

## 2.0 DATA SELECTION METHODOLOGY

This section details the methodology of data selection for use in SCDM. It describes the literature sources, guidance documents, and databases from which data are collected to populate SCDM. It also details the calculations used by SCDM for output values. This section specifies the data source hierarchies and how the HRS data selection hierarchies are applied for each data type collected. This section is primarily organized by each data element.

Section 2.1 describes hazardous substance identification protocols and how they relate to special cases. Sections 2.2 through 2.9 specify the references used to obtain the data for SCDM 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. As different compilations of data become available, different criteria may be considered.

### 2.1 Hazardous Substance Identities and SCDM Protocols

Compiling data for SCDM requires determining which data reasonably apply to a hazardous substance. Occasionally data in the references cited in Sections 2.2 through 2.9 are available for only classes and mixtures of hazardous substances, but not for the individual substances that make up that mixture.

This section describes how to assign particular values to members of classes of hazardous substances in SCDM. In general, if any member of these classes is present at a hazardous waste site, it is assumed that the most toxic, most persistent, or most bioaccumulative member of the class is present. In other words, from among the data given in the specified references for members of these classes, SCDM contains those data resulting in the greatest HRS factor values as specified by the HRS [e.g., lowest Reference Dose (RfD), highest cancer slope factor, longest half-life, greatest bioaccumulation factor].

#### 2.1.1 Generic Values

SCDM contains generic values for the following classes of compounds:

- chromium (III and VI oxidation states)
- mercury (elemental and inorganic compounds)
- polychlorinated biphenyls (PCBs) (various congeners and Aroclors)
- endosulfans (I and II)
- chlordane ( $\alpha$  and  $\gamma$ ).

Each compound is discussed individually below:

### Chromium

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 used the RfD from Chromium VI to assign toxicity data to total chromium.

### Mercury

For mercury, SCDM contains data for elemental and inorganic species. The oral RfD is for mercuric chloride, and the inhalation RfD is for elemental mercury vapor. Vapor pressure, Henry’s Law constant, and distribution coefficient are for the elemental mercury.

### Polychlorinated biphenyls (PCBs)

PCBs are represented as a class of compounds in SCDM, with a single value used regardless of the mixture of compounds identified at a site. For PCBs, toxicity and chemical properties in SCDM are based on Arochlor 1254, which results in the most environmentally conservative bioaccumulation/human food chain-based factor values for this group of compounds. The following is EPA’s most recent reference on PCB risk assessment:

- U.S. EPA. 2000a. *EPA’s PCB Risk Assessment Review Guidance Document, Interim Draft*, January.

### Endosulfans

SCDM contains data for endosulfan and two endosulfan isomers (Endosulfan I and Endosulfan II). The oral RfD for endosulfan and its isomers is from endosulfan. SCDM contains vapor pressure and Henry’s Law constant for each isomer, but the distribution coefficient for endosulfan and the two isomers is from endosulfan.

### Chlordane

SCDM contains some data for the  $\alpha$  and  $\gamma$  isomers of chlordane; but most values represent a mixture of the isomers. When a reference with chlordane data does not identify if data were derived from a specific isomer or isomer concentration, SCDM uses the generic values.

## **2.1.2 Compound Classes with Values for Individual Substances**

SCDM contains values for the individual substances of the following classes of compounds:

- dichlorobenzenes
- dinitrotoluenes
- hexachlorocyclohexanes
- xylenes.

If no data can be found in the specified references for an individual substance in the class but data are available for the generic class, SCDM assigns the generic value to that substance. These

classes are all relatively small sets of isomers, which are likely to occur as mixtures. Furthermore, these classes are 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.

#### Polychlorinated dibenzo-*p*-dioxins

SCDM treats the following substances of the polychlorinated dibenzo-*p*-dioxins and polychlorinated dibenzofurans class of compounds individually:

- 2,3,7,8-tetrachlorodibenzo-*p*-dioxin (TCDD)
- 1,2,3,7,8-pentachlorodibenzo-*p*-dioxin
- 1,2,3,4,7,8-hexachlorodibenzo-*p*-dioxin
- 1,2,3,6,7,8-hexachlorodibenzo-*p*-dioxin
- 1,2,3,7,8,9-hexachlorodibenzo-*p*-dioxin
- 1,2,3,4,6,7,8-heptachlorodibenzo-*p*-dioxin
- 2,3,7,8-tetrachlorodibenzofuran
- 1,2,3,7,8-pentachlorodibenzofuran
- 2,3,4,7,8-pentachlorodibenzofuran
- 1,2,3,4,7,8-hexachlorodibenzofuran
- 1,2,3,6,7,8-hexachlorodibenzofuran
- 1,2,3,7,8,9-hexachlorodibenzofuran
- 2,3,4,6,7,8-hexachlorodibenzofuran
- 1,2,3,4,6,7,8-heptachlorodibenzofuran
- 1,2,3,4,6,7,9-heptachlorodibenzofuran.

SCDM contains the cancer slope factor for 2,3,7,8-tetrachlorodibenzo-*p*-dioxin (TCDD). For all other dioxins and dibenzofurans, the cancer slope for TCDD is multiplied by the *toxicity equivalence factor* (TEF) for each substance to give an estimated slope factor that is entered into SCDM for that substance. TEF values are obtained from the following references:

- U.S. EPA. 1989a. *Interim Procedures for Estimating Risks Associated with Mixtures of Chlorinated Dibenzo-*p*-Dioxins and Dibenzofurans (CDDs and CDFs) and 1989 Update*. Risk Assessment Forum, Washington, DC (EPA/625/3-89-016). Section 3, Table 2.
- U.S. EPA. 1994. *Estimating Exposure to Dioxin Like Compounds*. June. (EPA/600/6-88/005Ca).
- U.S. EPA. 2000b. Part III: *Integrated Summary and Risk Characterization for 2,3,7,8-Tetrachlorodibenzo-*p*-Dioxin (TCDD) and Related Compounds*. Office of Research and Development, National Center for Environmental Assessment. June. (EPA/600/P-00/Ag).
- U.S. EPA. 2000c. *Chapter 9: Toxicity Equivalence Factors (TEFs) for Dioxin and Related Compounds*. Office of Research and Development, National Center for Environmental Assessment. June.

