminants" as defined in CERCLA itself in section 101(33).

SCDM contains HRS factor values and benchmarks for those hazardous substances frequently found at sites that are evaluated using the HRS. SCDM also contains the physical, chemical, toxicological, and radiological input data used to calculate the factors and benchmarks. The input data presented in SCDM are taken directly from peer reviewed, generally accepted literature sources and databases and/or U.S. Environmental Protection Agency (EPA) developed literature sources and databases; or are calculated using procedures set forth by the EPA and in the HRS. Further HRS procedures are then applied to the input data to determine factor values and benchmarks, which include both risk-based screening concentrations and concentrations specified in regulatory limits for the hazardous substances.

This document explains the procedures used to provide chemical and physical properties, factor values and screening concentration benchmarks for substances listed in SCDM. The current factor values and benchmarks published in the SCDM Web Query and changes noted in the SCDM Change Control and Errata Sheet (described below) supersede any previous values provided by SCDM. These values and benchmarks reflect the EPA's methodology for determining risk, as described in the EPA's *Risk Assessment Guidance for Superfund (RAGS) Volume 1: Human Health Evaluation Manual, Part F: Supplemental Guidance for Inhalation Risk Assessment* and *Part B: Development of Risk-based Preliminary Remediation Goals* (EPA-540-R-070-002/OSWER 9285.7-82) and *Soil Screening Guidance: Technical Background Document* (EPA/540/R95/128).

Section 2.0 (Data Selection Methodology) of this document explains how data are selected and prioritized for use in assigning SCDM values. Section 3.0 (Calculation of Interim Values) describes how some values (e.g., half-lives, distribution coefficients, slope factors and water solubility for metals) are calculated using data and methodologies from published literature or regulatory guidance documents. Section 4.0 (Screening Concentration Benchmarks) describes how screening concentration benchmarks are calculated for air, water, soil, and human food chain exposures. Section 5.0 (SCDM Data Reporting and Web Query) describes how SCDM data, HRS factor values, and screening concentration benchmarks are presented.

Data inputs, factor values and benchmarks are listed, by substance and Chemical Abstracts Survey Registry Number (CASRN), in the SCDM Web Query (http://www.epa.gov/superfund/superfund-chemical-data-matrix-scdm-query).

2.0 DATA SELECTION METHODOLOGY

This section describes the methodology used for collecting and selecting data to determine factor values and screening concentration benchmarks for the substances listed in SCDM. It also specifies data source reference hierarchies and how the hierarchies are applied for each data type.

Section 2.1 describes hazardous substance identification protocols and how they relate to special cases. Sections 2.2 through 2.8 specify the references used to obtain data and the methodologies used to extract the data and assign values. The criteria described in these sections were developed based on the type and quality of data available in the current SCDM references; they are not intended to apply to all data in general.

The references listed throughout Section 2.2 of this methodology document were last accessed during August – November 2012, in preparation for a comprehensive update to SCDM, which was published in January 2014. Any changes or additions since then are noted in the SCDM Change Control and Errata Sheet (available at: https://www.epa.gov/superfund/superfund-chemical-data-matrix-scdm).

2.1 General Protocols for SCDM Data Collection

Compiling data for SCDM requires a determination of which data reasonably apply to each hazardous substance. In most cases, data are collected for each substance from the specific references identified in Sections 2.2 through 2.8. In some cases, however, data in the references cited are available only for a class or mixture of hazardous substances and not for the individual substances that are included in the class or that make up the mixture. In general, if any of these classes or mixtures is present at a hazardous waste site, it is assumed that the most toxic, most persistent, or most bioaccumulative component of the class or mixture is present. For these mixtures or classes, SCDM collects and uses those data resulting in the greatest HRS factor values as specified by the HRS (e.g., lowest Reference Dose [RfD], highest slope factor [SF], longest half-life and greatest bioaccumulation factor) from the data provided in the references used. In other cases, data that are specific to individual substances are used or substituted as representative for a class of substances. There are also cases where references or reference hierarchies other than those described in Section 2.2 are used. These special cases are described in Sections 2.1.1 through 2.1.6 below.

2.1.1 Generic Values

SCDM contains generic values for the following classes of compounds:

- Chlordane (alpha and gamma) – SCDM contains some data for the alpha and gamma isomers of chlordane, but most values represent a mixture of the two. When a reference does not specify whether chlordane data were derived from a specific isomer or isomer concentration, SCDM uses the generic values.

- Chromium (all oxidation states) – SCDM contains values for chromium III, chromium VI, and a "generic" total chromium value to be used only when the specific oxidation state is not known. SCDM assigns the RfD, reference concentration (RfC), SF and inhalation unit risk (IUR) values from chromium VI to total chromium.

- Endosulfans – SCDM contains data for an endosulfan mixture and two endosulfan isomers (endosulfan I and endosulfan II). The RfD and distribution coefficient data are collected for endosulfan and applied to the endosulfan mixture and its isomers. SCDM contains a vapor pressure and Henry's Law Constant for each isomer.

- Polychlorinated biphenyls (PCBs) – PCBs are represented as a single class of compounds, regardless of the PCB mixture or mixtures that may be identified at a site. For PCBs, toxicity in SCDM is based on Aroclor 1254, which results in the most environmentally conservative screening concentration benchmarks and bioaccumulation/human food chain-based factor values for this group of compounds.

2.1.2 Use of Compound Classes to Assign Values for Individual Substances

SCDM assigns substance class data to the substances listed below. If no data can be found in the specified references for an individual substance, but data are available for the generic class to which the substance belongs, SCDM assigns the generic value to that substance. These substance classes contain relatively small sets of isomers, which are likely to occur as mixtures, and are well defined, in that the generic class typically refers to a mixture of all members of the class (e.g., o-, m-, p-xylenes). Members of these classes are also expected to have similar chemical behavior.

- Polyaromatic hydrocarbons (PAHs) – SCDM contains SF and IUR values for benzo(a)pyrene. When a SF and/or IUR are not available for similar PAHs listed in SCDM, SCDM applies relative potency factors (RPFs) to determine values for these substances. PAH-specific RPFs are obtained from EPA's *Provisional Guidance for Quantitative Risk Assessment of Polycyclic Aromatic Hydrocarbons* (EPA/600/R-93/089), July 1993. RPFs are not used to generate non-cancer values for PAHs (e.g., RfD or RfC).

- Polychlorinated dibenzo-dioxins and furans – SCDM contains SF, IUR, RfD, and RfC values for 2,3,7,8-tetrachlorodibenzo-p-dioxin (TCDD). When a substance-specific SF, IUR, chronic RfD and/or chronic RfC are not available for similar dioxins and furans listed in SCDM, SCDM applies toxicity equivalence factors (TEFs) to determine the values for these substances. For RfDs and RfCs, when neither a substance-specific chronic RfD/RfC nor a TEF is available, subchronic values may be considered. Substance-specific TEFs are obtained from EPA's *Recommended Toxicity Equivalence Factors (TEFs) for Human Health Risk Assessments of 2,3,7,8-Tetrachlorodibenzo-p-dioxin and Dioxin-Like Compounds* (EPA/100/R 10/005), December 2010. All members of this class are assigned the weight of evidence (WOE) assigned to TCDD, which is currently B2.

- Xylenes – Values are provided for o-xylene, m-xylene, and p-xylene. If no data can be found in the specified references for the individual substances, but data are available for the generic class of xylenes, SCDM assigns the generic value to the individual substances. The class of xylenes is a relatively small set of isomers that are likely to occur as mixtures. The class also is well defined in that the generic class (e.g., xylenes) almost always refers to a mixture of all members of the class (o-, m-, and p-xylene). The expected similarity in chemical behavior for members of each class, as well as the likelihood that they will occur as mixtures, makes using data from mixtures reasonable.

2.1.3 Substitution Classes

In some cases, SCDM uses data from a parent substance class, for particular substances of that class. SCDM contains three major classes of data for which data substitution may be applied: (1) toxicity, (2) ground water mobility and (3) other. All toxicity data used to determine human- or eco-toxicity factor values can be substituted. Ground water mobility data substitutions include water solubility, geometric mean water solubility and soil/water distribution coefficient (K_d). Parent class data also may be used for hydrolysis, biodegradation, photolysis, and volatilization half-lives, as well as bioconcentration factor (BCF) and logarithm of the n-octanol-water partition coefficient (Log K_{ow}).

Currently in SCDM, two groups of substances inherit data from a parent substance: metals and radioactive substances. Generally, metal-containing substances inherit data for ground water mobility values with the

elemental metal as the class parent. Radioactive isotopes may inherit data from the primary radioactive element. Substitute data are not applied to radioactive isotope decay chains.

2.1.4 Substances with Unique Value Selection

- Ammonium perfluoro-2-methyl-3-oxahexanoate.
  - SCDM assigns a freshwater ecological LC50 value for hexafluoropropylene oxide dimer acid to ammonium perfluoro-2-methyl-3-oxahexanoate using the following molecular weight conversion of the LC50 assigned to hexafluoropropylene oxide dimer acid: LC50 (ammonium perfluoro-2-methyl-3-oxahexanoate) = LC50 (hexafluoropropylene oxide dimer acid) x [molecular weight (ammonium perfluoro-2-methyl-3-oxahexanoate) / molecular weight (hexafluoropropylene oxide dimer acid)].
  - SCDM assigns a freshwater human food chain BCF value for hexafluoropropylene oxide dimer acid to ammonium perfluoro-2-methyl-3-oxahexanoate.
  - SCDM assigns a freshwater ecological BCF value for hexafluoropropylene oxide dimer acid to ammonium perfluoro-2-methyl-3-oxahexanoate.
  - SCDM assigns a K_{OC} value for hexafluoropropylene oxide dimer acid to ammonium perfluoro-2-methyl-3-oxahexanoate.

- Ammonium perfluorobutanoate.
  - SCDM assigns an RfD for perfluorobutanoic acid to ammonium perfluorobutanoate using the following molecular weight conversion of the RfD assigned to perfluorobutanoic acid: RfD (ammonium perfluorobutanoate) = RfD (perfluorobutanoic acid) x [molecular weight (ammonium perfluorobutanoate) / molecular weight (perfluorobutanoic acid)].
  - SCDM assigns a freshwater ecological BCF value for perfluorobutanoic acid to ammonium perfluorobutanoate.
  - SCDM assigns a freshwater ecological LC50 for perfluorobutanoic acid to ammonium perfluorobutanoate using the following molecular weight conversion of the LC50 assigned to perfluorobutanoic acid: LC50 (ammonium perfluorobutanoate) = LC50 (perfluorobutanoic acid) x [molecular weight (ammonium perfluorobutanoate) / molecular weight (perfluorobutanoic acid)].
  - SCDM assigns a K_{OC} value for perfluorobutanoic acid to ammonium perfluorobutanoate.
  - SCDM assigns WOE values for perfluorobutanoic acid to ammonium perfluorobutanoate.

- Ammonium perfluorohexanoate.
  - SCDM assigns an RfD for perfluorohexanoic acid to ammonium perfluorohexanoate using the following molecular weight conversion of the RfD assigned to perfluorohexanoic acid: RfD (ammonium perfluorohexanoate) = RfD (perfluorohexanoic acid) x [molecular weight (ammonium perfluorohexanoate) / molecular weight (perfluorohexanoic acid)].
  - SCDM assigns a freshwater ecological LC50 for perfluorohexanoic acid to ammonium perfluorohexanoate using the following molecular weight conversion of the LC50 assigned to perfluorohexanoic acid: LC50 (ammonium perfluorohexanoate) = LC50 (perfluorohexanoic acid) x [molecular weight (ammonium perfluorohexanoate) / molecular weight (perfluorohexanoic acid)].
  - SCDM assigns a K_{OC} value for perfluorohexanoic acid to ammonium perfluorohexanoate.
  - SCDM assigns a log K_{OW} value for perfluorohexanoic acid to ammonium perfluorohexanoate.

  - SCDM assigns WOE values for perfluorohexanoic acid to ammonium perfluorohexanoate.

- Asbestos and Lead – The HRS specifies that a human toxicity factor of 10,000 be assigned to asbestos, lead, and lead compounds. Asbestos also receives a K_d value of 1,000, as stated in the HRS.

- Bromodichloromethane – SCDM assigns an MCL to bromodichloromethane based on the MCL listed for total trihalomethanes (including bromodichloromethane, bromoform, dibromochloromethane, and chloroform). Concentrations of trihalomethanes can be added to determine if drinking water is at or above the MCL.

- Cadmium – For cadmium, the Integrated Risk Information System (IRIS) contains two RfD values: one for drinking water and one for dietary exposure. Because SCDM calculates RfD-based, non-cancer screening concentration benchmarks for both drinking water and dietary exposures, the more conservative value is used; therefore, SCDM uses the drinking water RfD for cadmium.

- Chloroform – SCDM assigns an MCL to chloroform based on the MCL listed for total trihalomethanes (including bromodichloromethane, bromoform, dibromochloromethane, and chloroform). Concentrations of trihalomethanes can be added to determine if drinking water is at or above the MCL.

- Copper – SCDM uses a HEAST water quality standard of 1.3 mg/L to determine an RfD for copper, based on drinking water exposure assumptions of 80 kg body mass, 30 years exposure, and 2.5 L/day ingestion.

- Dibutyltin compounds – SCDM assigns an RfD for dibutyltin dichloride using the following molecular weight conversion of the RfD assigned to dibutyltin: RfD (dibutyltin dichloride) = RfD (dibutyltin) x [molecular weight (dibutyltin dichloride) / molecular weight (dibutyltin)].

- Hexafluoropropylene oxide dimer acid.
  - SCDM assigns a saltwater human food chain BCF value for ammonium perfluoro-2-methyl-3-oxahexanoate to hexafluoropropylene oxide dimer acid.
  - SCDM assigns a saltwater ecological BCF value for ammonium perfluoro-2-methyl-3-oxahexanoate to hexafluoropropylene oxide dimer acid.

- Mercuric chloride – SCDM assigns an RfC for mercuric chloride using the following molecular weight conversion of the RfC assigned to mercury: RfC (mercuric chloride) = RfC (elemental mercury) x [molecular weight (mercuric chloride) / molecular weight (elemental mercury)]. SCDM also assigns an MCL for mercuric chloride using the following molecular weight conversion of the MCL assigned to mercury: MCL (mercuric chloride) = MCL (elemental mercury) x [molecular weight (mercuric chloride) / molecular weight (elemental mercury)].

- Perfluorobutanesulfonic acid – SCDM assigns freshwater and saltwater ecological LC_{50} values for potassium perfluorobutanesulfonate to perfluorobutanesulfonic acid using the following molecular weight conversion of the LC_{50} assigned to potassium perfluorobutanesulfonate: LC_{50} (perfluorobutanesulfonic acid) = LC_{50} (potassium perfluorobutanesulfonate) x [molecular weight (perfluorobutanesulfonic acid) / molecular weight (potassium perfluorobutanesulfonate)].

- Perfluorooctanesulfonic acid.
  - SCDM assigns BCF values for potassium perfluorooctanesulfonate to perfluorooctanesulfonic acid for freshwater human food chain BCF, freshwater ecological BCF, and saltwater ecological BCF.

- SCDM assigns a freshwater ecological LC_{50} for the perfluorooctanesulfonate anion to perfluorooctanesulfonic acid using the following molecular weight conversion of the LC_{50} available for the perfluorooctanesulfonate anion: LC_{50} (perfluorooctanesulfonic acid) = LC_{50} (perfluorooctanesulfonate anion) x [molecular weight (perfluorooctanesulfonic acid) / molecular weight (perfluorooctanesulfonate anion)].
- SCDM assigns a saltwater ecological LC_{50} for potassium perfluorooctanesulfonate to perfluorooctanesulfonic acid using the following molecular weight conversion of the LC_{50} assigned to potassium perfluorooctanesulfonate: LC_{50} (perfluorooctanesulfonic acid) = LC_{50} (potassium perfluorooctanesulfonate) x [molecular weight (perfluorooctanesulfonic acid) / molecular weight (potassium perfluorooctanesulfonate)].

- Potassium perfluorobutanesulfonate – SCDM assigns a K_{OC} for perfluorobutanesulfonic acid to potassium perfluorobutanesulfonate.

- Potassium perfluorobutanoate.
  - SCDM assigns an RfD for perfluorobutanoic acid to potassium perfluorobutanoate using the following molecular weight conversion of the RfD assigned to perfluorobutanoic acid: RfD (potassium perfluorobutanoate) = RfD (perfluorobutanoic acid) x [molecular weight (potassium perfluorobutanoate) / molecular weight (perfluorobutanoic acid)].
  - SCDM assigns a freshwater ecological BCF value for perfluorobutanoic acid to potassium perfluorobutanoate.
  - SCDM assigns a freshwater ecological LC50 for perfluorobutanoic acid to potassium perfluorobutanoate using the following molecular weight conversion of the LC50 assigned to perfluorobutanoic acid: LC50 (potassium perfluorobutanoate) = LC50 (perfluorobutanoic acid) x [molecular weight (potassium perfluorobutanoate) / molecular weight (perfluorobutanoic acid)].
  - SCDM assigns a K_{OC} value for perfluorobutanoic acid to potassium perfluorobutanoate.
  - SCDM assigns WOE values for perfluorobutanoic acid to potassium perfluorobutanoate.

- Potassium perfluorooctanesulfonate.
  - SCDM assigns a BCF value for perfluorooctanesulfonic acid to potassium perfluorooctanesulfonate for the saltwater human food chain BCF.
  - SCDM assigns lake and river hydrolysis half-life values for perfluorooctanesulfonic acid to potassium perfluorooctanesulfonate.
  - SCDM assigns a K_{OC} for perfluorooctanesulfonic acid to potassium perfluorooctanesulfonate.
  - SCDM assigns an RfD for perfluorooctanesulfonic acid to potassium perfluorooctanesulfonate using the following molecular weight conversion of the RfD assigned to perfluorooctanesulfonic acid: RfD (potassium perfluorooctanesulfonate) = RfD (perfluorooctanesulfonic acid) x [molecular weight (potassium perfluorooctanesulfonate) / molecular weight (perfluorooctanesulfonic acid)].

- Radium 226 (+D) and Radium 228 (+D) – SCDM assigns an MCL to radium 226 and radium 228 based on the combined MCL listed for radium 226 and radium 228. Concentrations of radium 226 and radium 228 can be added to determine if drinking water is at or above the combined MCL.

- Radium 228 (+D) – SCDM assigns the UMTRCA soil standard of 5 pCi/g for radium 226 to radium 228 based on 40 CFR Part 192 Subpart E, as well as the explanation from: U.S. EPA. February 12, 1998. *Use of*

Soil Cleanup Criteria in 40 CFR Part 192 as Remediation Goals for CERCLA Sites. Office of Radiation and Indoor Air, Washington, DC. https://nepis.epa.gov/Exe/ZyPDF.cgi/9101NOM6.PDF?Dockey=9101NOM6.PDF.

