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Screening Level Ecological Risk Assessment Protocol for Hazardous Waste Combustion Facilities

Volume Two
Appendix A

Peer Review Draft

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APPENDIX A

CHEMICAL-SPECIFIC DATA

Screening Level Ecological Risk Assessment Protocol

August 1999

APPENDIX A-1

INFORMATION ON COMPOUNDS OF POTENTIAL INTEREST

TABLE A-1

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APPENDIX A-1

COMPOUNDS OF POTENTIAL INTEREST

REFERENCES AND DISCUSSION

This discussion lists reference documents for each of the columns in Table A1-1 and briefly describes the quality of data associated with these references. This information is only presented for informational purposes to assist in planning data collection.

A1.1 COLUMN 1: CHEMICAL ABSTRACTS SERVICE (CAS) NUMBER

The CAS number is a unique number assigned to each compound in the table. Compounds are listed by CAS number, in ascending order, to prevent problems with alphabetization procedures or differences in common nomenclature.

A1.2 COLUMN 2: COMPOUND NAME

The most common compound name is listed. Where appropriate, common synonyms are also listed to aid the user in identifying particular compounds.

A1.3 COLUMN 3: COMPOUNDS LISTED IN 40 CFR PART 261 APPENDIX VII OR VIII

Appendix VII of Title 40 Code of Federal Regulations (40 CFR) Part 261 identifies compounds for which specific hazardous wastes, from specific and nonspecific sources, are listed (U.S. EPA 1995). Appendix VIII of 40 CFR Part 261 identifies acute hazardous wastes and toxic hazardous wastes associated with commercial chemical products, manufacturing chemical intermediates, and off-specification commercial chemical products (U.S. EPA 1995). This column lists hazardous waste codes for the associated compounds. This list is provided for reference purposes only, because it is commonly cited by other U.S. EPA combustion risk assessment documents as an original source of the product of incomplete combustion (PIC) lists. An explanation of the reasons for including a COPC on this list is beyond the scope of this guidance.

A1.4 COLUMN 4: CHEMICAL-SPECIFIC DATA AVAILABLE

This column lists those compounds for which the following are available (as presented in Appendix A-2): (1) chemical-specific physical and chemical information, and (2) chemical-specific fate-and-transport information.

A1.5 COLUMN 5: PICS RECOMMENDED BY U.S. EPA (1994a) FOR SCREENING LEVEL RISK ASSESSMENTS

Compounds in this column marked with an "X" in the appropriate cells identified by U.S. EPA (1994a) as PICs to be included in screening level risk assessments. U.S. EPA (1994a) does not describe the basis or references for the inclusion of these PICs in screening level risk assessments. More information regarding some of these compounds is presented in Chapter 2.

A1.6 COLUMN 6: PICS IDENTIFIED IN COMBUSTION UNIT EMISSIONS (U.S. EPA 1993)

Compounds in this column marked with an "X" in the appropriate cells are identified in U.S. EPA (1993) as PICs. The source documents for these tables cited by U.S. EPA (1993) are described in the following subsections. These references have been cited by this and other U.S. EPA reference documents as "sources" of information regarding PIC emissions from hazardous waste combustion units. This document─U.S. EPA (1993)─has, in turn, been cited by later guidance documents as a "source" of information regarding PIC emissions from hazardous waste combustion units. However, as is indicated by the listing of the references from Dempsey and Oppelt (1993) (which is a summary of existing

Standards are technology-based, not risk-based.

- U.S. EPA (1990a) describes amendments to the hazardous waste incinerator regulations for the following purpose:

> Improve control of toxic metal emissions, HCl emissions, and residual organic emissions; amend the definitions of incinerators and industrial furnaces; propose definitions for plasma arc incinerators and infrared incinerators; propose to regulate carbon regeneration units as thermal treatment devices; and make a number of minor revisions to permitting procedures.

U.S. EPA (1990a) also states the following:

> The database on PIC emissions is limited therefore, the risk assessments may under-estimate risk. The assessments consider only the organic compounds that have been actually identified and quantified. Zero to 60 percent of total unburned hydrocarbon emissions have been chemically identified at any particular facility. Thus, the bulk of the hydrocarbon emissions have not been considered in those risk assessments. Although many of the unidentified, unquantified organic compounds may be non-toxic, some fraction of the organic emissions is undoubtedly toxic. . . .data on typical PIC emissions from hazardous waste combustion sources were compiled and assessed in recent EPA studies. These studies identified 37 individual compounds in the stack gas of the eight full-scale hazardous waste incinerators tested, out of which 17 were volatile compounds and 20 semivolatile compounds. Eight volatile compounds (benzene, toluene, chloroform, trichloroethylene, carbon tetrachloride, tetrachloroethylene, chlorobenzene, and methylene chloride), and one semivolatile compound (naphthalene) were identified most frequently in more than 50 percent of the tests. Some of these compounds are carcinogenic.

The sources for these statements appear to be Wallace and others (1986) and Trenholm and Lee (1986).

Trenolm and Lee (1986), prepared by Andrew R. Trenholm of Midwest Research Institute and C.C. Lee at the U.S. EPA Hazardous Waste Engineering Research Laboratory, discussed that emissions from incinerators are only characterized for constituents listed in Appendix VIII. However, constituents not listed in Appendix VIII are also emitted from the stacks.

Data was obtained from HWERL-sponsored tests at eight hazardous waste incinerators, nine boilers that co-fired hazardous wastes, and five mineral processing kilns that fired hazardous wastes as fuel. In addition, SVOC emissions data for two municipal solid waste incinerators and seven coal-fired power plants were also reviewed. The common PICs are presented in the following table:

addressed, including issues concerning the combustion and incineration of hazardous waste. Major findings of the committee were as follows:

  - Fugitive emissions and spills may release as much or more material to the environment than the direct emissions from waste incineration processes.

  - Numerous PICs are formed during combustion processes. However, only a fraction of them are identified or detected. It is possible that the aggregate of all compound emissions that are not categorized as other POHCs or PICs can be more toxic and pose greater risks than those listed. Although 99.99 percent DRE has been claimed, if the unburned or undetected hydrocarbon output is included, the DRE may actually be less than 99.99 percent. Therefore, the concept of destruction efficiency used by EPA was found to be incomplete and not useful for subsequent exposure assessments. All emissions and effluents must be identified and quantified, including their physical form and characteristics.

  - Local site-specific conditions must be used in characterizing exposure to receptors from waste incinerator emissions.

  - The evaluation of exposure durations and concentrations should be based on a detailed assessment of transport processes and the habits of the exposed organisms. The role of food chains needs particular attention.

  - At a minimum, the toxicities of representative emissions and effluents from incinerators should be tested on sensitive life stages of representative aquatic and terrestrial vertebrates, invertebrates, and plants of ecological importance.

- U.S. EPA (1990b) does not include a list of PICs from combustion sources. It was prepared by the PIC subcommittee of the Science Advisory Board to review the OSW proposal to control emissions of PICs from hazardous waste incinerators by instituting process controls that are based on CO and THC emission concentrations. U.S. EPA risk assessments indicate that emissions of PICs at currently measured levels are not likely to produce unacceptable risks. However, because the current DRE standard applies only to designated POHCs, 99.99 percent DRE does not preclude the possibility that emission of PICs could present significant risk. The following summarizes the major findings of the subcommittee review.

  - The concept of using CO and THC as guidance for incinerator operational control is reasonable.

  - At low CO levels, CO correlates well with THC; therefore, limiting CO in order to ensure high combustion efficiency and low THC levels is reasonable. At high CO concentrations, CO and THC do not correlate well; therefore, relying solely on the controlling of CO may not provide a reasonable control for THC. Continuous emissions monitoring of THC is preferred. Quantification of PICs alone is not practical with the sampling techniques that are available, primarily because PICs are normally emitted in the range of parts per billion (ppb) to parts per trillion (ppt).

  - A 100-ppmv limit for CO is reasonable. However, supporting documentation does not demonstrate that a CO concentration of 100 ppmv is better than 50 ppmv or 150 ppmv.

  - Continuous emissions monitoring of THC with a cold system appears to be practical for routine operations. However, a hot transfer line produces better analysis of THC concentrations and detection of a larger fraction of the THCs emitted.

  - The database characterizing PICs in emissions would not allow a correlation to be established with CO or THC levels for various combustion devices and conditions. Limited data introduces large uncertainties into U.S. EPA's risk assessment. Therefore, U.S. EPA's site-specific risk assessment process is limited in its usefulness in establishing acceptable THC levels. However, the risk assessment procedures are risk-based.

- U.S. EPA (1987) is a report prepared by Andrew R. Trenholm, Acurex Corporation, California, and staff members from the U.S. EPA Hazardous Waste Engineering Research Laboratory in Cincinnati, Ohio. The paper discussed the lack of information on total emissions from combustion of hazardous wastes, particularly under conditions of less than optimal performance. The focus issue was whether additional constituents that are listed in Appendix VIII or not listed in Appendix VIII which were not identified in early tests might be emitted from hazardous waste combustion units. To address this issue and related issues, U.S. EPA initiated this project to qualitatively and quantitatively study the characteristics of all possible effluents, under steady-state and transient conditions. The following summarizes the major findings:

  - THC emissions detected as specific compounds ranged from 50 to 67 percent for five runs and were 91 percent for one run. The fraction of THC not detected is most likely explained by uncertainty in the measurements or other analytical problems.

  - Methane accounted for the largest fraction of THC.

  - Oxygenated aliphatic compounds made up the largest class of compounds among the SVOCs, both in total mass and number of compounds.

  - Transient upsets did not cause significant increases in the concentration of SVOCs or most VOCs. Three VOCs that were increased were methane, methylene chloride, and benzene.

  - Particulate and HCl emissions did not change between the steady-state and transient test runs.

- Duval and Rubey (1976) was prepared by D.S. Duval and W.A. Rubey of the University of Dayton Research Institute, Ohio. The objective of the study was to provide data from which requirements can be assigned for the thermal disposal of kepone. This report was primarily concerned with the high-temperature destruction of kepone, with DDT and Mirex used as comparative Analog. Laboratory tests were conducted to establish destruction temperature characteristics of the vaporized pesticides at preselected residence times. The following summarizes the major findings.

  - Kepone was essentially destroyed at a 1-second residence time and a temperature range of 500°C to 700°C, depending on the pesticide.
  - Major decomposition products detected were hexachlorocyclopentadiene and hexachlorobenzene for both kepone and Mirex. These products were formed in different thermal regions.
  - The study demonstrated that the chemical nature of the effluent products depends on the temperature and residence time that the basic molecule experiences.

- Duval and Rubey (1977) discusses the experimental destruction temperature and residence time relationships for various PCB compounds and mixtures of PCBs. The document states that "upon thermal stressing in air, PCBs decomposes to low-molecular-weight products." However, the document does not identify any of these low-molecular-weight products. In fact, the document states directly that the products were not identified in the study. It further recommends that additional research be conducted on the "degradation products and effluents."

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model based on laboratory studies conducted by using the nonflame mode of hazardous waste thermal decomposition. The results of these studies were compared to the flame-mode studies and field tests to evaluate the incineration model proposed. The model was based on the premise that incinerators do not operate continuously at optimum conditions. As a result, 1 percent or more of the feed and its flame treatment products must undergo further decomposition in the nonflame region to meet the DRE criterion of greater than 99.99 percent.

In the past, several methods were used to rank the incinerability of compounds. Nonflame studies, however, indicated that tests on compounds conducted at low oxygen concentrations provided a better correlation with field tests to determine the relative incinerability of compounds. Four experimental studies were conducted to develop and expand the database on POHCs and PICs.

Studies were conducted on individual compounds to evaluate degradation compounds and PICs from the original parent compound. The thermal degradation of 2,3’,4,4’,5-PCB was studied under four reaction atmospheres (at varying levels of oxygen) at a constant gas phase residence time of 2.0 seconds. Tests were conducted at temperatures ranging from 500^oC to 1,000^oC. Tests indicated that the yield of combustion products decreased with increased oxygen levels. Numerous major degradation products were identified from the thermal degradation of 2,3’,4,4’,5-PCB, including:

- Penta-, tetra-, and trichlorodibenzofurans
- Tetra- and trichlorobiphenyls
- Tri- and dichlorobenzene
- Tetra- and trichloronaphthalene
- Tri- and dichlorochlorophenylethlyene
- Tetrachlorobiphenylenes
- C_9H_8OCl
- $C_{10}H_3Cl_3$

Thermal decomposition of chloroform was studied. Numerous decomposition products were identified, including:

- CCl_4
- $C_2H_4Cl_2$
- C_2HCl_3
- C_2HCl_5
- C_2Cl_2
- C_2Cl_4
- C_3Cl_4
- C_4Cl_6

Thermal decomposition of polychlorinated phenols was studied in nitrogen (N_2) and oxygen atmospheres because of the potential formation of polychlorinated dibenzodioxins. Pentachlorophenol (PCP) thermal decomposition was studied. Numerous decomposition products of PCP were identified in N_2 and/or air atmospheres, including:

- Dichlorobutadiyne (in N_2)
- Tetrachloroethylene (in air)
- Tetrachloropropyne (in air)
- Trichlorofuran (in air)
- Tetrachlorofuran (in air)
- Trichlorobenzene (in N_2 and air)
- Tetrachlorobenzene (in N_2 and air)
- Pentachlorobenzene (in N_2 and air)
- Hexachlorobenzene (in N_2)
- Octachlorostyrene (in N_2)
- Hexachlorodihydronaphthalene (in N_2 and air)

The paper concluded that PICs in the air atmosphere may have formed directly from the parent material, whereas, in the nitrogen atmosphere, the principal PICs may have evolved from the thermal decomposition of other PICs.

- Kramlich, Seeker, and Heap (1984) does not include a list of PICs from combustion sources. It was prepared by J.C. Kramlich, W.R. Seeker, and M.P. Heap of Energy and Environmental Research Corporation, California; and C.C. Lee of the Industrial Waste Combustion Group, U.S. EPA. This paper presented a research program to study the flame-mode incineration of hazardous waste liquids in laboratory scale reactors. The objective of this study was to supply the flame-mode data that will be used in evaluating the applicability of various approaches to ranking the ease of incinerability.

  Five compounds were tested—chloroform, 1,1-dichloroethane, benzene, acrylonitrile, and chlorobenzene—because (1) their range of incinerabilities is broad, and (2) they are representative of liquid hazardous wastes. The following summarizes the findings.

  - The flame section of the incinerator destroys greater than 99.995 percent of the wastes.

  - The post-flame region destroys the remainder of the wastes.

  - The destruction efficiency is reduced because of flame-related failures.

  - Incinerability ranking depends on actual failure condition.

  - No incinerability ranking system completely predicts the destruction efficiency of the compounds tested for all failure conditions.

- Trenholm and Hathaway (1984) was prepared by Andrew Trenholm and Roger Hathaway of Midwest Research Institute (MRI) in Missouri, and Don Oberacker, U.S. EPA, Cincinnati, Ohio. PICs were defined as any Appendix VIII hazardous organic constituent detected in the stack gas but not present in the waste feed at a concentration of 100 micrograms per gram or higher. Benzene and chloroform were the most commonly found PICs. PIC emissions were comparable to POHC emissions in concentration and total mass output. This document discussed PIC formation mechanisms and criteria for PIC formations.