- U.S. EPA. 2000d. *Exposure and Health Reassessment of 2,3,7,8-Tetrachlorodibenzo-p-Dioxin (TCDD) and Related Compounds*. Office of Research and Development, National Center for Environmental Assessment. March/May. (EPA/600/P-00/001Ab-Ae).

All members of this class are assigned the weight-of-evidence for TCDD, which is currently B2. Please note that this weight-of-evidence characterization may change when EPA's recent *Integrated Risk Information System (IRIS)* change in the weight-of-evidence classification becomes final. (See Section 2.2.2, *Carcinogenicity Information*, for weight-of-evidence details.)

### 2.1.3 Substances with Unique Value Selection Protocol

#### Cadmium

For cadmium, *IRIS* contains two RfD values: one for drinking water and one for dietary exposure. Because SCDM calculates RfD-based screening concentrations for both drinking water and dietary exposure, the more conservative value is used; therefore, SCDM uses the drinking water RfD for cadmium.

#### Asbestos and Lead

The HRS specifies that a human toxicity factor of 10,000 be assigned to asbestos, lead and lead compounds. SCDM does this automatically within the computer code. Asbestos also receives a  $K_a$  value of 1,000, as stated in the HRS. Please note that the toxicity value listed in the Appendix A report is not an inhalation slope factor, but rather a unit risk factor value.

## 2.2 Toxicity Information

This section details how to compile the data used for determining the human toxicity values. The calculations presented in this section are taken directly from EPA's *Risk Assessment Guidance for Superfund* (1989b). Human toxicity values, specifically RfD, RfC, cancer slope factor, inhalation unit risk, Lethal Dose with 50% Mortality ( $LD_{50}$ ), Lethal Concentration with 50% Mortality ( $LC_{50}$ ), and the Effective Dose ( $ED_{10}$ ), (i.e. the dose corresponding to a 10% increase in an adverse effect, relative to the control response), are used in SCDM to determine the Human Toxicity Factor (HTF) value. The RfD, RfC, cancer slope factor, inhalation unit risk, and  $ED_{10}$  are used to calculate the air, drinking water, human food chain and soil screening benchmarks. This section details the SCDM selection and use protocol.

## 2.2.1 Non-Carcinogenic Toxicity Values

These values are used to determine the Human Toxicity Factor values for non-carcinogenic, non-radionuclide substances in accordance with procedures set forth in the HRS.

### 2.2.1.1 Reference Dose (RfD) - Oral; Reference Concentration (RfC) - Inhalation

SCDM contains RfD values for oral toxicity and RfC values for inhalation toxicity. In addition to determining the Human Toxicity Factor value, the RfD values are used to calculate the non-carcinogenic screening benchmarks for drinking water, food chain, soil ingestion, and air pathway threats. The RfC values are translated into inhalation RfD values for determining the human toxicity factor values and for calculating the air pathway benchmarks.

RfD values are obtained from several references (listed in order of preference), EPA's *Integrated Risk Information System (IRIS)*, EPA's *Superfund Technical Support Center Provisional Toxicity Values (STSCPTV)*, and EPA's *Health Effects Assessment Summary Tables (HEAST)*. SCDM ranks reference data according to the reference hierarchy; regardless of reference, chronic data are preferred over subchronic data. *IRIS* data are preferred over *STSCPTV* data, which are preferred over *HEAST* data. All three databases are available via the Internet, with *IRIS* having unrestricted public access. The other two (*STSCPTV* and *HEAST*) are password-protected and are accessible only to those with EPA approval. *STSCPTV* and *HEAST* may become publicly available at a later date; all references are listed below:

- U.S. EPA. 2003a. *Integrated Risk Information System (IRIS)*. Office of Research and Development, Cincinnati, OH. Accessed November 2003. (<http://www.epa.gov/iris>).
- U.S. EPA. 2001a. *Superfund Technical Support Center Provisional Toxicity Issue Papers (STSCPTV)*. Office of Radiation and Indoor Air, Washington, DC. February. Accessed November 2003. (<http://epa-heat.ornl.gov/provisional.html>).
- U.S. EPA. 2001b. *Health Effects Assessment Summary Tables (HEAST): Summary of HEAST Values*. Office of Radiation and Indoor Air, Washington, DC. February. Accessed November 2003. (<http://epa-heat.ornl.gov>).

Converting Inhalation RfC to Inhalation RfD

Inhalation data values from *IRIS* are typically given as reference concentrations (RfCs) that are equivalent to dose rather than an RfD. The RfC is converted to an RfD by the following equation (EPA, 1989b):

$$RfD_{inhal} = \frac{RfC \times IR \times AR}{BW \times 100} \quad (1)$$

where:

<i>RfC</i>	= Reference Concentration in Air (mg/m <sup>3</sup> )
<i>IR</i>	= Inhalation Rate (20 m <sup>3</sup> /day)
<i>AR</i>	= Absorption Rate (100% assumed unless otherwise specified)
<i>BW</i>	= Adult Body Weight (70 kg)

Using the default exposure assumptions listed above, Equation (1) may be simplified as:

$$RfD_{inhal} (mg / kg - day) = RfC_{inhal} \times AR \times 2.857 \times 10^{-3} \quad (2)$$

Equation (2) is used to convert an RfC to an inhalation RfD within SCDM. The resulting RfD inhalation value is used to calculate the air pathway screening benchmark for non-carcinogens and to determine an HTF if it is the lowest reference dose available. If the reference providing the value does not provide an absorption rate, it is assumed to be 100 percent.

