SUPERFUND CHEMICAL DATA MATRIX (SCDM) METHODOLOGY

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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 Registration Number
CCC	Criteria Continuous Concentration
CERCLA	Comprehensive Environmental Response, Compensation, and Liability Act
CFR	Code of Federal Regulations
CMC	Criteria 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
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
NJDEP	New Jersey Department of Environmental Protection
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
PPRTV	Provisional Peer Reviewed Toxicity Values

PRG	Preliminary Remediation Goals
RBA	Relative Bioavailability Adjustment
REL	Reference Exposure Level
RfC	Reference Concentration
RfD	Reference Dose
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 (Cancer)
SPHEM	Superfund Public Health Evaluation Manual
SRC	Syracuse Research Corporation
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

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METHODOLOGY

[June 2016]

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 51583) to evaluate potential National Priorities List (NPL) sites. The HRS assigns factor values for toxicity, gas migration potential, gas and ground water mobility, surface water persistence, 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 factor values and benchmarks supersede any previous values provided by SCDM, beginning June 2016. These new 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 Abstract 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 cancer 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 (III and VI 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 oral RfD and reference concentration (RfC) 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 Arochlor 1254, which results in the most environmentally conservative screening concentration benchmarks and bioaccumulation/human food chain-based factor values for this group of compounds. EPA's most recent reference on PCB risk assessment is "EPA's *PCB Risk Assessment Review Guidance Document, Interim Draft*," 2000a.

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 cancer slope factor and IUR values for benzo(a)pyrene. When a slope factor and/or IUR are not available for similar PAHs listed in SCDM, SCDM applies TEFs to determine values for these substances. PAH-specific TEFs are obtained from EPA's *Provisional Guidance for Quantitative Risk Assessment of Polycyclic Aromatic Hydrocarbons* (EPA/600/R-93/089), July 1993.

- Polychlorinated dibenzo-dioxins and furans – SCDM contains cancer slope factor, inhalation unit risk (IUR) and RfD values for 2,3,7,8-tetrachlorodibenzo-p-dioxin (TCDD). When a slope factor, IUR and/or RfD are not available for similar dioxins and furans listed in SCDM, SCDM applies toxicity equivalence factors (TEFs) to determine the values for these substances. 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.
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- 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

- 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.

- 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.

- 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 70 kg body mass, 30 years exposure, and 2 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)].

- 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)].

- 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

- Chromium VI – An oral cancer slope factor was selected from: New Jersey Department of Environmental Protection (NJDEP), Division of Science, Research and Technology. *Derivation of Ingestion-Based Soil Remediation Criterion for Cr+6 Based on the NTP Chronic Bioassay Data for Sodium Dichromate Dihydrate*. April 2009. (http://www.state.nj.us/dep/dsr/chromium/soil-cleanup-derivation.pdf).

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.

- 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.

- *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. http://hhpprtv.ornl.gov.

- The Agency for Toxic Substances and Disease Registry (ATSDR) minimal risk levels (MRLs). http://www.atsdr.cdc.gov/mrls/mrllist.asp (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. Main database. http://oehha.ca.gov/risk/chemicalDB/index.asp.

- PPRTV Appendix Screening Toxicity Values. http://hhpprtv.ornl.gov/quickview/pprtv_papers.php.

- 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/.

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.

- *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. http://hhpprtv.ornl.gov.

- The California Environmental Protection Agency (CALEPA) Office of Environmental Health Hazard Assessment's (OEHHA) Chronic Reference Exposure Levels (RELS) and Cancer Potency Values. Main database. http://oehha.ca.gov/risk/chemicalDB/index.asp.

- PPRTV Appendix. http://hhpprtv.ornl.gov/quickview/pprtv_compare.php.

- 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). If only an oral WOE classification is provided for a substance that is identified as carcinogenic via inhalation, the oral WOE is recorded for the inhalation cancer risk value. 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, cancer 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. http://www.acgih.org/tlv-bei-guidelines/policies-procedures-presentations/overview.

- 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

When a cancer SF with WOE is not available, SCDM uses ED_{10} oral and inhalation values to calculate cancer SF (see Section 3.3 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 Information

Vapor pressures and Henry's Law Constants are used to determine the gas migration potential and gas mobility potential for each substance. 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:

- PHYSPROP Database. Syracuse Research Corporation (SRC). 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.

- 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.