MRI conducted a series of tests at eight operating hazardous waste incineration facilities and analyzed the collected samples for PICs. These tests were conducted as part of the technical support of U.S. EPA's preparation of a regulatory impact analysis for hazardous waste incinerators. Each incinerator had a liquid injection burner, and some facilities also included a rotary kiln or hearth. Three incinerators had no air pollution control devices. The remaining five had wet scrubbers for HCl control, and four of these had other particulate control devices. Twenty-nine compounds were classified as PICs from the eight incinerator tests and are presented in Table A1.6-1. In general, PIC concentrations were slightly higher than POHC concentrations, although this ratio varied from site to site. PIC output rate very rarely exceeded 0.01 percent of the POHC input rate. The document stated that the measurement of Appendix VIII compounds at low concentrations in the waste feed, auxiliary fuel, and inflow streams to control systems is often necessary to explain the presence of PICs.

- Olexsey, Huffman, and Evans (1985) was prepared by Robert A. Olexsey and others of the U.S. EPA Hazardous Waste Engineering Research Laboratory in Cincinnati, Ohio. This document discussed PIC generation mechanisms and criteria for PIC formations. The paper provided data on emissions of PICs during full-scale tests conducted on incinerators and boilers burning hazardous waste (Trenholm and others 1984; Castaldini and others 1984). The documents referenced by this paper summarized a series of full-scale tests conducted on seven incinerators and five boilers conducted by U.S. EPA to support its regulatory development for incinerators and boilers. Commonly found PICs identified in these tests are presented in Tables A1.6-2 and A1.6-3.

TABLE A1.6-1

PICS IDENTIFIED BY TRENHOLM AND HATHAWAY (1984)

PICs Found In Stack Effluents			
PIC	Number of Facilities	Low Concentration (ng/L)	High Concentration (ng/L)
Benzene	6	12	670
Chloroform	5	1	1,330
Bromodichloromethane	4	3	32
Dibromochloromethane	4	1	12
Naphthalene	3	5	100
Bromoform	3	0.2	24
Chlorobenzene	3	1	10
Tetrachloroethylene	3	0.1	2.5
1,1,1,-Trichloroethane	3	0.1	1.5
Toluene	2	2	75
o-Nitrophenol	2	2	50
Methylene chloride	2	2	27
Phenol	2	4	22
2,4,6-Trichlorophenol	1	110	110
Carbon disulfide	1	32	32
o-Chlorophenol	1	22	22
2,4-Dimethylphenol	1	21	21
Methylene bromide	1	18	18
Bromochloromethane	1	14	14
Trichlorobenzene	1	7	7
Hexachlorobenzene	1	7	7
Diethyl phthalate	1	7	7
Pentachlorophenol	1	6	6
Dichlorobenzene	1	4	4
Chloromethane	1	3	3
Methyl ethyl ketone	1	3	3
Bromomethane	1	1	1
Pyrene	1	1	1
Fluoranthene	1	1	1

Notes:

ng/L = Nanograms per liter
PIC = Product of incomplete combustion

- From the U.S. EPA-sponsored tests, (1) volatile compounds listed in Appendix VIII identified were only a fraction—sometimes about one-half—of the total organic compounds identified, and (2) semivolatile compounds not listed in Appendix VIII identified were three to 30 times the quantity of organic compounds listed in Appendix VIII . Table A1.6-4 lists the compounds identified by the U.S. EPA-sponsored tests.

- A study of hazardous waste incinerator stack effluent was conducted to characterize the types of compounds emitted. Twenty-nine compounds were identified at a concentration range of 0.1 to 980 nanograms per liter. Methane, chloromethane, and chloroform accounted for more than one-half of the total mass of VOCs detected. Other than methane, oxygenated aliphatic hydrocarbons formed the highest fraction of the total emissions.

- Based on the incinerator stack effluent study, it was found that as combustion

TABLE A1.6-4

MOST FREQUENTLY IDENTIFIED PICS
(TRENHOLM, KAPELLA, AND HINSHAW 1992)

Appendix VIII Volatile Organic Compounds	Appendix VIII Semivolatile Organic Compounds	Compounds Not Listed in Appendix VIII
1,1,1-Trichloroethane	Bis(2-Ethylhexyl)phthalate	1,1'-(1,4-Phenylene)bisethanone
Benzene	Butylbenzylphthalate	Acetone
Carbon tetrachloride	Dibutylphtahlate	Acetophenone
Chlorobenzene	Diethylphthalate	Benzaldehyde
Chloroform	Naphthalene	Benzenedicarboxaldehyde
Methylene chloride	Phenol	Benzoic acid
Tetrachloroethylene		Cyclohexanol
Toluene		Chlorocyclohexanol
Trichloroethylene		Cyclohexane
		Ethylbenzene
		Ethylbenzoic acid
		Ethylphenol
		Ethylphenyl-ethanone
		Ethynylbenzene
		Phenylpropenol
		Propenylmethylbenzene
		Tetramethyloxirane
		Trimethylhexane

TABLE A1.6-5

COPCS IDENTIFIED BY CARB (1990b)

COPC		
Ammonia	1,2-Dibromoethane	Nickel
Arsenic	Dichloroethane	Nitrogen oxides
Benzene	Dichloromethane	PM
Bromodichloromethane	1,2-Dichloropropane	PAHs
Cadmium	Ethylbenzene	Sulfur dioxide
Carbon dioxide	Freon	Tetrachloroethene
Carbon monoxide	Hydrocarbon, total	Tetratrichloromethylene
Carbon tetrachloride	Hydrogen chloride	Toluene
Chlorobenzenes	Hydrogen fluoride	Tribromomethane
Chlorodibromomethane	Iron	Trichlorethane
Chloroform	Lead	1,1,1-Trichloroethane
Chlorophenols	Manganese	Trichloroethylene
Chromium, hexavalent	Mercury	Trichlorotrifluroethane
Chromium, total	Mesitylene	Vinyl chloride
Copper	Methyl isobutyl ketone	Xylenes
Cumene	Napthalene	Zinc

Notes:

PAH = Polynuclear aromatic hydrocarbons
PM = Particulate matter

TABLE A1.6-6

STACK GAS ANALYSIS DATA
(CARB 1991)

(Page 2 of 2)

Notes:

✔ = Detected in at least one emission test
ND = Not detected in any emission test
NA = No analysis

[a] Number in parentheses indicates the number of facilities for which data were tabulated.
[b] Isomers and/or homologues that were not detected were added to total values at one-half the detection limit; pollutant may not have actually been detected.

A1.6.5 U.S. EPA (1988)

This document, referenced by some documents as a 1989 document, was prepared in 1988.

U.S. EPA prepared "Hospital Waste Combustion Study: Data Gathering Phase" to assemble available information on hospital waste combustion so that U.S. EPA can evaluate whether airborne pollutant emissions from hospital waste combustion should be regulated. While preparing this document, U.S. EPA reviewed the pertinent literature to determine which studies would be helpful in completing the

- California HSC 44321(c): CARB
- California HSC 44321(d): Hazard Evaluation System and Information Service
- California HSC 44321(e): U.S. EPA
- California HSC 44321(f): California HSC

The lists of toxic substances presented in the document are not restricted to incinerator facilities, but apply to any facility discharging airborne pollutants to the atmosphere. The document also removes numerous substances, primarily medicinal compounds, from lists of toxic chemicals that must always be evaluated, and places them on lists of toxic compounds that require evaluation only if a facility manufactures that substance.

A1.7 COLUMN 7: U.S. EPA-RECOMMENDED AND POTENTIAL PICS (1994a; 1994b)

Compounds marked with an "X" in the appropriate cells are identified in U.S. EPA (1994a and 1994b). Based on information presented in U.S. EPA (1994b), these tables were developed from available U.S. EPA data and from lists of toxic compounds from various U.S. EPA programs. Because the source lists were not developed as lists of toxic PICs, U.S. EPA deleted compounds that were not appropriate (U.S. EPA 1994b). U.S. EPA acknowledged the importance of using focused studies to develop a PIC list that is (1) appropriately protective of the environment, and (2) not excessively burdensome on the regulated community. Nevertheless, Tables 1 and 2 in U.S. EPA (1994b) were compiled as draft lists for use during the interim period. Tables in U.S. EPA (1994b) were to be revised as additional PIC data were collected. U.S. EPA Permits and State Program Division is currently updating these tables; however, a target completion date is not available. Tables 1 and 2 are based on the following (U.S. EPA 1994b):

- Hazardous waste constituent list in 40 CFR Part 261, Appendix VIII
- hazardous air pollutants (HAP) list
- Office of Research and Development list of organic compounds found in combustion devices developed for U.S. EPA (1993)

The following compounds were deleted from this list:

- Pesticide compounds not likely to be a PIC
- Federal Drug Administration-regulated drugs
- Carcinogenic sugar substitutes
- Compounds without chemical-specific listings (for example, "coal tar")
- Compounds without U.S. EPA-established sampling and analysis methods
- Metallic compounds (because of difficulty in analyzing the specific compounds; metals are still included in elemental totals)

- Compounds with low octanol-water partition coefficients and no inhalation toxicity data
- Compounds with low toxicity values
- Naturally-occurring plant toxins

Specific compounds were retained on Tables 1 and 2 on the following basis:

- Pesticides with a molecular structure simple enough to be of concern as a PIC

California Air Resources Board (CARB). 1990a. "Health Risk Assessment Guidelines for Nonhazardous Waste Incinerators." Prepared by the Stationary Source Division of the CARB and the California Department of Health Services.

CARB. 1990b. "Technical Support Document of Proposed Dioxins Control Measures for Medical Waste Incinerators." May 25.

CARB. 1991. "Air Pollution Control at Resource Recovery Facilities. Update."

CARB. 1996. "Proposed Amendments to the Emission Inventory Criteria and Guidelines Report Published in Accordance with the Air Toxics ‘Hot Spots’ Information and Assessment Act of 1987." May.

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Kramlich, J.C., W.R. Seeker, and M.P. Heap. 1984. "Laboratory-Scale Flame Mode Study of Hazardous Waste Incineration." *Proceedings of the Ninth Annual Research Symposium on Incineration and Treatment of Hazardous Waste*. Fort Mitchell, Kentucky. May 2 through 4, 1983. EPA-600/9-84/015. NTIS PB-84-234525. Pages 79-94. July.

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U.S. EPA. 1985. *Report on the Incineration of Liquid Hazardous Wastes.* Science Advisory Board. Environmental Effects, Transport, and Fate Committee. April.

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U.S. EPA. 1990a. "Standards for Owners and Operators of Hazardous Waste Incinerators and Burning of Hazardous Wastes in Boilers and Industrial Furnaces; Proposed Rule, Supplemental Proposed Rule, Technical Corrections, and Request for Comments." *Federal Register.* 55(82):17862-17921. April 27.

U.S. EPA. 1990b. *Report of the Products of Incomplete Combustion Subcommittee of the Science Advisory Board; Review of OSW Proposed Controls for Hazardous Waste Incineration Products of Incomplete Combustion.* EPA-SAB EC-90-004. October 24.

U.S. EPA. 1993. *Review Draft Addendum to the Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions*. OHEA. ORD. EPA-600-AP-93-003. November 10.

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APPENDIX A-2

COMPOUND SPECIFIC PARAMETER VALUES

Screening Level Ecological Risk Assessment Protocol

August 1999

Screening Level

APPENDIX A-2

LIST OF VARIABLES AND COMPOUND-SPECIFIC PARAMETERS

ρ_{air} = Density of air (g/cm^3)
ρ_{forage} = Density of forage (g/cm^3)

Ba_{beef} = Biotransfer factor in beef (mg COPC/kg FW tissue)/(mg COPC/day) OR (day/kg FW tissue)
$Ba_{chicken}$ = Biotransfer factor in chicken (mg COPC/kg FW tissue)/(mg COPC/day) OR (day/kg FW tissue)
Ba_{egg} = Biotransfer factor in eggs (mg COPC/kg FW tissue)/(mg COPC/day) OR (day/kg FW tissue)
Ba_{milk} = Biotransfer factor in milk (mg COPC/kg FW tissue)/(mg COPC/day) OR (day/kg FW tissue)
Ba_{pork} = Biotransfer factor in pork (mg COPC/kg FW tissue)/(mg COPC/day) OR (day/kg FW tissue)
BAF_{fish} = Bioaccumulation factor in fish (mg COPC/kg FW tissue)/(mg COPC/L total water column) OR (L water/kg FW tissue)
BCF_{fish} = Bioconcentration factor in fish (L/kg FW OR unitless)
Br_{ag} = Plant-soil bioconcentration factor in aboveground produce (µg COPC/g DW plant)/(µg COPC/g DW soil)—unitless
$Br_{forage/silage}$ = Plant-soil bioconcentration factor in forage and silage (µg COPC/g DW plant)/(µg COPC/g DW soil)—unitless
Br_{grain} = Plant-soil bioconcentration factor in grain (µg COPC/g DW grain)/(µg COPC/g DW soil)—unitless
$\mathrm{Br}_{\mathrm{rootveg}}$ = Plant-soil bioconcentration factor for belowground produce (µg COPC/g DW plant)/(µg COPC/g DW soil)—unitless
$BSAF_{fish}$ = Biota-sediment accumulation factor in fish (mg COPC/kg lipid tissue)/(mg COPC/kg sediment)—unitless
B_{vol} = Volumetric air-to-leaf biotransfer factor in leaf (µg COPC/L FW plant)/(µg COPC/L air)—unitless
Bv_{ag} = COPC air-to-plant biotransfer factor for aboveground produce (µg COPC/g DW plant)/(µg COPC/g air)—unitless
$Bv_{forage/silage}$ = Air-to-plant biotransfer factor in forage and silage (µg COPC/g DW plant)/(µg COPC/g air)—unitless

c = Junge constant = 1.7×10^{-04} (atm-cm)

D_a = Diffusivity of COPC in air (cm^2/s)
D_w = Diffusivity of COPC in water (cm^2/s)

$f_{oc,bs}$ = Fraction of organic carbon in bottom sediment (unitless)
$f_{oc,s}$ = Fraction of organic carbon in soil (unitless)
$f_{oc,sw}$ = Fraction of organic carbon in suspended sediment (unitless)
f_{water} = Fraction of COPC in water (unitless)

F_v = Fraction of COPC air concentration in vapor phase (unitless)
Fw = Fraction of wet deposition that adheres to plant surfaces (unitless)

H = Henry's law constant

Inhalation CSF = Inhalation cancer slope factor (mg/kg-day)$^{-1}$
Inhalation URF = Inhalation unit risk factor (µg/m^3)$^{-1}$

Kd_s = Soil-water partition coefficient (mL water/g soil OR cm^3 water/g soil)
Kd_{sw} = Suspended sediment-surface water partition coefficient
(L water/kg suspended sediment OR cm^3 water/g suspended sediment)
Kd_{bs} = Bed sediment-sediment pore water partition coefficient
(L water/kg bottom sediment OR cm^3 water/g bottom sediment)
K_{ow} = Octanol/water partitioning coefficient
(mg COPC/L octanol)/(mg COPC/L octanol)—unitless
K_{oc} = Soil organic carbon-water partition coefficient (mL water/g soil)
ksg = COPC soil loss constant due to biotic and abiotic degradation (yr^{-1})

MW = Molecular weight of COPC (g/mole)

p°_{L} = Liquidphase vapor pressure of COPC (atm)
p°_{S} = Solid-phase vapor pressure of COPC (atm)

Oral CSF = Oral cancer slope factor (mg/kg-day)$^{-1}$

R = Universal gas constant (atm-m^3/mol-K)
RCF = Root concentration factor
(µg COPC/g DW plant)/(µg COPC/mL soil water)
RfC = Reference concentration (mg/m^3)
RfD = Reference dose (mg/kg/day)
Rp = Interception factor of edible portion of plant (unitless)

S = Solubility of COPC in water (mg COPC/L water)
ΔS_f = Entropy of fusion [$\Delta S_f/R$ = 6.79 (unitless)]
S_T = Whitby's average surface area of particulates (aerosols)
= 3.5 x 10^{-06} cm^2/cm^3 air for background plus local sources
= 1.1 x 10^{-05} cm^2/cm^3 air for urban sources

$t_{1/2}$ = Half-time of COPC in soil (days)
T_a = Ambient air temperature (K)
T_m = Melting point temperature (K)
TEF = Toxicity equivalency factor (unitless)

Vp = Vapor pressure of COPC (atm)

APPENDIX A-2

The following sections provide the methodology and rationale followed for the selection or development of compound-specific parameter values recommended by U.S. EPA OSW. Compound-specific values are provided for (1) physical and chemical properties, (2) fate-and-transport parameters, and (3) health benchmarks. A summary table of all compound-specific parameter values is provided at the end of this appendix, followed by individual parameter-value tables for each compound. The individual parameter-value tables cite sources for each parameter value.