**2.2.1.2 LD<sub>50</sub> - Oral, Dermal; LC<sub>50</sub> - Inhalation**

When a reference dose or cancer slope factor with weight-of-evidence is not available, SCDM uses the LD<sub>50</sub> (oral, dermal) or LC<sub>50</sub> (inhalation) to assign human toxicity factor values. The lowest of the two values is selected. These values are not used to calculate benchmarks. The reference hierarchy is as follows:

- American Conference of Governmental Industrial Hygienists (ACGIH). 2001. *Documentation of the Threshold Limit Value and Biological Exposure Indices*. 7<sup>th</sup> Edition. ACGIH, Cincinnati, OH.
- National Institute for Occupational Safety and Health (NIOSH). 2002. *Registry of Toxic Effects of Chemical Substances (RTECS)*. Accessed November 2002. (<http://grc.ntis.gov>).

- C-E Environmental, Inc. 1990. *The Identification of Health Effects Data for Chemicals Contained in the Clean Air Act Amendments: Final Report to Dr. John Vanderbury*. U.S. Environmental Protection Agency, Research Triangle Park, NC.

SCDM contains the lowest LD<sub>50</sub> or LC<sub>50</sub> value for any mammalian species by the specified route of exposure (i.e., oral or dermal) in controlled dose studies in laboratory animals. Human lethality data (i.e., data from suicide and worker poisonings) are not used due to the associated inaccuracy of the dosage estimates. Data from former Eastern Bloc countries (such as the former Soviet Union) are not used due to the typically poor data quality. Only data for exposure durations <24 hours are used. If the LD<sub>50</sub> value is not given, SCDM uses the Lethal Dose- Low or (LD<sub>Lo</sub>) (i.e., the lowest dose corresponding to an adverse effect relative to the control response) value if it: (1) is for the same exposure route, (2) has an exposure duration <24 hours, and (3) is reasonable relative to the other values (e.g., relative to chronic values) given for that substance and exposure route.

### 2.2.2 Carcinogenic Toxicity

These values are used to determine the Human Toxicity Factor values for carcinogenic substances in accordance with procedures set forth in the HRS.

#### 2.2.2.1 Cancer Slope Factor (SF) and Weight-of-Evidence - Oral; Unit Risk Factor (URF) and Weight-of-Evidence - Inhalation

SCDM contains SF values for oral toxicity and URF for inhalation toxicity. In addition to determining the Human Toxicity Factor value, the SF values are used to calculate the carcinogenic screening benchmarks for drinking water, food chain, soil ingestion, and air pathway threats. The URF values are translated into inhalation SF values for determining the human toxicity factor value and for calculating the air pathway benchmark.

The cancer slope factor with the weight-of-evidence classification for oral toxicity and the unit risk factor with the weight-of-evidence classification for inhalation toxicity are obtained from several references, which are listed below in order of preference. Cancer slope and unit risk values are obtained from several references (listed in order of preference), EPA's *Integrated Risk Information System (IRIS)*, EPA's *Superfund Technical Support Center Provisional Toxicity Values (STSCPTV)*, and EPA's *Health Effects Assessment Summary Tables (HEAST): Summary of HEAST Values*. SCDM ranks reference data according to the reference hierarchy. *IRIS* data are preferred over *STSCPTV* data, which are preferred over *HEAST* data. All three databases are available via the Internet, with *IRIS* having unrestricted public access. The other two (*STSCPTV* and *HEAST*) are password-protected and are accessible only to those with EPA approval. *STSCPTV* and *HEAST* may become publicly available at a later date.

For obtaining cancer slope factors for radionuclides, SCDM uses EPA's *HEAST Radionuclide Table: Carcinogenicity - Slope Factors* – (formerly known as Table 4), which is publicly available via the Internet or through the *HEAST* link at the EPA Office of Research and Development (ORD) password-protected

Web site at (<http://epa-heat.ornl.gov>). The ORD Web site is where the most current data will be made available. All references are listed below:

- U.S. EPA. 2003a. *Integrated Risk Information System (IRIS)*. Office of Research and Development, Cincinnati, OH. Accessed November 2003. (<http://www.epa.gov/iris>).
- U.S. EPA. 2001a. *Superfund Technical Support Center Provisional Toxicity Issue Papers (STSCPVT)*. Office of Research and Development, Washington, DC. February. Accessed November 2003. (<http://epa-heat.ornl.gov/provinsional.html>).
- U.S. EPA. 2001b. *Health Effects Assessment Summary Tables (HEAST): Summary of HEAST Values*. Office of Radiation and Indoor Air, Washington, DC. February. Accessed November 2003. (<http://epa-heat.ornl.gov>).
- U.S. EPA. 2001c. *HEAST Radionuclide Table: Carcinogenicity - Slope Factors*. Office of Radiation and Indoor Air, Washington, DC. April. Accessed November 2003. (<http://www.epa.gov/radiation/heat/index.html>).

#### Converting Unit Risk Factor to Inhalation Slope Factor

Carcinogenic inhalation data values from *IRIS* are typically given as unit risk factors. The URFs can be converted to an inhalation cancer slope factor by the following equation (this applies to non-radionuclides only) (EPA, 1989b):

$$SF_{inhal} = \frac{URF \times BW \times CF \times 100}{IR \times AR} \quad (3)$$

where:

- $SF$  = Cancer Slope Factor (mg/kg-day)<sup>-1</sup>  
 $URF$  = Unit Risk Factor (µg/m<sup>3</sup>)<sup>-1</sup>  
 $BW$  = Adult Body Weight (70 kg)  
 $CF$  = Conversion Factor (1,000 µg/mg)  
 $IR$  = Inhalation Rate (20 m<sup>3</sup>/day)  
 $AR$  = Absorption Rate (100% assumed unless otherwise specified)