- PHYSPROP Database. Syracuse Research Corporation (SRC). 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.

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:

- PHYSPROP Database. Syracuse Research Corporation (SRC). 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:

- PHYSPROP Database. Syracuse Research Corporation (SRC). 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.

- 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:

- PHYSPROP Database. Syracuse Research Corporation (SRC). 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.

- 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.

- PHYSPROP Database. Syracuse Research Corporation (SRC). 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 3.7 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 3.7 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 3.7 (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.

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 3.7 of this methodology document).

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

2.4 Persistence Information

The evaluation of persistence is based primarily on the half-life of hazardous substances in surface water and (for non-radionuclides) secondarily on the sorption of the hazardous substances to sediments. Persistence information is used to determine the surface water persistence factor value.

2.4.1 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. http://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm.

- 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 3.4 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 Volatilization Half-Lives

SCDM estimates volatilization half-lives for organic substances in both rivers and lakes, using the equations and procedures described in Section 3.5 of this methodology document. Volatilization half-lives are not collected or estimated for inorganic substances.

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

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.

- PHYSPROP Database. Syracuse Research Corporation (SRC). 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.

- 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. If values are obtained from CHEMFATE, the recommended values are 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) Criteria Maximum Concentration (CMC), to be used in place of what was previously acute AWQC, and (2) Criteria Continuous Concentration (CCC), to be used in place of what was previously chronic AWQC. 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. http://water.epa.gov/scitech/swguidance/standards/current/index.cfm#altable.

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/dwstandardsregulations.

- 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. http://www.fda.gov/food/guidanceregulation/ucm077969.htm.

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

SCDM contains hazardous substance physical property data including, but not limited to, chemical formula, molecular weight, density, boiling point and melting point. SCDM applies yes/no flags to classify physical property data into the four substance categories defined below.

Organic Substances ("Organic"): "Y" indicates that the substance is organic, and "N" 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.

Metal-Containing Substances ("Metal Contain"): "Y" indicates that the substance is a metal or metalloid or an inorganic compound that contains a metal or metalloid. "N" 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.

Radioactive Isotope ("Radionuclide"): "Y" indicates that the substance is a specific radioactive isotope, and "N" 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"): "Y" indicates that the substance is a radioactive element, and "N" 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.

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.

- PHYSPROP Database. Syracuse Research Corporation (SRC). 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:

- PHYSPROP Database. Syracuse Research Corporation (SRC). 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.

- 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.

- PHYSPROP Database. Syracuse Research Corporation (SRC). 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.

- 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.

- PHYSPROP Database. Syracuse Research Corporation (SRC). 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.

- 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 RfC to RfD_{inhal}

SCDM contains RfD values for oral toxicity and RfC values for inhalation toxicity that are used to determine HTF values and screening concentration benchmarks. SCDM must convert RfC to RfD_{inhal}, for use in these determinations. RfC values are converted from concentrations into inhalation dosages (RfD_{inhal}) values for determining HTF values using the following equation:

$$RFD_{inhal} = \frac{RFC \times IR \times AR}{BM} \quad (1)$$

Where:
RFD_{inhal} = Calculated Reference Dose in Air (mg/kg-day)
RFC = Reference Concentration in Air (mg/m^3)
IR = Inhalation Rate (20 m^3/day)
AR = Absorption (100% assumed unless otherwise specified)
BM = Adult Body Mass (80 kg)

Equation (1) is used to convert RfCs to inhalation RfDs. The resulting RfD_{inhal} values are used to determine HTF values (see HRS Section 2.4.1.1, Table 2-4 [40 CFR Part 300]). If the reference source used to provide the RfD or RfC does not provide a corresponding absorption, it is assumed to be 100.

3.2 IUR to Inhalation Slope Factor

SCDM contains slope factors for oral toxicity and IUR values for inhalation toxicity. IUR values are converted into inhalation slope factors (SF_{inhal}) for use in determining HTF values. SCDM converts IUR values to calculated SF_{inhal} before assigning HTF values, using the following equation:

$$SF_{inhal} = \frac{IUR \times BM \times CF}{IR \times AR} \quad (2)$$

Where:
SFinhal = Cancer Slope Factor $(mg/kg\text{-}day)^{-1}$
IUR = Inhalation Unit Risk $(\mu g/m^3)^{-1}$
BM = Adult Body Mass (80 kg)
CF = Conversion Factor (1,000 µg/mg)
IR = Inhalation Rate (20 m^3/day)
AR = Absorption (100% assumed unless otherwise specified)

Equation (2) is used to convert the IUR value to an inhalation cancer SF, and the resulting inhalation cancer SF is evaluated with a corresponding WOE (see Section 2.2.2.1 above) to assign an HTF value based on HRS Table 2-4 (40 CFR Part 300).