A2.1 PRIMARY GUIDANCE DOCUMENTS

Throughout Appendix A-2, the following guidance documents are referenced as the primary sources for the development and comparision of compound-specific parameter values, and used to the fullest extent possible to provide consistency. Therefore, in this appendix, the term **primary guidance documents** refers to the following documents:

- U.S. EPA. 1994f. *Revised Draft Guidance for Performing Screening Level Risk Analyses at Combustion Facilities Burning Hazardous Wastes: Attachment C, Draft Exposure Assessment Guidance for RCRA Hazardous Waste Combustion Facilities*. Office of Emergency and Remedial Response (OERR). Office of Solid Waste. December 14.

- U.S. EPA. 1995b. *Review Draft Development of Human Health Based and Ecologically Based Exit Criteria for the Hazardous Waste Identification Project*. Volumes I and II. Office of Solid Waste. March 3.

- North Carolina Department of Environment, Health, and Natural Resources (NC DEHNR). 1997. *North Carolina Protocol for Performing Indirect Exposure Risk Assessments for Hazardous Waste Combustion Units*. January.

To ensure consistency, sources referenced in the primary guidance documents were also evaluated. Information for certain compounds like PCDDs, PCDFs, and mercury were obtained from the following documents:

- U.S. EPA. 1994a. *Estimating Exposure to Dioxin-Like Compounds*. External Review Draft Report. Volumes I-III. Office of Research and Development. Washington, DC. EPA/600/6-88/005Ca,b,c.

- U.S. EPA. 1997g. *Mercury Study Report to Congress. Volume III: Fate and Transport of Mercury in the Environment.* Office of Air Quality Planning and Standards and Office of Research and Development. EPA-452/R-97-005. December.

U.S. EPA (1994a) provides various parameter values for (but are not limited to) PCDDs, PCDFs, and PCBs. U.S. EPA (1997g) provides various parameter values for mercuric compounds including elemental mercury, mercuric chloride, and methyl mercury.

A2.2 GENERAL ANALYSIS AND METHODOLOGY

This section describes the general analysis and methodology followed for the development of compound-specific parameter values presented. Compound-specific parameter values in the primary guidance documents and other sources generally were evaluated as follows:

1. Compound-specific values for each parameter were compared among the primary guidance documents and the following observations were noted:

    a. Parameter values provided in U.S. EPA (1994f) are limited to 24 compounds. For these compounds, sources were referenced specifically to each parameter, in addition to the methodology used to obtain the respective values.

    b. U.S. EPA (1995b) provides various parameter values for a comprehensive list of compounds. The methodology used for determining values was covered in detail. However, parameter values for each compound were not referenced to a specific source. Although a comprehensive list of sources was provided, it is difficult to determine which parameter value for a compound was obtained from which source.

    c. NC DEHNR (1997) provides various parameter values for a comprehensive list of compounds, including congeners of polychlorinated dibenzo(p)dioxins (PCDDs) and polychlorinated dibenzofurans (PCDFs). However, the sections citing the methodology and sources of values in the NC DEHNR (1997) were reproduced directly from U.S. EPA (1994f). Therefore, in NC DEHNR (1997), the compound-specific parameter values that were provided did not correlate with the sections citing the methodology and sources of values. In addition, only a partial list of sources was provided for the values. Therefore, it was not possible to determine the actual source of values with certainty.

2. Sources of values referenced in the primary guidance documents were further researched and evaluated. Observations affecting usability are included in parameter-specific discussions for each compound, as appropriate.

3. Values provided in the primary guidance documents were used only when the sources and applicability of such values could be verified. Additional sources of parameter values were evaluated, used, and referenced when technically justified.

documents, U.S. EPA (1994a), and U.S. EPA (1997g) are recommended.

3. If unable to obtain acceptable values from published literature or the primary guidance

A2.3.2 Melting Point Temperature (T_m)

Melting point temperature (T_m) is the temperature of the compound (in degree Kelvin [K]) at which the solid state of the compound undergoes a phase change to a liquid phase. At ambient temperatures and at an atmpospheric pressure of 1 atmosphere, compounds are either in a solid or liquid state. The compound liquid or solid state is provided in the summary tables of compound-specific parameter values.

Organics and Metals

from 20°C to 30°C, U.S. EPA (1994c) states that *S* values were not corrected to 25°C, because the variability in solubilities measured at 20°C to 25°C was within the overall range of measured values.

U.S. EPA (1994c) is the preferred source, because (1) sources and the conditions at which each value was obtained are provided, and (2) values were provided to 2 significant figures. Also, U.S. EPA (1994c) provides multiple *Vp* and *S* values for each compound from several different literature sources; providing a recent, more comprehensive compilation of reported literature values. *Vp* and *S* values from U.S. EPA (1994c) were generally consistent with those provided in U.S. EPA (1994f), U.S. EPA (1995b), and NC DEHNR (1997).

When *Vp* and *S* values were not available in U.S. EPA (1994c), they were obtained from one of three sources, in the following order of preference:

1. U.S. EPA (1994f)

2. U.S. EPA (1995b); values from which were obtained from one of three sources:

    a. Mackay, D., W.Y. Shiu, and K.C. Ma. 1992. *Illustrated Handbook of Physical-Chemical Properties and Environmental fate for Organic Chemicals. Volume I - Monoaromatic Hydrocarbons, Chlorobenzenes, and PCBs. Volume II-Polynuclear Aromatic Hydrocarbons, Polychlorinated Dioxins and Dibenzofurans. Volume III - Volatile Organic Chemicals.* Lewis Publishers. Boca Raton, Florida.

    b. Howard, P.H. 1989-1993. *Handbook of Environmental Fate and Exposure Data For Organic Chemicals*. *Volumes I: Large Production and Priority Pollutants (1989). Volume II: Solvents (1990). Volume III: Pesticides (1991). Volume IV: Solvents2 (1993).* Lewis Publishers. Chelsea, Michigan.

    c. Other referenced literature sources, when values were not available in Mackay, Shiu, and Ma (1992) or Howard (1989-1993).

3. U.S. EPA. 1994b. *Superfund Chemical Data Matrix (SCDM).* Office of Emergency and Remedial Response. Washington, DC. June.

Vp and *S* values in U.S. EPA (1994f) were geometric mean values obtained from various literature sources. References specific to sources of values for each compound were provided in U.S. EPA (1994f) and were, therefore, preferred over U.S. EPA (1995b) values.

Most *Vp* and *S* values in U.S. EPA (1995b) were obtained from Mackay, Shiu, and Ma (1992) or Howard (1989-1993). Mackay, Shiu, and Ma (1992) and Howard (1989-1993) obtain the "best" values after evaluation of various literature sources.

Vp values in U.S. EPA (1994b) were obtained from various literature sources. *S* values in U.S. EPA (1994b) were the geometric mean of values obtained from various literature sources.

PCDDs and PCDFs *Vp* and *S* values for PCDDs and PCDFs were obtained from U.S. EPA (1994a). *Vp* and *S* values were either (1) measured, or (2) estimated by using the homologue (compound class with the same amount of chlorination) average method.

NOTE: The phase—solid or liquid—of *Vp* values for all organics, including PCDDs and PCDFs, was indicated. This is based on whether the compound is in the solid or liquid phase at ambient soil temperatures.

Metals As cited in the primary guidance documents and in the literature, metals—except mercury—are considered (1) nonvolatile at ambient temperatures, and (2) insoluble in water, except as certain weak acids. Therefore, *Vp* and *S* values were not available for all metals (except mercury) in any of the literature sources reviewed.

Mercuric Compounds Mercury is a relatively volatile compound. *Vp* and *S* values for elemental mercury were obtained from Budavari, O'Neil, Smith, and Heckelman (1989); and are comparable to the values in the primary guidance documents. *Vp* and *S* values for mercuric chloride were obtained from U.S. EPA (1997g) and Budavari, O'Neil, Smith, and Heckelman (1989), respectively. *Vp* and *S* values for methyl mercury were not found in the literature.

A2.3.4 Henry's Law Constant (*H*)

Henry's Law constant (*H*) is also referred to as the air-water partition coefficient, and is defined as the ratio of the partial pressure of a compound in air to the concentation of the compound in water at a given temperature under equilibrium conditions. Henry's Law constant values generally can be (1) calculated from the theoretical equation defining the constant, (2) measured, or (3) estimated from the compound structure. Experimental and estimated *H* values from literature reports, however, are (1) very temperature-dependent and difficult to measure, (2) generally obtained from various literature sources that use different experimental and estimation methods, and (3) available for only a limited number of compounds.

Organics For organics (excluding PCDDs and PCDFs), *H* values were calculated from the following theoretical equation (Lyman, Reehl, and Rosenblast 1982) for consistency, using recommended *MW, S,* and *Vp* values provided in this SLERAP:

$$H = \frac{Vp \cdot MW}{S} \qquad \text{Equation A2-1}$$

H = Henry's Law constant (atm-m^3/mole)
Vp = Vapor pressure of COPC (atm)
S = Solubility of COPC in water (mg COPC/L water)

The primary guidance documents also used theoretical Equation A-3-1 to calculate *H* values.

PCDDs and PCDFs *H* values for PCDDs and PCDFs are calculated values obtained from U.S. EPA (1994a).

Metals For all metals (except mercury), *H* is zero, because *Vp*—because of the nonvolatile nature of the metals—and *S* are assumed to be zero.

Mercuric Compounds *H* values for elemental mercury, mercuric chloride, and methyl mercury were obtained from U.S. EPA (1997g).

A2.3.5 Diffusivity of COPCs in Air (D_a) and Water (D_w)

Diffusivity or diffusion coefficients in air (D_a) and water (D_w) are used to calculate the liquid or gas phase transfer of a COPC into a waterbody.

Organics For organics (except PCDDs and PCDFs), diffusivity values were obtained directly from the CHEMDAT8 model chemical properties database (Worksheet DATATWO.WK1):

- U.S. EPA. 1994d. *CHEM8—Compound Properties Estimation and Data*. Version 1.00. CHEMDAT8 Air Emissions Program. Prepared for Chemicals and Petroleum Branch, OAQPS. Research Triangle Park. North Carolina. November 18.

The U.S. EPA (1994d) database uses empirical correlations with compound density and molecular weight to calculate diffusivity values. For compounds not in the U.S. EPA (1994d) database, diffusivity values were obtained by using the WATER8 model correlation equations for air and water diffusivities:

- U.S. EPA. 1995d. *WATER8—Air Emissions Models Wastewater Treatment*. Version 4.0. OAQPS. Research Triangle Park. North Carolina. May 1.

U.S. EPA(1995d) database values were predicted by using chemical-structural relationships. Diffusivity values for all compounds in the U.S. EPA (1994d) and (1995d) databases were either predicted or estimated. The primary guidance documents also recommended U.S. EPA (1994d) and (1995d) database model values. More recent documents, including the following, also recommended these values:

- U.S. EPA. 1996. *Soil Screening Guidance: Technical Background Document and User's Guide*. Office of Solid Waste and Emergency Response. Washington, DC. EPA/540/R-95/128. May.

For diffusivity values that were not available in these databases, D_w and D_a values were calculated using the following equations cited and recommended for use in U.S. EPA (1997g):

$$D_{a,i} = \frac{1.9}{(MW_i)^{2/3}} \qquad \text{Equation A2-2a}$$

$$D_{w,i} = \frac{22\times10^{-5}}{(MW_i)^{2/3}} \qquad \text{Equation A2-2b}$$

U.S. EPA (1995b) recommended the use of standard default diffusivity values. U.S. EPA (1995b) stated that the diffusivity parameters vary slightly, and default values appear to be within the range of typical values. Values for diffusivity in air range from about 0.01 to 0.1 square centimeters per second (cm^2

PCDDs and PCDFs Diffusivity values in air and water for (1) 2,3,7,8-TCDD were obtained from U.S. EPA (1994e), and (2) 2,3,7,8-TCDF were obtained from U.S. EPA (1995d). For all other congeners of PCDDs and PCDFs, (1) a default *Dw* value of 8 x 10^{-06} cm^2/s was used, and (2) *Da* values were calculated using the following equation recommended by U.S. EPA (1994a):

$$\frac{D_x}{D_y} = \left(\frac{MW_y}{MW_x}\right)^{0.5} \qquad \text{Equation A2-2c}$$

where

D

3. U.S. EPA (1995b), values from which were obtained from one of three sources:

    a. Mackay, D., W.Y. Shiu, and K.C. Ma. 1992. *Illustrated Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals. Volume I - Monoaromatic Hydrocarbons, Chlorobenzenes, and PCBs. Volume II - Polynuclear Aromatic Hydrocarbons, Polychlorinated Dioxins and Dibenzofurans. Volume III - Volatile Organic Chemicals.* Lewis Publishers. Boca Raton, Florida.

    b. Howard, P.H. 1989-1993. *Handbook of Environmental Fate and Exposure Data For Organic Chemicals*. *Volumes I: Large Production and Priority Pollutants (1989). Volume II: Solvents (1990). Volume III: Pesticides (1991). Volume IV: Solvents2 (1993).* Lewis Publishers. Chelsea, Michigan.

    c. Other literature sources, when values were not available in Mackay, Shiu, and Ma (1992) and Howard (1989-1993).

U.S. EPA (1994c) is the preferred source of values because (1) sources were provided, (2) several literature values were provided, some of which are also cited by the primary guidance documents and Karickhoff and Long (1995), and (3) the values were provided to 2 significant figures.

U.S. EPA (1994f) is the second-choice source of K_{ow} values recommended; and provides geometric mean values obtained from various literature sources. Karickhoff and Long (1995) recommended arithmetic mean values obtained from various literature sources and was, therefore, preferred as the third-choice source of K_{ow} values when values were not available from the first two sources.