Using the assumptions listed above reduces Equation (3) to the following equation:

$$SF_{inhal} (mg / kg - day)^{-1} = \frac{URF \times 3.50 \times 10^5}{AR} \quad (4)$$

Equation (4) is used to convert the unit risk factor to an inhalation cancer slope factor in SCDM. The resulting inhalation cancer slope factor is used to determine the HTF and the air pathway screening benchmark for non-radionuclide carcinogens. If *IRIS*, *STSCPVT*, or *HEAST* does not provide an absorption rate, it is assumed to be 100 percent. The risk calculations used in SCDM are intended to reflect EPA's current risk assessment practices and methodology as set forth in the EPA's recommended guidance documents, such as *Risk Assessment Guidance for Superfund (RAGS), Volume 1, Part A* (EPA 1989b) and *Part B* (EPA 1991), *Soil Screening Guidance: Technical Background Document* (EPA, 1996), and *Supplemental Guidance for Developing Soil Screening Levels for Superfund Sites* (Peer Review Draft) (EPA, 2001d).

#### Weight-of-Evidence

The HRS uses the weight-of-evidence combined with the cancer slope factor to determine the human toxicity factor value. (See HRS, Section 2.4.1.1). SCDM uses the weight-of-evidence classification from the same reference that provides the corresponding slope factor. The weight-of-evidence classification for most carcinogenic substances in SCDM is obtained from *IRIS*.

The weight-of-evidence value most closely described to the specified route of exposure is recorded separately for the oral weight-of-evidence and the inhalation weight-of-evidence. If only one weight-of-evidence is given, it is recorded for both the oral and inhalation values. In *HEAST*, there are usually two values listed, one for oral and one for inhalation. Usually these values are identical; *SCDM* records each value separately.

Please note the following: Recently *IRIS* proposed to adopt the weight-of-evidence criteria from what is now the *Draft Guidelines for Carcinogenic Risk Assessment* (U.S. EPA, 1999). This proposed *IRIS* revision will modify how carcinogenic weight-of-evidence classifications are presented and defined. This may eventually directly impact how the HRS determines the HTF (U.S. EPA *Guidelines for Carcinogenic Risk Assessment*. Review Draft. July 1999). Although *IRIS* is currently using the this proposed 1999 weight-of-evidence classification method as individual substances are reviewed, it currently retains the 1986 weight-of-evidence classifications. The 1986 weight-of-evidence classifications were A, B1, B2, C, and D. The 1999 (henceforth referred to as "new") proposed weight-of-evidence classifications are presented in a narrative fashion according to EPA's 1999 *Guidelines for Carcinogenic Risk Assessment*. These new classifications do not directly correspond to the 1986 A, B, C classifications. It has not yet been determined exactly when or if the 1986 weight-of-evidence classifications will no longer be consider valid. *IRIS* recommends using the new classifications over the 1986 ones; however, the HRS does not accommodate determining the HTF using the new weight-of-evidence classifications. SCDM will retain and use the old weight-of-evidence classifications, but also record the new weight-of-evidence classifications for future use. It is expected that the weight-of-evidence preference will change to the new weight-of-evidence in the near future as individual *IRIS* substances undergo review.

### 2.2.2.2 ED<sub>10</sub> and Weight-of-Evidence - Oral, Inhalation

When cancer slope factors with weight-of-evidence are not available, SCDM uses an ED<sub>10</sub> to calculate a cancer slope factor. SCDM uses data from the following references, listed in order of preference for oral and inhalation ED<sub>10</sub> and the associated weights-of-evidence:

- U.S. EPA. 1988. *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), (OWSER Directive 9285.4-1).

In the first reference (EPA, 1988) the values are reported as a single potency factor for oral and inhalation. This value is the reciprocal of an ED<sub>10</sub>. Therefore, the oral and inhalation ED<sub>10</sub> values for SCDM are calculated by taking the reciprocal of the (reported value) potency factor (that is, ED<sub>10</sub> = 1/potency factor).

## 2.3 Mobility Information

Vapor pressure and Henry's Law Constant are used to determine the gas migration potential and gas mobility potential. Water solubility and the soil/water distribution coefficient are used to determine the ground water mobility factor.

### 2.3.1 Vapor Pressure

SCDM uses data from the following references, which are listed in order of preference, for vapor pressure values:

- Syracuse Research Corporation (SRC). 2003a. *CHEMFATE Database*. SRC. Syracuse, NY. Accessed October 2003. (<http://esc.syrres.com/efdb/chemfate.htm>).
- Syracuse Research Corporation (SRC). 2003b. *PHYSPROP Database*. SRC. Syracuse, NY. Accessed October 2003. (<http://esc.syrres.com/interkow/physdemo.htm>).
- Lide, D.R. (Ed.). 2002-2003. *CRC Handbook of Chemistry and Physics*, 83<sup>rd</sup> Edition. CRC Press, Boca Raton, FL.
- O'neil, M., and A. Smith (Eds). 2001. *The Merck Index*, 13<sup>th</sup> Edition. Merck & Co., Inc., Rahway, NJ.
- CHEMCAL data file developed from:
  - Research Triangle Institute (RTI). 1996. *Chemical Properties for SCDM Development*. Prepared for U.S. EPA Office of Emergency and Remedial Response, Washington DC.Using procedures set forth by:
  - Lyman et al. 1990. *Handbook of Chemical Property Estimation Methods*. American Chemical Society, Washington, DC.

*CHEMFATE* contains recommended values, which are preferred over estimated or calculated values for use in SCDM. If more than one recommended value is in *CHEMFATE*, the highest is selected. 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, values determined within the range of 20 to 30°C are used. 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 in *CHEMFATE* for all vapor pressure measurements for a substance, SCDM uses the highest value.