- Sodium perfluorobutanoate.
  - SCDM assigns an RfD for perfluorobutanoic acid to sodium perfluorobutanoate using the following molecular weight conversion of the RfD assigned to perfluorobutanoic acid: RfD (sodium perfluorobutanoate) = RfD (perfluorobutanoic acid) x [molecular weight (sodium perfluorobutanoate) / molecular weight (perfluorobutanoic acid)].
  - SCDM assigns a freshwater ecological BCF value for perfluorobutanoic acid to sodium perfluorobutanoate.
  - SCDM assigns a freshwater ecological LC50 for perfluorobutanoic acid to sodium perfluorobutanoate using the following molecular weight conversion of the LC50 assigned to perfluorobutanoic acid: LC50 (sodium perfluorobutanoate) = LC50 (perfluorobutanoic acid) x [molecular weight (sodium perfluorobutanoate) / molecular weight (perfluorobutanoic acid)].
  - SCDM assigns a K_{OC} value for perfluorobutanoic acid to sodium perfluorobutanoate.
  - SCDM assigns WOE values for perfluorobutanoic acid to sodium perfluorobutanoate.
- Sodium perfluorohexanoate.
  - SCDM assigns an RfD for perfluorohexanoic acid to sodium perfluorohexanoate using the following molecular weight conversion of the RfD assigned to perfluorohexanoic acid: RfD (sodium perfluorohexanoate) = RfD (perfluorohexanoic acid) x [molecular weight (sodium perfluorohexanoate) / molecular weight (perfluorohexanoic acid)].
  - SCDM assigns a freshwater ecological LC50 for perfluorohexanoic acid to sodium perfluorohexanoate using the following molecular weight conversion of the LC50 assigned to perfluorohexanoic acid: LC50 (sodium perfluorohexanoate) = LC50 (perfluorohexanoic acid) x [molecular weight (sodium perfluorohexanoate) / molecular weight (perfluorohexanoic acid)].
  - SCDM assigns a K_{OC} value for perfluorohexanoic acid to sodium perfluorohexanoate.
  - SCDM assigns a log K_{OW} value for perfluorohexanoic acid to sodium perfluorohexanoate.
  - SCDM assigns WOE values for perfluorohexanoic acid to sodium perfluorohexanoate.
- Tributyltin compounds – SCDM assigns an RfD for tributyltin chloride using the following molecular weight conversion of the RfD assigned to tributyltin: RfD (tributyltin chloride) = RfD (tributyltin) x [molecular weight (tributyltin chloride) / molecular weight (tributyltin)].
- Vanadium – SCDM assigns an RfD for vanadium using the following molecular weight conversion of the RfD available for vanadium pentoxide: RfD (vanadium) = RfD (vanadium pentoxide) x [molecular weight (vanadium) / molecular weight (vanadium pentoxide)].

2.1.5 Substances with Unique Reference Hierarchy Selections

- All PFAS substances – For multiple physical/chemical parameters (boiling point, density, HLC, K_{OC}, log K_{OW}, melting point, solubility, and vapor pressure) the following is considered the primary reference for PFAS substances: 3M. January 2021. *Summary of Physical/Chemical and Environmental Parameters for*

PFAS: Subject to Interim Special Order by Consent No. 20-086- CWP/AP/GW/HW/DW/SW, paragraph 37(J)(3). Environmental Studies Report E21-0037. https://semspub.epa.gov/src/document/HQ/100002785.

- Ammonium perfluoro-2-methyl-3-oxahexanoate – Formula, K_{OC}, molecular weight, RfD, solubility, and WOE values were selected from U.S. EPA. October 2021. *Human Health Toxicity Values for Hexafluoropropylene Oxide (HFPO) Dimer Acid and Its Ammonium Salt (CASRN 13252-13-6 and CASRN 62037-80-3), Also Known as "GenX Chemicals*." Office of Water, Health and Ecological Criteria Division. Washington, D.C. https://www.epa.gov/system/files/documents/2021-10/genx-chemicals-toxicity-assessment_tech-edited_oct-21-508.pdf.

- Ammonium perfluoro-2-methyl-3-oxahexanoate, hexafluoropropylene oxide dimer acid, and perfluorooctanoic acid – A hydrolysis half-life was selected from: 3M. January 2021. *Summary of Physical/Chemical and Environmental Parameters for PFAS: Subject to Interim Special Order by Consent No. 20-086- CWP/AP/GW/HW/DW/SW, paragraph 37(J)(3)*. Environmental Studies Report E21-0037. https://semspub.epa.gov/src/document/HQ/100002785.

- Ammonium perfluorobutanoate, perfluorobutanoic acid, perfluorooctanoic acid, potassium perfluorobutanoate, sodium perfluorobutanoate – A log K_{OW} value was selected from: Ding, Guanghui, and Peijnenburg, Willie J. G. M. 2013. *Physicochemical Properties and Aquatic Toxicity of Poly- and Perfluorinated Compounds*. Critical Reviews in Environmental Science and Technology. 43:6, 598-678.

- Ammonium perfluorobutanoate – Boiling point, formula, melting point, molecular weight, and vapor pressure values were selected from: CompTox Chemicals Dashboard. https://comptox.epa.gov/dashboard/.

- Ammonium perfluorohexanoate – Boiling point, density, melting point, and vapor pressure values were selected from: CompTox Chemicals Dashboard. https://comptox.epa.gov/dashboard/.

- Hexafluoropropylene oxide dimer acid – Boiling point, melting point, RfD, and WOE values were selected from U.S. EPA. October 2021. *Human Health Toxicity Values for Hexafluoropropylene Oxide (HFPO) Dimer Acid and Its Ammonium Salt (CASRN 13252-13-6 and CASRN 62037-80-3), Also Known as "GenX Chemicals*." Office of Water, Health and Ecological Criteria Division. Washington, D.C. https://www.epa.gov/system/files/documents/2021-10/genx-chemicals-toxicity-assessment_tech-edited_oct-21-508.pdf.

- Perfluorobutanesulfonic acid and potassium perfluorobutanesulfonate – River and lake hydrolysis half-life values were selected from: Australian Government, Department of Health and Ageing. November 2005. *Existing Chemical Hazard Assessment Report. Potassium Perfluorobutane Sulfonate*. National Industrial Chemicals Notification and Assessment Scheme. https://www.industrialchemicals.gov.au/sites/default/files/Potassium%20perfluorobutane%20sulfonate.pdf.

- Perfluorobutanesulfonic acid, perfluorobutanoic acid, perfluorohexanesulfonic acid, and perfluorohexanoic acid – K_{OC} values were selected from Guelfo, Jennifer L, and Higgins, Christoper P. 2013. *Subsurface Transport Potential of Perfluoroalkyl Acids at Aqueous Film-Forming Foam (AFFF) - Impacted Sites*. Environmental Science & Technology. 47: 4164-4171, and Supporting Information document (supporting information document available at https://pubs.acs.org/doi/suppl/10.1021/es3048043/suppl_file/es3048043_si_001.pdf).

- Perfluorobutanoic acid and perfluorooctanoic acid – An HLC value was selected from: ATSDR. Toxicological Profiles. https://www.atsdr.cdc.gov/toxprofiledocs/index.html.

- Perfluorooctanesulfonic acid – A melting point value was selected from: CompTox Chemicals Dashboard. https://comptox.epa.gov/dashboard/.

- Perfluorooctanesulfonic acid, perfluorooctanoic acid and potassium perfluorooctanesulfonate – WOE values were selected from: U.S. EPA. *EPA Non-Regulatory Health-Based Drinking Water Levels*, Health Effects Support Documents (HESD). Office of Water. Washington, DC. https://www.epa.gov/sdwa/epa-non-regulatory-health-based-drinking-water-levels.

- Perfluorooctanoic acid – A molecular weight value was selected from: U.S. National Library of Medicine. Bethesda, MD. *Hazardous Substances Data Bank (HSDB)*. (HSDB data accessed through the PubChem database at https://pubchem.ncbi.nlm.nih.gov/.)

- Perfluorononanoic acid – A solubility value was selected from: CompTox Chemicals Dashboard. https://comptox.epa.gov/dashboard/.

- Perfluorononanoic acid and perfluorooctanoic acid – K_{OC} values were selected from Higgins, Christopher P., and Luthy, Richard G. 2006. Sorption of Perfluorinated Surfactants on Sediments. Environ. Sci. Technol. 40(23): 7251-7256.

- Perfluorooctanoic acid – An SF value was selected from: U.S. EPA. *EPA Non-Regulatory Health-Based Drinking Water Levels*, Health Effects Support Documents (HESD). Office of Water. Washington, DC. https://www.epa.gov/sdwa/epa-non-regulatory-health-based-drinking-water-levels.

- Potassium perfluorooctanesulfonate – An HLC value and melting point value were selected from: Beach, Susan A, John L. Newsted, Katie Coady, and John P. Giesy. 2006. *Ecotoxicological Evaluation of Perfluorooctanesulfonate (PFOS)*, Reviews of Environmental Contamination and Toxicology. 186: 133-174. https://www.researchgate.net/publication/7103955_Ecotoxicological_Evaluation_of_Perfluorooctanesulfonate_PFOS.

- Potassium perfluorobutanoate – Boiling point, density, formula, melting point, molecular weight, and vapor pressure values were selected from: CompTox Chemicals Dashboard. https://comptox.epa.gov/dashboard/.

- Potassium perfluorooctanesulfonate – Vapor pressure and water solubility values were selected from: U.S. National Library of Medicine. Bethesda, MD. *Hazardous Substances Data Bank (HSDB)*. (HSDB data accessed through the PubChem database at https://pubchem.ncbi.nlm.nih.gov/.)

- Sodium perfluorobutanoate – Boiling point, density, melting point, and vapor pressure values were selected from: CompTox Chemicals Dashboard. https://comptox.epa.gov/dashboard/.

- Sodium perfluorohexanoate – Boiling point, density, melting point, and vapor pressure values were selected from: CompTox Chemicals Dashboard. https://comptox.epa.gov/dashboard/.

- Uranium – An ATSDR intermediate oral minimal risk level for "uranium, soluble salts" is selected for an RfD, in accordance with the December 21, 2016 U.S. EPA memorandum *Considering a Noncancer Oral Reference Dose for Uranium for Superfund Human Health Risk Assessments* (available at: https://semspub.epa.gov/src/document/HQ/196808).

- The following subchronic values are selected in accordance with the May 2021 U.S. EPA memorandum *Recommendations on the Use of Chronic or Subchronic Noncancer Values for Superfund Human Health Risk Assessments* (available at: https://semspub.epa.gov/src/document/HQ/100002839).

- An ATSDR intermediate-duration oral minimal risk level is selected for an RfD for:
  - Atrazine
  - Cadmium
  - Heptachlor
  - Lindane (gamma-hexachlorocyclohexane)
- A PPRTV subchronic RfD is selected for an RfD for:
  - Bromodichloromethane
  - 4-methylphenol
  - Ethylbenzene
  - Hexachlorobenzene
  - 1,2,4,5-Tetrachlorobenzene
- An ATSDR intermediate-duration inhalation minimal risk level is selected for an RfC for vinyl chloride.
- A PPRTV subchronic RfC is selected for an RfC for ethyl chloride.

2.1.6 Substances with Unique Identifiers

There is no CASRN specific to uranium 238 (+D) (radionuclide). Therefore, the EPA identification number of E1734789 is used in its place. Information regarding EPA identification numbers may be found from the EPA Substance Registry Service (SRS, accessible online at http://ofmpub.epa.gov/sor_internet/registry/substreg/home/overview/home.do).

2.2 Data Used to Determine Human Toxicity Factor Values and Screening Concentration Benchmarks

Section 2.2 details how data are obtained for determining human toxicity factor (HTF) values and screening concentration benchmarks. RfD, RfC, SF, IUR, lethal dose with 50% mortality (LD_{50}), lethal concentration with 50% mortality (LC_{50}) and effective dose (ED_{10}) values are identified and used to determine the HTF value for each substance according to HRS Section 2.4.1.1. The RfD, RfC, SF, IUR values are also used to determine screening concentration benchmarks (see Section 4.0 of this document).

Non-carcinogenic data (RfD, RfC, LD_{50} and LC_{50}) and carcinogenic data (IUR, SF and ED_{10}) are selected for each substance according to a hierarchy of references. Of the values selected, the most conservative (i.e., most protective of human health) is used to determine the HTF, regardless of exposure route or whether the value represents a non-cancer or cancer effect.

2.2.1 SF, IUR, RfD and RfC Data Collection

SCDM does not assign RfD or RfC data to radionuclides. SF values (inhalation, oral and external exposure) are obtained for radionuclides from the following references, listed in order of preference:

- U.S. EPA *Preliminary Remediation Goals (PRGs) for Radionuclides*. Office of Superfund Remediation and Technology Innovation (OSRTI). http://epa-prgs.ornl.gov/radionuclides/download.html. Primary PRG source documents include:

  - Oak Ridge National Laboratory. September 2014. *Calculation of Slope Factors and Dose Coefficients*. ORNL/TM-2013/00. https://epa-prgs.ornl.gov/radionuclides/SlopesandDosesFinal.pdf.
  - Oak Ridge National Laboratory. January 2017. *Radon Cancer Risk Coefficients & Age-Specific Effective Dose Coefficients*. ORNL/TM-2017/47. https://epa-prgs.ornl.gov/radionuclides/RadonDoseandRiskCoefficientReport.pdf.

- U.S. EPA. *Health Effects Assessment Summary Tables (HEAST)*. Office of Research and Development/Office of Emergency and Remedial Response, Washington, DC. http://www.epa.gov/sites/production/files/2015-02/documents/heast2_table_4-d2_0401.pdf.

Accompanying area correction factors (ACFs) and decay constants (lambda) are also collected from the PRG source cited above.

For all other substances, RfD and RfC values are obtained from the following references, listed in order of preference:

- U.S. EPA. *Integrated Risk Information System (IRIS)*. Office of Research and Development, Cincinnati, OH. http://www.epa.gov/iris.

- U.S. EPA. *Provisional Peer Reviewed Toxicity Values for Superfund (PPRTVs)* derived by the EPA's Superfund Health Risk Technical Support Center (STSC) for the EPA Superfund program. https://www.epa.gov/pprtv.

- The Agency for Toxic Substances and Disease Registry (ATSDR) minimal risk levels (MRLs). https://www.atsdr.cdc.gov/mrls/index.html (non-cancer data only)

- The California Environmental Protection Agency (CALEPA) Office of Environmental Health Hazard Assessment's (OEHHA) Chronic Reference Exposure Levels (RELS) and Cancer Potency Values. Toxicity Criteria Database, and main chemical database. https://data.ca.gov/dataset/toxicity-criteria-database and http://oehha.ca.gov/risk/chemicalDB/index.asp.

- U.S. EPA. PPRTV Appendix Screening Toxicity Values (Derivation Support Documents). https://www.epa.gov/pprtv.

- U.S. EPA. *Health Effects Assessment Summary Tables (HEAST)*. Office of Research and Development/Office of Emergency and Remedial Response, Washington, DC.

ATSDR provides MRLs for acute (1 – 14 days), intermediate (>14 – 364 days), and chronic (365 days and longer) exposure durations. SCDM does not use MRLs that are based on acute exposure. Similarly, PPRTV, PPRTV Appendix, and HEAST provide RfD and RfC values (or PPRTV Appendix screening levels) for chronic and subchronic exposure durations. During SCDM data collection, preference is given to values that are based on chronic exposure. SCDM may use intermediate MRLs or subchronic RfDs or RfCs only if no chronic value is available from any reference in the above hierarchy.

Where intermediate MRLs are used in SCDM, the reference provided in the SCDM Web Query report is "ATSDR-Int." Where subchronic RfDs or RfCs from PPRTV or HEAST, or subchronic PPRTV Appendix screening levels, are used in SCDM, the reference provided in the SCDM Web Query report is "PPRTV-Sub," "HEAST-Sub" or "PPRTV_APP-Sub."

For non-radionuclide substances, SF and IUR values are obtained from the following references, listed in order of preference:

- U.S. EPA. *Integrated Risk Information System (IRIS)*. Office of Research and Development, Cincinnati, OH. http://www.epa.gov/iris.

- U.S. EPA. *Provisional Peer Reviewed Toxicity Values for Superfund (PPRTVs)* derived by the EPA's Superfund Health Risk Technical Support Center (STSC) for the EPA Superfund program. https://www.epa.gov/pprtv.

- The California Environmental Protection Agency (CALEPA) Office of Environmental Health Hazard Assessment's (OEHHA) Chronic Reference Exposure Levels (RELS) and Cancer Potency Values. Toxicity Criteria Database, and main chemical database. https://data.ca.gov/dataset/toxicity-criteria-database and http://oehha.ca.gov/risk/chemicalDB/index.asp.

- U.S. EPA. PPRTV Appendix (Derivation Support Documents). https://www.epa.gov/pprtv.

- U.S. EPA. *Health Effects Assessment Summary Tables (HEAST)*. Office of Research and Development/Office of Emergency and Remedial Response, Washington, DC. http://epa-heast.ornl.gov/.

2.2.2 Weight of Evidence (WOE)

When available, a carcinogenic risk WOE classification is collected from the same reference that provided the corresponding cancer risk value (e.g., IUR or SF). Where a WOE classification is available without a corresponding cancer risk, the available WOE will still be collected. If a WOE classification is available for one route (oral or inhalation) but not the other, it is applied to both routes unless reference information indicates a route restriction. In some instances, two or more WOE assessments are provided in a single reference. In these cases, the WOE assessment associated with the selected risk value is used; typically, this is the most recent WOE assessment.

2.2.3 LD_{50} – Oral, Dermal; LC_{50} - Inhalation

When no RfD, RfC, SF with WOE or IUR with WOE are available, SCDM uses an LD_{50} (oral, dermal) or LC_{50} (dust and gas inhalation) to assign HTF values. The lowest value is used to determine the HTF. LD_{50} and LC_{50} values are not used to calculate screening concentration benchmarks.

SCDM does not assign LD_{50} and LC_{50} values to radionuclides. The references used to collect these data for other substances are listed below, in order of preference:

- American Conference of Governmental Industrial Hygienists (ACGIH). 2012. *Threshold Limit Values and Biological Exposure Indices*, ACGIH, Cincinnati, OH.ISBN: 978-1-607260-48-6. https://www.acgih.org/.

- National Institute for Occupational Safety and Health (NIOSH). 2012. *Registry of Toxic Effects of Chemical Substances* (RTECS). http://www.cdc.gov/niosh/rtecs/.

SCDM contains the lowest LD_{50} or LC_{50} value for any mammalian species by the oral and dermal exposures, in controlled dose studies, with durations of less than 24 hours. LD_{50} and LC_{50} data that are reported in the references as less than or greater than a particular value are considered non definitive and are not used in SCDM.

2.2.4 ED_{10} and Weight-of-Evidence – Oral, Inhalation

In cases where neither a slope factor with WOE nor IUR with WOE is available for a substance, SCDM uses ED_{10} oral and inhalation values to calculate cancer SF (see Section 3.1 of this methodology document). SCDM does not assign ED_{10} values to radionuclides. For all other substances, SCDM uses data from the following references, listed in order of preference for oral and inhalation ED_{10} and associated WOEs:

- U.S. EPA. 1989. *Methodology for Evaluating Potential Carcinogenicity in Support of Reportable Quantity Adjustments Pursuant to CERCLA Section 102* (EPA_ED10), Office of Health and Environmental Assessment, Washington DC (EPA/600/8-89/053).

- U.S. EPA. 1986. *Superfund Public Health Evaluation Manual* (SPHEM), Office of Emergency and Remedial Response, Washington DC (EPA/540/1-86/060) (OSWER Directive 9285, 4-1).

ED_{10} data that are reported in the references as less than or greater than a particular value are considered non definitive and are not used in SCDM. Values that are included in EPA_ED10 are provided as potency factors; the reciprocal of these potency factors are used as ED_{10} values in SCDM.

2.3 Mobility/Volatility Information

Vapor pressures and Henry's Law Constants are used to determine the gas migration potential, gas mobility potential, and whether a substance is treated as a gas and/or particulate for the air migration pathway. They are also used to determine the vapor migration potential and whether a substance is considered volatile for the SsI component. Water solubility and soil/water distribution coefficients are used to determine ground water mobility factor values. Henry's Law Constants are also used to determine volatilization half-life.

2.3.1 Vapor Pressure

SCDM uses data from the following references to obtain vapor pressures for organic compounds, listed in order of preference:

- Syracuse Research Corporation (SRC). PHYSPROP Database. Syracuse, NY. http://www.srcinc.com/what-we-do/environmental/scientific-databases.html.