3.3 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 a slope factor and/or IUR is not available for a substance, SCDM uses ED10 values, when available, to calculate oral and inhalation slope factors (SF_{oral} and SF_{inhal}), as follows:

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

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

3.4 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

3.5 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:

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

[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.

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:

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

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:

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

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

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

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:

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

- 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.

3.5.1 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)

3.5.2 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)

3.6 Overall Half-Lives

3.6.1 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

3.6.2 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

3.7 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:
>
> $$K_d = (K_{OC})(f_S) \quad (25)$$
>
> *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:

$$\text{Log } K_{OC} = 0.00028 + (0.983 \text{ Log } K_{OW}) \quad (26)$$

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):

$$\text{Log } K_{OC} = 0.0784 + (0.7919 \text{ Log } K_{OW}) \quad (27)$$

[Note: SCDM applied the following criteria to define a substance as volatile: 1) vapor pressure greater than 1 mm Hg or 2) Henry's Law Constant greater than 0.00001 atm-m^3/mole. These criteria are based on EPA Office of Solid Waste and Emergency Response's (OSWER) "OSWER Technical Guide for Assessing and Mitigating the Vapor Intrusion Pathway from Subsurface Vapor Sources to Indoor Air," Publication 9200.2-154, June 2015.]

3.8 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:

$$\text{Geometric Mean Solubility} = \sqrt{(\text{low water solubility}) \times (\text{high water solubility})} \quad (28)$$

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

The following equations are used to determine air inhalation screening concentration benchmarks for the air migration pathway. 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 *Handbook for Implementing the Supplemental Cancer Guidance at Waste and Cleanup Sites*. Equations used for radionuclides are provided in Section 4.1.5.

4.1.1 Non-carcinogenic – Air, Inhalation

$$SC_{nc-air} = \frac{THQ \times (AT \times ED) \times \left(\frac{1000\ \mu g}{mg}\right)}{EF \times ED \times ET \times \left(\frac{1\ day}{24\ hours}\right) \times \frac{1}{RfC}} \quad (29)$$

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 = Inhalation reference concentration (mg/m^3)

Using the exposure assumptions listed above, Equation (29) can be simplified as:

$$SC_{nc-air} = 1042.857 \times RfC \quad (30)$$

4.1.2 Carcinogenic – Air, Inhalation

$$SC_{c-air} = \frac{TR \times (AT \times LT)}{EF \times ED \times ET \times \left(\frac{1\ day}{24\ hours}\right) \times IUR} \quad (31)$$

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 (31) can be simplified as:

$$SC_{c-air} = \frac{2.808 \times 10^{-6}}{IUR} \tag{32}$$

4.1.3 Carcinogenic – Air, Inhalation – Asbestos

$SC_{c\text{-}air\text{-}asbestos}$ (fibers/mL) = *TR / (IUR x TWF)* (33)

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, Inhalation

$$SC_{mu-air} = \frac{TR \times (AT \times LT)}{EF \times ET \times \left(\frac{1\ day}{24\ hours}\right) \times [(ED_{0-2} \times IUR \times 10) + (ED_{2-6} \times IUR \times 3) + (ED_{6-16} \times IUR \times 3) + (ED_{16-26} \times IUR \times 1)]} \tag{34}$$

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 (34) can be simplified as:

$$SC_{mu-air} = \frac{1.014 \times 10^{-6}}{IUR} \quad (35)$$

4.1.4.1 Vinyl Chloride – Air, Inhalation

$$SC_{mu-vc} = \frac{TR}{IUR + \left[\frac{IUR \times EF \times ED \times ET \times (1\ day / 24\ hours)}{(AT \times LT)}\right]} \quad (36)$$

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 (36) can be simplified as:

$$SC_{mu-vc} = \frac{7.374 \times 10^{-7}}{IUR} \quad (37)$$

4.1.4.2 Trichloroethylene – Air, 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.

$$SC_{mu-tce} = \frac{TR \times (AT \times LT)}{EF \times ET \times (1\ day/24\ hours) \times [(ED_{0-2} \times IUR_{kidney} \times 10) + (ED_{2-6} \times IUR_{kidney} \times 3) + (ED_{6-16} \times IUR_{kidney} \times 3) + (ED_{16-26} \times IUR_{kidney} \times 1)]} \quad (38)$$