In order to reference specific sources of K_{ow} values for each compound, values from U.S. EPA (1995b) and NC DEHNR (1997) were used only when values were not available in the literature sources reviewed.

PCDDs and PCDFs K_{ow} values for the PCDDs and PCDFs were obtained from either U.S. EPA (1994a) or U.S. EPA (1992d). U.S. EPA (1994a) and U.S. EPA (1992d) provide K_{ow} values for PCDDs and PCDFs that were either measured values obtained from the literature or calculated by averaging the literature values within the homologue group. According to U.S. EPA (1994a), K_{ow} values for hexachlorodibenzofurans were not available in the literature. Therefore, as recommended in U.S. EPA (1994a), due to lack of data, homologue group average values for hexachlorodibenzodioxins were applied to hexachlorodibenzofurans.

Metals No K_{ow} values were available for metals, either in the literature or in the primary guidance documents. K_{ow} values for the metals were assumed to be zero, because the affinity of the metals to the octanol is almost zero.

Mercuric compounds No K_{ow} values were available in the literature for mercury and methyl mercury. For mercuric chloride, the K_{ow} value was obtained from U.S. EPA (1997g).

A2.3.7 Soil Organic Carbon-Water Partition Coefficient (K_{oc})

The soil organic carbon-water partition coefficient (K_{oc}) or the organic carbon normalized soil sorption coefficient is defined as the ratio of adsorbed compound per unit weight of organic carbon to the aqueous solute concentration (Montgomery and Welkom 1991).

Organics Because of the soil mechanisms that are inherently involved, K_{oc} values for the ionizing organics and nonionizing organics are discussed separately.

A2.3.7.1 Ionizing Organic Compounds

Ionizing organic compounds include amines, carboxylic acids, and phenols. These compounds contain the functional groups that ionize under specific pH conditions, and include the following:

- Organic acids (2,4,6-trichlorophenol; pentachlorophenol; 2,3,4,5-tetrachlorophenol; 2,3,4,6-tetrachlorophenol; 2,4,5-trichlorophenol; 2,4-dichlorophenol; 2-chlorophenol; phenol; 2,4-dimethylphenol; 2-methylphenol; 2,4-dinitrophenol; and benzoic acid)

- Organic bases—n-nitroso-di-n-propylamine; n-nitrosodiphenylamine, and 4-chloroaniline)

K_{oc} values for ionizing organic compounds were obtained from U.S. EPA (1994c). U.S. EPA (1994c) provides K_{oc} values for the ionizing organic compounds that have been estimated on the basis of the degree of ionization and the relative proportions of neutral and ionized species. The primary guidance documents cite one value for the ionizing organics, independent of the pH. The primary guidance documents calculate K_{oc} values for the ionizing organics by using correlation equations containing K_{ow} that are applicable to nonionizing organics. However, K_{oc} values for ionizing compounds can vary vastly, depending on the pH conditions in the environment. Therefore, for the aforementioned ionizing organic compounds, this SLERAP prefers and provides estimated K_{oc} values that are based on pH.

K_{oc} values were estimated on the basis of the assumption that the sorption of ionizing organic compounds is similar to hydrophobic organic sorption, because the soil organic carbon is the dominant sorbent. According to U.S. EPA (1994c), for low pH conditions, these estimated values may overpredict sorption coefficients, because they ignore sorption to components other than organic carbon.

A2.3.7.2 Nonionizing Organic Compounds

Nonionizing organic compounds are all other organic compounds not listed earlier as ionizing. They

NC DEHNR (1997) and U.S. EPA (1994f) use the following correlation equation to calculate K_{oc} from K_{ow} for all organics:

$$\log K_{oc} = 0.88 (\log K_{ow}) + 0.114 \qquad (r^2 = 0.96) \qquad \text{Equation A-2-3}$$

- Research Triangle Institute (RTI). 1992. *Preliminary Soil Action Level for Superfund Sites, Draft Interim Report.* Prepared for U.S. EPA Hazardous Site Control Division, Remedial Operations Guidance Branch. Arlington, Virginia. December.

However, according to U.S. EPA (1994c), the correlation between K_{oc} and K_{ow} can be improved considerably by performing separate linear regressions on two chemical groups. U.S. EPA (1994c) derives the following correlation equations from measured K_{oc} values cited in U.S. EPA (1994c) and U.S. EPA (1996b):

For phthalates and PAHs

$$\log K_{oc} = 0.97 (\log K_{ow}) - 0.094 \qquad (r^2 = 0.99) \qquad \text{Equation A-2-4}$$

For all organics except phthalates, PAHs, PCDDs, and PCDFs

$$\log K_{oc} = 0.78 (\log K_{ow}) + 0.151 \qquad (r^2 = 0.98) \qquad \text{Equation A-2-5}$$

Because of the improved regressions (r^2), U.S. EPA (1994c) recommended that correlation Equations A-2-4 and A-2-5 be used instead of correlation Equation A-2-3. U.S. EPA (1995b) also recommended that correlation Equations A-2-4 and A-2-5 be used.

Although U.S. EPA (1995b) recommended the use of correlation Equations A-2-4 and A-2-5, the following correlation equation was used by that document to calculate K_{oc} values for all organics except PCDDs and PCDFs:

$$\log K_{oc} = 0.983 (\log K_{ow}) + 0.0002 \qquad \text{Equation A-2-6}$$

- DiToro, D.M., C.S. Zarba, D.J. Hansen, W.J. Berry, R.C. Swartz, C.E. Cowan, S.P. Pavlou, H.E. Allen, N.A. Thomas, and P.R. Paquin. 1991. "Technical Basis for

Establishing Sediment Quality Criteria for Nonionic Compounds Using Equilibrium Partitioning." *Environmental Toxicology and Chemistry*. 10:1541-1583

For the purposes of this SLERAP, values obtained by using correlation Equations A-2-3 through A-2-6, were compared. In general, more of the K_{oc} values obtained by using correlation Equations A-2-4 and A-2-5 were within the range of measured values in the literature than those obtained by using correlation Equations A-2-3 and A-2-6. Therefore, when measured K_{oc} values were not available, values were estimated, for all nonionizing organic compounds except PCDDs and PCDFs, by using the appropriate correlation Equation A-2-4 or A-*2-5.*

PCDDs and PCDFs For PCDDs and PCDFs, the following correlation equation (Karickhoff, Brown, and Scott 1979) was used to calculate K_{oc} values, as cited by U.S. EPA (1994a).

$$\log K_{oc} = \log K_{ow} - 0.21 \qquad (n = 10,\ r^2 = 1.0)$$ Equation A-2-7

- Karickhoff, S.W., D.S. Brown, and T.A. Scott. 1979. "Sorption of Hydrophobic Pollutants on Natural Sediments." Water Resources. 13:241-248.

Metals For metals, no

$$Kd_s = f_{oc,s} \cdot K_{oc} \qquad \text{Equation A-2-8a}$$

$$Kd_{sw} = f_{oc,sw} \cdot K_{oc} \qquad \text{Equation A-2-8b}$$

$$Kd_{bs} = f_{oc,bs} \cdot K_{oc} \qquad \text{Equation A-2-8c}$$

- U.S. EPA. 1993d. Review Draft Addendum to the Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions. Office of Health and Environmental Assessment. Office of Research and Development. EPA-600-AP-93-003. November 10.

U.S. EPA (1993d), from literature searches, states that f_{OC} could range as follows:

- 0.002 to 0.024 in soils—for which a mid-range value of $f_{oc,s}$ = 0.01 generally can be used.
- 0.05 to 0.1 in suspended sediments—for which a mid-range value of $f_{oc,sw}$ = 0.075 generally can be used.
- 0.03 to 0.05 in bottom sediments—for which a mid-range value of $f_{oc,bs}$ = 0.04 generally can be used.

Consistent with the primary guidance documents, this SLERAP uses mid-range f_{oc} values recommended by U.S. EPA (1993d). *Kd* values were calculated using K_{oc} values recommended for each compound in this SLERAP.

Metals For metals (except mercury), *Kd* is governed by factors other than organic carbon, such as pH, redox, iron content, cation exchange capacity, and ion-chemistry. Therefore, *Kd* values for metals cannot be calculated using the same correlation equations specified for organic compounds. Instead, *Kd* values for the metals must be obtained directly from literature sources. *Kd* values for all metals, except lead, were obtained from U.S. EPA (1996b). U.S. EPA (1996b) provides values for *Kd* that are based on pH, and are estimated by using the MINTEQ2 model, which is a geochemical speciation model. The MINTEQ2 model analyses were conducted under a variety of geochemical conditions and metal concentrations. The MINTEQ2 pH-dependent *Kd* values were estimated by holding constant the iron oxide at a medium value and the f_{oc} at 0.002. For arsenic, hexavalent chromium, selenium, and thallium, empirical pH-dependent *Kd* values were used.

U.S. EPA (1995b) also recommended *Kd* values estimated using the MINTEQ2 model. U.S. EPA (1994f) and NC DEHNR (1997) provided *Kd* values obtained from several literature sources, depending on the compound; however, the *Kd* values are identical in all of the primary guidance documents.

The MINTEQ2 model values in U.S. EPA (1996b) were comparable to the values in the primary guidance documents. In addition, because organic carbon does not play a major role in partitioning for the metals, U.S. EPA (1994f) assumed that the partitioning is the same, regardless of the soil, suspended sediment, or bottom sediment phase. Therefore, in this SLERAP, values for partitioning coefficients Kd_s, Kd_{sw}, and Kd_{bs} for the metals are assumed to be the same.

Kd value for lead was obtained from the following:

- Baes, C.F., R.D. Sharp, A.L. Sjoreen, and R.W. Shor. 1984. "Review and Analysis of Parameters and Assessing Transport of Environmentally Released Radionuclides Through Agriculture." Oak Ridge National Laboratory, Oak Ridge, Tennessee.

Mercuric Compounds Kd_s, Kd_{sw}, and Kd_{bs} values for mercury, mercuric chloride, and methyl mercury were obtained from U.S. EPA (1996b). Kd values for mercuric chloride and methyl mercury were obtained from U.S. EPA (1997g).

A2.3.9 Soil Loss Constant Due to Degradation *(ksg)*

Soil loss constant due to degradation *(ksg)* reflects loss of a compound from the soil by processes other than leaching. Degradation rates in the soil media include biotic and abiotic mechanisms of transformation. Abiotic degradation includes photolysis, hydrolysis, and redox reactions. Hydrolysis and redox reactions can be significant abiotic mechanisms in soil (U.S. EPA 1990).

The following document states that degradation rates can be assumed to follow first order kinetics in a homogenous media:

- Lyman , W.J., W.F. Reehl, and D.H. Rosenblatt. 1982. *Handbook of Chemical Property Estimation Methods: Environmental Behavior of Organic Compounds.* McGraw-Hill Book Company. New York, New York.

Therefore, the half-life $(t_{½})$ of compounds can be related to the degradation rate constant (*ksg*) as follows:

$$ksg = \frac{0.693}{t_{½}} \qquad \text{Equation A-2-9}$$

Ideally, *ksg* is the sum of all biotic and abiotic rate constants in the soil. Therefore, if the $t_{½}$ for all of the mechanisms of transformation are known, the degradation rate can be calculated using Equation A-2-9. However, literature sources generally do not provide sufficient data for all such mechanisms, especially for soil.

Organics For organics (except PCDDs and PCDFs), *ksg* values were calculated using half-life soil values obtained from the following document:

- Howard, P.H., Boethling, R.S., Jarvis, W.F., Meylan, W.M., and Michalenko, E.M. 1991. *Handbook of Environmental Degradation Rates.* Lewis Publishers. Chelsea, Michigan.

Half-life values provided in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991) indicate the disappearance of a substance in ground water or soil; with the principal degradation mechanisms being biodegradation and hydrolysis. Values reported were highly variable because of the different methods used for measurements, in addition to the various controlling factors that could affect them. Therefore, Howard, Boethling, Jarvis, Meylan, and Michalenko (1991) provided a range of half-life values found in the literature, usually for the fastest reaction mechanism,. *Ksg* values recommended in this SLERAP were calculated with the high-end half-life values.

U.S. EPA (1994b) also cited values obtained from Howard, Boethling, Jarvis, Meylan, and Michalenko (1991). NC DEHNR (1997) cited values that are comparable to *ksg* values calculated by using half-life values obtained from Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).

PCDDs and PCDFs For PCDDs and PCDFs, *ksg* values were calculated from half-life values in soil obtained from Mackay, Shiu, and Ma (1992). For 2,3,7,8-TCDD, *ksg* value was obtained from U.S. EPA (1994a); which discussed experimental studies that were conducted on PCDDs and PCDFs degradation mechanisms. U.S. EPA (1994a) summarized the degradation of PCDDs and PCDDs as follows:

- A few experimental studies have shown possible biological degradation of TCDDs. However, the studies conclude that microbial action is very slow for PCDDs under optimum conditions, with the degradation rates probably higher with decreasing chlorination. PCDFs were found to be extremely stable to biological degradation.

- Abiotic degradation, such as photolysis, appears to be the most significant natural degradation mechanism for PCDDs and PCDFs. Experimental studies have shown that PCDDs and PCDFs undergo photolysis in the presence of a suitable hydrogen donor. No information was available to show that other abiotic degradation mechanisms, such as oxidation and hydrolysis, are important under environmentally relevant conditions.

Metals For the metals, NC DEHNR (1997) cites *ksg* values of zero. Literature states that the metals are transformed, but not degraded, by such mechanisms; therefore, *ksg* values are not applicable to metals.

Mercuric Compounds For mercury, mercuric chloride, and methylmercury, U.S. EPA (1997g) recommended *ksg* values of zero.

