17.0 Chemical Properties

Chemical properties are required by most of the modules of the 3MRA modeling system. This section describes how chemical properties were collected for the representative national data set included in the modeling system.

17.1 Parameters Collected

The chemical properties used by the 3MRA modeling system are listed in Table 17-1 along with the modules that use them.[1] Chemical properties are applied nationally and adjusted based on site-specific or regional pH and temperature conditions.

17.2 Data Sources and Methodology

The chemical property values used in the 3MRA modeling system were obtained through a combination of modeling, existing databases, and literature review. Table 17-2 summarizes how the various chemical properties were obtained. Certain metal partition coefficients, biodegradation rates, and hydrolysis rate constants were collected through literature surveys for measured values. Thermodynamic properties and partition coefficients for organic chemicals were calculated using the SPARC (System Performs Automated Reasoning in Chemistry) model and metal sorption isotherms were calculated using the MINTEQA2 geochemical speciation model. These models are described briefly below, along with their application for 3MRA modeling system.

SPARC. EPA developed the predictive modeling system SPARC to help meet the growing need for chemical-specific inputs for multimedia, multipathway, multireceptor risk assessment tools such as the 3MRA modeling system. SPARC (U.S. EPA, 2003) calculates a large number of physical and chemical parameters from chemical molecular structure and basic information about the environment (media, temperature, pressure, pH, etc.). For the 3MRA modeling system, SPARC is used to estimate solubility, vapor pressure, Henry's law constant, octanol/water partition coefficient, air diffusivity, water diffusivity, and ionization potential at a standard temperature and pH. These properties are contained in the 3MRA modeling system in text files. The Chemical Properties Processor (CPP; U.S. EPA, 1999d) reads those files to prepare the input files for the system modules. Prior to creating the input data sets, the CPP

[1] Chemical-specific bio-uptake, bioconcentration, and bioaccumulation factors used by the food web modules (Farm Food Chain, Terrestrial Food Web, and Aquatic Food Web Modules) are described in Chapter 10 of this volume.

Table 17-1. Chemical Properties by Module

Chemical property	CPP[a]	Source Modules					Media Modules			Food Modules	
		Surface Imp.	Aerated Tank	Land-fill	Waste-pile	LAU	Water-shed	Surface Water	Vadose/ Aquifer	TFW/ FFC[b]	AFW[c]
Thermodynamic Properties (organic chemicals)											
Molecular weight	●							●			
Density	●							●			
Molecular volume	●							●			
Boiling point	●										
Vapor pressure	○							●			
Solubility	○	●	●	●		●	●	●			
Air diffusivity	○	●	●	●		●	●	●			
Water diffusivity	○	●	●	●		●	●	●			
Ionization coefficient	●										
Partition Coefficients (organic chemicals)											
Henry's law constant	○	●	●	●	●	●	●	●		●	
Octanol-water partition coefficient	○							●		●	●
Soil-water partition coefficient	○	●	●	●	●	●	●	●	●	●	
Degradation Constants (organic chemicals)											
Hydrolysis rates	○	●	●	●	●	●	●	●	●		
Aerobic biodegradation rates	●	●	●	●	●	●	●	●	●		
Anaerobic biodegradation rates	●	●	●	●	●	●	●	●	●		
Partition Coefficients (metals)											
Partition coefficients (waste, soil, surface water, sediment)	●	●	●	●	●	●	●	●			
Sorption isotherms									●		

[a] Chemical Properties Processor
[b] TFW = terrestrial food web
FFC = farm food chain
[c] AFW = aquatic food web
○ calculated and/or adjusted for media pH and temperature conditions by the CPP
● used directly without adjustment

adjusts the SPARC-calculated properties to the temperature and pH conditions for the site and media being modeled. The CPP also calculates soil-water partition coefficients from octanol-water partition coefficients. U.S. EPA (1999c) describes the algorithms used within the CPP for these adjustments and calculations.

Table 17-2. Methodology and Data Sources for 3MRA Chemical Properties

Property	Methodology	References
Organic Chemicals		
Thermodynamic properties and partition coefficients[a]	SPARC-calculated values, adjusted by CPP for temperature and pH	U.S. EPA (2003) U.S. EPA (1999c)
Hydrolysis rates	Measured or estimated rate constants adjusted by CPP for temperature and pH	U.S. EPA (1996) U.S. EPA (1999c)
Aerobic biodegradation rates	Measured values from literature, grouped by pH and temperature regimes	Aronson et al. (1999)
Anaerobic biodegradation rates	Measured values from literature, grouped by pH, temperature, and redox regimes	U.S. EPA (1999a)
Soil/water partition coefficients	Calculated from Kow by CPP	U.S. EPA (1999c)
Metals		
Partition coefficients (waste, soil, surface water, sediment)	Measured or estimated values, presented as national distributions	U.S. EPA (1999e)
Sorption isotherms	MINTEQA2 model	U.S. EPA (1998, 1999b)

[a] molecular weight, density, volume, vapor pressure, boiling point, air and water diffusion coefficients, solubility, Henry's law constant, octanol/water partition coefficient (Kow), ionization coefficient

MINTEQA2. The MINTEQA2 model was used to develop metal sorption isotherms that are contained within the Vadose Zone and Aquifer Modules and used to provide the pH and concentration-adjusted soil-water partition coefficients needed to estimate sorption of metal contaminants in the subsurface. MINTEQA2 is a equilibrium speciation model that calculates the equilibrium composition of dilute aqueous solutions in the laboratory or in natural aqueous systems. The model can calculate the equilibrium mass distribution among dissolved species, adsorbed species, and multiple solid phases under a variety of conditions, including a gas phase with constant partial pressure. For more information on MINTEQA2, see U.S. EPA (1998) and U.S. EPA (1999b).