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 (38) can be simplified as:

$$SC_{m\text{-}air} = 1.014 \times 10^{-6} / IUR_{kidney} \quad (39)$$

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

$$SC_{c-tce} = \frac{TR \times (AT \times LT)}{EF \times ED \times ET \times (1\ day/24\ hours) \times IUR_{NHL\ and\ Liver}} \quad (40)$$

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 (40) can be simplified as:

$$SC_{c\text{-}air} = 2.81 \times 10^{-6} / IUR_{NHL\ and\ liver} \quad (41)$$

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.

$$SC_{mu-c-tce} = \frac{1}{\left(\frac{1}{SC_{m-air}}\right) + \left(\frac{1}{SC_{c-air}}\right)} \quad (42)$$

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

$$SC_{mu-c-tce} = \frac{1}{9.86 \times 10^{5}\, IUR_{kidney} + 3.56 \times 10^{5}\, IUR_{NHL\ and\ Liver}} \quad (43)$$

4.1.5 Carcinogenic – Air, Inhalation, Radionuclides

$$SC_{c\text{-}air\text{-}rad} = \frac{TR}{ET \times \left(\frac{1\ day}{24\ hr}\right) \times EF \times ED \times SF_i \times IFA_{r\text{-}adj}} \quad (44)$$

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 (1×10^{-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 (44) can be simplified as:

$$SC_{c\text{-}air\text{-}rad} = 6.21 \times 10^{-12} / SF_i \quad (45)$$

4.2 Screening Concentration Benchmarks for the Soil Exposure Pathway

The following equations are used to determine soil ingestion screening concentration benchmarks for the soil exposure pathway. 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 *Handbook for Implementing the Supplemental Cancer Guidance at Waste and Cleanup Sites*. 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

$$SC_{res\text{-}sol\text{-}nc\text{-}ing} = \frac{THQ \times AT \times ED_C \times BM_C}{EF \times ED_C \times \left(\frac{1}{RfD}\right) \times IRS_C \times \frac{10^{-6}\ kg}{mg}} \quad (46)$$

Where:

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

RfD = Oral 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 (46) can be simplified as:

$$SC_{res-sol-nc-ing} = 78214.29 \times RfD \quad (47)$$

4.2.2 Carcinogenic – Soil, Ingestion

$$SC_{res-sol-ca-ing} = \frac{TR \times AT \times LT}{SF \times EF \times IFS \times \frac{10^{-6}\,kg}{mg}} \quad (48)$$

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 = Chronic oral cancer 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 – 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 (48) can be simplified as:

$$SC_{res-sol-ca-ing} = \frac{0.695}{SF} \quad (49)$$

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

$$SC_{res-sol-mu-ing} = \frac{TR \times AT \times LT}{SF \times EF \times IFSM \times \frac{10^{-6}\,kg}{mg}} \quad (50)$$

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 = Chronic oral cancer 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 (50) can be simplified as:

$$SC_{res\text{-}sol\text{-}mu\text{-}ing} = \frac{0.153}{SF} \tag{51}$$

4.2.3.1 Vinyl Chloride – Soil, Ingestion

$$SC_{res\text{-}sol\text{-}ca\text{-}vc\text{-}ing} = \frac{TR}{\left[\left(\frac{SF \times EF \times IFS \times \frac{10^{-6}\,kg}{mg}}{AT \times LT}\right) + \left(\frac{SF \times IRS_C \times \frac{10^{-6}\,kg}{mg}}{BM_C}\right)\right]} \tag{52}$$

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 = Chronic oral cancer 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 (52) can be simplified as:

$$SC_{res\text{-}sol\text{-}ca\text{-}vc\text{-}ing} = \frac{0.068}{SF} \tag{53}$$

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.

$$SC_{sol\text{-}mu\text{-}tce\text{-}ing} = \frac{TR \times AT \times LT}{SF_{kidney} \times EF \times IFSM \times \frac{10^{-6}\,kg}{mg}} \tag{54}$$

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} = Chronic oral 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 (54) can be simplified as:

$$SC_{soil\text{-}mu\text{-}tce\text{-}ing} = \frac{0.153}{SF_{kidney}} \tag{55}$$