A2.3.10 Fraction of Pollutant Air Concentration in the Vapor Phase (F_v)

Organics

$$Fv = 1 - \frac{c\ S_T}{p^\circ_L + c\ S_T} \qquad \text{Equation A-2-10}$$

$$\ln \left(\frac{p^{\circ}_{L}}{p^{\circ}_{S}}\right.$$

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TABLES OF COMPOUND-SPECIFIC PARAMETER VALUES

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TABLE A-2-1

CHEMICAL-SPECIFIC INPUTS FOR ACENAPHTHENE (83-32-9)

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TABLE A-2-2

CHEMICAL-SPECIFIC INPUTS FOR ACETALDEHYDE (75-07-0)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	44.05
T_m (K)	Montgomery and Welkom (1991)	149.6
Vp (atm)	--	ND
S (mg/L)	--	ND
H (atm·m^3/mol)	--	ND
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.72E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.33E-05
K_{ow} (unitless)	Recommended K_{ow} value cited in Karickhoff and Long (1995).	6.02E-01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	9.53E-01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K	

TABLE A-2-3

CHEMICAL-SPECIFIC INPUTS FOR ACETONE (67-64-1)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	58.08
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	179.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	2.99E-01 at 25

TABLE A-2-4

CHEMICAL-SPECIFIC INPUTS FOR ACETONITRILE (75-05-8)

(Page 1 of 1)

TABLE A-2-5

CHEMICAL-SPECIFIC INPUTS FOR ACETOPHENONE (98-86-2)

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TABLE A-2-6

CHEMICAL-SPECIFIC INPUTS FOR ACROLEIN (107-02-8)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	56.06
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	185.1
Vp (atm)	*Vp* value cited in U.S. EPA (1995b).	3.50E-01 at 25ºC (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	2.10E+05
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	9.34E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.92E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.22E-05
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	9.80E-01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all	

TABLE A-2-7

CHEMICAL-SPECIFIC INPUTS FOR ACRYLONITRILE (107-13-1)

(Page 1 of 1)

TABLE A-2-8

CHEMICAL-SPECIFIC INPUTS FOR ALDRIN (309-00-2)

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TABLE A-2-8a

CHEMICAL-SPECIFIC INPUTS FOR ALUMINUM (7429-90-5)

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TABLE A-2-9

CHEMICAL-SPECIFIC INPUTS FOR ANILINE (62-53-3)

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TABLE A-2-10

CHEMICAL-SPECIFIC INPUTS FOR ANTHRACENE (120-12-7)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	178.22
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	491.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	3.35E-08 at 25ºC (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	5.37E-02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.11E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	3.24E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.74E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c)	2.95E+04
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	2.35E+04
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.35E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.76E+03
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	9.40E+02
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	5.50E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-11

CHEMICAL-SPECIFIC INPUTS FOR ANTIMONY (7440-36-0)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	121.75
T_m (^oK)	Budavari, O'Neil, Smith, and Heckelman (1989)	903.1
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	NA
H (atm·m^3/mol)	H value is assumed to be zero, because the Vp and S values are zero for all metals, except mercury.	0.0
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	7.73E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	8.96E-06
K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (mL/g)	Kd_s value was obtained from U.S. EPA (1996b), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model.	45 at pH=6.8
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	45 at pH=6.8
Kd_{bs} (mL/g)	Kd_{bs} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	45 at pH=6.8
ksg (year)$^{-1}$	--	ND
Fv (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	0.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-12

CHEMICAL-SPECIFIC INPUTS FOR AROCLOR 1016 (12674-11-2)

(Page 1 of 1)

TABLE A-2-13

CHEMICAL-SPECIFIC INPUTS FOR AROCLOR 1254 (11097-69-1)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	327.0
T_m (K)	Montgomery and Welkom (1991)	283.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1.16E-07 at 25ºC (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	5.15E-02
H (atm·m^3/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	7.37E-04
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	4.00E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	4.64E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	1.61E+06
K_{oc}		

TABLE A-2-14

CHEMICAL-SPECIFIC INPUTS FOR ARSENIC (7440-38-2)

(Page 1 of 1)

TABLE A-2-15

CHEMICAL-SPECIFIC INPUTS FOR ATRAZINE (1912-24-9)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	215.68
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	444.1
Vp (atm)	Vp value cited in Budavari, O'Neil, Smith, and Heckelman (1989)	3.66×10^{-10} at 25ºC (solid)
S (mg/L)	S value cited in Howard and others 1989 - 1993	3.00E+01
H (atm·m^3/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	2.63E-09
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.80E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.03E-06
K_{ow} (unitless)	log K_{ow} value cited in Karickhoff and Long (1995).	4.07E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.54E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.54E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.15E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with	

TABLE A-2-16

CHEMICAL-SPECIFIC INPUTS FOR BARIUM (7440-39-3)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	137.33
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	983
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	0.0
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	0.0
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	7.14E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	8.26E-06
K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (mL/g)	Kd_s value was obtained from U.S. EPA (1996b), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model.	11 at pH=4.9; 41 at pH=6.8; 52 at pH=8.0
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	11 at pH=4.9; 41 at pH=6.8; 52 at pH=8.0
Kd_{bs} (mL/g)	Kd_{bs} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	11 at pH=4.9; 41 at pH=6.8; 52 at pH=8.0
ksg (year)$^{-1}$	--	ND
Fv (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	0.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-17

CHEMICAL-SPECIFIC INPUTS FOR BENZALDEHYDE (100-52-7)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	106.12
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	329.6
Vp (atm)	*Vp* value cited in NC DEHNR (1997).	1.30E-03 at 25ºC (solid)
S (mg/L)	*S* value cited in NC DEHNR (1997).	3.30E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.18E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.07E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.48E-06
K_{ow} (unitless)		

TABLE A-2-18

CHEMICAL-SPECIFIC INPUTS FOR BENZENE (71-43-2)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	78.11
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	278.6
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1.25E-01 at 25ºC (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.78E+03
H (atm·m^3/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	5.49E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.17E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.02E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	137
K_{oc} (mL/g)	Geometric mean of measured values was obtained from U.S. EPA (1996b).	6.20E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	6.20E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	4.65E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the	

TABLE A-2-19

CHEMICAL-SPECIFIC INPUTS FOR BENZO(A)ANTHRACENE (56-55-3)

(Page 1 of 1)

TABLE A-2-20

CHEMICAL-SPECIFIC INPUTS FOR BENZO(A)PYRENE (50-32-8)

(**Page 1 of 1**)

Parameter	Reference and Explanation	Value
	Chemical/Physical Properties	
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	252.3
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	452
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	6.43E-12 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	1.94E-03
H (atm·m^3/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S and Vp values that are provided in this table.	8.36E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database in U.S. EPA (1994d).	2.18E-02
D_w (cm^2/s)	D	

TABLE A-2-21

CHEMICAL-SPECIFIC INPUTS FOR BENZO(B)FLUORANTHENE (205-99-2)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	252.32
T_m (K)	Montgomery and Welkom (1991)	441
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	1.06E-10 at 25ºC (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	4.33E-03
H (atm·m^3/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S and Vp values that are provided in this table.	6.18E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database U.S. EPA (1994d).	2.28E-02
D_w		

TABLE A-2-22

CHEMICAL-SPECIFIC INPUTS FOR BENZO(K)FLUORANTHENE (207-08-9)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	252.32
T_m (K)	Montgomery and Welkom (1991)	490
Vp (atm)	U.S. EPA (1994b)	1.32E-12 at 25ºC (solid)
S (mg/L)	U.S. EPA (1994b)	8.0E-04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW, S* and *Vp* values that are provided in this table.	4.15E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database U.S. EPA (1994d).	2.28E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database U.S. EPA (1994d).	5.49E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995)	1.56E+06
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	8.32E+05
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	8.32E+03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	6.24E+04
Kd_{bs} (mL/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.33E+04
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Lyman, Reehl, and Rosenblatt (1991).	1.18E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	0.149

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-23

CHEMICAL-SPECIFIC INPUTS FOR BENZOIC ACID (65-85-0)

(Page 1 of 2)

TABLE A-2-23

CHEMICAL-SPECIFIC INPUTS FOR BENZOIC ACID (65-85-0)

(Page 2 of 2)

Parameter	Reference and Explanation	Value
ksg $(\text{year})^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited Howard (1989-1993).	1.26E+02
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-24

CHEMICAL-SPECIFIC INPUTS FOR BENZONITRILE (100-47-0)

(Page 1 of 1)

TABLE A-2-25

CHEMICAL-SPECIFIC INPUTS FOR BENZYL ALCOHOL (100-51-6)

(Page 1 of 1)

TABLE A-2-26

CHEMICAL-SPECIFIC INPUTS FOR BENZYL CHLORIDE (100-44-7)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	126.58
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	225.1
Vp (atm)	*Vp* value cited in U.S. EPA (1995b).	1.60E-03 at 25ºC (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	4.90E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.13E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.43E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.80E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	2.00E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with	

TABLE A-2-27

CHEMICAL-SPECIFIC INPUTS FOR BERYLLIUM (7440-41-7)

(Page 1 of 1)

TABLE A-2-28

CHEMICAL-SPECIFIC INPUTS FOR ALPHA-BHC (319-84-6)

(Page 1 of 1)

TABLE A-2-29

CHEMICAL-SPECIFIC INPUTS FOR BETA-BHC (319-85-7)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	290.83
T_m (K)	Montgomery and Welkom (1991)	582.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	6.45E-10 at 25ºC (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	5.42E-01
H (atm·m^3/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	3.46E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.9E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.40E-06
K_{ow} (unitless)	Geometric mean value cited in Karickoff and Long (1995).	6.81E+03
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	2.14E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.14E+01
Kd		

TABLE A-2-30

CHEMICAL-SPECIFIC INPUTS FOR BIS(2-CHLORETHYL)ETHER (111-44-4)

(Page 1 of 1)

TABLE A-2-31

CHEMICAL-SPECIFIC INPUTS FOR BROMODICHLOROMETHANE (75-27-4)

(Page 1 of 1)

TABLE A-2-32

CHEMICAL-SPECIFIC INPUTS FOR BROMOFORM (75-25-2)

(Page 1 of 1)

TABLE A-2-33

CHEMICAL-SPECIFIC INPUTS FOR 4-BROMOPHENYL-PHENYLETHER (101-55-3)

(Page 1 of 1)

TABLE A-2-34

CHEMICAL-SPECIFIC INPUTS FOR BUTYLBENZYLPHTHALATE (85-68-7)

(Page 1 of 1)

TABLE A-2-35

CHEMICAL-SPECIFIC INPUTS FOR CADMIUM (7440-43-9)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	112.41
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	594.1
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	0.0
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp*	

TABLE A-2-36

CHEMICAL-SPECIFIC INPUTS FOR CARBON DISULFIDE (75-15-0)

(Page 1 of 1)

TABLE A-2-37

CHEMICAL-SPECIFIC INPUTS FOR CARBON TETRACHLORIDE (56-23-5)

(Page 1 of 1)

TABLE A-2-38

CHEMICAL-SPECIFIC INPUTS FOR CHLORDANE (57-74-9)

(Page 1 of 1)

TABLE A-2-39

CHEMICAL-SPECIFIC INPUTS FOR CHLORINE (7782-50-5)

(Page 1 of 1)

TABLE A-2-40

CHEMICAL-SPECIFIC INPUTS FOR 4-CHLORO-3-METHYLPHENOL (59-50-7)

(Page 1 of 1)

TABLE A-2-41

CHEMICAL-SPECIFIC INPUTS FOR P-CHLOROANILINE (106-47-8)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	127.57
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	345.6
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	3.09E-05 at 25ºC (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	3.36E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.17E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.80E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.02E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	7.40E+01
K_{oc} (mL/g)	For all ionizing organics, K_{oc} values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c).	K_{oc} is 41 for pH range of 4.9 to 8
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s	

TABLE A-2-42

CHEMICAL-SPECIFIC INPUTS FOR CHLOROBENZENE (108-90-7)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	112.56
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	228.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1.59E-02 at 25ºC (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	4.09E+02
H (atm·m^3/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	4.38E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.35E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.49E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c)	6.16E+02
K_{oc}		

TABLE A-2-43

CHEMICAL-SPECIFIC INPUTS FOR CHLOROBENZILATE (510-15-6)

(Page 1 of 1)

TABLE A-2-44

CHEMICAL-SPECIFIC INPUTS FOR CHLORODIFLUOROMETHANE (75-45-6)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Howard 1989-1993	86.47
T_m (K)	Howard 1989-1993	126.6
Vp (atm)	Vp value cited in Howard 1989-1993.	5.63 at 25ºC (liquid)
S (mg/L)	Howard 1989-1993	2.90E+03
H (atm·m^3/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	1.68E-01
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	9.72E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	1.13E-05
K_{ow} (unitless)	Calculated using the log K_{ow} value cited in Howard 1989-1993.	1.20E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	9.83E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	9.83E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	7.38E-01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.93E-01
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991) OR Howard (1989-1993) OR Mackay, Shiu, and Ma (1992).	0.0
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in the table.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-45

CHEMICAL-SPECIFIC INPUTS FOR CHLOROETHANE (75-00-3)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	64.52
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	441.8
Vp (atm)	*Vp* value cited in Lucius et al. (1992).	159.88 at 25ºC (solid)
S (mg/L)	*S* value cited in U.S. EPA (1994a)	5.74E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.80
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.27E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.53E-06
K_{ow} (unitless)	K_{ow} value calculated from log K_{ow} value cited in U.S. EPA (1995a).	1.26E+03
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	3.71E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Kd_s value was calculated by using the K_{oc} value that is provided in this table.	3.71E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.78E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with *K*	

TABLE A-2-46

CHEMICAL-SPECIFIC INPUTS FOR CHLOROFORM (67-66-3)

(Page 1 of 1)

TABLE A-2-47

CHEMICAL-SPECIFIC INPUTS FOR (BIS)-1,2-CHLOROISOPROPYLETHER (39638-32-9)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	171.07
T_m (K)	Montgomery and Welkom (1991)	369.9
Vp (atm)	Montgomery and Welkom (1991)	7.00E-03 at 25ºC (solid)
S (mg/L)	Montgomery and Welkom (1991)	1.70E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	7.04E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	3.61E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.38E-06
K_{ow} (unitless)	K_{ow} value cited in Howard (1989 - 1993).	3.80E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.46E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.46E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw}	

TABLE A-2-48

CHEMICAL-SPECIFIC INPUTS FOR 2-CHLORONAPHTHALENE (91-58-7)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	162.61
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	332.6
Vp (atm)	Vp value cited in U.S. EPA (1995b).	1.05E-05 at 25ºC (solid)
S (mg/L)	S value cited in U.S. EPA (1995b).	1.20E+01
H (atm·m^3/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	1.43E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	3.64E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.24E-06
K_{ow} (unitless)	Montgomery and Welkom (1991)	1.17E+04
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	7.14E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Kd_s value was calculated by using the K_{oc} value that is provided in this table.	7.14E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	5.36E+02
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K	

TABLE A-2-49

CHEMICAL-SPECIFIC INPUTS FOR 2-CHLOROPHENOL (95-57-8)

(Page 1 of 2)

TABLE A-2-49

CHEMICAL-SPECIFIC INPUTS FOR 2-CHLOROPHENOL (95-57-8)

(Page 2 of 2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties (Continued)		
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table for a pH of 7.0.	2.90E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table for a pH of 7.0.	1.55E+01
ksg $(year)^{-1}$	*Ksg* value was assumed to be 0 due to a lack of data.	0.0
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-50

CHEMICAL-SPECIFIC INPUTS FOR 4-CHLOROPHENYL-PHENYLETHER (7005-72-3)

(Page 1 of 1)

		[redacted]

TABLE A-2-51

CHEMICAL-SPECIFIC INPUTS FOR CHLOROPYRIFOS (2921-88-2)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	350.59
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	314.6
Vp (atm)	*Vp* value cited in Howard (1989-1993).	1.32E-03 at 25ºC (solid)
S (mg/L)	*S* value cited in Howard (1989-1993).	5.00E+00
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	9.26E-02
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	3.82E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	4.42E-06
K_{ow} (unitless)	Recommended K_{ow} value cited in Karickhoff and Long (1995).	1.82E+05
K_{oc} (mL/g)	K_{oc}	

TABLE A-2-52

CHEMICAL-SPECIFIC INPUTS FOR CHROMIUM (7440-47-3)

(Page 1 of 1)

TABLE A-2-53

CHEMICAL-SPECIFIC INPUTS FOR HEXAVALENT CHROMIUM (18540-29-9)

(Page 1 of 1)

TABLE A-2-54

CHEMICAL-SPECIFIC INPUTS FOR CHRYSENE (218-01-9)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)		

TABLE A-2-54a

CHEMICAL-SPECIFIC INPUTS FOR COPPER (7440-50-8)