Other chemical properties were obtained from literature sources or estimated using empirical methods and expert judgment. Anaerobic and aerobic biodegradation rates and degradation products were collected using preestablished criteria for the evaluation of field and laboratory studies (U.S. EPA, 1999a; Aronson et al., 1999). The collected biodegradation rates are grouped by pH and temperature regimes and the CPP selects the appropriate value depending on media pH and temperature conditions at a site, or within a waste management unit. Anaerobic degradation rates are also grouped by redox regime (reducing, sulfate reducing, and methanogenic), which can be randomly selected during Monte Carlo runs.

Hydrolysis rates were compiled by EPA scientists along with probable pathways and degradation products for the hydrolysis reactions in question (U.S. EPA, 1996). EPA used literature sources where available, and supplemented these published data with laboratory experiments and expertise in structure activity relationships as needed. The overall hydrolysis rate constants used by the 3MRA modeling system are calculated by the CPP as a summation of the rate constants for acid, neutral, and base hydrolysis, using site-specific pH and temperature conditions in the media being modeled (U.S. EPA, 1999c).

The metal sorption coefficients for surface soils, surface water, sediments, and wastes were collected from literature where available, or estimated using a combination of empirical relationships with available literature values, geochemical modeling using MINTEQA2, and expert judgment. The methodology employed to collect or estimate these metal Kd values is described in detail in U.S. EPA (1999e). To represent the nationwide variability in sorption coefficients, the metal Kd values for each media are contained within the 3MRA modeling system as distributions that are randomly sampled by the CPP during model execution.

17.3 Quality Assurance/Quality Control

Quality assurance/quality control (QA/QC) protocols were developed and followed for each chemical property data collection effort. These QA/QC protocols are described in the documents referenced in Section 17.2.

17.4 Results

Appendix 17A provides the chemical property values included in the 3MRA modeling system for the 46 chemicals in the representative national data set. These values are contained in a set of text (.csv) files. During model execution, these files are read by the CPP to provide the appropriate chemical property data to each module. Table 17-3 lists the text files and the chemical properties that they contain.

Table 17-3. Chemical Property Files Contained within 3MRA Modeling System

File Name	Contents
AerBio.csv	Aerobic biodegradation rate constants (minimum, maximum, central tendency, standard deviation, and distribution type); reaction products
AnaBio.csv	Anaerobic biodegradation rate constants (minimum, maximum, central tendency, standard deviation, and distribution type); reaction products
AnaRed.csv	Anaerobic biodegradation rate constants, reducing redox regime (minimum, maximum, central tendency, standard deviation, and distribution type); reaction products
CAT.csv	Catalyzed acid, neutral, and base hydrolysis rates; reaction products
MethBio.csv	Anaerobic biodegradation rate constants, methanogenic redox regime (minimum, maximum, central tendency, standard deviation, and distribution type); reaction products
MICP.csv	Metal sorption coefficients (minimum, maximum, central tendency, standard deviation, and distribution type)
OCP.csv	Organic chemical thermodynamic properties and partition coefficients
SO4Bio.csv	Anaerobic biodegradation rate constants, sulfate-reducing redox regime (minimum, maximum, central tendency, standard deviation, and distribution type); reaction products

17.5 Issues and Uncertainties

Issues and uncertainties associated with the various chemical properties in the representative national data set can be found in the documentation listed for each property in Section 17.2.

17.6 References

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U.S. EPA (Environmental Protection Agency). 1996. *Environmental Fate Constants for Organic Chemicals under Consideration for EPA's Hazardous Waste Identification Rule.* Office of Research and Development. Athens, GA.

U.S. EPA (Environmental Protection Agency). 1998. *MINTEQA2/PRODEFA2, A Geochemical Assessment Model for Environmental Systems: User Manual Supplement for Version 4.0*. Prepared for the U.S. Environmental Protection Agency by HydroGeoLogic, Inc., Contract No. 68-C6-0020.

U.S. EPA (Environmental Protection Agency). 1999a. *Anaerobic Biodegradation of Organic Chemicals in Groundwater: Summary of Field and Laboratory Studies*. Office of Solid Waste. Washington, DC.

U.S. EPA (Environmental Protection Agency). 1999b. *Changes in the MINTEQA2 Modeling Procedure for Estimating Metal Partition Coefficients in Groundwater*, prepared by HydroGeoLogic, Inc. for the U.S. Environmental Protection Agency, Washington, DC.

U.S. EPA (Environmental Protection Agency). 1999c. *Chemical Database for HWIR99.* Office of Solid Waste. Athens, GA.

U.S. EPA (Environmental Protection Agency). 1999d. *Documentation for the FRAMES-HWIR Technology Software System, Volume 13: Chemical Properties Processor*. Office of Research and Development. Athens, GA.

U.S. EPA (Environmental Protection Agency). 1999e. *Surface Water, Soil, and Waste Partition Coefficients for Metals*. Office of Solid Waste. Washington, DC.

U.S. EPA (Environmental Protection Agency). 2003. *Prediction of Chemical Reactivity Parameters and Physical Properties of Organic Compounds from Molecular Structure Using SPARC*. Internal Report. Ecosystems Research Division, National Exposure Research Laboratory, Athens, GA. March.