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

$$SC_{sol-ca-tce-ing} = \frac{TR \times AT \times LT}{SF_{NHL\ and\ Liver} \times EF \times IFS \times \frac{10^{-6}\ kg}{mg}} \quad (56)$$

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:

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

$SF_{NHL\ and\ liver}$ = Chronic oral cancer 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)

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 (56) can be simplified as:

$$SC_{soil-ca-tce-ing} = \frac{0.695}{SF_{NHL\ and\ Liver}} \quad (57)$$

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.

$$SC_{soll-ca-mu-tce-ing} = \frac{1}{\left(\frac{1}{SC_{soil-ca-ing}} \right) + \left(\frac{1}{SC_{soil-mu-ing}} \right)} \quad (58)$$

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:

$$SC_{soil-ca-mu-tce-ing} = \frac{1}{1.44\ SF_{NHL\ and\ Liver} + 6.54\ SF_{kidney}} \quad (59)$$

4.2.4 Carcinogenic – Soil, Radionuclides

4.2.4.1 Oral

$$SC_{c\text{-}sol-rad} = \frac{TR\ x\ t_r\ x\ \lambda}{\left((1-e^{-\lambda t_r})\ x\ SF_s\ x\ IFS_{r-adj}\ x\ EF_r\ x\ ED_r\ x\left(\frac{g}{1000mg}\right)\right)} \quad (60)$$

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 (60) can be simplified as:

$$SC_{c\text{-}sol\text{-}rad} = 2.32 \times 10^{-8} \times \lambda / [(1 - e^{-26\lambda}) \times SF_s] \quad (61)$$

4.2.4.2 External Exposure (gamma emitters)

$$SC_{ext\text{-}rad} = \frac{TR \times t_r \times \lambda}{(1\text{-}e^{-\lambda t_r}) \times SF_{ext} \times ACF \times EF \times \left(\frac{1\ year}{365\ days}\right) \times ED \times [ET_{r\text{-}o} \times GSFo + (ET_{r\text{-}i} \times GSF_i)]} \quad (62)$$

Where:

$SC_{ext\text{-}rad}$ = Screening concentration benchmark – radiochemical, external (pCi/g)
SFext = Slope factor – external exposure – substance specific) (risk/yr per pCi/g)
TR = Target risk (= 1×10^{-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 (62) can be simplified as:

$$SC_{ext-rad} = \frac{2.60 \text{ x } 10^{-6} \text{ x } \lambda}{[(1 - e^{-26\lambda}) \text{ x } SF_{ext} \text{ x } ACF]} \quad (63)$$

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 *Handbook for Implementing the Supplemental Cancer Guidance at Waste and Cleanup Sites*. Equations used for radionuclides are provided in Section 4.3.4.

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

$$SC_{water-nc-ing} = \frac{THQ \times AT \times ED_C \times BM_C \times 1000 \ \mu g/mg}{EF \times ED_C \times \left(\frac{1}{RfD} \right) \times IRW_C} \quad (64)$$

<u>*Where*</u>:
$SC_{water-nc-ing}$ = Ground Water/Drinking Water Screening Concentration, Non-Carcinogenic (µg/L)
RfD = Oral 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 (64) can be simplified as:

$$SC_{water-nc-ing} = 20054.95 \times RfD \quad (65)$$

4.3.2 Carcinogenic – Ground Water and Drinking Water, Ingestion

$$SC_{water-ca-ing} = \frac{TR \times AT \times LT \times 1000 \ \mu g/mg}{SF \times EF \times IFW} \quad (66)$$

<u>*Where*</u>:
$SC_{water-ca-ing}$ = 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 = Chronic oral slope factor (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 (66) can be simplified as:

$$SC_{water\text{-}ca\text{-}ing} = \frac{0.0779}{SF} \tag{67}$$

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

$$SC_{water\text{-}mu\text{-}ing} = \frac{TR \times AT \times LT \times 1000\ \mu g/mg}{SF \times EF \times IFWM} \tag{68}$$