TABLE A-2-55

CHEMICAL-SPECIFIC INPUTS FOR M-CRESOL (108-39-4)

(Page 1 of 1)

TABLE A-2-56

CHEMICAL-SPECIFIC INPUTS FOR O-CRESOL (95-48-7)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	108.13
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	303.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	4.16E-04 at 25ºC (solid)
S		

TABLE A-2-57

CHEMICAL-SPECIFIC INPUTS FOR P-CRESOL (106-44-5)

(Page 1 of 1)

TABLE A-2-58

CHEMICAL-SPECIFIC INPUTS FOR CUMENE (ISOPROPYLBENZENE) (98-82-8)

(Page 1 of 1)

TABLE A-2-59

CHEMICAL-SPECIFIC INPUTS FOR CYANIDE (57-12-5)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S.EPA (1992a)	26.017
T_m (K)	--	ND
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1.82E-02 at 25ºC (solid)
S (mg/L)	--	ND
H (atm·m^3/mol)	--	ND
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	5.48E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	2.10E-05
K_{ow} (unitless)	--	ND
K_{oc} (mL/g)	--	ND
Kd_s (cm		

TABLE A-2-60

CHEMICAL-SPECIFIC INPUTS FOR 4,4’-DDD (72-54-8)

(Page 1 of 1)

TABLE A-2-61

CHEMICAL-SPECIFIC INPUTS FOR 4,4'-DDE (72-55-9)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	319.03
T_m (K)	Montgomery and Welkom (1991)	361.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	7.45E-09 at 25ºC (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.92E-02
H (atm·m^3/mol)	*H*	

TABLE A-2-62

CHEMICAL-SPECIFIC INPUTS FOR 4,4’-DDT (50-29-3)

(Page 1 of 1)

TABLE A-2-63

CHEMICAL-SPECIFIC INPUTS FOR DI-N-BUTYL PHTHALATE (84-74-2)

(Page 1 of 1)

TABLE A-2-64

CHEMICAL-SPECIFIC INPUTS FOR DI-N-OCTYLPHTHALATE (117-84-0)

(Page 1 of 1)

TABLE A-2-65

CHEMICAL-SPECIFIC INPUTS FOR DIAZINON (333-41-5)

(Page 1 of 1)

TABLE A-2-66

CHEMICAL-SPECIFIC INPUTS FOR DIBENZ(A,H)ANTHRACENE (53-70-3)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	278.33
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	539.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	2.70E-14 at 25ºC (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	6.70E-04
H (atm·m^3/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S and Vp values that are provided in this table.	1.12E-08
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	1.80E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	6.01E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	3.53E+06
K_{oc} (mL/g)	Geometric mean of measured values was obtained from U.S. EPA (1996b).	1.79E+06
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.79E+04
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.34E+05
Kd_{bs} (mL/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	7.16E+04
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	2.69E-01
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using S, T_m, and Vp values that are provided in this table. Vp value for this compound was converted to a liquid phase value before being used in the calculations.	0.011

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-67

CHEMICAL-SPECIFIC INPUTS FOR 1,2-DIBROMO-3-CHLOROPROPANE (96-12-8)

(Page 1 of 1)

TABLE A-2-68

CHEMICAL-SPECIFIC INPUTS FOR DIBROMOCHLOROMETHANE (124-48-1)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O’Neil, Smith, and Heckelman (1989)	208.3
[redacted]		
[redacted]		
[redacted]		
[redacted]		
[redacted]		
[redacted]		
[redacted]		
[redacted]		
[redacted]		
[redacted]		
[redacted]		
[redacted]		
[redacted]		

TABLE A-2-69

CHEMICAL-SPECIFIC INPUTS FOR 1,2-DICHLOROBENZENE (95-50-1)

(Page 1 of 1)

TABLE A-2-70

CHEMICAL-SPECIFIC INPUTS FOR 1,3-DICHLOROBENZENE (541-73-1)

(Page 1 of 1)

TABLE A-2-71

CHEMICAL-SPECIFIC INPUTS FOR 1,4-DICHLOROBENZENE (106-46-7)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)		

TABLE A-2-72

CHEMICAL-SPECIFIC INPUTS FOR 3,3’-DICHLOROBENZIDINE (91-94-1)

TABLE A-2-73

CHEMICAL-SPECIFIC INPUTS FOR DICHLORODIFLUOROMETHANE (75-71-8)

(Page 1 of 1)

TABLE A-2-74

CHEMICAL-SPECIFIC INPUTS FOR 1,1-DICHLOROETHANE (75-34-3)

(Page 1 of 1)

TABLE A-2-75

CHEMICAL-SPECIFIC INPUTS FOR 1,2-DICHLOROETHANE (107-06-2)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	98.96
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	233.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1.07E-01 at 25ºC (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	8.31E+03
H (atm·m^3/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	1.27E-03
D_a (cm^2/s)	D_a	

TABLE A-2-76

CHEMICAL-SPECIFIC INPUTS FOR 1,1-DICHLOROETHYLENE (75-35-4)

(Page 1 of 1)

TABLE A-2-77

CHEMICAL-SPECIFIC INPUTS FOR (CIS)-1,2-DICHLOROETHYLENE (156-59-2)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Howard (1989-1993)	96.94
T_m (K)	Howard (1989-1993)	192.6
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	2.30E-01 at 25ºC (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	4.94E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.51E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.36E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.13E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	9.60E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	4.98E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.98E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.73+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited	

TABLE A-2-78

CHEMICAL-SPECIFIC INPUTS FOR (TRANS)-1,2-DICHLOROETHYLENE (156-60-5)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	96.95
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	223.7
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	4.63E-01 at 25ºC (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	6.03E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	7.44E-03
D_a (cm		

TABLE A-2-79

CHEMICAL-SPECIFIC INPUTS FOR 2,4-DICHLOROPHENOL (120-83-2)

(Page 1 of 2)

TABLE A-2-79

CHEMICAL-SPECIFIC INPUTS FOR 2,4-DICHLOROPHENOL (120-83-2)

(Page 2 of 2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties (Continued)		
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	5.58E+00
ksg (year)$^{-1}$	ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	3.61E+00
Fv (unitless)	Fv	

TABLE A-2-80

CHEMICAL-SPECIFIC INPUTS FOR 1,2-DICHLOROPROPANE (78-87-5)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O’Neill, Smith, and Heckelman (1989)	112.99
T_m (K)	Montgomery and Welkom (1991)	172.7
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	6.66E-02 at 25ºC (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	2.68E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.81E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.21E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.71E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	1.78E+02
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	4.70E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.70E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.53E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with $K_{\text{52j re f 39.09 270.69 44di0 0 5an vao cmean8 -0.}}$	

TABLE A-2-81

CHEMICAL-SPECIFIC INPUTS FOR (CIS)-1,3-DICHLOROPROPENE (542-75-6)

(Page 1 of 1)

TABLE A-2-82

CHEMICAL-SPECIFIC INPUTS FOR DICHLORVOS (62-73-7)

(Page 1 of 1)

TABLE A-2-83

CHEMICAL-SPECIFIC INPUTS FOR DIELDRIN (60-57-1)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	380.93
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	449.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	1.31E-09 at 25ºC (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	1.87E-01
H (atm·m^3/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	2.66E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	1.36E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	4.29E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c)	1.86E+05
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	2.55E+04
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.55E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.91E+03
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.02E+03
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991)	2.34E+00
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	0.9860

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-84

CHEMICAL-SPECIFIC INPUTS FOR DIETHYL PHTHALATE (84-66-2)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	222.24
T_m (K)	Montgomery and Welkom (1991)	232.6
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	2.17E-06 at 25ºC (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	8.80E+02
H (atm·m^3/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	5.48E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.56E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.35E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	2.73E+04
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	8.20E+01
Kd_s (cm^3/g)	Kd	

TABLE A-2-85

CHEMICAL-SPECIFIC INPUTS FOR DIMETHYL PHTHALATE (131-11-3)

(Page 1 of 1)

TABLE A-2-86

CHEMICAL-SPECIFIC INPUTS FOR 2,4-DIMETHYLPHENOL (105-67-9)

(Page 1 of 2)

TABLE A-2-86

CHEMICAL-SPECIFIC INPUTS FOR 2,4-DIMETHYLPHENOL (105-67-9)

(Page 2 of 2)

Parameter	Reference and Explanation	Value

TABLE A-2-87

CHEMICAL-SPECIFIC INPUTS FOR 3,3’-DIMETHYOXYBENZIDINE (119-90-4)

(Page 1 of 1)

TABLE A-2-88

CHEMICAL-SPECIFIC INPUTS FOR 1,3-DINITROBENZENE (99-65-0)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	168.11
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	363
Vp (atm)	Geometric mean value cited in U.S. EPA (1994f).	4.0E-07 at 25ºC (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994f).	5.4E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S* and *Vp* values that are provided in this table.	1.25E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	3.18E-02
D_w (cm^2		

TABLE A-2-89

CHEMICAL-SPECIFIC INPUTS FOR 2,4-DINITROPHENOL (51-28-5)

(Page 1 of 2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	184.11
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	385.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1.52E-07 at 25ºC (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	5.8E+03
H (atm·m^3/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	4.82E-09
D_a (cm^2/s)	D	

TABLE A-2-89

CHEMICAL-SPECIFIC INPUTS FOR 2,4-DINITROPHENOL (51-28-5)

(Page 2 of 2)

Parameter	Reference and Explanation	Value

TABLE A-2-90

CHEMICAL-SPECIFIC INPUTS FOR 2,4-DINITROTOLUENE (121-14-2)

(Page 1 of 1)

TABLE A-2-91

CHEMICAL-SPECIFIC INPUTS FOR 2,6-DINITROTOLUENE (606-20-2)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Howard (1989-1993)	182.15
T_m (K)	Howard (1989-1993)	339
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	7.47E-07 at 25ºC (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	1.05E+03
H (atm·m^3/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S and Vp values that are provided in this table.	1.30E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database U.S. EPA (1994d).	3.11E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database U.S. EPA (1994d).	7.76E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	7.70E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	4.19E+01
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.19E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.14E+00
Kd_{bs} (mL/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.68E+00
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.41E+00
Fv (unitless)	Fv	

TABLE A-2-92

CHEMICAL-SPECIFIC INPUTS FOR 1,4-DIOXANE (123-91-1)

(Page 1 of 1)

[redacted]

TABLE A-2-93

CHEMICAL-SPECIFIC INPUTS FOR 1,2-DIPHENYLHYDRAZINE (122-66-7)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	184.24
T_m (K)	Montgomery and Welkom (1991)	401.1
Vp (atm)	*Vp* value cited in U.S. EPA (1995b)	4.74E-08 at 25ºC (solid)
S (mg/L)	*S* value cited in U.S. EPA (1995b)	6.80E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.28E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.95E-02
D		

TABLE A-2-94

CHEMICAL-SPECIFIC INPUTS FOR DISULFOTON (298-04-4)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	274.38
T_m (K)	T_m value cited in U.S. EPA (1995b).	248
Vp (atm)	*Vp* value cited in U.S. EPA (1995b).	3.7E-07 at 25ºC (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	1.6E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.12E-06
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	4.50E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	5.21E-06
K_{ow} (unitless)	Recommended K_{ow} value cited in Karickhoff and Long (1995).	9.55E+03
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.80E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.80E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction oF 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.35E+02
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	7.20E+01
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.20E+01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	0.998

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-95

CHEMICAL-SPECIFIC INPUTS FOR ENDOSULFAN I (115-29-7)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	406.95
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	343.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	1.31E-08 at 25ºC (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	2.31E-01
H (atm·m^3/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	2.31E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.59E-03
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.76E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	3.02E+03
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	2.04E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.04E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.53E+02
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	8.16E+01
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	2.78E+01
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid phase value before being used in the calculations.	0.9839

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-96

CHEMICAL-SPECIFIC INPUTS FOR ENDRIN (72-20-8)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	380.93
T_m (K)	U.S.EPA (1992a)	473.1
Vp (atm)	Vp value cited in U.S. EPA (1992a)	7.68E-10 at 25ºC (solid)
S (mg/L)	S value cited in U.S. EPA (1992a)	2.46E-01
H (atm·m^3/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	1.19E-06
D_a		

TABLE A-2-97

CHEMICAL-SPECIFIC INPUTS FOR EPICHLOROHYDRIN (106-89-8)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	92.53
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	247.5
Vp (atm)	Vp value cited in U.S. EPA (1995b).	2.20E-02 at 25ºC (liquid)
S (mg/L)	S value cited in U.S. EPA (1995b).	6.60E+04
H (atm·m^3/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	3.08E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.13E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.10E-05
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	1.78E+00
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.22E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.22E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.66E-01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	8.88E-02
ksg (year)$^{-1}$	ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	9.03E+00
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-98

CHEMICAL-SPECIFIC INPUTS FOR ETHYL METHACRYLATE (97-63-2)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	*MW* value cited in U.S. EPA (1995b)	114.14
T_m (K)	--	NA
Vp (atm)	*Vp* value cited in U.S. EPA (1995b).	2.30E-02 at 25ºC
S (mg/L)	*S* value cited in U.S. EPA (1995b).	1.90E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.38E-04
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	8.07E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	9.35E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	3.89E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.46E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.46E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.85E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	9.80E-01
ksg (year)$^{-1}$	*Ksg* value was assumed to be 0 due to a lack of data.	0.0
Fv (unitless)	*Fv* value cited in NC DEHNR (1997).	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-99

CHEMICAL-SPECIFIC INPUTS FOR ETHYL METHANESULFONATE (62-50-0)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	124.15
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	373.0
Vp (atm)		

TABLE A-2-100

TABLE A-2-101

CHEMICAL-SPECIFIC INPUTS FOR ETHYLENE DIBROMIDE (106-93-4)

(Page 1 of 1)

TABLE A-2-102

CHEMICAL-SPECIFIC INPUTS FOR ETHYLENE OXIDE (75-21-8)

(Page 1 of 1)

TABLE A-2-103

CHEMICAL-SPECIFIC INPUTS FOR BIS(2-ETHYLHEXYL)PHTHALATE (117-81-7)

(Page 1 of 1)

TABLE A-2-104

CHEMICAL-SPECIFIC INPUTS FOR FLUORANTHENE (206-44-0)

(Page 1 of 1)

TABLE A-2-105

CHEMICAL-SPECIFIC INPUTS FOR FLUORENE (86-73-7)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	166.22
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	389.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	8.17E-07 at 25ºC (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	1.86E+00
H (atm·m^3/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	7.30E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	3.63E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	7.88E-06
K_{ow} (unitless)	K_{ow} value cited in U.S. EPA (1995b)	1.47E+04
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	7.71E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	7.71E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction oF 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	5.78E+02
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.08E+02
ksg (year)$^{-1}$	Ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	4.22E+00
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid phase value before being used in the calculations.	0.9999

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-106

CHEMICAL-SPECIFIC INPUTS FOR FORMALDEHYDE (50-00-0)

(Page 1 of 1)

TABLE A-2-107

CHEMICAL-SPECIFIC INPUTS FOR FORMIC ACID (64-18-6)

(Page 1 of 1)

TABLE A-2-108

CHEMICAL-SPECIFIC INPUTS FOR
1,2,3,4,6,7,8-HEPTACHLORODIBENZO(P)DIOXIN (35822-46-9)