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Appendix 17A

Chemical Properties Values in the 3MRA Modeling System Representative National Data Set

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Table 17A-1. Organic Chemical Properties

Chemical	MW	AirDif	Volume	VP	Ka1	Sol	HLC	Kow
	g/mole	cm^2/s	mL	torr	mg/L	mg/L	atm m^3/mol	mL/mL
Acetonitrile	41.05	2.37E-06	2.57E+01	8.96E+00	NA	4.80E+00	2.89E+00	1.61E+00
Acrylonitrile	53.06	1.59E-06	3.94E+01	1.14E+01	NA	6.12E+00	4.08E+00	1.57E+00
Aniline	93.13	1.30E-06	7.28E+01	8.54E+00	0.234	7.51E+00	1.16E-01	-9.47E-01
Benzene	78.11	1.71E-06	5.72E+01	8.17E+00	NA	5.78E+00	1.40E+00	3.80E-01
Benzo(a)pyrene	252.31	5.14E-07	1.99E+02	-4.60E+00	NA	3.33E+00	-8.30E+00	4.67E+00
Bis-(2-ethylhexyl) phthalate	390.56	4.07E-07	3.24E+02	-7.20E+00	NA	3.64E+00	-1.04E+01	3.55E+00
Carbondisulfide	76.14	2.19E-06	4.26E+01	7.51E+00	NA	1.63E+00	1.58E+00	4.41E-01
Chlorobenzene	112.56	1.34E-06	7.22E+01	7.21E+00	NA	5.52E+00	8.59E-01	6.06E-01
Chloroform	119.38	1.76E-06	4.87E+01	7.78E+00	NA	5.27E+00	1.71E+00	1.62E-01
Dibenz(a,h)anthracene	278.35	4.75E-07	2.13E+02	-2.07E+01	NA	-6.00E-01	-1.94E+01	7.78E+00
2,4-D [2,4-Dichlorophenoxyacetic acid]	221.04	7.96E-07	1.25E+02	6.90E+00	3.74	7.08E+00	-7.04E-01	-5.35E-02
Ethylenedibromide	187.86	1.36E-06	6.18E+01	8.12E+00	NA	5.86E+00	1.66E+00	-1.28E-01
Hexachloro-1,3-butadiene	260.76	8.30E-07	1.17E+02	7.66E+00	NA	5.02E+00	2.17E+00	1.02E-01
Methoxychlor	345.65	5.23E-07	2.16E+02	-7.25E-01	NA	4.50E+00	-5.53E+00	4.27E+00
Methylethylketone	72.11	1.70E-06	5.41E+01	7.81E+00	NA	3.28E+00	3.51E+00	1.54E+00
Methylmethacrylate	100.12	1.40E-06	7.22E+01	7.95E+00	NA	4.05E+00	3.02E+00	1.05E+00
Methylenechloride	84.93	2.15E-06	3.70E+01	7.57E+00	NA	4.31E+00	1.31E+00	1.42E-01
Nitrobenzene	123.11	1.15E-06	7.78E+01	8.21E+00	NA	5.89E+00	1.53E+00	1.47E+00
Pentachlorophenol	266.34	8.25E-07	1.24E+02	7.32E+00	4.47	3.70E+00	3.15E+00	7.29E-01
Phenol	94.11	1.33E-06	7.04E+01	1.03E+01	4.47	9.60E+00	-1.45E-01	-2.00E+00

(continued)

Table 17A-1. (continued)

Chemical	MW	AirDif	Volume	VP	Ka1	Sol	HLC	Kow
	g/mole	cm^2/s	mL	torr	mg/L	mg/L	atm m^3/mol	mL/mL
Pyridine	79.1	1.62E-06	5.45E+01	8.22E+00	2.58	4.23E+00	3.01E+00	8.22E-01
2,3,7,8-Tetrachlorodibenzo-p-dioxin [2,3,7,8-TCDD]	321.97	6.10E-07	1.75E+02	-2.68E+00	NA	1.64E+00	-4.90E+00	5.01E+00
Tetrachloroethylene	165.83	1.37E-06	7.31E+01	7.77E+00	NA	4.67E+00	2.44E+00	6.63E-01
Thiram	240.44	5.67E-07	1.70E+02	8.08E+00	NA	4.63E+00	2.94E+00	-1.09E-01
Toluene	92.14	1.42E-06	7.19E+01	7.86E+00	NA	5.60E+00	1.34E+00	3.89E-01
1,1,1-Trichloroethane	133.4	1.56E-06	6.95E+01	7.56E+00	NA	5.16E+00	1.65E+00	2.80E-01
Trichloroethylene	131.39	1.60E-06	6.11E+01	7.68E+00	NA	4.65E+00	2.27E+00	6.72E-01
Vinylchloride	62.5	2.57E-06	3.62E+01	7.17E+00	NA	4.87E-01	1.55E+00	5.55E-01

Properties generated by SPARC chemical properties estimator
MW = molecular weight; AirDif = air diffusivity; Volume = molar volume; VP = vapor pressure; Ka1 = ionization coefficient
Sol = solubility; HLC = Henry's Law constant; Kow = octanol/water partition coefficient; Koc = soil / water partition coefficient
NA = not available

Table 17A-2a. Chemical Properties for Metals (MICP.csv)