- The Estimation Programs Interface (EPI) Suite™ (experimental values). Developed by the U.S. Environmental Protection Agency's Office of Pollution Prevention and Toxics and Syracuse Research Corporation (SRC). http://www.epa.gov/tsca-screening-tools/epi-suitetm-estimation-program-interface.

- Perry's Chemical Engineers' Handbook, 8th Edition. 2008. Perry, Roberts H., Green, Don W., McGraw-Hill, ISBN: 978-0-07-142294-9.

- CRC Handbook of Chemistry and Physics, 93rd Edition. 2012 – 2013. W.M. Haynes, National Institute of Standards and Technology, CRC Press, Boulder, Colorado. ISBN-10: 1439855110/ISBN-13: 978-1439855119. Alternatively, values may be collected from the online CRC. https://hbcp.chemnetbase.com/.

- O'Neil, M., and A. Smith (Eds). 2012. The Merck Index, 14th Edition. Merck & Co., Inc., Rahway, NJ.

SCDM uses data from the following references to obtain vapor pressures for non-organic compounds, listed in order of preference:

- CRC Handbook of Chemistry and Physics, 93rd Edition. 2012 – 2013. W.M. Haynes, National Institute of Standards and Technology, CRC Press, Boulder, Colorado. ISBN-10: 1439855110/ISBN-13: 978-1439855119. Alternatively, values may be collected from the online CRC. https://hbcp.chemnetbase.com/.

- Syracuse Research Corporation (SRC). PHYSPROP Database. Syracuse, NY. http://www.srcinc.com/what-we-do/environmental/scientific-databases.html.

- Lange's Handbook of Chemistry. 16th Edition. 2004. Speight, James G., McGraw-Hill, ISBN-10:0071432205 / ISBN-13: 978-0071432207.

- Perry's Chemical Engineers' Handbook, 8th Edition. 2008. Perry, Roberts H., Green, Don W., McGraw-Hill, ISBN: 978-0-07-142294-9.

- O'Neil, M., and A. Smith (Eds). 2012. The Merck Index, 14th Edition. Merck & Co., Inc., Rahway, NJ.

If a recommended vapor pressure is not provided in the references, SCDM uses a value measured at 25°C. If more than one vapor pressure measured at 25°C is available, SCDM uses the highest value. If no value is available at 25°C, the value determined at a temperature closest to 25°C is selected. If no temperature is specified for all vapor pressure measurements for a substance, SCDM uses the highest value.

If no vapor pressure values are available in any of the references listed or if the referenced value is suspect, a value may be either selected from a data source outside the hierarchy or estimated. For any given substance, suspect values are identified by comparison with other vapor pressure values in SCDM data sources or other sources of chemical property data. The procedures described in Lyman *et al*. (1990) are used to estimate vapor pressure. RTI (1996) describes the use of these procedures for specific hazardous substances.

- Estimation procedures set forth by Lyman *et al*. 1990. Handbook of Chemical Property Estimation Methods. American Chemical Society, Washington, DC, as described in Research Triangle Institute (RTI). 1996. Chemical Properties for SCDM Development, Prepared for U.S. EPA Office of Emergency and Remedial Response.

For organic substances, if a vapor pressure is not available, a normal boiling point is obtained from the reference hierarchy listed in Section 2.8.1. If the boiling point at 1 atmosphere (atm) is <25°C, a default vapor pressure of 760 Torr is used with the assumption that the substance is a gas at 25°C—this approach is applied for the purposes of determining whether a substance qualifies as a gas and/or particulate for the air migration pathway and assigning a vapor pressure value in evaluating the air migration pathway gas migration potential factor value.

If no vapor pressure is available for a substance and the normal boiling point is ≥25°C, SCDM assumes that the substance is in a particulate form, rather than a gaseous form, and no vapor pressure is assigned. This assumption is made because the absence of a vapor pressure value often reflects an extremely low and difficult to measure (under standard conditions) value for nongaseous substances.

2.3.2 Henry's Law Constant

SCDM uses data from the following references to obtain Henry's Law Constants (HLC) for organic compounds, listed in order of preference:

- Syracuse Research Corporation (SRC). PHYSPROP Database. Syracuse, NY. http://www.srcinc.com/what-we-do/environmental/scientific-databases.html.

- EPI Suite™ (experimental values). Developed by the US Environmental Protection Agency's Office of Pollution Prevention and Toxics and Syracuse Research Corporation (SRC). http://www.epa.gov/tsca-screening-tools/epi-suitetm-estimation-program-interface.

SCDM uses data from the following references to obtain HLC's for inorganic compounds, listed in order of preference:

- Syracuse Research Corporation (SRC). PHYSPROP Database. Syracuse, NY. http://www.srcinc.com/what-we-do/environmental/scientific-databases.html.

- CRC Handbook of Chemistry and Physics. 93rd Edition. 2012 – 2013. W.M. Haynes, National Institute of Standards and Technology, CRC Press, Boulder, Colorado. ISBN-10: 1439855110/ISBN-13: 978-1439855119. Alternatively, values may be collected from the online CRC. https://hbcp.chemnetbase.com/.

- Lange's Handbook of Chemistry. 16th Edition. 2004. Speight, James G., McGraw-Hill, ISBN-10:0071432205 / ISBN-13: 978-0071432207.

- Perry's Chemical Engineers' Handbook, 8th Edition. 2008. Perry, Roberts H., Green, Don W., McGraw-Hill, ISBN: 978-0-07-142294-9.

- O'Neil, M., and A. Smith (Eds). 2012. The Merck Index, 14th Edition. Merck & Co., Inc., Rahway, NJ.

If a recommended value is not available, SCDM uses a value measured at 25°C. If more than one value measured at 25°C is available, SCDM uses the highest one. If no value is available at 25°C, the value determined at a temperature closest to 25°C is selected. If more than one value measured at the same temperature is available and none is recommended, SCDM uses the highest value. If no temperature is specified for all Henry's Law Constants for a substance, SCDM uses the highest value.

2.3.3 Water Solubility

Water solubility is used, along with K_d values, to calculate the ground water mobility of hazardous substances that do not meet observed release criteria. All hazardous substances that are available to migrate from sources at a site to the ground water are evaluated for ground water mobility. Water solubility values are also used to assign BCF values for hazardous substances when BCF or Log K_{ow} data are not available.

2.3.3.1 Water Solubility - Organic Substances

SCDM obtains water solubility values for organic substances from the following references, listed in order of preference:

- Syracuse Research Corporation (SRC). PHYSPROP Database. Syracuse, NY. http://www.srcinc.com/what-we-do/environmental/scientific-databases.html.

- EPI Suite™ (experimental values) developed by the US Environmental Protection Agency's Office of Pollution Prevention and Toxics and Syracuse Research Corporation (SRC). http://www.epa.gov/tsca-screening-tools/epi-suitetm-estimation-program-interface.

- CRC Handbook of Chemistry and Physics. 93rd Edition. 2012 – 2013. W.M. Haynes, National Institute of Standards and Technology, CRC Press, Boulder, Colorado. ISBN-10: 1439855110/ISBN-13: 978-1439855119. Alternatively, values may be collected from the online CRC. https://hbcp.chemnetbase.com/.

- Perry's Chemical Engineers' Handbook, 8th Edition. 2008. Perry, Roberts H., Green, Don W., McGraw-Hill, ISBN: 978-0-07-142294-9.

- Lange's Handbook of Chemistry. 16th Edition. 2004. Speight, James G., McGraw-Hill, ISBN-10:0071432205 / ISBN-13: 978-0071432207.

- Estimation procedures set forth by Lyman *et al*. 1990. *Handbook of Chemical Property Estimation Methods*. American Chemical Society, Washington, DC, as described in Research Triangle Institute (RTI). 1996. Chemical Properties for SCDM Development, Prepared for U.S. EPA Office of Emergency and Remedial Response.

If a recommended value is not available, SCDM uses a value measured at 25°C. If more than one value measured at 25°C is available, SCDM uses the highest one. If no value is available at 25°C, the value determined at a temperature closest to 25°C is selected. If more than one value measured at the same temperature is available and none is recommended, SCDM uses the highest value. If no temperature is specified for all water solubility measurements for a substance, SCDM uses the highest value.

2.3.3.2 Water Solubility – Metals, Metalloids and Radionuclides

SCDM obtains water solubility values for metals and metalloid compounds from the following references, listed in order of preference:

- CRC Handbook of Chemistry and Physics. 93rd Edition. 2012 – 2013. W.M. Haynes, National Institute of Standards and Technology, CRC Press, Boulder, Colorado. ISBN-10: 1439855110/ISBN-13: 978-1439855119. Alternatively, values may be collected from the online CRC. https://hbcp.chemnetbase.com/.

- Syracuse Research Corporation (SRC). PHYSPROP Database. Syracuse, NY. http://www.srcinc.com/what-we-do/environmental/scientific-databases.html.

- Lange's Handbook of Chemistry. 16th Edition. 2004. Speight, James G., McGraw-Hill, ISBN-10:0071432205 / ISBN-13: 978-0071432207.

- Perry's Chemical Engineers' Handbook, 8th Edition. 2008. Perry, Roberts H., Green, Don W., McGraw-Hill, ISBN: 978-0-07-142294-9.

For a metal or metalloid substance, SCDM determines and assigns water solubility as the geometric mean of the highest and lowest water solubility values available for compounds containing the metal or metalloid, as defined in the HRS (see HRS Section 3.2.1.2, Mobility), and described in Section 3.8 of this document.

2.3.4 Soil/Water Distribution Coefficient (Kd); Soil Organic/Carbon Partition Coefficients (Koc and Log Kow)

K_d values are used to calculate ground water mobility for hazardous substances that do not meet observed release

criteria. If K_d values are not available, associated K_{oc} and Log K_{ow} values are used to calculate K_d. All hazardous substances that are available to migrate from sources at the site to ground water are evaluated for ground water mobility.

For organic substances, SCDM calculates the K_d according to HRS Section 3.2.1.2 (Mobility) and the relationship of $K_d = K_{oc} \times f_s$ (see Section 3.5 of this methodology document), where f_s is the sorbent content (fraction of clays plus organic carbon) and K_{oc} is obtained from the following references, listed in order of preference:

- EPI Suite™ (estimated values) developed by the U.S. Environmental Protection Agency's Office of Pollution Prevention and Toxics and Syracuse Research Corporation (SRC). http://www.epa.gov/tsca-screening-tools/epi-suitetm-estimation-program-interface.

- U.S. EPA. 2002. *Supplemental Guidance for Developing Soil Screening Levels for Superfund Sites* (Peer Review Draft), OSWER 9355.4-24. http://www.epa.gov/superfund/soil-screening-guidance.

- U.S. EPA. 1996. *Soil Screening Guidance: Technical Background Document*. EPA/540/R95/128. Office of Emergency and Remedial Response, Washington, DC. NTIS PB96-963502. http://www.epa.gov/superfund/soil-screening-guidance.

- Estimated as described in Section 3.5 of this methodology document

When using values from EPI Suite™, SCDM prefers K_{oc} values that are estimated using the Molecular Connectivity Index (MCI) method over K_{oc} values that are estimated by the Log K_{ow} method. When a K_{oc} is not available using the MCI method, SCDM uses the EPI Suite™ K_{oc} values estimated using the Log K_{ow} method. Information regarding collection of Log K_{ow} values is provided in Section 2.5.2 of this methodology document. Section 3.5 (Soil Water Distribution Coefficient [K_d]; Soil Organic/Carbon Partition Coefficients [K_{oc}]) of this document provides additional information regarding SCDM calculations of K_d and K_{oc} values.

The exceptions to this hierarchy are the K_{oc} values for ionizable organic substances that are included in Table 42 in Part 5 of the *Soil Screening Guidance: Technical Background Document* cited above (derivation of these values is provided in Appendix L of the same document). For these substances, the K_{oc} is assigned based on values listed for pH 6.8 in Table 42 of that document instead of values available in the above hierarchy.

SCDM obtains K_d values for inorganic substances from the following references, listed in order of preference:

- U.S. EPA. 2002. *Supplemental Guidance for Developing Soil Screening Levels for Superfund Sites* (Peer Review Draft), Office of Solid Waste and Emergency Response. 9355.4-24. http://www.epa.gov/superfund/soil-screening-guidance.

- U.S. EPA. 1996. *Soil Screening Guidance: Technical Background Document*. EPA/540/R95/128. Office of Emergency and Remedial Response, Washington, DC. NTIS PB96-963502. http://www.epa.gov/superfund/soil-screening-guidance.

- Baes, C.F. III, R.D. Sharp, and A.L. Sjoreen, and R.W. Shor. 1984. *A Review and Analysis of Parameters for Assessing Transportation of Environmentally Released Radionuclides through Agriculture*. Oak Ridge National Laboratory, TN. ORNL-5786.

- HRS Section 3.2.1.2 (See Section 3.5 of this methodology document).

SCDM contains values corresponding to typical subsurface pH (e.g., 6.8).

2.4 Persistence/Degradation Information

The evaluation of persistence for non-radionuclides in the surface water migration pathway is based primarily on hydrolysis, biodegradation, photolysis, and volatilization half-lives of hazardous substances in surface water and secondarily on the sorption of the hazardous substances to sediments; for radionuclides the evaluation is based on volatilization and radioactive half-lives. Persistence information is used to determine the surface water persistence factor value.

The evaluation of degradation for the subsurface intrusion component is based on the SsI hydrolysis and SsI biodegradation half-lives of hazardous substances in the subsurface for non-radionuclides, and on radioactive half-life for radionuclides. Degradation information is used with other site-specific information to determine site-specific SsI degradation factor values. These SsI degradation factor values are based on site conditions and therefore, not included in SCDM.

2.4.1 Surface Water Hydrolysis, Biodegradation and Photolysis Half-Lives

SCDM does not assign hydrolysis, biodegradation, or photolysis half-lives to radionuclides. SCDM obtains hydrolysis, biodegradation, and photolysis half-lives for all other substances from the following references, listed in order of preference:

- *Handbook of Environmental Degradation Rates* (HEDR). 1991. Howard, Phillip H., W.F. Jarvis, W.M. Meylan and E.M. Michalenko, Lewis Publishers, Inc. Chelsea, Michigan.

- Hazardous Substances Data Bank (HSDB). U.S. National Library of Medicine. Bethesda, MD. (HSDB data accessed through the PubChem database at https://pubchem.ncbi.nlm.nih.gov/.)

- EPI Suite™ (estimated values, HYDROWIN hydrolysis half-life estimates and BioHCwin biodegradation half-life estimates; does not apply to photolysis values) developed by the U.S. Environmental Protection Agency's Office of Pollution Prevention and Toxics and Syracuse Research Corporation (SRC). http://www.epa.gov/tsca-screening-tools/epi-suitetm-estimation-program-interface.

For collection of hydrolysis and biodegradation half-lives, SCDM uses aqueous half-life values. Only aerobic biodegradation half-lives are collected. If values are obtained from HEDR, SCDM uses only values listed as "first-order." If multiple values are provided from a given reference, the highest value is used. For photolysis half-life values collected from HEDR and HSDB, both direct photolysis and indirect photolysis (or photooxidation) half-lives are collected, if available. If only a direct or indirect photolysis value is available, that value is used as the SCDM final photolysis half-life. If both direct and indirect photolysis values are available from a given reference, a final photolysis half-life is calculated as described in Section 3.2 of this methodology document. For photolysis half-lives collected from HSDB, if the photolysis mechanism (direct or indirect) is unspecified, the value is used to determine a final photolysis half-life only if no direct and/or indirect photolysis half-life is available.

If the reference from which half-lives are collected contains half-lives that apply specifically and separately to rivers and lakes, the values are used for the specified water body in SCDM. If different values for each water body type are not available, the half-life value collected is applied to both rivers and lakes.

2.4.2 SsI Hydrolysis and SsI Biodegradation Half-Lives

SCDM assigns SsI hydrolysis and SsI biodegradation half-lives only to non-radionuclide substances that qualify as SsI volatile (see Section 2.8 of this methodology document regarding determination of SsI volatility). SsI hydrolysis and SsI biodegradation half-lives are obtained from the same reference hierarchy used in Section 2.4.1 of this methodology document.

SCDM assigns SsI hydrolysis the same values collected for lakes as described in Section 2.4.1 of this methodology document.

For collection of SsI biodegradation half-lives, SCDM employs the following procedure:

- Values are considered for the following four matrix/mechanism scenarios: aqueous/aerobic, aqueous/anaerobic, soil/aerobic, and soil/anaerobic.

- If multiple half-lives are available for a specific matrix/mechanism in a given reference, the longest value will be selected for that matrix/mechanism for further consideration. This will result in up to four matrix/mechanism values from the reference for further consideration (the longest aqueous/aerobic half-life, longest aqueous/anaerobic half-life, longest soil/aerobic half-life, and longest soil/anaerobic half-lives available in the reference).

- Of the possible four matrix/mechanism values selected in the step above from a given reference for further consideration, the shortest half-life will be collected as the SsI biodegradation half-life.

- SsI biodegradation half-life values will be collected from the most preferred reference from which any biodegradation data are available (i.e., an available half-life for one matrix/mechanism scenario from a more preferred reference will not be compared to a half-life value for another matrix/mechanism from a less preferred reference).

2.4.3 Volatilization Half-Lives

SCDM estimates volatilization half-lives for organic substances in both rivers and lakes, using the equations and procedures described in Section 3.3 of this methodology document. Volatilization half-lives are not collected or estimated for inorganic substances.

2.4.4 Radioactive Half-Lives

SCDM obtains radioactive half-lives for radioactive substances from the following references, listed in order of preference:

- International Commission on Radiological Protection (ICRP). *Nuclear Decay Data for Dosimetric Calculations*. ICRP Publication 107. Ann. ICRP 38 (3). http://www.icrp.org/publication.asp?id=ICRP%20Publication%20107.

- U.S. EPA. *Health Effects Assessment Summary Tables (HEAST)*. Office of Research and Development/Office of Emergency and Remedial Response, Washington, DC. http://www.epa.gov/sites/production/files/2015-02/documents/heast2_table_4-d2_0401.pdf.

- U.S. EPA. October 2000. *Soil Screening Guidance for Radionuclides: User's Guide*. EPA/540-R-00-007 PB2000 963307. http://nepis.epa.gov/Exe/ZyPURL.cgi?Dockey=P100A141.txt.

2.5 Bioaccumulation Potential Information

BCF values for freshwater and saltwater (one set each for the human food chain and environmental threats) are used to determine bioaccumulation potential factor values (40 CFR Part 300, Appendix A, Section 4.1.3.2.1.3). BCF values are selected based on edible species to determine bioaccumulation potential factor values for the human food chain threat. If BCF data are not available for organic substances, the Log K_{ow} is used to determine bioaccumulation potential factor values. Water solubility data are used if the Log K_{ow} exceeds 6.0, the substance is inorganic or there is no Log K_{ow}.

2.5.1 Bioconcentration

Bioaccumulation factor values in SCDM are preferentially based on actual measurements of bioconcentration in aquatic organisms. SCDM used BCF values from the following sources, listed in order of preference:

- U.S. EPA. ECOTOX Database. Environmental Research Laboratory, Duluth, MN. http://www.epa.gov/chemical-research/ecotoxicology-database.

- Versar, Inc. 1990. *Issue Paper: Bioaccumulation Potential Based on Ambient Water Quality Criteria Documents* (VER_BCF). Prepared for U.S. EPA Office of Emergency and Remedial Response, Washington, DC. Contract No. 68-W8-0098.

SCDM uses the highest measured value from ECOTOX. Measured values are preferred over calculated or estimated values. The Versar reference is a report of literature survey BCF values developed to obtain preliminary values for use when the initial HRS was being developed. When using data from this reference, SCDM also prefers the highest measured value to an estimated value. BCF data reported in the references as less than or greater than a particular value or data reported as approximations are considered non definitive and are not used in SCDM. SCDM uses BCF values derived from wet weight data. Values derived from dry weight data are not selected. When BCF values are reported as a range, the upper limit of the range is selected.