If vapor pressure values are not available in *CHEMFATE*, then they are taken from the *PHYSPROP*, *CRC Handbook of Chemistry and Physics*, or *The Merck Index*. If no vapor pressure values are available in any of these four references, the procedures described in Lyman et al. (1990) are used to calculate vapor pressure, which is entered in a SCDM data file called *CHEMCAL*. RTI (1996) describes the use of these procedures for specific hazardous substances found in SCDM.

The above hierarchy is superseded by values in SCDM's *LIVECHEM* data file. When a value selected by the hierarchy is suspect or a measured value is not available in the SCDM data sources, values may be selected or calculated from other data sources, regardless of the reference hierarchy, and entered into *LIVECHEM*. For a particular chemical, suspect values are identified by comparison with other vapor

pressure values in SCDM data sources or other sources of chemical property data. The *LIVECHEM* data file includes a comment field listing the source of each *LIVECHEM* value.

For nonmetallic substances, if vapor pressure is not available, a normal boiling point is obtained from the *CRC Handbook of Chemistry and Physics* (Lide, 2002-2003) and entered directly into the *Cheminfo* file via the Chemical Properties data entry screen. The *Cheminfo* file stores all the physical properties data for SCDM substances. If a boiling point is not available from Lide (2002-2003), a value is obtained from *The Merck Index*. If the boiling point at 1 atmosphere (atm) is  $<25^{\circ}\text{C}$ , a default vapor pressure of 760 Torr is entered into *LIVECHEM* (that is, the substance is assumed to be a gas at  $25^{\circ}\text{C}$ ).

If no vapor pressure is available for a substance and the normal boiling point is  $\geq 25^{\circ}\text{C}$ , 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, which are listed in order of preference, for Henry's Law Constant:

- Syracuse Research Corporation (SRC). 2003a. *CHEMFATE Database*. SRC. Syracuse, NY. Accessed October 2003. (<http://esc.syrres.com/efdb/chemfate.htm>).
- Syracuse Research Corporation (SRC). 2003b. *PHYSPROP Database*. SRC. Syracuse, NY. Accessed October 2003. (<http://esc.syrres.com/interkow/physdemo.htm>).
- CHEMCAL data file developed from:
  - Research Triangle Institute (RTI). 1996. *Chemical Properties for SCDM Development*. Prepared for U.S. EPA Office of Emergency and Remedial Response, Washington DC.Using procedures set forth by:
  - Lyman et al. 1990. *Handbook of Chemical Property Estimation Methods*. American Chemical Society, Washington, DC.

*CHEMFATE* contains recommended values, which are preferred over estimated or calculated values for use in SCDM. If more than one recommended value is in *CHEMFATE*, the highest is selected. If a recommended value is not available, SCDM uses a value measured at  $25^{\circ}\text{C}$ . If more than one value measured at  $25^{\circ}\text{C}$  is available, SCDM uses the highest one. If no value is available at  $25^{\circ}\text{C}$ , values determined within the range of  $20$  to  $30^{\circ}\text{C}$  are used. 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 in *CHEMFATE* for all Henry's Law constants for a substance, SCDM uses the highest value.

If no Henry's Law constant is available, the procedures described in Lyman et. al (1990) are used to calculate a Henry's Law constant, and the calculated values are placed in the SCDM *CHEMCAL* data file.

The above hierarchy is superseded by values in SCDM's *LIVECHEM* data file when a value selected by the hierarchy is suspect or a measured value is not available in the SCDM data sources. For a particular chemical, suspect values are identified by comparison with other Henry's Law constant values in SCDM data sources or other sources of chemical property data. The *LIVECHEM* data file includes a comment field listing the source of each *LIVECHEM* value.

### 2.3.3 Water Solubility

Water solubility values and distribution coefficient ( $K_d$ ) values are used 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 a bioaccumulation potential factor value for hazardous substances when bioconcentration factor (BCF) data or logarithm of the n-octanol-water partition coefficient ( $\log K_{ow}$ ) data are not available.

#### 2.3.3.1 Water Solubility - Nonmetallic Compounds

The SCDM obtains water solubility values for nonmetallic substances from the following references:

- Syracuse Research Corporation (SRC). 2003a. *CHEMFATE Database*. SRC. Syracuse, NY. Accessed October 2003. (<http://esc.syrres.com/efdb/chemfate.htm>).
- Syracuse Research Corporation (SRC). 2003b. *PHYSPROP Database*. SRC. Syracuse, NY. Accessed October 2003. (<http://esc.syrres.com/interkow/physdemo.htm>).
- Dean, J.A. (Ed.). 2002. *Lange's Handbook of Chemistry*, 15<sup>th</sup> Edition. McGraw-Hill, New York.
- CHEMCAL data file developed from:
  - Research Triangle Institute (RTI). 1996. *Chemical Properties for SCDM Development*. Prepared for U.S. EPA Office of Emergency and Remedial Response, Washington DC.Using procedures set forth by:
  - Lyman et al. 1990. *Handbook of Chemical Property Estimation Methods*. American Chemical Society, Washington, DC.

*CHEMFATE* contains recommended values, which are preferred over estimated or calculated values for use in SCDM. If more than one recommended value is in *CHEMFATE*, the highest is selected. 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, values determined within the range of 20 to 30°C are used. 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 in *CHEMFATE* for all water solubilities for a substance, SCDM uses the highest value.

If water solubility values are not available in *CHEMFATE*, *PHYSPROP* or *Lange's Handbook of Chemistry*, the procedures described in Lyman et al. (1990) are used to calculate water solubility. RTI (1996) describes the use of these procedures for specific hazardous substances found in SCDM.

The above hierarchy is superceded by values in SCDM's *LIVECHEM* data file when a value selected by the hierarchy is suspect or a measured value is not available in the SCDM data sources. For a particular chemical, suspect values are identified by comparison with other water solubility values in SCDM data sources or other sources of chemical property data. The *LIVECHEM* data file includes a comment field listing the source of each *LIVECHEM* value.