Chemical	MW	Wdiff (mean)	Wdiff (min)	Wdiff (max)	Wdiff (dist)	Sol
	g/mole	cm^2/s	cm^2/s	cm^2/s	-	mg/L
Antimony	121.75	-	1.00E-04	1.00E-02	Uniform	1.00E+05
Arsenic	74.92	-	1.00E-04	1.00E-02	Uniform	1.00E+05
Barium	137.33	-	1.00E-04	1.00E-02	Uniform	1.00E+05
Beryllium	9.01218	-	1.00E-04	1.00E-02	Uniform	1.00E+05
Cadmium	112.4	-	1.00E-04	1.00E-02	Uniform	1.00E+05
Chromium III	52	-	1.00E-04	1.00E-02	Uniform	1.00E+05
Chromium VI	52	-	1.00E-04	1.00E-02	Uniform	1.00E+05
Lead	207.2	-	1.00E-04	1.00E-02	Uniform	1.00E+05
Divalent mercury	200	1.00E-04			Constant	1.00E+05
Elemental mercury	200	1.00E-04			Constant	2.50E-02
Methyl mercury	215	1.00E-04			Constant	1.00E+05
Nickel (+2)	58.7	-	1.00E-04	1.00E-02	Uniform	1.00E+05
Selenium (+6)	78.96	-	1.00E-04	1.00E-02	Uniform	1.00E+05
Silver	107.87	-	1.00E-04	1.00E-02	Uniform	1.00E+05
Thallium	204.37	-	1.00E-04	1.00E-02	Uniform	1.00E+05
Vanadium	50.9415	-	1.00E-04	1.00E-02	Uniform	1.00E+05
Zinc	65.38	-	1.00E-04	1.00E-02	Uniform	1.00E+05

MW = molecular weight; Wdiff = water diffusivity
Sol = solubility limit for sediment, soil, and wastes in LAUs, waste piles, surface impounments, and aerated tanks

Table 17A-2b. Metal Partition Coefficients (Kd values; MICP.csv)

Chemical	Statistic	Environmental Media Kd Values (L/kg)				Waste Kd Values (L/kg)				
		Organic carbon	Soil	Sediment	Surface Water	LAU	Waste Pile	Landfill	Surface Impoundment	Aerated Tank
Antimony	min	0	1.258925	3.981072	7943.282	1.00714	1.00714	1.00714	7943.282347	7943.282
	mean	5.01E+02	199.5262	3981.072	63095.73	159.621	159.621	159.621	63095.73445	63095.73
	max	2.00E+04	501.1872	63095.73	79432.82	400.9498	400.9498	400.9498	79432.82347	79432.82
	std. dev.		12.58925	63.09573	3.162278	10.0714	10.0714	10.0714	3.16227766	3.162278
	distrib.	constant	triangular	triangular	triangular	triangular	triangular	triangular	triangular	triangular
Arsenic	min		1.995262	39.81072	100	1.59621	1.59621	1.59621	100	100
	mean	0	1584.893	251.1886	7943.282	1267.915	1267.915	1267.915	7943.282347	7943.282
	max		19952.62	19952.62	1000000	15962.1	15962.1	15962.1	1000000	1000000
	std. dev.		5.011872	5.011872	3.162278	4.009498	4.009498	4.009498	3.16227766	3.162278
	distrib.	constant	triangular	triangular	triangular	triangular	triangular	triangular	triangular	triangular
Barium	min		5.011872	7.943282	794.3282	4.009498	4.009498	4.009498	794.3282347	794.3282
	mean	0	100	316.2278	10000	80	80	80	10000	10000
	max		2511.886	1584.893	31622.78	2009.509	2009.509	2009.509	31622.7766	31622.78
	std. dev.		5.011872	6.309573	2.511886	4.009498	4.009498	4.009498	2.511886432	2.511886
	distrib.	constant	triangular	triangular	triangular	triangular	triangular	triangular	triangular	triangular
Beryllium	min	1.00E+03	50.11872	6.309573	630.9573	40.09498	40.09498	40.09498	630.9573445	630.9573
	mean	3.16E+04	158.4893	630.9573	15848.93	126.7915	126.7915	126.7915	15848.93192	15848.93
	max	2.00E+05	12589.25	3162278	6309573	10071.4	10071.4	10071.4	6309573.445	6309573
	std. dev.		10	79.43282	5.011872	8	8	8	5.011872336	5.011872
	distrib.	constant	triangular	triangular	triangular	triangular	triangular	triangular	triangular	triangular

(continued)

Table 17A-2b. (continued)

Chemical	Statistic	Environmental Media Kd Values (L/kg)				Waste Kd Values (L/kg)				
		Organic carbon	Soil	Sediment	Surface Water	LAU	Waste Pile	Landfill	Surface Impoundment	Aerated Tank
Cadmium	min	2.51E+03	1.258925	3.162278	630.9573	1.00714	1.00714	1.00714	630.9573445	630.9573
	mean	1.58E+05	501.1872	1995.262	79432.82	400.9498	400.9498	400.9498	79432.82347	79432.82
	max	3.16E+05	100000	19952623	1995262	80000	80000	80000	1995262.315	1995262
	std. dev.		6.309573	63.09573	3.981072	5.047659	5.047659	5.047659	3.981071706	3.981072
	distrib.	constant	triangular	triangular	triangular	triangular	triangular	triangular	triangular	triangular
Chromium III	min		10	79.43282	7943.282	8	8	8	7943.282347	7943.282
	mean	0	6309.573	79432.82	125892.5	5047.659	5047.659	5047.659	125892.5412	125892.5
	max		50118.72	794328.2	1000000	40094.98	40094.98	40094.98	1000000	1000000
	std. dev.		2.511886	31.62278	2.511886	2.009509	2.009509	2.009509	2.511886432	2.511886
	distrib.	constant	triangular	triangular	triangular	triangular	triangular	triangular	triangular	triangular
Chromium VI	min		0.199526	1	3981.072	0.159621	0.159621	0.159621	3981.071706	3981.072
	mean	0	6.309573	50.11872	15848.93	5.047659	5.047659	5.047659	15848.93192	15848.93
	max		1995.262	25118.86	125892.5	1596.21	1596.21	1596.21	125892.5412	125892.5
	std. dev.		6.309573	25.11886	3.162278	5.047659	5.047659	5.047659	3.16227766	3.162278
	distrib.	constant	triangular	triangular	triangular	triangular	triangular	triangular	triangular	triangular
Divalent mercury	min	1.00E+04	158.4893	6309.573	15848.93	126.7915	126.7915	126.7915	15848.93192	15848.93
	mean	5.00E+04	3981.072	79432.82	199526.2	3184.857	3184.857	3184.857	199526.2315	199526.2
	max	1.00E+05	630957.3	1000000	7943282	504765.9	504765.9	504765.9	7943282.347	7943282
	std. dev.		5.011872	3.981072	2.511886	4.009498	4.009498	4.009498	2.511886432	2.511886
	distrib.	triangular	triangular	triangular	triangular	triangular	triangular	triangular	triangular	triangular