Environmental Threat: For the environmental threat, the highest value from any aquatic organism, regardless of whether it is consumed by humans, in each reference is used to establish environmental threat BCF values.

Human Food Chain Threat: The highest measured BCF for aquatic organisms typically known to be consumed by humans is used to obtain the human food chain threat BCF values. Table 1 includes a list of some of the organisms for which these BCF values may be taken. This list is intended to serve only as a guide to the SCDM data collector and hence, not all human food chain aquatic organisms are listed. Values from organisms not in this list may be used provided they are known to be consumed by humans.

Table 1. Examples of Human Food Chain Aquatic Organisms

American or Virginia oyster	Common limpet, flither	Japanese eel	Pinfish
Atlantic salmon	Common mud crab	Japanese littleneck clam	Pink salmon
Bay scallop	Common or edible winkle	Japanese whiting	Pink shrimp, common prawn
Bay shrimp, sand shrimp	Common rangia or clam	Lake trout, siscowet	Porcelain crab
Bent-nosed clam	Common shrimp, sand shrimp	Lake whitefish	Porgy
Bivalve	Crab	Lamp mussel	Rainbow trout
Bivalve/clam/mussel class	Crayfish	Largemouth bass	Red abalone
Black abalone	Daggerblade grass shrimp	Leopard frog	Red sea bream
Black bullhead	Dog whelk, Atlantic dogwinkle	Limpet	Red swamp crayfish
Blue crab	Dungeness or edible crab	Longnose killifish	River limpet
Bluegill	Eastern lamp mussel	Mangrove oyster	Rough periwinkle
Bony fishes	Edible or rock crab	Marine bivalve	Scallop
Brook silverside	European lobster	Marsh grass shrimp	Short-necked clam
Brook trout	Filefish	Marsh snail	Slipper limpet
Brown shrimp	Flat, native European oyster	Mediterranean mussel	Snail
Bullfrog	Freshwater crab	Minnow, carp family	Sole order
Carp	Freshwater mussel	Mozambique tilapia	Spot
Catfish	Fresh-water mussel	Mud crab	Starry flounder
Channel catfish	Gizzard shad	Mummichog	Striped mullet
Chinook salmon	Golden shiner	Mussel	Swan mussel
Clam	Grass shrimp, freshwater prawn	Mussel family	Taiwan abalone
Cockle	Great scallop	Mussel, eastern elliptio	Two spot goby
Coho salmon, silver salmon	Green mussel	Netted dog whelk	Unionid clam
Common bay mussel, blue mussel	Green or European shore crab	Northern krill	Wedge clam
Common carp	Green sunfish	Northern pink shrimp	White mullet
	Gudgeon	Opossum shrimp	Whitefish
		Oyster	Zebra mussel
		Pacific oyster	

2.5.2 Octanol/Water Partition Coefficient (Log K_{OW})

Log K_{OW} values are used to determine the bioaccumulation potential factor value for a hazardous substance for which BCF data are not available. SCDM may also use the log K_{OW} to estimate a log K_{OC} when a K_{OC} is not available (see Sections 2.3.4 and 3.2 of this methodology document). SCDM obtains n-octanol/water (log K_{OW}, also referred to as Log P) values from the following sources, listed in order of preference:

- EPI Suite™ (organic substances, experimental values) developed by the U.S. Environmental Protection Agency's Office of Pollution Prevention and Toxics and Syracuse Research Corporation (SRC). http://www.epa.gov/tsca-screening-tools/epi-suitetm-estimation-program-interface.

- Syracuse Research Corporation (SRC). PHYSPROP Database. Syracuse, NY. http://www.srcinc.com/what-we-do/environmental/scientific-databases.html.

- CRC Handbook of Chemistry and Physics. 93rd Edition. 2012 – 2013. W.M. Haynes, National Institute of Standards and Technology, CRC Press, Boulder, Colorado. ISBN-10: 1439855110/ISBN-13: 978-1439855119. Alternatively, values may be collected from the online CRC. https://hbcp.chemnetbase.com/.

- Research Triangle Institute (RTI). 1996. Chemical Properties for SCDM Development. Prepared for the U.S.

EPA Office of Emergency and Remedial Response, Washington, DC.

SCDM uses experimental values; estimated or calculated values are not used.

2.5.3 Water Solubility

Water solubility values are used to assign a bioaccumulation potential factor value for hazardous substances when BCF or log K_{OW} data are not available. See Sections 2.3.3.1 (Water Solubility – Organic Substances) and 2.3.3.2 (Water Solubility – Metals, Metalloids and Radionuclides) of this methodology document for the data collection protocol and guidance on water solubility values.

2.6 Ecotoxicity Parameters

Ecotoxicity data are used in the HRS scoring system to determine the Ecotoxicity Factor values (HRS; 40 CFR Part 300, Appendix A, Section 4.1.4.2.1.1). SCDM uses acute and chronic freshwater and saltwater criteria, and only uses those values specifically stated as criteria. If criteria are not available, then LC_{50} data are used.

2.6.1 Acute and Chronic Freshwater and Saltwater Criteria - CCC, CMC

The HRS (Section 4.1.4.2.1.1, Ecosystem Toxicity) uses the EPA Ambient Water Quality Criteria (AWQC) and Ambient Aquatic Life Advisory Concentrations (AALAC) for assigning ecosystem toxicity factor values. The acute and chronic AWQC have been replaced by a new set of criteria, and the AALAC values no longer exist. The new criteria replacing the AWQC for both freshwater and saltwater are labeled as (1) Criterion Maximum Concentration (CMC), to be used in place of what was previously acute AWQC, and (2) Criterion Continuous Concentration (CCC), to be used in place of what was previously chronic AWQC (acknowledged in HRS Section 1.1 [Definitions] in the 2017 HRS SsI Addition, 82 FR 2760). These new values closely correspond to the old acute and chronic AWQC values, respectively; however, some values have been re-derived using different methodology. Therefore, the resulting values must be used as directed by the EPA. Many of the CMC and CCC values have associated endnotes regarding how the value was derived and how it should be used. Some CMC and CCC values are baseline values that must be adjusted using the information specified in the endnotes. The CMC and CCC values are taken from:

- U.S. EPA. National Recommended Water Quality Criteria. Office of Water. Washington, DC. https://www.epa.gov/wqc/national-recommended-water-quality-criteria-aquatic-life-criteria-table.

2.6.2 LC_{50} - Freshwater, Saltwater

SCDM obtains LC_{50} data from the ECOTOX database for both freshwater and saltwater.

- U.S. EPA. 2012. ECOTOX Database. Environmental Research Laboratory, Duluth, MN. http://www.epa.gov/chemical-research/ecotoxicology-database.

SCDM uses the lowest acute LC_{50} value found for any aquatic organism in the specified environment with an acute exposure duration of ≥1 day and ≤ 4 days. When no duration or environment is given, LC_{50} values are not entered into SCDM. SCDM does not use ecological LC_{50} results that are qualified as labile, dissolved, or unionized. Data that are reported in the references as less than or greater than a particular value or data reported as approximations are considered non definitive and are not used in SCDM. When LC_{50} values are presented as a range, the lowest value is collected.

2.7 Regulatory Benchmarks

The HRS assigns extra weight to targets with exposure to hazardous substances at levels that are at or above regulatory benchmark values. This section describes the sources for regulatory limits that the HRS uses as health-based or ecological-based benchmarks.

2.7.1 National Ambient Air Quality Standards (NAAQS)

National Ambient Air Quality Standards (NAAQS) are used to establish Level I concentrations. Targets exposed to concentrations at or above the NAAQS are scored as Level I targets. SCDM uses data from the following source to obtain NAAQS:

- 40 CFR Part 50. National Ambient Air Quality Standards. https://www.epa.gov/criteria-air-pollutants/naaqs-table.

2.7.2 National Emissions Standards for Hazardous Air Pollutants (NESHAPs)

National Emission Standards for Hazardous Air Pollutants (NESHAPs) are used to establish Level I concentrations. Targets exposed to concentrations at, or above NESHAPs are scored as Level I targets. SCDM uses data from the following source to obtain NESHAPs and uses only those values that are reported in ambient concentration units ($\mu g/m^3$):

- 40 CFR Part 61 and Part 63. National Emission Standards for Hazardous Air Pollutants. http://www.epa.gov/enforcement/air-enforcement.

2.7.3 Maximum Contaminant Levels (MCLs) and Maximum Contaminant Level Goals (MCLGs)

Maximum Contaminant Levels (MCLs) and Maximum Contaminant Level Goals (MCLGs) are used to establish Level I concentrations. Targets exposed to concentrations at or above MCLs and MCLGs are scored as Level I targets. SCDM uses data from the following sources for MCLs and MCLGs:

- U.S. EPA. Drinking Water Contaminants – Standards and Regulations. Office of Water. Washington, DC. https://www.epa.gov/ground-water-and-drinking-water/national-primary-drinking-water-regulations.

- U.S. EPA. October 2000. *Soil Screening Guidance for Radionuclides: User's Guide* (EPA/540-R-00-007, PB2000 963307). http://nepis.epa.gov/Exe/ZyPURL.cgi?Dockey=P100A141.txt.

(Although NPDWS is the primary source of MCLs, MCLs for beta-emitting radionuclides are collected from the Soil Screening Guidance document where the NPDWS values in units of millirem/year are converted to pCi/L.)

SCDM uses only MCLs that are reported in units of concentration (mg/L, µg/L, or pCi/L) and only non-zero MCLGs that are reported in units of concentration (mg/L or µ/L). Where available, both MCLs and MCLGs are collected for non-radionuclide substances; only MCL values are collected for radionuclide substances.

2.7.4 FDA Action Levels (FDAALs)

Food and Drug Administration Action Levels (FDAAL) are used to establish Level I concentrations. Targets exposed to concentrations at or above FDAALs are scored as Level I targets. SCDM contains FDAALs for fish

and shellfish only, and obtains the FDAAL values from the following reference:

- U.S. Food and Drug Administration. 2000. Action Levels for Poisonous or Deleterious Substances in Human and Animal Feed. Center for Food Safety and Applied Nutrition, Washington, D.C. https://www.fda.gov/regulatory-information/search-fda-guidance-documents/guidance-industry-action-levels-poisonous-or-deleterious-substances-human-food-and-animal-feed.

2.7.5 Ecological Based Benchmarks

See Section 2.6.1 of this document for information regarding acute CMC and chronic CCC for freshwater and saltwater.

2.7.6 Uranium Mill Tailings Radiation Control Act Standards (UMTRCA)

Uranium Mill Tailings Radiation Control Act (UMTRCA) standards are used to establish Level I concentrations. Targets exposed to concentrations at or above UMTRCA standards are scored as Level I targets. SCDM extracts UMTRCA data directly from 40 CFR Part 192 (Uranium Mill Tailings Radiation Control Act Standards). http://www.ecfr.gov/cgi-bin/text-idx?SID=2315f900f6e83727c94c050ced329934&mc=true&node=pt40.25.192&rgn=div5#se40.25.192_102.

2.8 Physical Properties and Other Data

SCDM contains hazardous substance physical property data including, but not limited to, chemical formula, molecular weight, density, boiling point, and melting point. SCDM also includes several other parameters used to classify substances based on physical properties and other aspects as described below:

Metal-Containing Substances ("Metal Contain"): "Yes" indicates that the substance is a metal or metalloid or an inorganic compound that contains a metal or metalloid. "No" indicates that the substance is not, or does not contain, a metal or metalloid. This flag is used to determine factor values for ground water mobility and surface water persistence.

Organic Substances ("Organic"): "Yes" indicates that the substance is organic, and "No" indicates an inorganic substance. This flag is used to determine factor values for ground water mobility and bioaccumulation potential. These flags influence the SCDM calculation of K_d values.

Air Pathway Gas: "Yes" indicates that the vapor pressure for the substance is greater than or equal to 10^{-9} torr, and that the substance may be evaluated as a gas in the HRS air migration pathway under HRS Section 6.1.2.1 (Gas potential to release). "No" indicates that the vapor pressure for the substance does not meet this criterion, or that a vapor pressure value is not available. For organic substances, if a vapor pressure is not available, for the purpose of determining the Air Pathway Gas value, a normal boiling point is obtained from the reference hierarchy listed in Section 2.8.1. If the boiling point at 1 atm is <25°C, the substance is assumed to be a gas at 25°C and a value of "Yes" is assigned. For decay chain (+D) radionuclide substances, available vapor pressure and boiling point information for the non-decay chain radionuclide or elemental counterpart are considered in assigning this flag.

Air Pathway Particulate: "Yes" indicates that the vapor pressure for the substance is less than or equal to 10^{-1} torr, and that the substance may be evaluated as a particulate in the HRS air migration pathway under HRS Section 6.1.2.2 (Particulate potential to release). "No" indicates that the vapor pressure for the substance does not meet this criterion. For organic substances, if a vapor pressure is not available, for the purpose of determining the

Air Pathway Particulate value, a normal boiling point is obtained from the reference hierarchy listed in Section 2.8.1. If the boiling point at 1 atm is ≥25°C, the substance is assumed to be a particulate at 25°C and a value of "Yes" is assigned. If no vapor pressure/boiling point information is available, then the substance is assigned a "Yes" for the air pathway particulate flag. For decay chain (+D) radionuclide substances, available vapor pressure and boiling point information for the non-decay chain radionuclide or elemental counterpart are considered in assigning this flag.

SsI Volatile: "Yes" indicates that the substance meets the following SsI component criteria for volatility: vapor pressure greater than or equal to one torr or an HLC greater than or equal to 10^{-5} atm-m^3/mol. "No" indicates that neither the HLC nor the vapor pressure meet these criteria, or that neither a HLC nor a vapor pressure is available for the substance. This flag is used to indicate a substance's eligibility in several aspects of the SsI component evaluation; this flag also determines whether some SsI-related values are populated, e.g., vapor migration potential, SsI hydrolysis, SsI biodegradation, and SsI overall half-lives. [Note that, as previously described, substitute chemical data are generally not applied to radioactive isotope decay chains ("+D" substances); therefore, these substances do not have HLC, or vapor pressure data listed in SCDM. For guidance on SsI component scoring of decay chain substances, please contact EPA Headquarters.]

Radioactive Isotope ("Radionuclide"): "Yes" indicates that the substance is a specific radioactive isotope, and "No" indicates that it is not. In SCDM, a substance cannot be both a radioactive element and a specific radioactive isotope. This flag is used to determine factor values for human toxicity, ecosystem toxicity and surface water persistence.

Radioactive Element ("Rad. Element"): "Yes" indicates that the substance is a radioactive element, and "No" indicates that it is not. In SCDM, a substance cannot be both a radioactive element and a specific radioactive isotope. This flag determines which HRS factor values and benchmarks will be included in the SCDM Web Query.

Mutagen: "Yes" indicates that the substance is known to be carcinogenic by a mutagenic mode of action. This flag affects the selection of equations for calculating screening concentration benchmarks. Information on substances considered carcinogenic by a mutagenic mode of action is obtained from the following sources:

- U.S. EPA. 2005. Supplemental Guidance for Assessing Susceptibility from Early-Life Exposure to Carcinogens (EPA/630/R-03/003F). https://epa-prgs.ornl.gov/chemicals/help/documents/CHILDRENS_SUPPLEMENT_FINAL_%5b1%5d.pdf.
- U.S. EPA. *Integrated Risk Information System (IRIS)*. Office of Research and Development, Cincinnati, OH. http://www.epa.gov/iris.
- U.S. EPA. *Provisional Peer Reviewed Toxicity Values for Superfund (PPRTVs), Derivation Support Documents*. https://www.epa.gov/pprtv.
- U.S. EPA. 1993. *Provisional Guidance for Quantitative Risk Assessment of Polycyclic Aromatic Hydrocarbons*, Office of Health and Environmental Assessment. EPA/600/R-93/089. http://epa-prgs.ornl.gov/chemicals/help/documents/600R93089.pdf.
- California Environmental Protection Agency (CALEPA). Public Health Goals For Chemicals In Drinking Water. Hexavalent Chromium (Cr VI). July 2011. https://oehha.ca.gov/media/downloads/water/chemicals/phg/cr6phg072911.pdf.
- U.S. EPA. 2009. *An Evaluation of the Mode of Action Framework for Mutagenic Carcinogens Case Study II: Chromium (VI)*. Office of Pesticide Programs. Environmental and Molecular Mutagenesis. https://rais.ornl.gov/documents/McCarroll_et_al_2009.pdf.

- U.S. EPA. Framework for Determining a Mutagenic Mode of Action for Carcinogenicity. Office of the Science Advisor. https://archive.epa.gov/osa/mmoaframework/web/html/index.html.

K_{OC} Equation: For organic substances, this flag determines which equation will be used to calculate a K_{OC} from a K_{OW} when a K_{OC} is not available in references. See Section 3.5 of this methodology document describing the specific equations. A value of 1 indicates the first equation is used, applying to most organic substances. A value of 2 indicates the second equation is used, applying to some volatile organic compounds, chlorinated benzenes, and certain chlorinated pesticides as specified in the Soil Screening Guidance Technical Background Document (EPA, 1996). This field is populated as follows:

- If the substance is listed in the Soil Screening Guidance Technical Background Document Table 39, SCDM assigns the K_{OC} Equation value from that table.

- If the substance is not in Soil Screening Guidance Technical Background Document Table 39 and is a chlorobenzene (a benzene with one or more chlorines and no other functional groups), SCDM assigns a K_{OC} Equation value of 2.

- If neither of the above applies, and the substance is listed as a volatile organic compound in Contract Laboratory Program analytical methodology at the time of the Soil Screening Guidance document (OLM03.1), SCDM assigns a K_{OC} Equation value of 2.

- If none of the above applies, SCDM assigns a K_{OC} Equation value of 1.

2.8.1 Chemical Formula, Boiling Point and Melting Point

Chemical formula, boiling point and melting point data are extracted for inorganic substances, from the following sources in order of preference:

- CRC Handbook of Chemistry and Physics. 93rd Edition. 2012 – 2013. W.M. Haynes, National Institute of Standards and Technology, CRC Press, Boulder, Colorado. ISBN-10: 1439855110/ISBN-13: 978-1439855119. Alternatively, values may be collected from the online CRC. https://hbcp.chemnetbase.com/.

- Syracuse Research Corporation (SRC). PHYSPROP Database. Syracuse, NY. http://www.srcinc.com/what-we-do/environmental/scientific-databases.html.

- Lange's Handbook of Chemistry. 16th Edition. 2004. Speight, James G., McGraw-Hill, ISBN-10:0071432205 / ISBN-13: 978-0071432207.

- Perry's Chemical Engineers' Handbook, 8th Edition. 2008. Perry, Roberts H., Green, Don W., McGraw-Hill, ISBN: 978-0-07-142294-9.

- O'Neil, M., and A. Smith (Eds). 2012. The Merck Index, 14th Edition. Merck & Co., Inc., Rahway, NJ.

Chemical formula, boiling point and melting point data are extracted for all other substances, from the following sources in order of preference:

- Syracuse Research Corporation (SRC). PHYSPROP Database. Syracuse, NY. http://www.srcinc.com/what-we-do/environmental/scientific-databases.html.

- CRC Handbook of Chemistry and Physics. 93rd Edition. 2012 – 2013. W.M. Haynes, National Institute of Standards and Technology, CRC Press, Boulder, Colorado. ISBN-10: 1439855110/ISBN-13: 978-1439855119. Alternatively, values may be collected from the online CRC. https://hbcp.chemnetbase.com/.

- EPI Suite™ (experimental values) developed by the U.S. Environmental Protection Agency's Office of Pollution Prevention and Toxics and Syracuse Research Corporation (SRC). http://www.epa.gov/tsca-screening-tools/epi-suitetm-estimation-program-interface.