### 2.3.3.2 Water Solubility - Metals and Metalloids

SCDM obtains water solubility values for metals and metalloid compounds from the following references:

- Lide, D.R. (Ed.). 2002-2003. *CRC Handbook of Chemistry and Physics*, 83<sup>rd</sup> Edition. CRC Press, Boca Raton, FL.
- Dean, J.A. (Ed.). 2002. *Lange's Handbook of Chemistry*, 15<sup>th</sup> ed. McGraw-Hill, New York.

SCDM contains the geometric mean water solubility values for metals and metalloids as defined in the HRS as the geometric mean of the highest and lowest water solubility values available for any inorganic compound containing the metal or metalloid.

### 2.3.4 Soil/Water Distribution Coefficient ( $K_d$ ); Soil Organic/Carbon Partition Coefficients ( $K_{oc}$ )

The soil/water distribution coefficient ( $K_d$ ) values (and associated  $K_{oc}$  and  $\text{Log } K_{ow}$  if there is no  $K_d$  value) are used to calculate ground water mobility for hazardous substances that do not meet observed release criteria. All hazardous substances that are available to migrate from sources at the site to a ground water are evaluated for ground water mobility.

The present SCDM obtains soil/water distribution coefficient ( $K_d$ ) values for metals and radionuclides from the following references:

- U.S. EPA. 2001d. *Supplemental Guidance for Developing Soil Screening Levels for Superfund Sites* (Peer Review Draft), OSWER 9355.4-24. March. Accessed October 2003. (<http://www.epa.gov/superfund/resources/soil/index.htm>).
- U.S. EPA. 2000e. *Soil Screening Guidance for Radionuclides: User's Guide*. EPA/540-R-00-007 PB2000 963307. Accessed October 2003. (<http://www.epa.gov/superfund/resources/radiation/radssg.htm>).
- 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. Accessed October 2003. (<http://www.epa.gov/superfund/resources/soil/index.htm>).
- 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.
- Research Triangle Institute (RTI). 1996. *Chemical Properties for SCDM Development*. Prepared for U.S. EPA Office of Emergency and Remedial Response, Washington, DC.

### Metals

For metals, SCDM uses  $K_d$  values contained EPA's *Soil Screening Guidance* (EPA, 2001). These were estimated using the MINTEQA2 aqueous speciation geochemical model. When the required thermodynamic data were not available in the MINTEQA2 database, the empirical pH-dependent relationships developed by the EPA's Office of Research and Development laboratory in Athens, Georgia, are used (RTI, 1996). SCDM contains values corresponding to typical subsurface pH (6.8).

### Organic Substances

For organic hazardous substances, SCDM calculates the  $K_d$  according to the HRS Section 3.2.1.2, *Mobility*, and the relationship  $K_d = K_{oc} \times f_s$ , where  $K_{oc}$  is also calculated following directions from the *Soil Screening Guidance* (EPA, 1996) and Di'Toro (1985).  $K_{oc}$  values are also obtained from the *Soil Screening Guidance* and the *Supplemental Guidance for Developing Soil Screening Levels for Superfund Sites* (EPA, 2001d). See Section 3.2, Soil Water Distribution Coefficient ( $K_d$ ); Soil Organic/Carbon Partition Coefficients ( $K_{oc}$ ), of this document for more on SCDM calculations for  $K_d$  and  $K_{oc}$  values.

## **2.4 Persistence Information**

The evaluation of persistence is based primarily on the half-life of the hazardous substance in surface water and secondarily on the sorption of the hazardous substance to sediments. Persistence information is used to determine the surface water persistence factor.

### 2.4.1 Hydrolysis, Biodegradation, and Photolysis Half-Lives

The present SCDM obtains hydrolysis, biodegradation, and photolysis half-lives from the following references:

- Syracuse Research Corporation (SRC). 2003a. *CHEMFATE Database*. SRC. Syracuse, NY. Accessed October 2003. (<http://esc.syrres.com/efdb/chemfate.htm>).
- Howard, Philip H., W.F. Jarvis, W.M. Meylan, and E.M. Michalenko. 1991. *Handbook of Environmental Degradation Rates*. (FATERATE) Lewis Publishers, Inc. Chelsea, Michigan.
- Syracuse Research Corporation (SRC). 2003b. *PHYSPROP Database*. SRC. Syracuse, NY. Accessed October 2003. (<http://esc.syrres.com/interkow/physdemo.htm>).

SCDM uses only those values listed as “first-order” in *FATERATE*. If high and low values are provided, the highest value is used. SCDM only uses measured values from the *CHEMFATE* database. Estimated or calculated values are not used in SCDM. If more than one recommended value is in *CHEMFATE*, the highest is selected. 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, values determined within the range of 20 to 30°C are used. If more than one value measured at the same temperature and none is recommended, SCDM uses the highest value. If no half-life value is specified in *CHEMFATE*, the half-life used in SCDM is calculated based on the percent change over time by assuming a first-order rate law.

### 2.4.2 Radioactive Half-Life

The radioactive half life is used to determine the persistence of the radionuclide. The persistence of a hazardous substance is assigned according to HRS Table 4-10 *Persistence Factor Values - Half-Life* (40 CFR Part 300, Appendix A, Section 4.1.2.2.1.2).

SCDM obtains radioactive half-life values from the following references listed in order of preference:

- U.S. EPA. 2000e. *Soil Screening Guidance for Radionuclides: User's Guide*. EPA/540-R-00-007 PB2000 963307. Accessed October 2003. (<http://www.epa.gov/superfund/resources/radiation/radssg.htm>).
- International Commission on Radiological Protection (ICRP). 1983. *Radionuclide Transformations: Energy and Intensity of Emissions*. ICRP Publication No. 38. Pergamon Press, NY.