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 = Chronic oral slope factor (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 (68) can be simplified as:

$$SC_{water\text{-}mu\text{-}ing} = \frac{0.0251}{SF} \quad (69)$$

4.3.3.1 Vinyl Chloride – Ground Water and Drinking Water, Ingestion

$$SC_{res\text{-}water\text{-}ca\text{-}vc\text{-}ing} = \frac{TR}{\left[\left(\frac{SF \times EF \times IFW \times \frac{mg}{1000\ \mu g}}{AT \times LT}\right) + \left(\frac{SF \times IRW_C \times \frac{mg}{1000\ \mu g}}{BM_C}\right)\right]} \quad (70)$$

<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 = Chronic oral 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 (70) can be simplified as:

$$SC_{res\text{-}water\text{-}ca\text{-}vc\text{-}ing} = \frac{0.0154}{SF} \quad (71)$$

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.

$$SC_{water\text{-}mu\text{-}tce\ \ ing} = \frac{TR \times AT \times LT \times 1000\,\mu g/mg}{SF_{kidney} \times EF \times IFWM} \quad (72)$$

<u>*Where*</u>:
$SC_{water\text{-}mu\text{-}tce\text{-}ing}$ = 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} = Chronic oral cancer 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_{0-2} = Exposure duration – resident ages 0-2 (= 2 years)
ED_{2-6} = Exposure duration – resident ages 2-6 (= 4 years)
ED_{6-16} = Exposure duration – resident ages 6-16 (= 10 years)
ED_{16-26} = 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 (72) can be simplified as:

$$SC_{water\text{-}mu\text{-}tce\text{-}ing} = 0.0251 / SF_{kidney} \quad (73)$$

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

$$SC_{water\text{-}ca\text{-}tce-ing} = \frac{TR \times AT \times LT \times 1000\ \mu g/mg}{SF_{NHL\ and\ Liver} \times EF \times IFW} \quad (74)$$

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:

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

$SF_{NHL\ and\ liver}$ = Chronic oral cancer 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)
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 (74) can be simplified as:

$SC_{water\text{-}ca\text{-}tce\text{-}ing} = 0.0779 / SF_{NHL\ and\ liver}$ (75)

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.

$$SC_{water-ca-mu-tce-ing} = \frac{1}{\left(\frac{1}{SC_{water\text{-}ca\text{-}ing}}\right) + \left(\frac{1}{SC_{water\text{-}mu\text{-}ing}}\right)} \quad (76)$$

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:

$$SC_{water-ca-mu-tce-ing} = \frac{1}{12.82\, SF_{NHL\,and\,Liver} + 39.84\, SF_{kidney}} \quad (77)$$

4.3.4 Carcinogenic – Ground Water and Drinking Water, Radionuclides

$$SC_{c-water-rad} = \frac{TR}{EF_r \; x \; ED_r \; x \; SF_w \; x \; IFW_{r-adj}} \quad (78)$$

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 (78) can be simplified as:

$SC_{c\text{-}water\text{-}rad} = 5.23 \times 10^{-11} / SF_w$ (79)

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

$$SC_{res\text{-}fsh\text{-}nc\text{-}ing} = \frac{THQ \times AT \times ED_r \times BM_a}{EF \times ED_r \times \left(\frac{1}{RfD}\right) \times IRF \times \frac{10^{-6}\,kg}{mg}} \quad (80)$$

<u>*Where*</u>:
$SC_{res\text{-}fsh\text{-}nc\text{-}ing}$ = Human Food Chain Screening Concentration, Fish Ingestion, Non-Carcinogenic (mg/kg)
RfD = Oral 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 x 10^4 mg / day)
THQ = Target hazard quotient (=1)

Using the exposure assumptions listed above, Equation (80) can be simplified as:

$$SC_{res\text{-}fsh\text{-}nc\text{-}ing} = 1540 \times RfD \quad (81)$$

4.4.2 Carcinogenic – Human Food Chain, Fish Ingestion

$$SC_{res-fsh\text{-}ca\text{-}ing} = \frac{TR \times AT \times LT \times BM_a}{EF \times ED_r \times SF \times IRF \times \frac{10^{-6}\,kg}{mg}} \quad (82)$$

<u>*Where*</u>:
$SC_{res\text{-}fsh\text{-}ca\text{-}ing}$ = Human Food Chain Screening Concentration, Fish Ingestion, Carcinogenic (mg/kg)
SF = Chronic oral cancer slope factor $(mg/kg\text{-}day)^{-1}$
TR = Target risk (= 1 x 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 (82) can be simplified as:

$$SC_{res\text{-}fsh-ca\text{-}ing} = \frac{0.00416}{SF} \quad (83)$$

4.4.3 Carcinogenic – Human Food Chain, Fish Ingestion, Radionuclides

$$SC_{C\text{-}fish-rad} = \frac{TR}{EF_r \times ED \times SF_f \times IRF \; x \frac{g}{1000\,mg}} \quad (84)$$