- Perry's Chemical Engineers' Handbook, 8th Edition. 2008. Perry, Roberts H., Green, Don W., McGraw-Hill, ISBN: 978-0-07-142294-9.

2.8.2 Molecular Weight

Molecular weight data are collected for inorganic substances, from the following sources in order of preference:

- CRC Handbook of Chemistry and Physics. 93rd Edition. 2012 – 2013. W.M. Haynes, National Institute of Standards and Technology, CRC Press, Boulder, Colorado. ISBN-10: 1439855110/ISBN-13: 978-1439855119. Alternatively, values may be collected from the online CRC. https://hbcp.chemnetbase.com/.

- Syracuse Research Corporation (SRC). PHYSPROP Database. Syracuse, NY. http://www.srcinc.com/what-we-do/environmental/scientific-databases.html.

- Lange's Handbook of Chemistry. 16th Edition. 2004. Speight, James G., McGraw-Hill, ISBN-10:0071432205 / ISBN-13: 978-0071432207.

- Perry's Chemical Engineers' Handbook, 8th Edition. 2008. Perry, Roberts H., Green, Don W., McGraw-Hill, ISBN: 978-0-07-142294-9.

- O'Neil, M., and A. Smith (Eds). 2012. The Merck Index, 14th Edition. Merck & Co., Inc., Rahway, NJ.

Molecular weight data are collected for all other substances, from the following sources in order of preference:

- EPI Suite™ (experimental values) developed by the U.S. Environmental Protection Agency's Office of Pollution Prevention and Toxics and Syracuse Research Corporation (SRC). http://www.epa.gov/tsca-screening-tools/epi-suitetm-estimation-program-interface.

- CRC Handbook of Chemistry and Physics. 93rd Edition. 2012 – 2013. W.M. Haynes, National Institute of Standards and Technology, CRC Press, Boulder, Colorado. ISBN-10: 1439855110/ISBN-13: 978-1439855119. Alternatively, values may be collected from the online CRC. https://hbcp.chemnetbase.com/.

- Perry's Chemical Engineers' Handbook, 8th Edition. 2008. Perry, Roberts H., Green, Don W., McGraw-Hill, ISBN: 978-0-07-142294-9.

- Lange's Handbook of Chemistry. 16th Edition. 2004. Speight, James G., McGraw-Hill, ISBN-10:0071432205 / ISBN-13: 978-0071432207.

2.8.3 Density

Density data are collected for inorganic substances, from the following sources in order of preference:

- CRC Handbook of Chemistry and Physics. 93rd Edition. 2012 – 2013. W.M. Haynes, National Institute of Standards and Technology, CRC Press, Boulder, Colorado. ISBN-10: 1439855110/ISBN-13: 978-1439855119. Alternatively, values may be collected from the online CRC. https://hbcp.chemnetbase.com/.

- Syracuse Research Corporation (SRC). PHYSPROP Database. Syracuse, NY. http://www.srcinc.com/what-we-do/environmental/scientific-databases.html.

- Lange's Handbook of Chemistry. 16th Edition. 2004. Speight, James G., McGraw-Hill, ISBN-10:0071432205 / ISBN-13: 978-0071432207.

- Perry's Chemical Engineers' Handbook, 8th Edition. 2008. Perry, Roberts H., Green, Don W., McGraw-Hill, ISBN: 978-0-07-142294-9.

- O'Neil, M., and A. Smith (Eds). 2012. The Merck Index, 14th Edition. Merck & Co., Inc., Rahway, NJ.

Density data are collected for all other substances, from the following sources in order of preference:

- CRC Handbook of Chemistry and Physics. 93rd Edition. 2012 – 2013. W.M. Haynes, National Institute of Standards and Technology, CRC Press, Boulder, Colorado. ISBN-10: 1439855110/ISBN-13: 978-1439855119. Alternatively, values may be collected from the online CRC. https://hbcp.chemnetbase.com/.

- Perry's Chemical Engineers' Handbook, 8th Edition. 2008. Perry, Roberts H., Green, Don W., McGraw-Hill, ISBN: 978-0-07-142294-9.

- Lange's Handbook of Chemistry. 16th Edition. 2004. Speight, James G., McGraw-Hill, ISBN-10:0071432205 / ISBN-13: 978-0071432207.

3.0 CALCULATION OF INTERIM VALUES

SCDM calculates specific chemical properties for some of the following cases:

- when all preferred references do not contain a property value for a given chemical
- the property value or values from a given reference cannot be used because they are suspect or
- the EPA specifies that a value be calculated

3.1 Using ED10 to estimate a Slope Factor for either oral or inhalation pathways

SCDM uses slope factors and IUR values to determine human toxicity factor values and screening concentration benchmarks. In cases where neither a slope factor with WOE nor IUR with WOE is available for a substance, SCDM uses ED10 values, when available, to calculate oral and inhalation slope factors (SF_{oral} and SF_{inhal}) as shown below. These ED10-determined slope factors are used to determine human toxicity factor values; they are not used in determining screening concentration benchmarks.

$$SF_{oral} = 1 / (6 * ED10_{oral}) \quad (3)$$

$$SF_{inhal} = 1 / (6 * ED10_{inhal}) \quad (4)$$

3.2 Photolysis Half-Life

In instances where both direct and indirect photolysis half-lives are available, SCDM combines the two to calculate a final photolysis half-life for lakes (Equation 5) or rivers (Equation 6) as follows:

$$PHALFL\_FINAL = \frac{1}{\frac{1}{PHALFL\_D} + \frac{1}{PHALFL\_I}} \quad (5)$$

Where:
PHALFL_FINAL = Final photolysis half-life in lakes
PHALFL_D = Direct photolysis half-life in lakes
PHALFL_I = Indirect photolysis half-life in lakes

$$PHALFR\_FINAL = \frac{1}{\frac{1}{PHALFR\_D} + \frac{1}{PHALFR\_I}} \quad (6)$$

Where:
PHALFR_FINAL = Final photolysis half-life in rivers
PHALFR_D = Direct photolysis half-life in rivers
PHALFR_I = Indirect photolysis half-life in rivers

3.3 Volatilization Half-Life

SCDM estimates the volatilization half-life in surface water for organic substances using Equation 7 (presented as Equation 15-12 in the "Handbook of Chemical Property and Estimation Methods," Lyman, *et al*).[1] In this method, the volatilization half-life ($T_{1/2}$) can be expressed as follows:

$$T_{1/2}\,(\text{hr}) = \left[\frac{Z \times \ln 2}{K_L}\right] \tag{7}$$

Where:
Z = Mean water body depth (cm)
K_L = Overall liquid-phase mass transfer coefficient
ln 2 = Natural logarithm of 2 (~0.693147)

The following expression gives the overall liquid-phase mass transfer coefficient:

$$K_L\,(\text{cm/hr}) = \frac{(H/RT)k_g \times k_l}{(H/RT)k_g + k_l} \tag{8}$$

Where:
H = Henry's Law Constant (atm·m^3/mol)
R = Universal gas constant (8.20×10^{-5} atm·m^3/mol·K)
T = Temperature (K; ºC + 273)
k_g = Gas-phase exchange coefficient
k_l = Liquid-phase exchange coefficient

The gas-phase exchange coefficient expression depends on the molecular weight (MW) of the compound.

- If MW is <65 g/mol, the following equation is used:

$$k_g\,(\text{cm/hr}) = 3{,}000 \times (18/\text{MW})^{1/2} \tag{9}$$

- If MW is ≥65 g/mol, the following equation is used:

$$k_g\,(\text{cm/hr}) = 1{,}137.5 \times (V_{wind} + V_{curr})(18/\text{MW})^{1/2} \tag{10}$$

Where:
V_{wind} = Wind velocity (m/s)
V_{curr} = Current velocity (m/s)

The liquid-phase exchange coefficient expression also depends on the molecular weight of the compound.

- If MW is <65 g/mol, the following equation is used:

[1] Thomas, R.G. 1990. "Volatilization from Water." In Handbook of Chemical Property Estimation Methods. W.J. Lyman, W.F. Reehl, D.H. Rosenblatt, Eds. American Chemical Society, Washington, DC, 15:9–28. 0-ISBN 8412-1761-0.

$$k_1\,(\text{cm/hr}) = 20 \times (44 / MW)^{1/2} \quad (11)$$

- If MW is ≥65 g/mol, the expression also depends on the wind and current velocities; the following equation is used when V_{wind} is ≤1.9 m/sec and MW is ≥65 g/mol:

$$k_l(m/s) = 23.51 \times (V_{curr}^{0.969} / (Z \times 1m/100cm)^{0.673}) \times (32/MW)^{1/2} \quad (12)$$

The following equation is used when V_{wind} is >1.9 m/sec and ≤5 m/sec, and MW is ≥65 g/mol:

$$k_l(m/s) = 23.51 \times (V_{curr}^{0.969} / (Z \times 1m/100cm)^{0.673}) \times (32/MW)^{1/2} e^{0.526(V_{wind}-1.9)} \quad (13)$$

No liquid-phase exchange coefficient equation is provided in Thomas (1990) for wind velocities >5 m/sec.

Combining Equations (7), (8), (9), and (10) into a single equation for estimating volatilization half-life ($T_{1/2}$) for compounds with MW <65 g/mol gives the following equation:

$$T_{1/2}\,(\text{days}) = (1day/24hr) \times (Z \times \ln 2) \times \{[(1/20) \times (MW/44)^{1/2}] + [RT/(H \times 3000) \times (MW/18)^{1/2}]\} \quad (14)$$

The following equation, combining Equations (7), (8), (9), and (11), can be used to estimate the volatilization half-life ($T_{1/2}$) for compounds with MW ≥65 g/mol if the wind velocity is ≤1.9 m/sec:

$$T_{1/2}\,(\text{days}) = (1day/24hr) \times Z \times \ln 2 \times \{[(Z \times 1m/100cm)^{0.673} / (23.51 \times V_{curr}^{0.969}) \times (MW/32)^{1/2}] + [RT/((H \times 1{,}137.5) \times (V_{wind} + V_{curr})) \times (MW/18)^{1/2}]\} \quad (15)$$

The following equation, combining Equations (7), (8), (9), and (12), can be used to estimate the volatilization half-life ($T_{1/2}$) for compounds with MW ≥65 g/mol if the wind velocity is >1.9 m/sec and ≤5 m/sec:

$$T_{1/2}\,(\text{days}) = (1day/24hr) \times Z \times \ln 2 \times \{[(Z \times 1m/100cm)^{0.673} / (23.51 \times V_{curr}^{0.969}) \times (MW/32)^{1/2}]\, e^{0.526(1.9-V_{wind})} + [RT/((H \times 1{,}137.5) \times (V_{wind} + V_{curr})) \times (MW/18)^{1/2}]\} \quad (16)$$

If H is $<10^{-7}$ atm·m^3/mol, the substance is less volatile than water and its concentration will increase as the water evaporates. The substance is considered essentially nonvolatile (Thomas, 1990, pp. 15-9 to 15-28) and no volatilization half-life is estimated for rivers or lakes.

3.3.1 Volatilization Half-Life for Rivers, Oceans, Coastal Tidal Waters, and the Great Lakes

To calculate the volatilization half-life for rivers, oceans, coastal tidal waters and the Great Lakes, the mean water body depth is taken as 100 cm, the temperature as 298 K, the wind velocity as 0.5 m/sec and the current velocity as 1 m/sec. Using these values, Equations (14) and (15) reduce to the following:

- If MW <65 g/mol:

$$T_{1/2}\,(\text{days}) = 2.89 \times \{[0.05 \times (MW/44)^{1/2}] + [(8.1 \times 10^{-6}/H) \times (MW/18)^{1/2}]\} \quad (17)$$

- If MW ≥65 g/mol:

$$T_{1/2}\,(\text{days}) = 2.89 \times \{[0.0425 \times (MW/32)^{1/2}] + [(1.4 \times 10^{-5}/H) \times (MW/18)^{1/2}]\} \quad (18)$$

Where:
H = Henry's Law Constant (atm·m^3/mol)
MW = Molecular Weight (g/mol)

3.3.2 Volatilization Half-Life for Lakes

To calculate the volatilization half-life for lakes, the mean water body depth is taken as 100 cm, the temperature as 298 K, the wind velocity as 0.5 m/sec and the current velocity as 0.05 m/sec. Using these values, Equations (14) and (15) reduce to the following:

- If MW <65 g/mol:

$$T_{1/2}\,(\text{days}) = 2.89 \times \{[0.05 \times (MW/44)^{1/2}] + [(8.1 \times 10^{-6}/H) \times (MW/18)^{1/2}]\} \quad (19)$$

- If MW ≥65 g/mol:

$$T_{1/2}\,(\text{days}) = 2.89 \times \{[0.775 \times (MW/32)^{1/2}] + [(3.9 \times 10^{-5}/H) \times (MW/18)^{1/2}]\} \quad (20)$$

Where:
H = Henry's Law Constant (atm·m^3/mol)
MW = Molecular Weight (g/mol)

3.4 Overall Half-Lives

3.4.1 Surface Water Persistence Overall Half-Lives for Non-radionuclides

Overall half-lives are estimated for non-radioactive substances, in rivers and lakes, as follows:

$$HALF\_LAK = \frac{1}{\frac{1}{HHALFL} + \frac{1}{BHALFL} + \frac{1}{PHALFL} + \frac{1}{VHALFL}} \quad (21)$$

Where:
HHALFL = Hydrolysis half-life in lakes
BHALFL = Biodegradation half-life in lakes
PHALFL = Photolysis half-life in lakes
VHALFL = Volatilization half-life in lakes

$$HALF\_RIV = \frac{1}{\frac{1}{HHALFR} + \frac{1}{BHALFR} + \frac{1}{PHALFR} + \frac{1}{VHALFR}} \quad (22)$$

Where:
HHALFR = Hydrolysis half-life in rivers

BHALFR = Biodegradation half-life in rivers
PHALFR = Photolysis half-life in rivers
VHALFR = Volatilization half-life in rivers

3.4.2 Surface Water Persistence Overall Half-Lives for Radionuclides

SCDM estimates overall half-lives of radionuclides in rivers and lakes as follows (this calculation is similar to the equation used for non-radioactive substances, but considers only radioactive half-life and volatilization half-life):

$$HALF\_R\_LAK = \frac{1}{\frac{1}{RHALFL} + \frac{1}{VHALFL}} \quad (23)$$

Where:
RHALFL = Radioactive half-life in lakes
VHALFL = Volatilization half-life in lakes

$$HALF\_R\_RIV = \frac{1}{\frac{1}{RHALFR} + \frac{1}{VHALFR}} \quad (24)$$

Where:
RHALFR = Radioactive half-life in rivers
VHALFR = Volatilization half-life in rivers

3.4.3 SsI Degradation Overall Half-Lives for Non-radionuclides

SsI degradation overall half-lives are estimated for non-radioactive substances, as follows:

$$SSITHALF = \frac{1}{\frac{1}{SSIHHALF} + \frac{1}{SSIBHALF}} \quad (25)$$

Where:
SSIHHALF = SsI hydrolysis half-life
SSIBHALF = SsI biodegradation half-life

3.5 Soil Water Distribution Coefficient (K_d); Soil Organic/Carbon Partition Coefficients (K_{OC})

In the evaluation of the ground water migration pathway, a hazardous substance that does not meet the criteria for an observed release is assigned a mobility factor value from HRS Table 3-8 (Ground Water Mobility Factor Values) based on its K_d value and its water solubility value. K_d values that are not available in the references listed in Section 2.3.4 of this methodology document are calculated as detailed below:

HRS Section 3.2.1.2 (Mobility) states:

> For any hazardous substance that does not meet the criteria for an observed release by chemical analysis to at least one of the aquifers, assign that hazardous substance a mobility factor value from Table 3-8 for the aquifer being evaluated, based on its water solubility and distribution coefficient (K_d).… For any hazardous substance that is organic and that does not meet the criteria for an observed release by chemical analysis, establish a distribution coefficient for that hazardous substance as follows:
>
> Estimate K_d range for the hazardous substance using the following equation:
>
> $$K_d = (K_{OC})(f_S) \quad (26)$$
>
> *Where:*
> K_{OC} = Soil-water partition coefficient for organic carbon for the hazardous substance
> f_S = Sorbent content (fraction of clays plus organic carbon) in the subsurface
>
> > Use f_S values of 0.03 and 0.77 in the above equation to establish the upper and lower values of the K_d range for the hazardous substance.
> >
> > Calculate the geometric mean of the upper and lower K_d range values. Use this geometric mean as the distribution coefficient in assigning the hazardous substance a mobility factor value from [HRS] Table 3-8.

When a K_{OC} is not available to calculate K_d values, SCDM uses the Log P or Log K_{OW} to estimate K_{OC} values. To perform this calculation, SCDM uses the relationship determined by Di'Toro (1985) for semi-volatile organic compounds:

$$\text{Log } K_{OC} = 0.00028 + (0.983 \text{ Log } K_{OW}) \quad (27)$$

For volatile organic compounds, chlorinated benzenes, and certain chlorinated pesticides, SCDM uses the relationship derived in the Soil Screening Guidance Technical Background Document (EPA, 1996):

$$\text{Log } K_{OC} = 0.0784 + (0.7919 \text{ Log } K_{OW}) \quad (28)$$

The determination of which equation is applied to each substance is also described in Section 2.8 of this methodology document. A K_{OC} Equation field value of 1 indicates that Equation 27 is applied, and a value of 2 indicates Equation 28 is applied.

3.6 Water solubility for metals

If a water solubility value is not available for metal substances, it is calculated as the geometric mean of the highest water solubility and lowest water solubility of substances containing the metal, using the following equation:

$$\text{Geometric Mean Solubility} = \sqrt{(\text{low water solubility}) \times (\text{high water solubility})} \quad (29)$$

4.0 SCREENING CONCENTRATION BENCHMARKS

Section 4 details the equations and exposure assumptions that are used to determine screening concentration benchmarks for the substances contained in SCDM. The sources of data and determination of the substance-specific values used in these equations are detailed in Sections 2.0 and 3.0 of this methodology document.

4.1 Screening Concentration Benchmarks for the Air Migration Pathway and SsI Component

The following equations are used to determine air inhalation screening concentration benchmarks for the air migration pathway and SsI component. The benchmarks use exposure parameters and factors that represent Reasonable Maximum Exposure (RME) conditions for long-term/chronic exposures and are based on the methodology outlined in the EPA's *Risk Assessment Guidance for Superfund, Part B* (1991), *Risk Assessment Guidance for Superfund, Part F* (2009) and Exposure Factors Handbook (2011). General equations are provided in Section 4.1.1 (non-carcinogenic benchmarks) and Section 4.1.2 (carcinogenic benchmarks). An equation specific for asbestos is provided in Section 4.1.3. Equations that are specific for substances that are carcinogenic through a mutagenic mode of action, including vinyl chloride and trichloroethylene (TCE), are provided in Section 4.1.4; these equations are taken from EPA's *Supplemental Guidance for Assessing Susceptibility from Early-Life Exposure to Carcinogens*. Equations used for radionuclides are provided in Section 4.1.5.