(Page 1 of 1)

TABLE A-2-109

CHEMICAL-SPECIFIC INPUTS FOR
1,2,3,4,6,7,8-HEPTACHLORODIBENZO(P)FURAN (67562-39-4)

(Page 1 of 1)

TABLE A-2-110

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3,4,7,8,9-HEPTACHLORODIBENZO(P)FURAN (55673-89-7)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1994a)	409.31
T_m (K)	U.S. EPA (1994a)	494.1
Vp (atm)	U.S. EPA (1994a)	1.41E-13 at 25ºC (solid)
S (mg/L)	Homologue group average value obtained from U.S. EPA (1994a).	1.40E-06
H (atm·m^3/mol)	U.S. EPA (1994a)	5.30E-05
D_a (cm^2/s)	D_a value was calculated by using Equation A-3-2. Recommended value was calculated by using the MW and D_a values that are provided in the tables in Appendix A-2 for 2,3,7,8-TCDF.	1.55E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	3.99E-06
K_{ow} (unitless)	Homologue group average value obtained from U.S. EPA (1992d).	8.32E+07
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for dioxins and furans that is cited in U.S. EPA (1994a) and U.S. EPA (1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	5.13E+07
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	5.13E+05
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.85E+06
Kd_{bs} (cm^3		

TABLE A-2-111

CHEMICAL-SPECIFIC INPUTS FOR HEPTACHLOR (76-44-8)

(Page 1 of 1)

TABLE A-2-112

CHEMICAL-SPECIFIC INPUTS FOR HEPTACHLOR EPOXIDE (1024-57-3)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	389.32
T_m (K)	Montgomery and Welkom (1991)	430.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	5.71E-09 at 25ºC (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	2.68E-01
H (atm·m^3/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	8.29E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.32E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.23E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	5.62E+04
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates	

TABLE A-2-113

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3,4,7,8-HEXACHLORODIBENZO(P)DIOXIN (39227-28-6)

(Page 1 of 1)

TABLE A-2-114

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3,6,7,8-HEXACHLORODIBENZO(P)DIOXIN (57653-85-7)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1994a)	390.87
T_m (K)	U.S. EPA (1994a)	558.1
Vp (atm)	U.S. EPA (1994a)	4.74E-14 at 25°C (solid)
S (mg/L)	Homologue group average value obtained from U.S. EPA (1994a).	4.40E-06
H (atm·m^3/mol)	U.S. EPA (1994a)	1.20E-05
D_a (cm^2/s)	D_a value was calculated by using Equation A-3-2. Recommended value was calculated by using the MW and D_a values that are provided in the tables in Appendix A-2 for 2,3,7,8-TCDD.	1.15E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	4.12E-06
K_{ow} (unitless)	Homologue group average value obtained from U.S. EPA (1992d).	1.78E+07
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for dioxins and furans that is cited in U.S. EPA (1994a) and U.S. EPA (1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	1.10E+07
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.10E+05
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc}	

TABLE A-2-115

CHEMICAL-SPECIFIC INPUTS FOR
1,2,3,7,8,9-HEXACHLORODIBENZO(P)DIOXIN (19408-74-3)

(Page 1 of 1)

TABLE A-2-116

CHEMICAL-SPECIFIC INPUTS FOR
1,2,3,4,7,8-HEXACHLORODIBENZO(P)FURAN (70648-26-9)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1994a)	374.87
T_m (K)	U.S. EPA (1994a)	498.6
Vp (atm)	U.S. EPA (1994a)	3.16E-13 at 25ºC (solid)
S (mg/L)	U.S. EPA (1994a)	8.25E-06
H (atm·m^3/mol)	U.S. EPA (1994a)	1.40E-05
D_a (cm^2/s)	D_a value was calculated by using Equation A-3-2. Recommended value was calculated by using the MW and D_a values that are provided in the tables in Appendix A-2 for 2,3,7,8-TCDF.	1.62E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	4.23E-06
K_{ow} (unitless)	Homologue group average value obtained from U.S. EPA (1992d)	1.78E+07
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for dioxins and furans that is cited in U.S. EPA (1994a) and U.S. EPA (1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	1.10E+07
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.10E+05
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}	

TABLE A-2-117

CHEMICAL-SPECIFIC INPUTS FOR
1,2,3,6,7,8-HEXACHLORODIBENZO(P)FURAN (57117-44-9)

(Page 1 of 1)

TABLE A-2-118

CHEMICAL-SPECIFIC INPUTS FOR
1,2,3,7,8,9-HEXACHLORODIBENZO(P)FURAN (72918-21-9)

(Page 1 of 1)

TABLE A-2-119

CHEMICAL-SPECIFIC INPUTS FOR 2,3,4,6,7,8-HEXACHLORODIBENZO(P)FURAN (60851-34-5)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1994a)	374.87
T_m (K)	U.S. EPA (1994a)	512.1
Vp (atm)	U.S. EPA (1994a)	2.63E-13 at 25°C (solid)
S (mg/L)	Homologue group average value obtained from U.S. EPA (1994a).	1.30E-05
H (atm·m^3/mol)	U.S. EPA (1994a)	1.00E-05
D_a (cm^2/s)	D_a value was calculated by using Equation A-3-2. Recommended value was calculated by using the MW and D_a values that are provided in the tables in Appendix A-2 for 2,3,7,8-TCDF.	1.62E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	4.23E-06
K_{ow} (unitless)	Homologue group average value obtained from U.S. EPA (1992d).	1.78E+07
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for dioxins and furans that is cited in U.S. EPA (1994a) and U.S. EPA (1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	1.10E+07
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.10E+05
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	8.22E+05
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	4.39E+05
ksg (year)$^{-1}$	Ksg value was assumed to be 0 due to a lack of data.	0.0
Fv (unitless)	Fv value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and Vp values that are provided in this table. Vp value for this compound was converted to a liquid phase value before being used in the calculations.	5.47E-02

Note:
NA = Not Applicable
ND = No Data Available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-120

CHEMICAL-SPECIFIC INPUTS FOR HEXACHLORO-1,3-BUTADIENE (PERCHLOROBUTADIENE) (87-68-3)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	260.76
T_m (K)	Montgomery and Welkom (1991)	252.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	2.33E-04 at 25ºC (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	2.54E+00
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.39E-02
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.73E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.33E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	5.38E+04
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	6.94E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	6.94E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	5.20E+02
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	2.77E+02
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-121

CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROBENZENE (118-74-1)

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TABLE A-2-122

CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROCYCLOPENTADIENE (77-47-4)

(Page 1 of 1)

TABLE A-2-123

CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROETHANE (67-72-1)

(Page 1 of 1)

TABLE A-2-124

CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROPHENE (70-30-4)

(Page 1 of 1)

TABLE A-2-125

CHEMICAL-SPECIFIC INPUTS FOR HYDROGEN CHLORIDE (7647-01-0)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	36.47
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	158.9
Vp (atm)	U.S. EPA (1994b)	4.6E+01 (liquid)
S (mg/L)	--	ND
H (atm·m^3/mol)	--	ND
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	1.73E-01
D_w		

TABLE A-2-126

CHEMICAL-SPECIFIC INPUTS FOR INDENO(1,2,3-CD)PYRENE (193-39-5)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	276.34
T_m (K)	Montgomery and Welkom (1991)	435
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	1.88E-13 at 25ºC

TABLE A-2-127

TABLE A-2-128

CHEMICAL-SPECIFIC INPUTS FOR LEAD (7439-92-1)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	207.2
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	600.5
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	0.0
H (atm·m^3/mol)	H value is assumed to be zero, because the Vp and S	

TABLE A-2-129

CHEMICAL-SPECIFIC INPUTS FOR MALATHIONE (121-75-5)

(Page 1 of 1)

TABLE A-2-130

CHEMICAL-SPECIFIC INPUTS FOR MERCURIC CHLORIDE (7487-94-7)

(Page 1 of 1)

TABLE A-2-131

CHEMICAL-SPECIFIC INPUTS FOR MERCURY (7439-97-6)

(Page 1 of 1)

TABLE A-2-132

CHEMICAL-SPECIFIC INPUTS FOR METHACRYLONITRILE (126-98-7)

(Page 1 of 1)

TABLE A-2-133

CHEMICAL-SPECIFIC INPUTS FOR METHANOL (67-56-1)

(Page 1 of 1)

TABLE A-2-134

CHEMICAL-SPECIFIC INPUTS FOR METHOXYCHLOR (72-43-5)

(Page 1 of 1)

TABLE A-2-135

CHEMICAL-SPECIFIC INPUTS FOR METHYL ACETATE (79-20-9)

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TABLE A-2-136

TABLE A-2-137

CHEMICAL-SPECIFIC INPUTS FOR METHYL CHLORIDE (74-87-3)

(Page 1 of 1)

TABLE A-2-138

CHEMICAL-SPECIFIC INPUTS FOR METHYL ETHYL KETONE (78-93-3)

(Page 1 of 1)

TABLE A-2-139

CHEMICAL-SPECIFIC INPUTS FOR METHYL ISOBUTYL KETONE (108-10-1)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	100.16
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	188.4
Vp (atm)	*Vp* value cited in U.S. EPA (1995b).	2.50E-02 at 25ºC (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	2.00E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.25E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.59E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.36E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	1.55E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.20E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in	

TABLE A-2-140

CHEMICAL-SPECIFIC INPUTS FOR METHYL MERCURY (22967-92-6)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1997g)	216.0
T_m (ºK)	--	ND
Vp (atm)	--	ND
S (mg/L)	--	ND
H (atm·m^3		

TABLE A-2-141

CHEMICAL-SPECIFIC INPUTS FOR METHYL PARATHION (298-00-0)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	263.23
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	310.1
Vp (atm)	*Vp* value cited in U.S. EPA (1992a).	1.30E-08 at 25ºC (solid)
S (mg/L)	*S* value cited in U.S. EPA (1992a).	5.00E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	6.84E-08
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.87E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.43E-06
K_{ow} (unitless)	K_{ow} value cited in U.S. EPA (1995b).	7.20E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.40E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.40E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.80E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	9.59E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	7.03E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	0.966

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-142

CHEMICAL-SPECIFIC INPUTS FOR METHYLENE BROMIDE (74-95-3)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
	Chemical/Physical Properties	
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	173.86
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	220.4
Vp (atm)	*Vp* value cited in U.S. EPA (1995b).	2.20E+00 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	1.45E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.64E-02
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	6.10E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	7.06E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	4.17E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.60E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.60E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.95E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate *Kd*	

TABLE A-2-143

CHEMICAL-SPECIFIC INPUTS FOR METHYLENE CHLORIDE (75-09-2)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	84.94
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	178.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	4.87E-01 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.74E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.38E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database U.S. EPA (1994d).	8.69E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database U.S. EPA (1994d).	1.25E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	1.80E+01
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	1.00E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s	

TABLE A-2-144

CHEMICAL-SPECIFIC INPUTS FOR NAPHTHALENE (91-20-3)

(Page 1 of 1)

TABLE A-2-145

NICKEL (7440-02-0)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	58.69
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	1,828
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	0.0
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	0.0
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	1.26E-01
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	1.46E-05
K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (mL/g)	Kd_s value was obtained from U.S. EPA (1996b), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model.	16 at pH=4.9; 65 at pH=6.8; 1,900 at pH=8.0;
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	16 at pH=4.9; 65 at pH=6.8; 1,900 at pH=8.0;
Kd_{bs} (mL/g)	Kd_{bs} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	16 at pH=4.9; 65 at pH=6.8; 1,900 at pH=8.0;
ksg (year)$^{-1}$		

TABLE A-2-146

CHEMICAL-SPECIFIC INPUTS FOR 2-NITROANILINE (88-74-4)

(Page 1 of 1)

TABLE A-2-147

CHEMICAL-SPECIFIC INPUTS FOR 3-NITROANILINE (99-09-2)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	138.12
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	387.1
Vp (atm)	--	1.07E-05 at 25ºC (solid)
S (mg/L)	*S* value cited in Montgomery and Welcom (1991)	8.90E+02
H (atm·		

TABLE A-2-148

CHEMICAL-SPECIFIC INPUTS FOR 4-NITROANILINE (100-01-6)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	138.12
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	419.10
Vp (atm)		

TABLE A-2-149

CHEMICAL-SPECIFIC INPUTS FOR NITROBENZENE (98-95-3)

(Page 1 of 1)

TABLE A-2-150

CHEMICAL-SPECIFIC INPUTS FOR 2-NITROPHENOL (88-75-5)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	139.11
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	317.1
Vp (atm)	Vp value cited in Howard (1989-1993).	2.63E-04 at 25ºC (solid)
S (mg/L)	S value cited in Howard (1989-1993).	2.50E+03
H (atm·m^3/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	1.46E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.44E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.19E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	6.17E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	3.53E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited	

TABLE A-2-151

CHEMICAL-SPECIFIC INPUTS FOR 4-NITROPHENOL (100-02-7)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	139.11
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	386.1
Vp (atm)	*Vp* value cited in Howard (1989-1993).	1.32E-06 at 25ºC (solid)
S (mg/L)	*S* value cited in Howard (1989-1993).	2.50E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	7.32E-09
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.30E-02
D_w (cm		

TABLE A-2-152

CHEMICAL-SPECIFIC INPUTS FOR N-NITROSO-DI-N-BUTYLAMINE (924-16-3)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	*MW* value cited in U.S. EPA (1995b)	158.20
T_m (K)	--	NA
Vp (atm)	*Vp* value cited in U.S. EPA (1995b)	3.80E-04 at 25°C
S (mg/L)	*S* value cited in U.S. EPA (1995b)	1.10E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	5.47E-05
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	6.50E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	7.52E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995)	2.57E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.07E+02
Kd_s (cm^3/g)	Kd_s	

TABLE A-2-153

CHEMICAL-SPECIFIC INPUTS FOR *N*-NITROSODIPHENYLAMINE (86-30-6)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	198.23
T_m (K)	Montgomery and Welkom (1991)	339.6
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	1.32E-04 at 25°

TABLE A-2-154

CHEMICAL-SPECIFIC INPUTS FOR *N*-NITROSODIPROPYLAMINE (621-64-7)

(Page 1 of 1)

TABLE A-2-155

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3,4,6,7,8,9-OCTACHLORODIBENZO(P)DIOXIN (3268-87-9)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1994a)	460.76
T_m (K)	U.S. EPA (1994a)	598.1
Vp (atm)	U.S. EPA (1994a)	1.09E-15 at 25ºC (solid)
S (mg/L)	U.S. EPA (1994a)	7.40E-08
H (atm·m^3/mol)	U.S. EPA (1994a)	7.00E-09
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.06E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	3.69E-07
K_{ow} (unitless)	U.S. EPA (1994a)	3.89E+07
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for dioxins and furans that is cited in U.S. EPA (1994a; 1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	2.40E+07
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.40E+05
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.80E+06
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	9.60E+05
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	1.09E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	0.0017

Note:
NA = Not Applicable
ND = No Data Available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-156

CHEMICAL-SPECIFIC INPUTS FOR
1,2,3,4,6,7,8,9-OCTACHLORODIBENZO(P)FURAN (39001-02-0)