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

Using the exposure assumptions listed above, Equation (84) can be simplified as:

$$SC_{c\text{-}fish\text{-}rad} = 2.04 \times 10^{-12} / SF_f \quad (85)$$

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 truncated and reported to two significant figures.
- Screening concentration benchmarks are truncated to the number of significant figures contained in the data input variable (i.e., RfD, RfC, IUR, or cancer slope factor) used to determine each benchmark. For example, a screening concentration benchmark determined using a cancer slope factor of 2.81E-8, will be reported to three significant figures.
- 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 and 55 FR 51583.

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.

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 acronym describing the reference source of the information. Data are divided into six functional groups: toxicity, persistence, 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
Oral RfD	6.0E-02	mg/kg/day	IRIS
Inhal RfD	--	--	--
RfC	--	--	--
Oral Slope	--	--	--
Oral Wt-of-Evid	--	--	--
IUR	--	--	--
IUR Wt-of-Evid	--	--	--
Inhal Slope	--	--	--
Oral ED10	--	--	--
Oral ED10 Wgt	--	--	--
Inhal ED10	--	--	--
Inhal ED10 Wgt	--	--	--
Oral LD50	--	--	--
Dermal LD50	--	--	--
Gas Inhal LC50	--	--	--
Dust Inhal LC50	--	--	--
Acute, Fresh CMC	--	--	--
Acute, Salt CMC	--	--	--
Chronic, Fresh CCC	--	--	--
Chronic, Salt CCC	--	--	--
Fresh Ecol LC50	5.0E+01	µg/L	ECOTOX
Salt Ecol LC50	1.4E+02	µg/L	ECOTOX

Figure 2. Toxicity Table

The top half of this table contains the data used to determine the HTF value: reference dose (oral and inhalation), cancer slope factor (oral and 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 this 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 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- HALFLIVES			
Parameter	**Value**	**Unit**	**Source**
Hydrolysis	--	--	--
Volatility	1.1E+02	Days	THOMAS
Final Photolysis	2.5E+00	Days	HEDR
Direct Photolysis	--	Days	--
Indirect Photolysis	--	Days	--
Unspecified Photolysis	--	Days	--
Biodeg	1.0E+02	Days	HEDR
Radio	--	--	--
RIVER- HALFLIVES			
Parameter	**Value**	**Unit**	**Source**
Hydrolysis	--	--	--
Volatility	1.3E+00	Days	THOMAS
Final Photolysis	2.5E+00	Days	HEDR
Direct Photolysis	--	Days	--
Indirect Photolysis	--	Days	--
Unspecified Photolysis	--	Days	--
Biodeg	1.0E+02	Days	HEDR
Radio	--	--	--
OTHER			
Parameter	**Value**	**Unit**	**Source**
Log Kow	3.9E+00		EPI_EXP

Figure 3. Persistence Table

The mobility table (Figure 4) 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.

DATA ELEMENTS: MOBILITY
Acenaphthene [CASRN 000083-32-9]

Parameter	Value	Unit	Source
Vapor Press	2.1E-03	Torr	PHYSPROP
Henry's Law	1.8E-04	atm-m3/mol	PHYSPROP
Water Solub	3.9E+00	mg/L	PHYSPROP
Distrib Coef	7.6E+02	mL/g	CALC
Geo Mean Sol	--	--	--

Figure 4. Mobility Table

The bioaccumulation table (Figure 5) contains the human food chain and environmental bioaccumulation potential factor data compiled using the methodology described in Section 2.5. 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**
Fresh BCF	3.8E+02		ECOTOX
Salt BCF	--	--	--
ENVIRONMENTAL			
Parameter	**Value**	**Unit**	**Source**
Fresh BCF	3.8E+02		ECOTOX
Salt BCF	--	--	--
OTHER			
Parameter	**Value**	**Unit**	**Source**
Log Kow	3.9E+00		EPI_EXP
Water Solub	3.9E+00	mg/L	PHYSPROP
Geo Mean Sol	--	--	--

Figure 5. Bioaccumulation Table

The physical characteristics table (Figure 6) contains logical "yes/no" flags that classify the substance. The "metal contain" flag indicates that the hazardous substance is a metal or metalloid and is used to determine ground water mobility and surface water persistence factors. The "organic" and "inorganic" flags are used to determine ground water mobility and bioaccumulation. The "radionuclide" flag is used to determine the HTF, the ecosystem toxicity factor and the surface water persistence factor. The radioactive element flag ("rad. element") is used to determine which HRS factors and benchmarks may be included. The gas and particulate flags are used to determine mobility and likelihood of release for the air pathway. MW is used to determine volatilization half-life.