4.1.1 Non-carcinogenic – Air and SsI, Inhalation

$$SC_{nc-air} = \frac{THQ \times (AT \times ED) \times \left(\frac{1000\ \mu g}{mg}\right)}{EF \times ED \times ET \times \left(\frac{1\ day}{24\ hours}\right) \times \frac{1}{RfC}} \quad (30)$$

Where:
SC_{nc-air} = Air Inhalation Screening Concentration, Non-Carcinogenic (µg/m^3)
THQ = Target hazard quotient (=1), unitless
AT = Averaging time (365 days/year)
ED = Exposure duration (26 years)
EF = Exposure frequency (350 days/year)
ET = Exposure time (24 hours/day)
RfC = Reference concentration (mg/m^3)

Using the exposure assumptions listed above, Equation (30) can be simplified as:

$$SC_{nc-air} = 1042.857 \times RfC \quad (31)$$

4.1.2 Carcinogenic – Air and SsI, Inhalation

$$SC_{c-air} = \frac{TR \times (AT \times LT)}{EF \times ED \times ET \times \left(\frac{1\ day}{24\ hours}\right) \times IUR} \quad (32)$$

Where:
$SC_{c\text{-}air}$ = Air Inhalation Screening Concentration, Carcinogenic (µg/m^3)
TR = Target risk (1 x 10^{-6}) (unitless)
AT = Averaging time (365 days/year)
LT = Lifetime (70 years)
ED = Exposure duration (26 years)
EF = Exposure frequency (350 days/year)
ET = Exposure time (24 hours/day)
IUR = Inhalation unit risk (µg/m^3)$^{-1}$

Using the exposure assumptions listed above, Equation (32) can be simplified as:

$$SC_{c-air} = \frac{2.808 \times 10^{-6}}{IUR} \tag{33}$$

4.1.3 Carcinogenic – Air and SsI, Inhalation – Asbestos

$SC_{c\text{-}air\text{-}asbestos}$ (fibers/mL) = *TR / (IUR x TWF)* (34)

Where:
$SC_{c\text{-}air\text{-}asbestos}$ = Air Inhalation Screening Concentration, Carcinogenic, Asbestos (fibers/mL)
TR = Target risk (1 x 10^{-6}) (unitless)
IUR = Inhalation Unit Risk (fibers/mL)$^{-1}$
TWF = Time Weighting Factor = 350/365 = 0.96

4.1.4 Carcinogenic through a Mutagenic Mode of Action – Air and SsI, Inhalation

$$SC_{mu-air} = \frac{TR \times (AT \times LT)}{EF \times ET \times \left(\frac{1\ day}{24\ hours}\right) \times [(ED_{0-2} \times IUR \times 10) + (ED_{2-6} \times IUR \times 3) + (ED_{6-16} \times IUR \times 3) + (ED_{16-26} \times IUR \times 1)]} \tag{35}$$

Where:
$SC_{mu\text{-}air}$ = Air Inhalation Screening Concentration, Carcinogenic – Mutagenic Mode of Action (µg/m^3)
TR = Target risk (1 x 10^{-6}) (unitless)
AT = Averaging time (365 days/year)
LT = Lifetime (70 years)
$ED_{0\text{-}2}$ = Exposure duration – resident (2 years)
$ED_{2\text{-}6}$ = Exposure duration – resident (4 years)
$ED_{6\text{-}16}$ = Exposure duration – resident (10 years)
$ED_{16\text{-}26}$ = Exposure duration – resident (10 years)
EF = Exposure frequency – resident (350 days/year)
ET = Exposure time – resident (24 hours/day)
IUR = Inhalation unit risk (µg/m^3)$^{-1}$

Using the exposure assumptions listed above, Equation (35) can be simplified as:

$$SC_{mu-air} = \frac{1.014 \times 10^{-6}}{IUR} \quad (36)$$

4.1.4.1 Vinyl Chloride – Air and SsI, Inhalation

$$SC_{mu-vc} = \frac{TR}{IUR + \left[\frac{IUR \times EF \times ED \times ET \times (1\ day / 24\ hours)}{(AT \times LT)}\right]} \quad (37)$$

Where:
SC_{mu-vc} = Air Inhalation Screening Concentration, Vinyl Chloride (µg/m^3)
TR = Target risk (1 x 10^{-6})
AT = Averaging time (365 days/year)
LT = Lifetime (70 years)
ED = Exposure duration – resident (26 years)
EF = Exposure frequency – resident (350 days/year)
ET = Exposure time – resident (24 hours/day)
IUR = Inhalation unit risk (µg/m^3)$^{-1}$

Using the exposure assumptions listed above, Equation (37) can be simplified as:

$$SC_{mu-vc} = \frac{7.374 \times 10^{-7}}{IUR} \quad (38)$$

4.1.4.2 Trichloroethylene – Air and SsI, Inhalation

The following three steps are used to calculate an air inhalation cancer screening concentration benchmark for TCE.

Step 1. A mutagenic screening concentration (SC) is calculated using the kidney IUR and the mutagenic equation provided below.

$$SC_{mu-tce} = \frac{TR \times (AT \times LT)}{EF \times ET \times (1\ day/24\ hours) \times [(ED_{0-2} \times IUR_{kidney} \times 10) + (ED_{2-6} \times IUR_{kidney} \times 3) + (ED_{6-16} \times IUR_{kidney} \times 3) + (ED_{16-26} \times IUR_{kidney} \times 1)]} \quad (39)$$

Where:
SC_{mu-tce} = Air Inhalation Screening Concentration, Carcinogenic–Mutagenic Mode of Action (µg/m^3)
TR = Target risk (1 x 10^{-6}) (unitless)
AT = Averaging time (365 days/year)
LT = Lifetime (70 years)
ED_{0-2} = Exposure duration – resident (2 years)
ED_{2-6} = Exposure duration – resident (4 years)
ED_{6-16} = Exposure duration – resident (10 years)
ED_{16-26} = Exposure duration – resident (10 years)
EF = Exposure frequency – resident (350 days/year)
ET = Exposure time – resident (24 hours/day)

IUR_{kidney} = Inhalation unit risk, kidney $(\mu g/m^3)^{-1}$

Using the exposure assumptions listed above, Equation (39) can be simplified as:

$$SC_{m\text{-}air} = 1.014 \times 10^{-6} / IUR_{kidney} \quad (40)$$

Step 2. A cancer SC is calculated using the non-Hodgkin's lymphoma (NHL) and liver cancer IUR and the cancer equation provided below.

$$SC_{c-tce} = \frac{TR \times (AT \times LT)}{EF \times ED \times ET \times (1\ day/24\ hours) \times IUR_{NHL\ and\ Liver}} \quad (41)$$

Where:

$SC_{c\text{-}tce}$ = Air Inhalation Screening Concentration, Carcinogenic $(\mu g/m^3)$
TR = Target risk (1×10^{-6}) (unitless)
AT = Averaging time (365 days/year)
LT = Lifetime (70 years)
ED = Exposure duration – resident (26 years)
EF = Exposure frequency – resident (350 days/year)
ET = Exposure time – resident (24 hours/day)
$IUR_{NHL\ and\ liver}$ = Inhalation unit risk, NHL and liver $(\mu g/m^3)^{-1}$

Using the exposure assumptions listed above, Equation (41) can be simplified as:

$$SC_{c\text{-}air} = 2.81 \times 10^{-6} / IUR_{NHL\ and\ liver} \quad (42)$$

Step 3. A cumulative result of both the mutagenic and cancer screening concentrations calculated in Steps 1 and 2 above is then generated, and the resulting value reflects both the kidney cancer risk (mutagenic risk estimate) and the NHL and liver cancer risk.

$$SC_{mu-c-tce} = \frac{1}{\left(\frac{1}{SC_{m-air}}\right) + \left(\frac{1}{SC_{c-air}}\right)} \quad (43)$$

Substituting the simplified equations provided above, the following is an alternative equation for calculating Step 3 results:

$$SC_{mu-c-tce} = \frac{1}{9.86 \times 10^{5}\, IUR_{kidney} + 3.56 \times 10^{5}\, IUR_{NHL\ and\ Liver}} \quad (44)$$

4.1.5 Carcinogenic – Air, Inhalation and SsI, Radionuclides

$$SC_{c\text{-}air\text{-}rad} = \frac{TR}{ET \times \left(\frac{1\ day}{24\ hr}\right) \times EF \times ED \times SF_i \times IFA_{r\text{-}adj}} \quad (45)$$

Where:

$$IFA_{r\text{-}adj} = \frac{(IRA_c \times ED_c + IRA_{r\text{-}a} \times ED_{r\text{-}a})}{ED}$$

$SC_{c\text{-}air\text{-}rad}$ = Air inhalation screening concentration benchmark – radiochemical (pCi/m^3)
SF_i = Slope factor – inhalation, radiochemical – substance specific (pCi)$^{-1}$
TR = Target risk (1 x 10^{-6}), unitless
ET = Exposure time – resident (24 hours/day)
EF = Exposure frequency – resident (350 days/year)
ED = Exposure duration – resident (26 years)
IRA_c = Inhalation rate – resident child (10 m^3/day)
ED_c = Exposure duration – resident child (6 years)
$ED_{r\text{-}a}$ = Exposure duration – resident adult (20 years)
$IRA_{r\text{-}a}$ = Inhalation rate – resident adult (20 m^3/day)
$IFA_{r\text{-}adj}$ = Age-adjusted inhalation factor (18 m^3/day)

Using the exposure assumptions listed above, Equation (45) can be simplified as:

$$SC_{c\text{-}air\text{-}rad} = 6.21 \times 10^{-12} / SF_i \quad (46)$$

4.2 Screening Concentration Benchmarks for the Soil Exposure Component

The following equations are used to determine soil ingestion screening concentration benchmarks for the soil exposure component. The benchmarks use exposure parameters and factors that represent RME conditions for long-term/chronic exposures and are based on the methodology outlined in the EPA's *Risk Assessment Guidance for Superfund, Part B* (1991) and Exposure Factors Handbook (2011). General equations are provided in Section 4.2.1 (non-carcinogenic benchmarks) and Section 4.2.2 (carcinogenic benchmarks). Equations that are specific for substances that are carcinogenic through a mutagenic mode of action, including vinyl chloride and TCE, are provided in Section 4.2.3; these equations are taken from EPA's *Supplemental Guidance for Assessing Susceptibility from Early-Life Exposure to Carcinogens*. Equations used for radionuclides are provided in Section 4.2.4. When determining soil ingestion screening concentration benchmarks for arsenic, the SF and RfD are multiplied by a relative bioavailability adjustment (RBA) factor of 0.6 (EPA *Guidance for Evaluating the Oral Bioavailability of Metals in Soils for Use in Human Health Risk Assessment*).

4.2.1 Non-carcinogenic – Soil, Ingestion

$$SC_{res\text{-}sol\text{-}nc\text{-}ing} = \frac{THQ \times AT \times ED_C \times BM_C}{EF \times ED_C \times \left(\frac{1}{RfD}\right) \times IRS_C \times \frac{10^{-6}\ kg}{mg}} \quad (47)$$

Where:
$SC_{res\text{-}sol\text{-}nc\text{-}ing}$ = Soil Screening Concentration, Non-Carcinogenic (mg/kg)

RfD = Reference dose (in mg/kg-day)
AT = Averaging time – resident (365 days/year)
BM_c = Body mass – child (= 15 kg)
ED_c = Exposure duration – resident child (= 6 years)
EF = Exposure frequency – resident (= 350 days/year)
IRS_c = Resident soil ingestion rate – child (= 200 mg/day)
THQ = Target hazard quotient (=1)

Using the exposure assumptions listed above, Equation (47) can be simplified as:

$$SC_{res-sol-nc-ing} = 78214.29 \times RfD \quad (48)$$

4.2.2 Carcinogenic – Soil, Ingestion

$$SC_{res-sol-ca-ing} = \frac{TR \times AT \times LT}{SF \times EF \times IFS \times \frac{10^{-6}\,kg}{mg}} \quad (49)$$

Where:
$SC_{res-sol-ca-ing}$ = Soil Screening Concentration, Carcinogenic (mg/kg)
IFS = Soil ingestion rate – resident, age adjusted [= (105 mg-year) / (kg-day)], calculated as:

$$= \left(\frac{EDc \times IRS_c}{BM_c} \right) + \left[\frac{(ED_r - ED_C) \times IRS_a}{BM_a} \right]$$

SF = Slope factor $(mg/kg\text{-}day)^{-1}$
TR = Target risk ($= 1 \times 10^{-6}$)
AT = Averaging time – resident (= 365 days/year)
LT = Lifetime (= 70 years)
EF = Exposure frequency – resident (= 350 days/year)
ED_c = Exposure duration – resident child (= 6 years)
ED_r = Exposure duration – resident (= 26 years)
IRS_a = Resident soil ingestion rate – adult (= 100 mg/day)
IRS_c = Resident soil ingestion rate – child (= 200 mg/day)
BM_a = Body mass – adult (= 80 kg)
BM_c = Body mass – child (= 15 kg)

Using the exposure assumptions listed above, Equation (49) can be simplified as:

$$SC_{res-sol-ca-ing} = \frac{0.695}{SF} \quad (50)$$

4.2.3 Carcinogenic through a Mutagenic Mode of Action – Soil, Ingestion

$$SC_{res-sol-mu-ing} = \frac{TR \times AT \times LT}{SF \times EF \times IFSM \times \frac{10^{-6}\,kg}{mg}} \quad (51)$$

Where:
$SC_{res\text{-}sol\text{-}mu\text{-}ing}$ = Soil Screening Concentration, Carcinogenic – Mutagenic Mode of Action (mg/kg)
IFSM = Mutagenic soil ingestion rate – resident, age adjusted [= (476.7 mg-year) / (kg-day)], calculated as:

$$= \left(\frac{ED_{0-2} \times IRS_c \times 10}{BM_c} \right) + \left(\frac{ED_{2-6} \times IRS_c \times 3}{BM_c} \right) + \left(\frac{ED_{6-16} \times IRS_a \times 3}{BM_a} \right) + \left(\frac{ED_{16-26} \times IRS_a \times 1}{BM_a} \right)$$

SF = Slope factor $(mg/kg\text{-}day)^{-1}$
TR = Target risk (= 1×10^{-6})
AT = Averaging time – resident (= 365 days/year)
LT = Lifetime (= 70 years)
EF = Exposure frequency – resident (= 350 days/year)
$ED_{0\text{-}2}$ = Exposure duration – resident ages 0-2 (= 2 years)
$ED_{2\text{-}6}$ = Exposure duration – resident ages 2-6 (= 4 years)
$ED_{6\text{-}16}$ = Exposure duration – resident ages 6-16 (= 10 years)
$ED_{16\text{-}26}$ = Exposure duration – resident ages 16-26 (= 10 years)
IRS_a = Resident soil ingestion rate – adult (= 100 mg/day)
IRS_c = Resident soil ingestion rate – child (= 200 mg/day)
BM_a = Body mass – adult (= 80 kg)
BM_c = Body mass – child (= 15 kg)

Using the exposure assumptions listed above, Equation (51) can be simplified as:

$$SC_{res\text{-}sol\text{-}mu\text{-}ing} = \frac{0.153}{SF} \tag{52}$$

4.2.3.1 Vinyl Chloride – Soil, Ingestion

$$SC_{res\text{-}sol\text{-}ca\text{-}vc\text{-}ing} = \frac{TR}{\left[\left(\frac{SF \times EF \times IFS \times \frac{10^{-6}\,kg}{mg}}{AT \times LT} \right) + \left(\frac{SF \times IRS_C \times \frac{10^{-6}\,kg}{mg}}{BM_C} \right) \right]} \tag{53}$$

Where:
$SC_{res\text{-}sol\text{-}ca\text{-}vc\text{-}ing}$ = Soil Screening Concentration, Vinyl Chloride (mg/kg)
IFS = Soil ingestion rate – resident, age adjusted [= (105 mg-year) / (kg-day)], calculated as:

$$= \left(\frac{EDc \times IRS_c}{BM_c} \right) + \left[\frac{(ED_r - ED_c) \times IRS_a}{BM_a} \right]$$

SF = Slope factor $(mg/kg\text{-}day)^{-1}$
TR = Target risk (= 1×10^{-6})
AT = Averaging time – resident (= 365 days/year)
LT = Lifetime (= 70 years)
EF = Exposure frequency – resident (= 350 days/year)
ED_c = Exposure duration – child (= 6 years)
ED_r = Exposure duration – resident (= 26 years)
IRS_a = Resident soil ingestion rate – adult (= 100 mg/day)

IRS_c = Resident soil ingestion rate – child (= 200 mg/day)
BM_a = Body mass – adult (= 80 kg)
BM_c = Body mass – child (= 15 kg)

Using the exposure assumptions listed above, Equation (53) can be simplified as:

$$SC_{res\text{-}sol\text{-}ca\text{-}vc\text{-}ing} = \frac{0.068}{SF} \quad (54)$$

4.2.3.2 Trichloroethylene (TCE) – Soil, Ingestion

The following three steps were used to calculate a soil screening concentration benchmark reflecting exposure only via ingestion.

Step 1. A mutagenic screening concentration (SC) is calculated using the kidney cancer slope factor and the mutagenic equation provided below.

$$SC_{sol\text{-}mu\text{-}tce\text{-}ing} = \frac{TR \times AT \times LT}{SF_{kidney} \times EF \times IFSM \times \frac{10^{-6}\,kg}{mg}} \quad (55)$$

Where:
$SC_{\text{-}sol\text{-}mu\text{-}tce\text{-}ing}$ = Soil Screening Concentration, Mutagenic (mg/kg)
IFSM = Mutagenic soil ingestion rate–resident, age adjusted [= (476.7 mg-year)/(kg-day)], calculated as:

$$= \left(\frac{ED_{0-2} \times IRS_c \times 10}{BM_c}\right) + \left(\frac{ED_{2-6} \times IRS_c \times 3}{BM_c}\right) + \left(\frac{ED_{6-16} \times IRS_a \times 3}{BM_a}\right) + \left(\frac{ED_{16-26} \times IRS_a \times 1}{BM_a}\right)$$

SF_{kidney} = Slope factor, kidney $(mg/kg\text{-}day)^{-1}$
TR = Target risk (= 1×10^{-6})
AT = Averaging time – resident (= 365 days/year)
LT = Lifetime (= 70 years)
EF = Exposure frequency – resident (= 350 days/year)
$ED_{0\text{-}2}$ = Exposure duration – resident ages 0-2 (= 2 years)
$ED_{2\text{-}6}$ = Exposure duration – resident ages 2-6 (= 4 years)
$ED_{6\text{-}16}$ = Exposure duration – resident ages 6-16 (= 10 years)
$ED_{16\text{-}26}$ = Exposure duration – resident ages 16-26 (= 10 years)
IRS_a = Resident soil ingestion rate – adult (= 100 mg/day)
IRS_c = Resident soil ingestion rate – child (= 200 mg/day)
BM_a = Body mass – adult (= 80 kg)
BM_c = Body mass – child (= 15 kg)

Using the exposure assumptions listed above, Equation (55) can be simplified as:

$$SC_{soil\text{-}mu\text{-}tce\text{-}ing} = \frac{0.153}{SF_{kidney}} \quad (56)$$

Step 2. A cancer screening concentration (SC) is calculated using the NHL and liver cancer slope factor and the cancer equation provided below.

$$SC_{sol-ca-tce-ing} = \frac{TR \times AT \times LT}{SF_{NHL\ and\ Liver} \times EF \times IFS \times \frac{10^{-6}\ kg}{mg}} \quad (57)$$

Where:
$SC_{-sol-ca-tce-ing}$ = Soil Screening Concentration, Carcinogenic (mg/kg)
IFS = Soil ingestion rate – resident, age adjusted [= (105 mg-year) / (kg-day)], calculated as:

$$= \left(\frac{EDc \times IRS_c}{BM_c} \right) + \left[\frac{(ED_r - ED_C) \times IRS_a}{BM_a} \right]$$

$SF_{NHL\ and\ liver}$ = Slope factor, NHL, and liver $(mg/kg\text{-}day)^{-1}$
TR = Target risk (= 1×10^{-6})
AT = Averaging time – resident (= 365 days/year)
LT = Lifetime (= 70 years)
EF = Exposure frequency – resident (= 350 days/year)
ED_c = Exposure duration – child (= 6 years)
ED_r = Exposure duration – resident (= 26 years)
IRS_a = Resident soil ingestion rate – adult (= 100 mg/day)
IRS_c = Resident soil ingestion rate – child (= 200 mg/day)
BM_a = Body mass – adult (= 80 kg)
BM_c = Body mass – child (= 15 kg)