Multiple Values, Multiple Decay Modes

If more than one value is given for a single decay mode, SCDM uses the highest value. If values are given for more than one decay mode, the half-life of the isotope is computed from the values for all decay modes according to the following formula:

$$t_{1/2} = 1 / \left( 1/t_1 + 1/t_2 \dots + 1/t_n \right) \quad (5)$$

where:

- $t_{1/2}$  = Half-life of the isotope
- $t_1$  = Value given for the first decay mode
- $t_2$  = Value given for the second decay mode
- $t_n$  = Value given for the n-th decay mode.

## 2.5 Bioaccumulation Potential Information

Bioconcentration Factors (BCF) for freshwater and saltwater (one set for the human food chain threat and another set for the environmental threat), Log  $K_{ow}$ , and water solubility values are used to determine the bioaccumulation potential factor value (40 CFR Part 300, Appendix A, Section 4.1.3.2.1.3). If BCF data are not available, the Log  $K_{ow}$  is used. Water solubility data are used if the Log  $K_{ow}$  exceeds 6.0, or the substance is inorganic, or there is no Log  $K_{ow}$ .

### 2.5.1 Bioconcentration

The BCF values for freshwater and saltwater are used to determine the human food chain threat BCF and the environmental threat BCF. The BCF values in SCDM are preferentially based on literature values of actual measurements of bioconcentration in aquatic organisms. SCDM used BCF values from the following sources (listed in order of preference):

- U.S. EPA. 2003b. *ECOTOX Database*. Environmental Research Laboratory, Duluth, MN. Accessed December 2003. (<http://www.epa.gov/ecotox>).
- 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.

In SCDM, the highest measured value from *ECOTOX* is used. Measured values are preferred over calculated or estimated values. The above listed Versar reference is a report of a literature survey of BCF values developed for the purpose of obtaining preliminary values for use when the present HRS was being

developed. When using data from this reference, SCDM also prefers the highest measured value to an estimated value. All values where no environment (i.e., saltwater or freshwater) is specified but list NaCl as a control are considered as freshwater values.

Environmental Threat

For the environmental threat, the highest value from *any* aquatic organism (regardless if it is consumed by humans) in each reference is used to establish environmental threat BCF values.

Human Food Chain Threat

The highest measured value from aquatic organisms typically known to be consumed by humans in each reference is used to establish the human food chain threat BCF values. Nonhuman food chain aquatic organisms are not used for the food chain BCF. Table 1 includes a list of some of the organisms for which 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	lake trout (siscowet)
Asiatic clam	lake whitefish
Atlantic salmon	mangrove snapper
Atlantic silverside	mussel
black bullhead	northern pike
black crappie	pilchard sardine
black mussel	pinfish
blue crab	pink salmon
bluegill	rainbow trout
brook trout	red swamp crayfish
brown trout	rock bass
channel catfish	sauger
clam	shore crab
common bay mussel	spot
common mirror colored carp	striped bass
common shrimp	striped mullet
crayfish	swan mussel
dungeness or edible crab	tong sole
giant gourami	topmouth gudgeon (golden shiner)
gulf toadfish	white mullet
kiyi	Manila littleneck clam
northern anchovy	white sand mussel

**2.5.2 Octanol/Water Partition Coefficient Log K<sub>ow</sub>**

The n-octanol/water partition coefficient (log K<sub>ow</sub>) values are used to determine the bioaccumulation potential factor value for a hazardous substance for which bioconcentration factor (BCF) data are not available.

SCDM obtains n-octanol/water ( $\log K_{ow}$ , also referred to as Log P) values from the following sources:

- Syracuse Research Corporation (SRC). 2003a. *CHEMFATE Database*. SRC. Syracuse, NY. Accessed October 2003. (<http://esc.syrres.com/efdb/chemfate.htm>).
- Syracuse Research Corporation (SRC). 2003b. *PHYSPROP Database*. SRC. Syracuse, NY. Accessed October 2003. (<http://esc.syrres.com/interkow/physdemo.htm>).
- Lide, D.R. (Ed.). 2002-2003. *CRC Handbook of Chemistry and Physics*, 83<sup>rd</sup> Edition. CRC Press, Boca Raton, FL.
- Research Triangle Institute (RTI). 1996. *Chemical Properties for SCDM Development*. Prepared for U.S. EPA Office of Emergency and Remedial Response, Washington, DC.

The above references are listed in the preferential hierarchy for SCDM. While most of the hazardous substances in SCDM are addressed in RTI (1996), more recent data sources are preferred. If the more recent sources do not have data for specific substances, then the RTI (1996) reference will be used. Many of the RTI (1996) values were selected by EPA's Office of Research and Development (ORD) in Athens, Georgia, from a list of measured values compiled by RTI and from values calculated by ORD using the SPARC and CLOGP computer programs. Values not selected by ORD were selected by RTI from a separate compilation of measured values.

SCDM uses only recommended values from the *CHEMFATE* database. If estimated or calculated values are present, those values are not used in SCDM.

### 2.5.3 Water Solubility

Water solubility values are used to assign a bioaccumulation potential factor value for hazardous substances when bioconcentration factor (BCF) data or logarithm of the n-octanol-water partition coefficient ( $\log K_{ow}$ ) data are not available.

See Sections 2.3.3.1, *Water Solubility - Nonmetallic Compounds*, and 2.3.3.2, *Water Solubility - Metals and Metalloids*, of this SCDM methodology for the data collection protocol and guidance on water solubility values and low-solubility compounds.

## 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. SCDM uses only 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 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 do not exist. These new criteria are now labeled as Criteria Maximum Concentration (CMC) (to be used in place of what was previously acute AWQC) and Criteria Continuous Concentration (CCC) (to be used in place of what was previously chronic AWQC) for freshwater and saltwater. They closely correspond to the old acute and chronic AWQC values, respectively; however, some values have been re-derived using different methodology and, therefore, the resulting values must be used as directed by EPA. Many of the CMC and CCC values have associated endnotes regarding how the value was derived and how it should be used. SCDM also contains these endnotes. 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. 2002. *National Recommended Water Quality Criteria - 2002*. Office of Water. Washington, DC. November.