DATA ELEMENTS: PHYSICAL CHARACTERISTICS
Acenaphthene [CASRN 000083-32-9]

Parameter	Value	Unit
Metal Contain	No	
Organic	Yes	
Gas	Yes	
Particulate	Yes	
Radionuclide	No	
Rad. Element	No	
Molecular Weight	1.5E+02	
Density	1.2E+00	g/mL @ 20.0 °C

Figure 6. Physical Characteristics Table

The table labeled "other data" (Figure 7) contains values for melting points and boiling points (°C). The chemical formula is also listed here.

DATA ELEMENTS: OTHER DATA
Acenaphthene [CASRN 000083-32-9]

Parameter	Value	Unit
Melting Point	9.3E+01	°C
Boiling Point	2.7E+02	°C
Formula	C12H10	

Figure 7. Other Data Table

The class information table (Figure 8) 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.

Currently, only two groups of substances inherit data from a parent substance: 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 8. Class Information Table

The other two categories of SCDM Web Query tables—factor values and benchmarks—contain the factor values (Figures 9 through 12) and benchmarks (Figures 13 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, soil 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. 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. 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 Solub	3.9E+00
Distrib	7.6E+02
Geo Mean Sol	--
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 9. Ground Water Pathway Factor Values Table

FACTOR VALUES: SURFACE WATER PATHWAY
Acenaphthene [CASRN 000083-32-9]

DRINKING WATER	
Parameter	**Value**
Toxicity	10
Persistence, River	--
Persistence, Lake	--
HUMAN FOOD CHAIN	
Parameter	**Value**
Toxicity	10
Persistence, River	--
Persistence, Lake	--
Bioaccumulation, Fresh	500
Bioaccumulation, Salt	500
ENVIRONMENTAL	
Parameter	**Value**
Toxicity, Fresh	10000
Toxicity, Salt	1000
Persistence, River	--
Persistence, Lake	--
Bioaccumulation, Fresh	500
Bioaccumulation, Salt	500

Figure 10. Surface Water Pathway Factor Values Table

FACTOR VALUES: SOIL EXPOSURE PATHWAY
Acenaphthene [CASRN 000083-32-9]

Parameter	Value
Toxicity	10

Figure 11. Soil Pathway Factor Values Table

FACTOR VALUES: AIR PATHWAY
Acenaphthene [CASRN 000083-32-9]

Parameter	Value
Toxicity	10
Gas Mobility	0.2
Gas Migration	11

Figure 12. Air Pathway Factor Values Table

The benchmarks (Figures 13 through 17), like the factor values, are presented by pathway: ground water, surface water, soil 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	9E-01	mg/L

Figure 13. 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	9E-01	mg/L
HUMAN FOOD CHAIN		
Parameter	**Value**	**Unit**
FDAAL	--	--
Cancer Risk	--	--
Non-Cancer Risk	8E+01	mg/kg
ENVIRONMENTAL		
Parameter	**Value**	**Unit**
Acute, Fresh CMC	--	--
Acute, Salt CMC	--	--
Chronic, Fresh CCC	--	--
Chronic, Salt CCC	--	--

Figure 14. Surface Water Pathway Benchmarks Table

BENCHMARKS: SOIL EXPOSURE PATHWAY
Acenaphthene [CASRN 000083-32-9]

Parameter	Value	Unit
Cancer Risk	--	--
Non-Cancer Risk	4E+03	mg/kg

Figure 15. Soil Exposure Pathway Benchmarks Table

BENCHMARKS: AIR PATHWAY
Acenaphthene [CASRN 000083-32-9]

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

Figure 16. 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 Ing	--	--
Cancer Risk Soil Gam	--	--
AIR		
Parameter	**Value**	**Unit**
Cancer Risk	--	--

Figure 17. Radionuclide Benchmarks Table

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