(continued)

Table 17A-2b. (continued)

Chemical	Statistic	Environmental Media Kd Values (L/kg)				Waste Kd Values (L/kg)				
		Organic carbon	Soil	Sediment	Surface Water	LAU	Waste Pile	Landfill	Surface Impoundment	Aerated Tank
Elemental mercury	min	1.00E-03	158.4893	6309.573	15848.93	126.7915	126.7915	126.7915	15848.93192	15848.93
	mean	1.00E-03	3981.072	79432.82	199526.2	3184.857	3184.857	3184.857	199526.2315	199526.2
	max	1.00E+00	630957.3	1000000	7943282	504765.9	504765.9	504765.9	7943282.347	7943282
	std. dev.		3.162278	3.981072	2.511886	2.529822	2.529822	2.529822	2.511886432	2.511886
	distrib.	triangular	triangular	triangular	triangular	triangular	triangular	triangular	triangular	triangular
Lead	min	6.31E+03	5.011872	100	2511.886	4.009498	4.009498	4.009498	2511.886432	2511.886
	mean	1.26E+05	5011.872	39810.72	501187.2	4009.498	4009.498	4009.498	501187.2336	501187.2
	max	3.98E+05	100000	10000000	3162278	80000	80000	80000	3162277.66	3162278
	std. dev.		15.84893	79.43282	2.511886	12.67915	12.67915	12.67915	2.511886432	2.511886
	distrib.	constant	triangular	triangular	triangular	triangular	triangular	triangular	triangular	triangular
Methyl mercury	min	5.00E+04	19.95262	630.9573	15848.93	15.9621	15.9621	15.9621	15848.93192	15848.93
	mean	1.00E+05	501.1872	7943.282	79432.82	400.9498	400.9498	400.9498	79432.82347	79432.82
	max	5.00E+05	63095.73	100000	1584893	50476.59	50476.59	50476.59	1584893.192	1584893
	std. dev.		3.981072	3.162278	5.011872	3.184857	3.184857	3.184857	5.011872336	5.011872
	distrib.	Triangular	triangular	triangular	triangular	triangular	triangular	triangular	triangular	triangular
Nickel (+2)	min	5.01E+04	10	1.995262	3162.278	8	8	8	3162.27766	3162.278
	mean	1.26E+05	794.3282	7943.282	25118.86	635.4626	635.4626	635.4626	25118.86432	25118.86
	max	2.51E+05	6309.573	10000	501187.2	5047.659	5047.659	5047.659	501187.2336	501187.2
	std. dev.		3.981072	63.09573	2.511886	3.184857	3.184857	3.184857	2.511886432	2.511886
	distrib.	constant	triangular	triangular	triangular	triangular	triangular	triangular	triangular	triangular
Selenium (+6)	min		0.501187	10	6309.573	0.40095	0.40095	0.40095	6309.573445	6309.573
	mean	0	19.95262	3981.072	25118.86	15.9621	15.9621	15.9621	25118.86432	25118.86
	max		251.1886	10000	63095.73	200.9509	200.9509	200.9509	63095.73445	63095.73
	std. dev.		2.511886	15.84893	2.511886	2.009509	2.009509	2.009509	2.511886432	2.511886
	distrib.	constant	triangular	triangular	triangular	triangular	triangular	triangular	triangular	triangular

(continued)

Table 17A-2b. (continued)

Chemical	Statistic	Environmental Media Kd Values (L/kg)				Waste Kd Values (L/kg)				
		Organic carbon	Soil	Sediment	Surface Water	LAU	Waste Pile	Landfill	Surface Impoundment	Aerated Tank
Silver	min		10	125.8925	25118.86	8	8	8	25118.86432	25118.86
	mean	0	398.1072	3981.072	158489.3	318.4857	318.4857	318.4857	158489.3192	158489.3
	max		31622.78	630957.3	1995262	25298.22	25298.22	25298.22	1995262.315	1995262
	std. dev.		6.309573	12.58925	3.981072	5.047659	5.047659	5.047659	3.981071706	3.981072
	distrib.	constant	triangular	triangular	triangular	triangular	triangular	triangular	triangular	triangular
Thallium	min		0.063096	0.316228	1000	0.050477	0.050477	0.050477	1000	1000
	mean	0	3.162278	19.95262	12589.25	2.529822	2.529822	2.529822	12589.25412	12589.25
	max		31.62278	3162.278	31622.78	25.29822	25.29822	25.29822	31622.7766	31622.78
	std. dev.		7.943282	12.58925	10	6.354626	6.354626	6.354626	10	10
	distrib.	constant	triangular	triangular	triangular	triangular	triangular	triangular	triangular	triangular
Vanadium	min		3.162278	2.511886	316.2278	2.529822	2.529822	2.529822	316.227766	316.2278
	mean	0	50.11872	125.8925	5011.872	40.09498	40.09498	40.09498	5011.872336	5011.872
	max		316.2278	1584.893	31622.78	252.9822	252.9822	252.9822	31622.7766	31622.78
	std. dev.		31.62278	7.943282	3.981072	25.29822	25.29822	25.29822	3.981071706	3.981072
	distrib.	constant	triangular	triangular	triangular	triangular	triangular	triangular	triangular	triangular
Zinc	min	3.98E+04	0.1	31.62278	3162.278	0.08	0.08	0.08	3162.27766	3162.278
	mean	7.94E+04	501.1872	12589.25	100000	400.9498	400.9498	400.9498	100000	100000
	max	2.51E+06	100000	1584893	7943282	80000	80000	80000	7943282.347	7943282
	std. dev.		10	39.81072	3.162278	8	8	8	3.16227766	3.162278
	distrib.	constant	triangular	triangular	triangular	triangular	triangular	triangular	triangular	triangular