Using the exposure assumptions listed above, Equation (57) can be simplified as:

$$SC_{soil-ca-tce-ing} = \frac{0.695}{SF_{NHL\ and\ Liver}} \quad (58)$$

Step 3. A cumulative result of both the mutagenic and cancer screening concentrations, via oral ingestion, calculated in Steps 1 and 2 above is then generated and the resulting value reflects both the kidney cancer risk (mutagenic risk estimate) and the NHL and liver cancer risk.

$$SC_{soll-ca-mu-tce-ing} = \frac{1}{\left(\frac{1}{SC_{soil-ca-ing}} \right) + \left(\frac{1}{SC_{soil-mu-ing}} \right)} \quad (59)$$

Substituting the simplified equations provided above for obtaining Step 1 and Step 2 results, the following is an alternative equation for calculating Step 3 results:

$$SC_{soil-ca-mu-tce-ing} = \frac{1}{1.44\ SF_{NHL\ and\ Liver} + 6.54\ SF_{kidney}} \quad (60)$$

4.2.4 Carcinogenic – Soil, Radionuclides

4.2.4.1 Oral

$$SC_{c\text{-}sol-rad} = \frac{TR\,x\,t_r\,x\,\lambda}{\left((1-e^{-\lambda t_r})\,x\,SF_s\,x\,IFS_{r-adj}\,x\,EF_r\,x\,ED_r\,x\left(\frac{g}{1000mg}\right)\right)} \quad (61)$$

Where:

$IFS_{r\text{-}adj} = \frac{(IRS_c\,x\,ED_c + IRS_a\,x\,ED_{r\text{-}a})}{ED}$

$SC_{c\text{-}sol\text{-}rad}$ = Soil cancer screening concentration benchmark – radiochemical (pCi/kg)
SF_s = Slope factor – soil, radiochemical – substance specific $(pCi)^{-1}$
$IFS_{r\text{-}adj}$ = Resident soil ingestion factor (mg/day)
TR = Target risk (1×10^{-6})
t_r = Time (26 years)
λ = Lambda – substance specific
EF_r = Exposure frequency – resident (350 days/year)
ED_r = Exposure duration – resident (26 years)
IRS_a = Soil ingestion rate – adult (100 mg/day)
IRS_c = Soil ingestion rate – child (200 mg/day)
ED_c = Exposure duration – resident child (6 years)
$ED_{r\text{-}a}$ = Exposure duration – resident adult (20 years)

Using the exposure assumptions listed above, Equation (61) can be simplified as:

$$SC_{c\text{-}sol\text{-}rad} = 2.32 \times 10^{-8} \times \lambda / [(1 - e^{-26\lambda}) \times SF_s] \quad (62)$$

4.2.4.2 External Exposure (gamma emitters)

$$SC_{ext\text{-}rad} = \frac{TR \times t_r \times \lambda}{(1\text{-}e^{-\lambda t_r}) \times SF_{ext} \times ACF \times EF \times \left(\frac{1\text{ year}}{365\text{ days}}\right) \times ED \times [ET_{r\text{-}o} \times \mathrm{GSF}o + (ET_{r\text{-}i} \times GSF_i)]} \quad (63)$$

Where:

$SC_{ext\text{-}rad}$ = Screening concentration benchmark – radiochemical, external (pCi/g)
SF_{ext} = Slope factor – external exposure – substance specific) (risk/yr per pCi/g)
TR = Target risk ($= 1 \times 10^{-6}$)
t_r = Time (26 years)
λ = Lambda – substance specific
e = Euler's number (= 2.718281828)
ACF = Area correction factor – substance specific
EF = Exposure frequency – resident (350 days/year)
ED = Exposure duration – resident (26 years)
ED_c = Exposure duration – resident child (6 years)
$ED_{r\text{-}a}$ = Exposure duration – resident adult (20 years)
$ET_{r\text{-}o}$ = Exposure time – resident outdoor (0.073 hr/hr)

$ET_{r\text{-}i}$ = Exposure time – resident indoor (0.684 hr/hr)
GSF_i = Gamma shielding factor – indoor (0.4), unitless
GSF_o = Gamma shielding factor – outdoor (1), unitless

Using the exposure assumptions listed above, Equation (63) can be simplified as:

$$SC_{ext-rad} = \frac{2.60 \text{ x } 10^{-6} \text{ x } \lambda}{[(1 - e^{-26\lambda}) \text{ x } SF_{ext} \text{ x } ACF]} \quad (64)$$

4.3 Screening Concentration Benchmarks for Ground Water and Drinking Water

The following equations are used to determine water ingestion screening concentration benchmarks. The benchmarks use exposure parameters and factors that represent RME conditions for long-term/chronic exposures and are based on the methodology outlined in the EPA's *Risk Assessment Guidance for Superfund, Part B* (1991). General equations are provided in Section 4.3.1 (non-carcinogenic benchmarks) and Section 4.3.2 (carcinogenic benchmarks). Equations that are specific for substances that are carcinogenic through a mutagenic mode of action, including vinyl chloride and TCE, are provided in Section 4.3.3; these equations are taken from EPA's *Supplemental Guidance for Assessing Susceptibility from Early-Life Exposure to Carcinogens*. Equations used for radionuclides are provided in Section 4.3.4.

4.3.1 Non-carcinogenic – Ground Water and Drinking Water, Ingestion

$$SC_{water-nc-ing} = \frac{THQ \times AT \times ED_C \times BM_C \times 1000 \ \mu g/mg}{EF \times ED_C \times \left(\frac{1}{RfD}\right) \times IRW_C} \quad (65)$$

Where:
$SC_{water-nc-ing}$ = Ground Water/Drinking Water Screening Concentration, Non-Carcinogenic (µg/L)
RfD = Reference dose (in mg/kg-day)
AT = Averaging time – resident (365 days/year)
BM_c = Body mass – child (= 15 kg)
ED_c = Exposure duration – child (= 6 years)
EF = Exposure frequency – resident (= 350 days/year)
IRW_c = Drinking water ingestion rate – resident child (= 0.78 L/day)
THQ = Target hazard quotient (=1)

Using the exposure assumptions listed above, Equation (65) can be simplified as:

$$SC_{water-nc-ing} = 20054.95 \times RfD \quad (66)$$

4.3.2 Carcinogenic – Ground Water and Drinking Water, Ingestion

$$SC_{water-ca-ing} = \frac{TR \times AT \times LT \times 1000 \ \mu g/mg}{SF \times EF \times IFW} \quad (67)$$

Where:
$SC_{water\text{-}ca\text{-}ing}$ = Ground Water/Drinking Water Screening Concentration, Carcinogenic (µg/L)
IFW = Drinking water ingestion rate – Resident, adjusted [= (0.937 L-year) / (kg-day)], calculated as:

$$= \left(\frac{ED_C \times IRW_c}{BM_c} \right) + \left[\frac{(ED_r - ED_C) \times IRW_a}{BM_a} \right]$$

SF = Slope factor $(mg/kg\text{-}day)^{-1}$
TR = Target risk (= 1×10^{-6})
AT = Averaging time – resident (= 365 days/year)
LT = Lifetime (= 70 years)
EF = Exposure frequency – resident (= 350 days/year)
ED_c = Exposure duration – child (= 6 years)
ED_r = Exposure duration – resident (= 26 years)
IRW_a = Drinking water ingestion rate – resident adult (= 2.5 L/day)
IRW_c = Drinking water ingestion rate – resident child (= 0.78 L/day)
BM_a = Body mass – adult (= 80 kg)
BM_c = Body mass – child (= 15 kg)

Using the exposure assumptions listed above, Equation (67) can be simplified as:

$$SC_{water\text{-}ca\text{-}ing} = \frac{0.0779}{SF} \tag{68}$$

4.3.3 Carcinogenic through a Mutagenic Mode of Action – Ground Water and Drinking Water, Ingestion

$$SC_{water\text{-}mu\text{-}ing} = \frac{TR \times AT \times LT \times 1000\ \mu g/mg}{SF \times EF \times IFWM} \tag{69}$$

Where:
$SC_{water\text{-}mu\text{-}ing}$ = Ground Water/Drinking Water Screening Concentration, Mutagenic (µg/L)
IFWM = Mutagenic Drinking Water ingestion rate – resident, age adjusted [= (2.914 L-year) / (kg-day)], calculated as:

$$= \left(\frac{ED_{0-2} \times IRW_c \times 10}{BM_c} \right) + \left(\frac{ED_{2-6} \times IRW_c \times 3}{BM_c} \right) + \left(\frac{ED_{6-16} \times IRW_a \times 3}{BM_a} \right) + \left(\frac{ED_{16-26} \times IRW_a \times 1}{BM_a} \right)$$

SF = Slope factor $(mg/kg\text{-}day)^{-1}$
TR = Target risk (= 1×10^{-6})
AT = Averaging time – resident (= 365 days/year)
LT = Lifetime (= 70 years)
EF = Exposure frequency – resident (= 350 days/year)
$ED_{0\text{-}2}$ = Exposure duration – resident ages 0-2 (= 2 years)
$ED_{2\text{-}6}$ = Exposure duration – resident ages 2-6 (= 4 years)
$ED_{6\text{-}16}$ = Exposure duration – resident ages 6-16 (= 10 years)
$ED_{16\text{-}26}$ = Exposure duration – resident ages 16-26 (= 10 years)
IRW_a = Drinking water ingestion rate – resident adult (= 2.5 L/day)
IRW_c = Drinking water ingestion rate – resident child (= 0.78 L/day)
BM_a = Body mass – adult (= 80 kg)

BM_c = Body mass – child (= 15 kg)

Using the exposure assumptions listed above, Equation (69) can be simplified as:

$$SC_{water\text{-}mu\text{-}ing} = \frac{0.0251}{SF} \tag{70}$$

4.3.3.1 Vinyl Chloride – Ground Water and Drinking Water, Ingestion

$$SC_{res\text{-}water\text{-}ca\text{-}vc\text{-}ing} = \frac{TR}{\left[\left(\frac{SF \times EF \times IFW \times \frac{mg}{1000\ \mu g}}{AT \times LT}\right) + \left(\frac{SF \times IRW_C \times \frac{mg}{1000\ \mu g}}{BM_C}\right)\right]} \tag{71}$$

<u>*Where*</u>:
$SC_{res\text{-}water\text{-}nc\text{-}ing}$ = Ground Water/Drinking Water Screening Concentration, Vinyl Chloride (µg/L)
IFW = Drinking water ingestion rate – Resident, adjusted [= (0.937 L-year) / (kg-day)], calculated as:

$$= \left(\frac{ED_C \times IRW_C}{BM_C}\right) + \left[\frac{(ED_r - ED_C) \times IRW_a}{BM_a}\right]$$

SF = Slope factor $(mg/kg\text{-}day)^{-1}$
TR = Target risk (= 1×10^{-6})
AT = Averaging time – resident (= 365 days/year)
LT = Lifetime (= 70 years)
EF = Exposure frequency – resident (= 350 days/year)
ED_c = Exposure duration –child (= 6 years)
ED_r = Exposure duration – resident (= 26 years)
IRW_a = Drinking water ingestion rate – resident adult (= 2.5 L/day)
IRW_c = Drinking water ingestion rate – resident child (= 0.78 L/day)
BM_a = Body mass – adult (= 80 kg)
BM_c = Body mass – child (= 15 kg)

Using the exposure assumptions listed above, Equation (71) can be simplified as:

$$SC_{res\text{-}water\text{-}ca\text{-}vc\text{-}ing} = \frac{0.0154}{SF} \tag{72}$$

4.3.3.2 Trichloroethylene (TCE) – Ground Water and Drinking Water, Ingestion

The following three steps were used to calculate a drinking water screening concentration reflecting exposure only via ingestion.

<u>Step 1</u>. A mutagenic screening concentration (SC) is calculated using the kidney cancer slope factor and the equation provided below.

$$SC_{water\text{-}mu\text{-}tce\ \ ing} = \frac{TR \times AT \times LT \times 1000 \mu g/mg}{SF_{kidney} \times EF \times IFWM} \quad (73)$$

Where:
$SC_{water\text{-}mu\text{-}tce\text{-}ing}$ = Drinking Water Screening Concentration, Mutagenic Mode of Action (µg/L)
IFWM = Mutagenic Drinking Water ingestion rate – resident, age adjusted [= (2.914 L-year) / (kg-day)], calculated as:

$$= \left(\frac{ED_{0-2} \times IRW_c \times 10}{BM_c}\right) + \left(\frac{ED_{2-6} \times IRW_c \times 3}{BM_c}\right) + \left(\frac{ED_{6-16} \times IRW_a \times 3}{BM_a}\right) + \left(\frac{ED_{16-26} \times IRW_a \times 1}{BM_a}\right)$$

SF_{kidney} = Slope factor, kidney (mg/kg-day)$^{-1}$
TR = Target risk (= 1 x 10^{-6})
AT = Averaging time – resident (= 365 days/year)
LT = Lifetime (= 70 years)
EF = Exposure frequency – resident (= 350 days/year)
$ED_{0\text{-}2}$ = Exposure duration – resident ages 0-2 (= 2 years)
$ED_{2\text{-}6}$ = Exposure duration – resident ages 2-6 (= 4 years)
$ED_{6\text{-}16}$ = Exposure duration – resident ages 6-16 (= 10 years)
$ED_{16\text{-}26}$ = Exposure duration – resident ages 16-26 (= 10 years)
IRW_a = Drinking water ingestion rate – resident adult (= 2.5 L/day)
IRW_c = Drinking water ingestion rate – resident child (= 0.78 L/day)
BM_a = Body mass – adult (= 80 kg)
BM_c = Body mass – child (= 15 kg)

Using the exposure assumptions listed above, Equation (73) can be simplified as:

$$SC_{water\text{-}mu\text{-}tce\text{-}ing} = 0.0251 / SF_{kidney} \quad (74)$$

Step 2. A cancer SC is calculated using the NHL and liver cancer slope factor and equation provided below.

$$SC_{water\text{-}ca\text{-}tce\text{-}ing} = \frac{TR \times AT \times LT \times 1000\ \mu g/mg}{SF_{NHL\ and\ Liver} \times EF \times IFW} \quad (75)$$

Where:
$SC_{water\text{-}ca\text{-}tce\text{-}ing}$ = Drinking Water Screening Concentration, Carcinogenic (µg/L)
IFW = Drinking water ingestion rate – Resident, adjusted [= (0.937 L-year) / (kg-day)], calculated as:

$$= \left(\frac{ED_C \times IRW_c}{BM_c}\right) + \left[\frac{(ED_r - ED_C) \times IRW_a}{BM_a}\right]$$

$SF_{NHL\ and\ liver}$ = Slope factor, NHL, and liver (mg/kg-day)$^{-1}$
TR = Target risk (= 1 x 10^{-6})
AT = Averaging time – resident (= 365 days/year)
LT = Lifetime (= 70 years)
EF = Exposure frequency – resident (= 350 days/year)
ED_c = Exposure duration – child (= 6 years)
ED_r = Exposure duration – resident (26 years)

IRW_a = Drinking water ingestion rate – resident adult (= 2.5 L/day)
IRW_c = Drinking water ingestion rate – resident child (= 0.78 L/day)
BM_a = Body mass – adult (= 80 kg)
BM_c = Body mass – child (= 15 kg)

Using the exposure assumptions listed above, Equation (75) can be simplified as:

$$SC_{water\text{-}ca\text{-}tce\text{-}ing} = 0.0779 / SF_{NHL\ and\ liver} \tag{76}$$

Step 3. A cumulative result of both the oral mutagenic and oral cancer screening concentrations calculated in Steps 1 and 2 above is then generated and the resulting value reflects both the kidney cancer risk (mutagenic risk estimate) and NHL and liver cancer risk.

$$SC_{water-ca-mu-tce-ing} = \frac{1}{\left(\frac{1}{SC_{water\text{-}ca\text{-}ing}}\right) + \left(\frac{1}{SC_{water\text{-}mu\text{-}ing}}\right)} \tag{77}$$

Substituting the simplified equations provided above for obtaining Step 1 and Step 2 results, the following is an alternative to Equation 76 for calculating Step 3 results:

$$SC_{water-ca-mu-tce-ing} = \frac{1}{12.82\,SF_{NHL\,and\,Liver} + 39.84\,SF_{kidney}} \tag{78}$$

4.3.4 Carcinogenic – Ground Water and Drinking Water, Radionuclides

$$SC_{c-water-rad} = \frac{TR}{EF_r\ x\ ED_r\ x\ SF_w\ x\ IFW_{r-adj}} \tag{79}$$

Where:

$$IFW_{r\text{-}adj} = \frac{ED_c\ x\ IRW_c\ +\ ED_{r\text{-}a}\ x\ IRW_a}{ED_r}$$

$SC_{c\text{-}water\text{-}rad}$ = Drinking water screening concentration benchmark – radiochemical (pCi/L)
SF_w = Slope factor – drinking water – substance specific $(pCi)^{-1}$
TR = Target risk (1×10^{-6}), unitless
EF_r = Exposure frequency – resident (350 days/year)
ED_r = Exposure duration – resident (26 years)
IRW_a = Water ingestion rate – adult (2.5 L/day)
IRW_c = Water ingestion rate – child (0.78 L/day)
ED_c = Exposure duration – resident child (6 years)
$ED_{r\text{-}a}$ = Exposure duration – resident adult (20 years)
$IFW_{r\text{-}adj}$ = Age-adjusted water ingestion rate (2.1 L/day)

Using the exposure assumptions listed above, Equation (79) can be simplified as:

$$SC_{c\text{-}water\text{-}rad} = 5.23 \times 10^{-11} / SF_w \quad (80)$$

4.4 Screening Concentration Benchmarks for the Human Food Chain

The following equations are used to determine screening concentration benchmarks for the human food chain threat. The benchmarks use exposure parameters and factors that represent RME conditions for long-term/chronic exposures and are based on the methodology outlined in the EPA's *Risk Assessment Guidance for Superfund, Part B* (1991). General equations are provided in Section 4.4.1 (non-carcinogenic benchmarks) and Section 4.4.2 (carcinogenic benchmarks). Equations used for radionuclides are provided in Section 4.4.3.