### 2.6.2 LC<sub>50</sub> - Freshwater, Saltwater

SCDM obtains LC<sub>50</sub> data from the *ECOTOX* database, which includes a subset of data called AQUIRE.

- U.S. EPA. 2003b. *ECOTOX Database*. Environmental Research Laboratory, Duluth, MN. Accessed December 2003. (<http://www.epa.gov/ecotox>).

SCDM uses the lowest acute LC<sub>50</sub> value found for any aquatic organism in the specified environment with an acute exposure duration of >1 day and < 4 days. All LC<sub>50</sub> values where no environment is given but that use NaCl as a control are considered as freshwater LC<sub>50</sub> values. When no durations or environments are given, LC<sub>50</sub> values are not entered into SCDM.

## 2.7 Regulatory Benchmarks

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

### 2.7.1 National Ambient Air Quality Standards

The 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 for *NAAQS*:

- 40 CFR Part 50. 2001. *National Ambient Air Quality Standards*. November.

### 2.7.2 National Emissions Standards for Hazardous Air Pollutants

The 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.

- 40 CFR Part 61. 1994. *National Emission Standards for Hazardous Air Pollutants*.

SCDM lists only values that are reported in ambient concentration units ( $\mu\text{g}/\text{m}^3$ ).

### 2.7.3 Maximum Contaminant Levels and Maximum Contaminant Level Goals

The 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. 2003c. *National Primary Drinking Water Standards*. Accessed through *List of Drinking Water Contaminants and MCLs*. Office of Water, Washington, DC. (<http://www.epa.gov/safewater/mcl.htm>).
- U.S. EPA. 2000e. *Soil Screening Guidance for Radionuclides: User's Guide* (EPA/540-R-00-007, PB2000 963307). October. (<http://www.epa.gov/superfund/resources/radiation/radssg.htm>).

SCDM uses only MCLs that are reported in units of concentrations (mg/L,  $\mu\text{g}/\text{L}$ , or pCi/L). SCDM uses only nonzero MCLGs that are reported in units of concentration (mg/L or  $\mu\text{g}/\text{L}$ ). For substances where multiple values are listed due to lack of consensus on appropriate carcinogen class, SCDM contains the lowest number. For substances where both MCLs and MCLGs are reported but are different, SCDM selects the lower of the two values.

### 2.7.4 FDA Action Level

The 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 FDA Action Levels for fish and shellfish only. Data are extracted directly from the reference. SCDM obtains FDAALs from the following references:

- 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. Accessed September 2003. (<http://www.cfsan.fda.gov/~lrd/fdaact.html>).

### 2.7.5 Uranium Mill Tailings Radiation Control Act Standards

The Uranium Mill Tailings Radiation Control Act Standards (*UMTRCA*) standards are used to establish Level I concentrations. Targets exposed to concentrations at or above *UMTRCA* are scored as Level I targets. Data are extracted directly from the reference.

SCDM uses data from the following source for *UMTRCA* Levels:

- 40 CFR Part 192. 1994. Uranium Mill Tailings Radiation Control Act Standards.

### 2.7.6 Ecological Based Benchmarks

The acute and chronic AWQC have been replaced by a new set of criteria, and the AALAC values do not exist. These new criteria are now labeled as acute Criteria Maximum Concentration (CMC) and chronic Criteria Continuous Concentration (CCC) for freshwater and saltwater. They closely correspond to the old acute and chronic AWQC values, respectively; however, some values have been re-derived using different methodology and, therefore, the resulting values must be used as directed by EPA. Many of the CMC and CCC values have associated endnotes regarding how the value was derived and how it should be used. SCDM also contains these endnotes. 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. 2002. *National Recommended Water Quality Criteria - 2002*. Office of Water. Washington, DC. November.

## 2.8 Other Chemical Data

SCDM contains hazardous substance physical property data including, but not limited to, chemical formula, molecular weight, density, boiling point, and melting point.

### 2.8.1 Physical Properties

SCDM contains other chemical data and information that are not contained in other data files. This information is in the *Cheminfo* file and can be viewed through the Chemical Properties data entry screen. SCDM physical property data of hazardous substances is directly extracted from the following sources:

- Lide, D.R. (Ed.). 2002-2003. *CRC Handbook of Chemistry and Physics*, 83<sup>rd</sup> Edition. CRC Press, Boca Raton, FL.
- O'neil, M., and A. Smith (Eds). 2001. *The Merck Index*, 13<sup>th</sup> Edition. Merck & Co., Inc., Rahway, NJ.

### 2.8.2 Logical Fields

SCDM uses four logical (or boolean yes/no) flags to classify substances that are entered into *Cheminfo* using the Chemical Properties data entry screen. These classification definitions are strictly intended for use in SCDM and should not be referenced for any other purpose. These flags are described below:

- Organic Substance (“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. Volatile and semivolatile organics are indicated. These flags influence the SCDM calculation of  $K_d$  values.
- Metal-Containing Substance (“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 whether or not the HRS factors and benchmarks are printed in Appendix A.

### 2.8.3 Substitution Classes

SCDM contains fields for three major substitution classes: toxicity, ground water mobility, and other data. For a particular chemical, a parent CAS number can be entered for any of these three substitution classes and SCDM automatically copies the relevant data from the parent chemical to the chemical of interest. Toxicity class data include all toxicity and benchmark data used to determine human or ecotoxicity factor values. Ground water mobility class data include water solubility, geometric mean water solubility, and soil/water distribution coefficient ( $K_d$ ). “Other” class data include hydrolysis, biodegradation, photolysis,

and volatilization half-lives, as well as BCF and Log  $K_{ow}$ . For a particular substance, SCDM may also indicate specific fields for data to be substituted from the parent CAS number.

Currently 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 and "other" classes.