Table 17A-3. Aerobic Biodegradation Rates (AerBio.csv)

Name	Aerobic biodegradation rate (1/day)			Distribution type	Reaction product
	min	central	max.		
Acetone	0	0.035	1.2	Uniform	
Benzene	0	0.096	3.3	Uniform	
Benzo(a)anthracene	0.000096	0.0035	0.072	Uniform	
Benzo(a)pyrene	0	0.0027	0.057	Uniform	
Bis(2-ethylhexy)phthalate	0	0.0205	0.23	Uniform	
Chrysene	0	0.003	0.037	Uniform	
m-Cresol	0.0035	0.133	1.16	Uniform	
o-Cresol	0.069	0.4	4.61	Uniform	
p-Cresol	0.079	1.75	13.15	Uniform	
Dichloromethane	0.00362	0.0546	0.533	Uniform	
Ethylbenzene	0.003	0.113	4.8	Uniform	
Fluoranthene	0	0.0048	0.045	Uniform	
Fluorene	0.0018	0.015	0.33	Uniform	
Methanol	0	0.118	0.693	Uniform	
Methyl ethyl ketone	0.4	0.69	1.4	Uniform	
Naphthalene	0	0.308	5	Uniform	
Phenol	0.024	0.21	11	Uniform	
Pyrene	0	0.00345	0.052	Uniform	
Tetrachloroethylene	0	0	0.139	Uniform	
Toluene	0	0.2	42.5	Uniform	
m-Xylene	0	0.057	0.76	Uniform	
o-Xylene	0	0.054	7.625	Uniform	
p-Xylene	0	0.052	0.56	Uniform	
Divalent Mercury	1.00E-05	5.00E-04	5.00E-03	Triangular	Methyl Mercury
Methyl Mercury	1.00E-04	5.00E-03	5.00E-02	Triangular	Divalent Mercury

Table 17A-4. Anaerobic Biodegradation Rates (AnaBio.csv)

Chemical	Anaerobic Biodegradation Rate (k_bio, 1/day)[1]				Distribution Type	Reaction Product
	minimum	mean	maximum	std. dev.		
Acenaphthalene	0.0043	0.0043	0.0043		Constant	
Benzene	0	0	0.071	0.0152	Uniform	
1,1'-Biphenyl	0	0.00016	0.019	0.00944	Uniform	
Carbon tetrachloride	0	0.16343	1.73	0.572	Uniform	
Chloroform	0.004	0.0315	0.25	0.0884	Uniform	
m-Cresol	0.0029	0.029	0.033	0.0138	Uniform	
o-Cresol	0	0.005	0.034	0.0172	Uniform	
p-Cresol	0.035	0.037	0.048	0.007	Uniform	
Cumene	0	0	0		Constant	
Dichlorodifluoromethane (CFC-12)	0	0	0		Constant	
1,2-Dichloroethane	0.0076	0.0076	0.0076		Constant	
Dichloromethane	0.0064	0.0064	0.0064		Constant	
2,4-Dichlorophenol	0	0.016	0.12	0.0501	Uniform	
Dioxane	0	0	0		Constant	
Ethylbenzene	0	0.0031	0.46	0.0762	Uniform	
Fluorene	0	0.00015	0.00145	0.00069	Uniform	
Methanol	0	0.036	0.34	0.0697	Uniform	
1-Methylnaphthalene	0	0	0.057	0.0214	Uniform	
Naphthalene	0	0	0.03	0.00791	Uniform	
Nitrobenzene	0.0037	0.0037	0.1168	0.0427	Uniform	
Pentachlorophenol	0	0	0	0	Constant	
Phenol	0	0.032	0.2	0.0651	Uniform	
Pyridine	0	0.01	0.02	0.0102	Uniform	
Styrene	0	0	0		Constant	
Tetrachloroethylene	0	0.00186	0.071	0.0223	Uniform	
Toluene	0	0.02	0.186	0.0372	Uniform	
1,1,2-Trichloro-1,2,2-trifluoroethane (CFC-113)	0	0	0		Constant	
1,1,1-Trichloroethane	0	0.00355	0.041	0.013	Uniform	

(continued)

Table 17A-4. (continued)

Chemical	Anaerobic Biodegradation Rate (k_bio, 1/day)[1]				Distribution Type	Reaction Product
	minimum	mean	maximum	std. dev.		
Trichloroethylene	0.00082	0.0016	0.04	0.00889	Uniform	
Trichloroflouromethane (CFC-11)	0.0016	0.0016	0.0016		Constant	
1,3,5-Trimethylbenzene	0	0	0.0039	0.00174	Uniform	
Vinyl Chloride	0	0.00405	0.0582	0.0139	Uniform	
m-Xylene	0	0.006	0.32	0.0675	Uniform	
o-Xylene	0	0.004	0.21	0.0468	Uniform	
p-Xylene	0	0.0052	0.17	0.0367	Uniform	
Divalent mercury	1.00E-05	1.00E-04	1.00E-03		Triangular	Methyl mercury
Methyl mercury	5.00E-05	5.00E-04	5.00E-03		Triangular	Divalent mercury