4.4.1 Non-carcinogenic – Human Food Chain, Fish Ingestion

$$SC_{res\text{-}fsh\text{-}nc\text{-}ing} = \frac{THQ \times AT \times ED_r \times BM_a}{EF \times ED_r \times \left(\frac{1}{RfD}\right) \times IRF \times \frac{10^{-6}\,kg}{mg}} \quad (81)$$

Where:

$SC_{res\text{-}fsh\text{-}nc\text{-}ing}$ = Human Food Chain Screening Concentration, Fish Ingestion, Non-Carcinogenic (mg/kg)
RfD = Reference dose (in mg/kg-day)
AT = Averaging time – resident (365 days/year)
BM_a = Body mass – adult (= 80 kg)
ED_r = Exposure duration – resident (= 26 years)
EF = Exposure frequency – resident (= 350 days/year)
IRF = Fish ingestion rate (= 5.4×10^4 mg / day)
THQ = Target hazard quotient (=1)

Using the exposure assumptions listed above, Equation (81) can be simplified as:

$$SC_{res\text{-}fsh\text{-}nc\text{-}ing} = 1540 \times RfD \quad (82)$$

4.4.2 Carcinogenic – Human Food Chain, Fish Ingestion

$$SC_{res\text{-}fsh\text{-}ca\text{-}ing} = \frac{TR \times AT \times LT \times BM_a}{EF \times ED_r \times SF \times IRF \times \frac{10^{-6}\,kg}{mg}} \quad (83)$$

Where:

$SC_{res\text{-}fsh\text{-}ca\text{-}ing}$ = Human Food Chain Screening Concentration, Fish Ingestion, Carcinogenic (mg/kg)
SF = Slope factor $(mg/kg\text{-}day)^{-1}$
TR = Target risk ($= 1 \times 10^{-6}$)
AT = Averaging time – resident (= 365 days/year)
LT = Lifetime (= 70 years)
BM_a = Body mass – adult (= 80 kg)
EF = Exposure frequency – resident (= 350 days/year)
ED_r = Exposure duration – resident (= 26 years)

IRF = Fish ingestion rate (= 5.4 x 10^4 mg / day)

Using the exposure assumptions listed above, Equation (83) can be simplified as:

$$SC_{res-fsh-ca-ing} = \frac{0.00416}{SF} \quad (84)$$

4.4.3 Carcinogenic – Human Food Chain, Fish Ingestion, Radionuclides

$$SC_{C-fish-rad} = \frac{TR}{EF_r \times ED \times SF_f \times IRF \; x \frac{g}{1000\,mg}} \quad (85)$$

Where:
$SC_{c-fish-rad}$ = Human Food Chain Screening Concentration, Fish Ingestion – Radiochemical, Carcinogenic (pCi/g)
SF_f = Slope factor – drinking water – substance specific $(pCi)^{-1}$
TR = Target risk (1 x 10^{-6}), unitless
EF_r = Exposure frequency – resident (350 days/year)
ED = Exposure duration – resident (26 years)
ED_c = Exposure duration – resident child (6 years)
ED_{r-a} = Exposure duration – resident adult (20 years)
IRF = Fish ingestion rate (= 5.4 x 10^4 mg / day)

Using the exposure assumptions listed above, Equation (85) can be simplified as:

$$SC_{c-fish-rad} = 2.04 \times 10^{-12} / SF_f \quad (86)$$

5.0 SCDM DATA REPORTING and WEB QUERY

5.1 Data Reporting

Data are collected from the references identified in Section 2 of this document. With the exceptions cited in Section 2.1, the data are collected exactly as provided in the references and compiled into a SCDM data management tool. Once in the tool, converted values are generated to reflect the SCDM standard units for use in calculations, while the original values remain unchanged for transparency. Collected data and calculated results are maintained in the tool and are not rounded, truncated, or otherwise adjusted except for purposes of reporting in the SCDM Web Query.

The following rules are applied for purposes of reporting SCDM data in the SCDM Web Query:

- Substance characterization data and data that serve as inputs to benchmark and factor value formulas are rounded and reported to three figures.
- Screening concentration benchmarks are rounded and reported to three figures. Although this sometimes results in more figures than contained in the input variable (e.g., RfD, RfC, SF, or IUR) used to determine each benchmark, the additional figures are provided to assist users in checking the math.
- Factor values will be reported to the number of significant figures needed to support decision making as described at 40 CFR Part 300 Appendix A, 55 FR 51532, and 82 FR 2760.

5.2 SCDM Web Query

The SCDM Web Query (http://www.epa.gov/superfund/superfund-chemical-data-matrix-scdm-query) contains selected data, HRS factor values and benchmarks for each hazardous substance in SCDM. Information is provided in tables for each substance. These tables are divided into three categories of available information: factor values, benchmarks, and data elements.

Figure 1 presents an example of the header that appears on the SCDM Web Query report for each substance. The header contains the substance name, the substance CASRN, and the date the query is accessed.

Substance: Acenaphthene
[CASRN 000083-32-9]

Query Accessed: 3/20/2018

Figure 1. SCDM Web Query Report Heading

For each substance, the data elements tables contain all of the selected chemical data, the data units, and an abbreviation describing the reference source of the information. The reference source abbreviations are provided alongside corresponding reference list citations in Section 6 of this methodology document. A reference source value of "CALC" indicates that a value was calculated using other collected data, and a reference source value of "HRS" indicates a value prescribed by the HRS. Data are divided into seven functional groups: toxicity, persistence, SsI degradation, mobility, bioaccumulation, physical characteristics, other data, and class information.

The toxicity table (Figure 2) contains the acute, chronic, and carcinogenicity data that were compiled using the methodology described in Sections 2.2 and 2.6, and used to derive human toxicity and ecotoxicity factor values.

Data Elements: Toxicity
Acenaphthene [CASRN 000083-32-9]

Parameter	Value	Unit	Source
RfD	6.00E-02	mg/kg/day	IRIS
RfC	--	--	--
Slope Factor	--	--	--
Slope Factor WOE	--	--	--
IUR	--	--	--
IUR WOE	--	--	--
Oral ED_{10}	--	--	--
Oral ED_{10} WOE	--	--	--
Inhalation ED_{10}	--	--	--
Inhalation ED_{10} WOE	--	--	--
Oral LD_{50}	--	--	--
Dermal LD_{50}	--	--	--
Gas Inhalation LC_{50}	--	--	--
Dust Inhalation LC_{50}	--	--	--
Acute, Freshwater CMC	--	--	--
Acute, Saltwater CMC	--	--	--
Chronic, Freshwater CCC	--	--	--
Chronic, Saltwater CCC	--	--	--
Freshwater Ecological LC_{50}	5.00E+01	µg/L	ECOTOX
Saltwater Ecological LC_{50}	1.40E+02	µg/L	ECOTOX

Figure 2a. Non-radionuclide Toxicity Table

Data Elements: Toxicity
Cadmium 109 (radionuclide) [CASRN 014109-32-1]

Parameter	Value	Unit	Source
RfD	--	--	--
RfC	--	--	--
Oral Slope Factor, Food	6.70E-12	pCi^{-1}	OSRTI_PRG
Oral Slope Factor, Soil	1.07E-11	pCi^{-1}	OSRTI_PRG
Oral Slope Factor, Water	5.00E-12	pCi^{-1}	OSRTI_PRG
Oral Slope Factor WOE	A		HRS
IUR	--	--	--
IUR WOE	A	--	HRS
Inhalation Slope	2.20E-11	pCi^{-1}	OSRTI_PRG
External Exposure Slope	8.69E-09	$yr^{-1}/(pCi/g)$	OSRTI_PRG
Lambda	5.48E-01		OSRTI_PRG
Area Correction Factor	1.00E+00		OSRTI_PRG
Oral ED_{10}	--	--	--
Oral ED_{10} WOE	--	--	--
Inhalation ED_{10}	--	--	--
Inhalation ED_{10} WOE	--	--	--
Oral LD_{50}	--	--	--
Dermal LD_{50}	--	--	--
Gas Inhalation LC_{50}	--	--	--
Dust Inhalation LC_{50}	--	--	--
Acute, Freshwater CMC	--	--	--
Acute, Saltwater CMC	--	--	--
Chronic, Freshwater CCC	--	--	--
Chronic, Saltwater CCC	--	--	--
Freshwater Ecological LC_{50}	--	--	--
Saltwater Ecological LC_{50}	--	--	--

Figure 2b. Radionuclide Toxicity Table

The top half of the table shown in Figure 2a contains the data used for non-radionuclides to determine the HTF value: reference dose, reference concentration, slope factor, inhalation unit risk [IUR], ED_{10} (oral and inhalation), LD_{50} (oral and dermal) and LC_{50} (gas and dust inhalation). The bottom half of the Figure 2a table contains the data used to determine an ecotoxicity factor value: acute and chronic water quality criteria, CMC and CCC, for fresh and salt water as well as fresh and salt water LC_{50} values. Blank entries indicate that no value was found using the procedures and references specified. The table shown in Figure 2b includes similar parameters for radionuclides.

The persistence table (Figure 3) contains the surface water persistence data compiled using the methodology described in Section 2.4. Surface water persistence factors can also be determined using the logarithm of the *n*-

octanol/water partition coefficient (Log K_{OW} or Log P, Section 2.3) if, as specified in the HRS, this gives a higher factor value than the half-lives (or a default, if applicable).

Data Elements: Persistence
Acenaphthene [CASRN 000083-32-9]

LAKE HALF-LIVES			
Parameter	**Value**	**Unit**	**Source**
Hydrolysis	--	--	--
Volatility	6.71E+00	days	CALC
Final Photolysis	2.50E+00	days	CALC
Direct Photolysis	2.50E+00	days	HEDR
Indirect Photolysis	--	days	--
Unspecified Photolysis	--	days	--
Biodegradation	1.02E+02	days	HEDR
Radioactive	--	--	--
RIVER HALF-LIVES			
Parameter	**Value**	**Unit**	**Source**
Hydrolysis	--	--	--
Volatility	9.13E-01	days	CALC
Final Photolysis	2.50E+00	days	CALC
Direct Photolysis	2.50E+00	days	HEDR
Indirect Photolysis	--	days	--
Unspecified Photolysis	--	days	--
Biodegradation	1.02E+02	days	HEDR
Radioactive	--	--	--
OTHER			
Parameter	**Value**	**Unit**	**Source**
Log Kow	3.92E+00		EPI_EXP

Figure 3. Persistence Table

The SsI degradation table (Figure 4) contains the SsI degradation data compiled using the methodology described in Section 2.4 of this methodology document. Along with additional site-specific data, these parameters are used to generate site-specific SsI degradation factor values that are not included in SCDM.

Data Elements: SsI Degradation
Acenaphthene [CASRN 000083-32-9]

HALFLIVES			
Parameter	**Value**	**Unit**	**Source**
SsI Hydrolysis	--	--	--
SsI Biodegradation	1.02E+02	days	HEDR
SsI Overall	1.02E+02	days	CALC
Radioactive	--	--	--

Figure 4. SsI Degradation Table

The mobility table (Figure 5) contains the air and ground water mobility data compiled using the methodology described in Section 2.3. Vapor pressure and HLC are used to determine gas migration potential and gas mobility factors. HLC is also used to calculate the volatilization half-life. Water solubility and the soil/water distribution coefficient are used to determine the ground water mobility factor. Substance-specific water solubility is used for nonmetal and non-metalloid substances, whereas for metal-containing substances, the solubility value is the geometric mean of the available water solubilities for inorganic compounds containing the hazardous substance. K_{OC} is used in determining K_d.

Data Elements: Mobility/Migration Potential
Acenaphthene [CASRN 000083-32-9]

Parameter	Value	Unit	Source
Vapor Pressure	2.15E-03	Torr	PHYSPROP
Henry's Law Constant	1.84E-04	atm-m^3/mol	PHYSPROP
Water Solubility	3.90E+00	mg/L	PHYSPROP
Distribution Coefficient	7.64E+02	mL/g	CALC
Geometric Mean Solubility	--	--	--
K_{OC}	5.03E+03	mL/g	EPI_EST

Figure 5. Mobility Table

The bioaccumulation table (Figure 6) contains the human food chain and environmental bioaccumulation potential factor data compiled using the methodology described in Section 2.5 of this methodology document. BCFs are collected for fresh and saltwater for the human food chain and environmental threats. Log K_{OW} or water solubility is used to establish bioaccumulation potential when a BCF is not available.

Data Elements: Bioaccumulation
Acenaphthene [CASRN 000083-32-9]

FOOD CHAIN			
Parameter	**Value**	**Unit**	**Source**
Freshwater BCF	3.87E+02		ECOTOX
Saltwater BCF	--	--	--
ENVIRONMENTAL			
Parameter	**Value**	**Unit**	**Source**
Freshwater BCF	3.87E+02		ECOTOX
Saltwater BCF	--	--	--
OTHER			
Parameter	**Value**	**Unit**	**Source**
Log K_{OW}	3.92E+00		EPI_EXP
Water Solubility	3.90E+00	mg/L	PHYSPROP
Geometric Mean Solubility	--	--	--

Figure 6. Bioaccumulation Table

The physical characteristics table (Figure 7) contains logical "yes/no" flags that classify the substance based on physical properties and other aspects as described in Section 2.8 of this methodology document. MW is used to determine volatilization half-life.

Data Elements: Physical Characteristics
Acenaphthene [CASRN 000083-32-9]

Parameter	Value	Unit
Metal Containing	No	
Organic	Yes	
Air Pathway Gas	Yes	
Air Pathway Particulate	Yes	
SsI Volatile	Yes	
Radionuclide	No	
Radioactive Element	No	
Mutagen	No	
Molecular Weight	1.54E+02	
Density	1.22E+00	g/mL @ 20.0 °C

Figure 7. Physical Characteristics Table

The table labeled "other data" (Figure 8) contains values for melting points and boiling points (°C). The chemical formula is also listed here. Finally, the K_{OC} equation parameter identifies which equation is used in generating a K_{OC} from a K_{OW} when no K_{OC} is available from references.

Data Elements: Other Data
Acenaphthene [CASRN 000083-32-9]

Parameter	Value	Unit
Melting Point	9.34E+01	°C
Boiling Point	2.79E+02	°C
Formula	C12H10	
K_{OC} Equation	1	

Figure 8. Other Data Table

The class information table (Figure 9) lists parent substances for three data substitution classes: toxicity, ground water mobility and other data. The toxicity class includes all toxicity and benchmark data used to determine human or ecotoxicity factor values. The ground water mobility class includes water solubility, K_d, and geometric mean water solubility. The "other" class includes hydrolysis, biodegradation, photolysis, and volatilization half-lives, as well as BCFs and Log K_{OW}. This section may also list other class-parent chemical substitutions for specific data elements.

The two main groups of substances involved in the majority of instances of inheriting data from a parent substance are metals and radioactive substances. Generally, metal-containing substances inherit data for the ground water mobility class with the elemental metal as the class parent. Radioactive isotopes may inherit data from their primary radioactive element for the ground water mobility and "other" classes.

Data Elements: Class Information
Acenaphthene [CASRN 000083-32-9]

Parameter	Value
Parent Substance	--

Figure 9. Class Information Table

The other two categories of SCDM Web Query tables—factor values and benchmarks—contain the factor values (Figures 10 through 14) and benchmarks (Figures 15 through 17) required by the HRS. SCDM determines factor values using HRS methodologies from selected data in the data elements tables. The factor values are presented by HRS pathway: ground water, surface water, the two components of the soil exposure and subsurface intrusion pathway (soil exposure component and SsI component), and air. The surface water pathway is further subdivided by threat: drinking water, human food chain, and environmental. The toxicity factor value represents human toxicity and is the same for all pathways/components. The surface water environmental toxicity factor values are based on fresh and saltwater ecosystem toxicity data, and the surface water persistence factor values are based on BCFs for all aquatic species. The surface water human food chain factor values are based on human toxicity and BCFs for only those aquatic species consumed by humans. For the SsI component, vapor migration potential is used to determine likelihood of exposure, SsI overall half-life and radioactive half-life are used in determining the site-specific degradation factor value, and SsI volatility is used to indicate a substance's eligibility in several aspects of the SsI component evaluation. The air pathway gas migration factor value is used to determine

likelihood of release. For radioactive substances, human toxicity, ecosystem toxicity and surface water persistence factor values are determined as specified in Section 7 of the HRS.

Factor Values: Ground Water Pathway
Acenaphthene [CASRN 000083-32-9]

Parameter	Value
Toxicity	10
Water Solubility	3.90E+00
Distribution Coefficient	7.64E+02
Geometric Mean Solubility	--
Mobility: Liquid, Karst	1.0E+00
Mobility: Liquid, Non-Karst	1.0E-02
Mobility: Non-Liquid, Karst	2.0E-01
Mobility: Non-Liquid, Non-Karst	2.0E-03

Figure 10. Ground Water Pathway Factor Values Table

Factor Values: Surface Water Pathway
Acenaphthene [CASRN 000083-32-9]

DRINKING WATER	
Parameter	**Value**
Toxicity	10
Persistence, River	0.4
Persistence, Lake	0.07
HUMAN FOOD CHAIN	
Parameter	**Value**
Toxicity	10
Persistence, River	0.4
Persistence, Lake	0.07
Bioaccumulation, Freshwater	500
Bioaccumulation, Saltwater	500
ENVIRONMENTAL	
Parameter	**Value**
Toxicity, Freshwater	10000
Toxicity, Saltwater	1000
Persistence, River	0.4
Persistence, Lake	0.07
Bioaccumulation, Freshwater	500
Bioaccumulation, Saltwater	500

Figure 11. Surface Water Pathway Factor Values Table

Factor Values: Soil Exposure Component
Acenaphthene [CASRN 000083-32-9]

Parameter	Value
Toxicity	10

Figure 12. Soil Exposure Component Factor Values Table

Factor Values: Subsurface Intrusion Component
Acenaphthene [CASRN 000083-32-9]

Parameter	Value
Toxicity	10
Vapor Migration Potential	5
SsI Overall Half-life (days)	1.02E+02
Radioactive Half-life (days)	--
SsI Volatile	Yes

Figure 13. Subsurface Intrusion Component Factor Values Table

Factor Values: Air Pathway
Acenaphthene [CASRN 000083-32-9]

Parameter	Value
Toxicity	10
Gas Mobility	0.2
Gas Migration Potential	11

Figure 14. Air Pathway Factor Values Table

The benchmarks (Figures 15 through 20), like the factor values, are presented by pathway: ground water, surface water, the two components of the soil exposure and subsurface intrusion pathway (soil exposure component and SsI component), and air, as described in Sections 3 through 6 of the HRS. The surface water pathway is further subdivided by threat: drinking water, human food chain, and environmental. For HRS scoring, actual sample contaminant concentrations for a particular medium are compared to these benchmark concentrations to determine if the target will be scored as subject to Level I or Level II concentrations.

Benchmarks: Ground Water Pathway
Acenaphthene [CASRN 000083-32-9]

Parameter	Value	Unit
MCL	--	--
MCLG	--	--
Cancer Risk	--	--
Non-Cancer Risk	1.20E+00	mg/L

Figure 15. Ground Water Pathway Benchmarks Table

Benchmarks: Surface Water Pathway
Acenaphthene [CASRN 000083-32-9]

DRINKING WATER		
Parameter	**Value**	**Unit**
MCL	--	--
MCLG	--	--
Cancer Risk	--	--
Non-Cancer Risk	1.20E+00	mg/L
HUMAN FOOD CHAIN		
Parameter	**Value**	**Unit**
FDAAL	--	--
Cancer Risk	--	--
Non-Cancer Risk	9.27E+01	mg/kg
ENVIRONMENTAL		
Parameter	**Value**	**Unit**
Acute, Freshwater CMC	--	--
Acute, Saltwater CMC	--	--
Chronic, Freshwater CCC	--	--
Chronic, Saltwater CCC	--	--

Figure 16. Surface Water Pathway Benchmarks Table

Benchmarks: Soil Exposure Component
Acenaphthene [CASRN 000083-32-9]

Parameter	Value	Unit
Cancer Risk	--	--
Non-Cancer Risk	4.69E+03	mg/kg

Figure 17. Soil Exposure Component Benchmarks Table

Benchmarks: Subsurface Intrusion Component
Acenaphthene [CASRN 000083-32-9]

Parameter	Value	Unit
Cancer Risk	--	--
Non-Cancer Risk	--	--

Figure 18. Subsurface Intrusion Component Benchmarks Table

Benchmarks: Air Pathway
Acenaphthene [CASRN 000083-32-9]

Parameter	Value	Unit
NAAQS	--	--
NESHAPS	--	--
Cancer Risk	--	--
Non-Cancer Risk	--	--

Figure 19. Air Pathway Benchmarks Table

Benchmarks: Radionuclide
Acenaphthene [CASRN 000083-32-9]

DRINKING WATER		
Parameter	**Value**	**Unit**
MCL	--	--
Cancer Risk	--	--
HUMAN FOOD CHAIN		
Parameter	**Value**	**Unit**
Cancer Risk	--	--
SOIL		
Parameter	**Value**	**Unit**
UMTRCA	--	--
Cancer Risk Soil Ingestion	--	--
Cancer Risk Soil Gamma	--	--
SUBSURFACE INTRUSION		
Parameter	**Value**	**Unit**
Cancer Risk	--	--
AIR		
Parameter	**Value**	**Unit**
Cancer Risk	--	--

Figure 20. Radionuclide Benchmarks Table

6.0 REFERENCES

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