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TABLE A-2-157

CHEMICAL-SPECIFIC INPUTS FOR
1,2,3,7,8-PENTACHLORODIBENZO(P)DIOXIN (40321-76-4)

(Page 1 of 1)

TABLE A-2-158

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3,7,8-PENTACHLORODIBENZO(P)FURAN (57117-41-6)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1994a)	340.42
T_m (K)	U.S. EPA (1994a)	498.1
Vp (atm)	U.S. EPA (1994a)	3.58E-12 at 25ºC (solid)
S (mg/L)	Homologue group average value obtained from U.S. EPA (1994a).	2.40E-04
H (atm·m^3/mol)	U.S. EPA (1994a)	6.20E-06
D_a (cm^2/s)	D_a value was calculated by using Equation A-3-2. Recommended value was calculated by using the *MW* and D_a values that are provided in the tables in Appendix A-2 for 2,3,7,8-TCDF.	1.70E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	4.51E-06
K_{ow} (unitless)	U.S. EPA (1992d)	6.17E+06
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for dioxins and furans that is cited in U.S. EPA (1994a) and U.S. EPA (1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	3.80E+06
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic	

TABLE A-2-159

CHEMICAL-SPECIFIC INPUTS FOR 2,3,4,7,8-PENTACHLORODIBENZO(P)FURAN (57117-31-4)

(Page 1 of 1)

TABLE A-2-160

CHEMICAL-SPECIFIC INPUTS FOR PENTACHLOROBENZENE (608-93-5)

(Page 1 of 1)

TABLE A-2-161

CHEMICAL-SPECIFIC INPUTS FOR PENTACHLORONITROBENZENE (82-68-8)

(Page 1 of 1)

TABLE A-2-162

CHEMICAL-SPECIFIC INPUTS FOR PENTACHLOROPHENOL (87-86-5)

(Page 1 of 2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	266.35
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	463
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	7.11E-07 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	1.34E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW, S* and *Vp* values that are provided in this table.	1.41E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	1.56E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	8.01E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	1.20E+05
K_{oc} (mL/g)	For all ionizing organics, K_{oc} values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c).	pH K_{oc} 1 19,949 2 19,918 3 19,604 4 16,942 5 7,333 6 1,417 7 504.9 8 408.7 9 399.1 10 398.1 11 398.0 12 398.0 13 398.0 14 398.0
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	pH K_{oc} 1 199.5 2 199.2 3 196.0 4 169.4 5 73.33 6 14.17 7 5.05 8 4.09 9 3.99 10 3.98 11 3.98 12 3.98 13 3.98 14 3.98

TABLE A-2-162

CHEMICAL-SPECIFIC INPUTS FOR PENTACHLOROPHENOL (87-86-5)

(Page 2 of 2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties (Continued)		
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	pH K_{oc} 1 1,496 2 1,494 3 1,470 4 1,271 5 550.0 6 106.2 7 37.87 8 30.66 9 29.93 10 29.86 11 29.85 12 29.85 13 29.85 14 29.85
Kd_{bs} (mL/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should @88	

TABLE A-2-163

CHEMICAL-SPECIFIC INPUTS FOR PHENANTHRENE (85-01-8)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	178.22
T_m (K)	Montgomery and Welkom (1991)	371.1
Vp (atm)	Geometric mean value calculated from values cited in Montgomery and Welkom (1991).	1.35E-03 at 25ºC (solid)
S (mg/L)	S value cited in Lucius et al. (1992).	1.28E+00
H (atm·m^3/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	1.88E-01
D_a (cm^2/s)	D_a	

TABLE A-2-164

CHEMICAL-SPECIFIC INPUTS FOR PHENOL (108-95-2)

(Page 1 of 2)

TABLE A-2-164

CHEMICAL-SPECIFIC INPUTS FOR PHENOL (108-95-2)

(Page 2 of 2)

Parameter	Reference and Explanation	Value
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-165

CHEMICAL-SPECIFIC INPUTS FOR PHORATE (298-02-2)

(Page 1 of 1)

TABLE A-2-166

CHEMICAL-SPECIFIC INPUTS FOR PHTHALIC ANHYDRIDE (85-44-9)

(Page 1 of 1)

TABLE A-2-167

CHEMICAL-SPECIFIC INPUTS FOR PRONAMIDE (23950-58-5)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	256.13
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	428.1
Vp (atm)	Vp value cited in U.S. EPA (1995b)	5.30E-07 at 25ºC (solid)
S (mg/L)	S value cited in U.S. EPA (1995b)	1.50E+01
H (atm·m^3/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	9.05E-06
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	4.71E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	5.45E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995)	3.24E+03
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow}	

TABLE A-2-168

CHEMICAL-SPECIFIC INPUTS FOR PYRENE (129-00-0)

(Page 1 of 1)

TABLE A-2-169

CHEMICAL-SPECIFIC INPUTS FOR PYRIDINE (110-86-1)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	79.10
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	231.5
Vp (atm)	Vp value cited in U.S. EPA (1995b)	2.60E-02 at 25ºC (liquid)
S (mg/L)	S value cited in U.S. EPA (1995b)	3.00E+02
H (atm·m^3/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	6.86E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.10E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.08E-05
K_{ow}		

TABLE A-2-170

CHEMICAL-SPECIFIC INPUTS FOR RONNEL (299-84-3)

(Page 1 of 1)

TABLE A-2-171

CHEMICAL-SPECIFIC INPUTS FOR SAFROLE (94-59-7)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	162.18
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	284.1
Vp (atm)	Vp value cited in U.S. EPA (1995b).	1.10E-04 at 25°C (liquid)
S (mg/L)	S value cited in U.S. EPA (1995b).	1.50E+03
H (atm·m^3/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	1.19E-05
D_a (cm^2/s)	D_a value was obtained from WATER8 model database (U.S. EPA 1995d).	4.06E-02
D_w (cm^2/s)	D_w value was obtained from WATER8 model database (U.S. EPA 1995d).	7.16E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	4.57E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.68E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.68E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.26E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	6.73E+00
ksg (year)$^{-1}$	ksg value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	9.03E+00
Fv (unitless)	Fv value was calculated by using the equation cited in Junge (1977). Recommended value of Fv was calculated by using the Vp value that is provided in this table.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-172

CHEMICAL-SPECIFIC INPUTS FOR SELENIUM (7782-49-2)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	78.96
T_m (ºK)	Budavari, O'Neil, Smith, and Heckelman (1989)	490.1
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient	

TABLE A-2-173

CHEMICAL-SPECIFIC INPUTS FOR SILVER (7440-22-4)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	107.87
T_m (ºK)	Budavari, O'Neil, Smith, and Heckelman (1989)	1,233.6
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	0.0
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S*	

TABLE A-2-174

CHEMICAL-SPECIFIC INPUTS FOR STRYCHNINE (57-24-9)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	334.40
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	541.1
Vp (atm)	Vp value cited in U.S. EPA (1995b).	2.20E-13 at 25ºC (solid)
S (mg/L)	Montgomery and Welkom (1991)	1.50E+02
H (atm·m^3/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	4.90E-13
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.38E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.58E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	8.51E+01
K_{oc} (mL/g)	K_{oc}	

TABLE A-2-175

CHEMICAL-SPECIFIC INPUTS FOR STYRENE (100-42-5)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
	Chemical/Physical Properties	
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	104.14
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	242.5
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	8.21E-03 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	2.57E+02
H (atm·m^3/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	3.33E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.73E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.77E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	8.49E+02
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	9.12E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K	

TABLE A-2-176

CHEMICAL-SPECIFIC INPUTS FOR 2,3,7,8-TETRACHLORODIBENZO(P)DIOXIN (1746-01-6)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1994a)	321.98
T_m (K)	U.S. EPA (1994a)	578.1
Vp (atm)	U.S. EPA (1994a)	9.74E-13 at 25°C (solid)
S (mg/L)	U.S. EPA (1994a)	1.93E-05
H (atm·m^3/mol)	U.S. EPA (1994a)	1.60E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.27E-02
D_w (cm^2/s)		

TABLE A-2-177

CHEMICAL-SPECIFIC INPUTS FOR
2,3,7,8-TETRACHLORODIBENZO(P)FURAN (51207-31-9)

(Page 1 of 1)

TABLE A-2-178

CHEMICAL-SPECIFIC INPUTS FOR 1,2,4,5-TETRACHLOROBENZENE (95-94-3)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	215.89
T_m (K)	Montgomery and Welkom (1991)	411.1
Vp (atm)	*Vp* value cited in U.S. EPA (1995b).	7.1E-06 at 25ºC (solid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	1.30E+00
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.18E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.11E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.75E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	4.36E+04
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	5.89E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	5.89E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	4.42E+02
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	2.36E+02
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of	

TABLE A-2-179

CHEMICAL-SPECIFIC INPUTS FOR 1,1,1,2-TETRACHLOROETHANE (630-20-6)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	167.85
T_m (K)	Montgomery and Welkom (1991)	230.1
Vp (atm)	Vp value cited in U.S. EPA (1995b)	1.60E-02 at 25ºC (liquid)
S (mg/L)	S value cited in U.S. EPA (1995b)	1.10E+03
H (atm·m^3/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	2.44E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	3.15E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.30E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995)	4.27E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.59E+02
Kd_s (cm		

TABLE A-2-180

CHEMICAL-SPECIFIC INPUTS FOR 1,1,2,2-TETRACHLOROETHANE (79-34-5)

(Page 1 of 1)

TABLE A-2-181

CHEMICAL-SPECIFIC INPUTS FOR TETRACHLOROETHYLENE (127-18-4)

(Page 1 of 1)

TABLE A-2-182

CHEMICAL-SPECIFIC INPUTS FOR 2,3,4,6-TETRACHLOROPHENOL (58-90-2)

(Page 1 of 2)

TABLE A-2-182

CHEMICAL-SPECIFIC INPUTS FOR 2,3,4,6-TETRACHLOROPHENOL (58-90-2)

(Page 2 of 2)

Parameter	Reference and Explanation	Value

TABLE A-2-183

CHEMICAL-SPECIFIC INPUTS FOR TETRAHYDROFURAN (109-99-9)

(Page 1 of 1)

TABLE A-2-184

CHEMICAL-SPECIFIC INPUTS FOR THALLIUM (7440-28-0)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	204.38
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	576.6
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	0.0
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	0.0
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	5.48E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	6.34E-06
K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (mL/g)	Kd_s value was obtained from U.S. EPA (1996b), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model.	44 at pH=4.9; 71 at pH=6.8; 96 at pH=8.0
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	44 at pH=4.9; 71 at pH=6.8; 96 at pH=8.0
Kd_{bs} (mL/g)	Kd_{bs} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	44 at pH=4.9; 71 at pH=6.8; 96 at pH=8.0
ksg (year)$^{-1}$	--	ND
Fv (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	0.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-185

CHEMICAL-SPECIFIC INPUTS FOR TOLUENE (108-88-3)

(Page 1 of 1)

TABLE A-2-186

CHEMICAL-SPECIFIC INPUTS FOR O-TOLUIDINE (95-53-4)

(Page 1 of 1)

TABLE A-2-187

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3-TRICHLOROBENZENE (87-61-6)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	181.46
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	325.7
Vp (atm)	Geometric mean value calculated from values cited in Mackay, Shiu, and Ma (1991).	3.20E-04 at 25ºC (solid)
S (mg/L)	Geometric mean value calculated from values cited in Mackay, Shiu, and Ma (1991).	2.05E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.84E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	3.02E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.15E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	1.11E+04
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.02E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.02E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.52E+02
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	8.10E+01
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-188

TABLE A-2-189

CHEMICAL-SPECIFIC INPUTS FOR 1,1,1-TRICHLOROETHANE (71-55-6)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	133.42
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	242.7
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	1.63E-01 at 25ºC (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	1.17E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.86E-02
D_a (cm^2/s)	*D*	

TABLE A-2-190

CHEMICAL-SPECIFIC INPUTS FOR 1,1,2-TRICHLOROETHANE (79-00-5)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	133.42
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	238.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	3.31E-02 at 25ºC (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	4.40E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.00E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.51E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.0E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	1.25E+02
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	7.50E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	7.50E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended *Kd*	

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CHEMICAL-SPECIFIC INPUTS FOR TRICHLOROETHYLENE (79-01-6)

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TABLE A-2-192

CHEMICAL-SPECIFIC INPUTS FOR TRICHLOROFLUOROMETHANE (75-69-4)

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TABLE A-2-193

CHEMICAL-SPECIFIC INPUTS FOR 2,4,5-TRICHLOROPHENOL (95-95-4)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	197.46
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	340.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	2.15E-05 at 25ºC (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	7.53E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	5.64E-06

TABLE A-2-194

CHEMICAL-SPECIFIC INPUTS FOR 2,4,6-TRICHLOROPHENOL (88-06-2)

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TABLE A-2-194

CHEMICAL-SPECIFIC INPUTS FOR 2,4,6-TRICHLOROPHENOL (88-06-2)

(Page 2 of 2)

Parameter	Reference and Explanation	Value
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-195

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3-TRICHLOROPROPANE (96-18-4)

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TABLE A-2-196

CHEMICAL-SPECIFIC INPUTS FOR 1,3,5-TRIMETHYLBENZENE (108-67-8)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	120.19
T_m (K)	Montgomery and Welkom (1991)	287.9
Vp (atm)	*Vp* value cited in U.S. EPA (1992a).	1.30E-03 at 25ºC (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1992a).	2.00E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	7.81E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.48E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.86E-06
K_{ow} (unitless)	K_{ow} value cited in Howard (1989-1993).	2.63E+03
K_{oc} (mL/g)	K_{oc}	

TABLE A-2-197

CHEMICAL-SPECIFIC INPUTS FOR 1,3,5-TRINITROBENZENE (99-35-4)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	213.11
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	395.6
Vp (atm)	Vp value cited in U.S. EPA (1995b).	1.30E-07 at 25ºC (solid)
S (mg/L)	S value cited in U.S. EPA (1995b).	3.20E+02
H (atm·m^3/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the MW, S, and Vp values that are provided in this table.	8.66E-08
D_a (cm^2/s)	D_a value was obtained from WATER8 model database (U.S. EPA 1995d).	2.84E-02
D_w (cm^2/s)	D_w value was obtained from WATER8 model database (U.S. EPA 1995d).	6.08E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	1.51E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.18E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.18E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	8.84E-01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	4.72E-01C˝/F4as343474.00 9.11935.29 T

TABLE A-2-198

CHEMICAL-SPECIFIC INPUTS FOR 2,4,6 -TRINITROTOLUENE (118-96-7)

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TABLE A-2-199

CHEMICAL-SPECIFIC INPUTS FOR VINYL ACETATE (108-05-4)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	86.09
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	180.1
Vp		

TABLE A-2-200

CHEMICAL-SPECIFIC INPUTS FOR VINYL CHLORIDE (75-01-4)

(Page 1 of 1)

TABLE A-2-201

CHEMICAL-SPECIFIC INPUTS FOR *M*-XYLENE (108-38-3)

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CHEMICAL-SPECIFIC INPUTS FOR

TABLE A-2-203

CHEMICAL-SPECIFIC INPUTS FOR *P*-XYLENE (106-42-3)

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TABLE A-2-204

CHEMICAL-SPECIFIC INPUTS FOR ZINC (7440-66-6)

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