[1] Same rates for all pH and temperature regimes

Table 17A-5. Anaerobic Biodegradation Rates, Reducing Conditions (AnaRed.csv)

Chemical	Anaerobic biodegradation rate (k_bio, 1/d)				Degradation Product
	minimum	mean	maximum	distribution type	
Divalent mercury	5.00E-03	1.00E-02	1.00E-01	triangular	Elemental mercury
Methyl mercury	1.00E-05	1.00E-03	1.00E-02	triangular	Elemental mercury
Elemental mercury	1.00E-05	1.00E-03	1.00E-02	triangular	Divalent mercury

Table 17A-6a. Anaerobic Biodegradation Rates: Methanogenic Conditions (MethBio.csv)
[statistical distributions, all pH and temperature regimes]

Chemical	Distribution type	Anaerobic biodegradation rate (k_bio, 1/d)			
		minimum	mean	maximum	std. dev.
Acenaphthalene	Constant	0.0043	0.0043	0.0043	
1,1'-Biphenyl	Uniform	0	0.00016	0.019	0.00944
Carbon tetrachloride	Uniform	0	0.16343	1.73	0.572
m-Cresol	Uniform	0.0029	0.029	0.033	0.0138
o-Cresol	Uniform	0	0.005	0.034	0.0172
p-Cresol	Uniform	0.035	0.037	0.048	0.007
Cumene	Constant	0	0	0	
Dichlorodifluoromethane (CFC-12)	Constant	0	0	0	
1,2-Dichloroethane	Constant	0.0076	0.0076	0.0076	
2,4-Dichlorophenol	Uniform	0	0.016	0.12	0.0501
Dioxane	Constant	0	0	0	
Ethylbenzene	Uniform	0	0.0031	0.46	0.0762
Fluorene	Uniform	0	0.00015	0.00145	0.00069
Methanol	Uniform	0	0.036	0.34	0.0697
1-Methylnaphthalene	Uniform	0	0	0.057	0.0214
Naphthalene	Uniform	0	0	0.03	0.00791
Styrene	Constant	0	0	0	
1,1,2-Trichloro-1,2,2-trifluoroethane (CFC-113)	Constant	0	0	0	
Trichloroflouromethane (CFC-11)	Constant	0.0016	0.0016	0.0016	
1,3,5-Trimethylbenzene	Uniform	0	0	0.0039	0.00174
m-Xylene	Uniform	0	0.006	0.32	0.0675
o-Xylene	Uniform	0	0.004	0.21	0.0468
p-Xylene	Uniform	0	0.0052	0.17	0.0367

Table 17A-6b. Anaerobic Biodegradation Rates: Methanogenic Conditions (MethBio.csv)
[empirical distributions, by pH and temperature regime]

Chemical	Anaerobic biodegradation rate (k_bio, 1/d)													
	min.	mean	max.	std. dev.	p5	p6	p7	p8	p9	p10	p11	p12	p13	p14
T<15, pH<6														
Benzene	0	0												
Toluene	0.043	0												
Tetrachloroethylene		0												
1,1,1-Trichloroethane		0.011												
Trichloroethylene		0												
Nitrobenzene		0.0037												
Pentachlorophenol	1.41E-03	1.98E-03												
T<15, 6<=pH<=8														
Benzene	0	0	0	0	0	0	0.000108	0.0015	0.002	0.00714	0.017	0.031	0.052	0.071
Toluene	0	0	0	0.042	0.042	0.043	0.0532	0.093	0.1	0.186				
Tetrachloroethylene	0	0	0.000735	0.0109	0.071									
1,1,1-Trichloroethane	0	0.0013	0.0037	0.0375	0.041									
Trichloroethylene	0	0	0	0.00062	0.0023	0.0034								
Nitrobenzene														
Pentachlorophenol		1.97E-03						4.94E-03				0	5.09E-03	0
Phenol		0						0.13				0.57	0.1	
Pyridine												0.01		
Dichloromethane		0.0064												
Vinyl Chloride	0.00093	0.00297												

(continued)

Table 17A-6b. (continued)

Chemical	Anaerobic biodegradation rate (k_bio, 1/d)													
	min.	mean	max.	std. dev.	p5	p6	p7	p8	p9	p10	p11	p12	p13	p14
T<15, pH>8														
Pentachlorophenol		5.75E-03												
Vinyl chloride	0													
T>=15, pH<6														
Trichloroethylene		0												
T>=15, 6<=pH<=8														
Benzene	0	0	0	0	0	0.005	0.0074							
Toluene	0	0	0	0.003	0.0098	0.0115	0.018	0.028	0.032	0.034				
Tetrachloroethylene	0.0084	0.003												
1,1,1-Trichloroethane		0.0092												
Trichloroethylene	0.039	0.016	0.013											

Table 17A-7. Anaerobic Biodegradation Rates - Sulfate Reducing Conditions (SO4Bio.csv)

Chemical	Distribution type	Anaerobic biodegradation rates (k_bio, 1/d)				p5	p6	p7	p8
		minimum	mean	maximum	std. dev.				
All pH and Temperature conditions									
Acenaphthalene	Constant	0.0043	0.0043	0.0043					
1,1'-Biphenyl	Uniform	0	0.00016	0.019	0.00944				
Carbon Tetrachloride	Uniform	0	0.16343	1.73	0.572				
m-Cresol	Uniform	0.0029	0.029	0.033	0.0138				
o-Cresol	Uniform	0	0.005	0.034	0.0172				
p-Cresol	Uniform	0.035	0.037	0.048	0.007				
Cumene	Constant	0	0	0					
Dichlorodifluoromethane (CFC-12)	Constant	0	0	0					
1,2-Dichloroethane	Constant	0.0076	0.0076	0.0076					
2,4-Dichlorophenol	Uniform	0	0.016	0.12	0.0501				
Dioxane	Constant	0	0	0					
Ethylbenzene	Uniform	0	0.0031	0.46	0.0762				
Fluorene	Uniform	0	0.00015	0.00145	0.00069				
Methanol	Uniform	0	0.036	0.34	0.0697				
1-Methylnaphthalene	Uniform	0	0	0.057	0.0214				
Naphthalene	Uniform	0	0	0.03	0.00791				
Styrene	Constant	0	0	0					
1,1,2-Trichloro-1,2,2-trifluoroethane (CFC-113)	Constant	0	0	0					

(continued)

Table 17A-7. (continued)

Chemical	Distribution type	Anaerobic biodegradation rates (k_bio, 1/d)				p5	p6	p7	p8
		minimum	mean	maximum	std. dev.				
Trichloroflouromethane (CFC-11)	Constant	0.0016	0.0016	0.0016					
1,3,5-Trimethylbenzene	Uniform	0	0	0.0039	0.00174				
m-Xylene	Uniform	0	0.006	0.32	0.0675				
o-Xylene	Uniform	0	0.004	0.21	0.0468				
p-Xylene	Uniform	0	0.0052	0.17	0.0367				
T<15, pH<6									
Benzene	Demp		0						
Phenol	Demp		0.2						
Toluene	Demp		0						
T<15 6<=pH<=8									
Benzene	Demp	0	0	0.00134	0.0029	0.0041	0.0063	0.0065	0.047
NitroBenzene	Demp		0.00263						
Phenol	Demp	0	0.0135						
Tetrachloroethylene	Demp	0	0.00405						
Toluene	Demp	0.0045	0.0024	0.01	0.016	0.019	0.066	0.083	0.087
1,1,1-Trichloroethane	Demp	0	0	0.01					
Trichloroethylene	Demp	0.00086	0.00074	0.0013	0.00231	0.0033	0.0036	0.01	0.014
Vinyl Chloride	Demp		0.0008						

(continued)

Table 17A-7. (continued)

Chemical	Distribution type	Anaerobic biodegradation rates (k_bio, 1/d)				p5	p6	p7	p8
		minimum	mean	maximum	std. dev.				
T>=15, pH<6									
Benzene	Demp		0						
Chloroform	Demp		0.01562						
Pentachlorophenol	Demp		0						
Tetrachloroethylene	Demp		0.00073						
Toluene	Demp		0.0086						
Trichloroethylene	Demp	0	0.0011						
T>=15, 6<=pH<=8									
Benzene	Demp	0	0.003	0.0041	0.0237	0.0308			
Chloroform	Demp	0.03	0.142						
Pyridine	Demp		0.014						
Tetrachloroethylene	Demp	0.0065	0.054						
Toluene	Demp	0.011	0.018	0.027	0.0446	0.045	0.091	0.11	
1,1,1-Trichloroethane	Demp	0.003	0.0092	0.0099					
Trichloroethylene	Demp	0.00069	0.0015	0.00153	0.0029	0.003	0.009	0.01	
Vinyl Chloride	Demp	0.0069	0.0082						

Demp = empirical distribution

Table 17A-8. Catalyzed Hydrolysis Rates (CAT.csv)

Chemical	Hydrolysis rate	Reaction Products		
		1	2	3
Acid Hydrolysis Rates (k_HA, L/mole-day)				
Acrylonitrile	1.368925394	Acrylamide		
Neutral Hydrolysis Rates (k_HN, 1/day)				
Chloroform	0.000000274	Carbon monoxide	Hydrochloric acid	
Ethylene dibromide	0.001724846	Hydrobromic acid	Vinyl bromide	2-Bromoethanol
Methoxychlor	0.001889117	2,2-Bis(p-methoxyphenyl)-1,1-dichloroethylene	Anisoin	Hydrochloric acid
Methylene chloride	0.00000274	Formaldehyde	Hydrochloric acid	
Thiram	0.119917864	--		
1,1,1-Trichloroethane	0.001752225	1,1-Dichloroethylene	Acetic acid	Hydrochloric acid
Base Hydrolysis Rates (k_HB, L/mole-day)				
Acetonitrile	0.123203285	Acetamide		
Acrylonitrile	14.23682409	Acrylamide		
Bis-(2-ethylhexyl) phthalate	3.832991102	2-Ethylhexanol	2-Ethylhexyl hydrogen phthalate	
Carbon disulfide	86.24229979	Carbonyl sulfide		
Chloroform	7.501711157	Carbon monoxide	Hydrochloric acid	
Methoxychlor	32.85420945	2,2-Bis(p-methoxyphenyl)-1,1-dichloroethylene	Anisoin	Hydrochloric acid
Methyl methacrylate	5201.916496	Methacrylic acid	Methanol	
Methylene chloride	0.00164271	Formaldehyde	Hydrochloric acid	
Thiram	99657.76865	--		
1,1,1-Trichloroethane	6570.841889	1,1-Dichloroethylene	Acetic acid	Hydrochloric acid