Part 5: CHEMICAL-SPECIFIC PARAMETERS

Chemical-specific parameters required for calculating soil screening levels include the organic carbon normalized soil-water partition coefficient for organic compounds (K_{oc}), the soil-water partition coefficient for inorganic constituents (K_d), water solubility (S), Henry's law constant (HLC, H'), air diffusivity ($D_{i,a}$), and water diffusivity ($D_{i,w}$). In addition, the octanol-water partition coefficient (K_{ow}) is needed to calculate K_{oc} values. This part of the background document describes the collection and compilation of these parameters for the SSL chemicals.

With the exception of values for air diffusivity ($D_{i,a}$), water diffusivity ($D_{i,w}$), and certain K_{oc} values, all of the values used in the development of SSLs can be found in the Superfund Chemical Data Matrix (SCDM). SCDM is a computer code that includes more than 25 datafiles containing specific chemical parameters used to calculate factor and benchmark values for the Hazard Ranking System (HRS). Because SCDM datafiles are regularly updated, the user should consult the most recent version of SCDM to ensure that the values are up to date.

5.1 Solubility, Henry's Law Constant, and K_{ow}

Chemical-specific values for solubility, Henry's law constant (HLC), and K_{ow} were obtained from SCDM. In the selection of the value for SCDM, measured or analytical values are favored over calculated values. However, in the event that a measured value is not available, calculated values are used. Table 36 presents the solubility, Henry's law constant, and K_{ow} values taken from SCDM and used to calculate SSLs.

Henry's law constant values were available for all but two of the constituents of interest. Henry's law constants could not be obtained from the SCDM datafiles for either carbazole or mercury. As a consequence, this parameter was calculated according to the following equation:

$$HLC = (VP)(M)/(S) \tag{68}$$

where

HLC = Henry's law constant (atm-m^3/mol)
VP = vapor pressure (atm)
M = molecular weight (g/mol)
S = solubility (mg/L or g/m^3).

The SSL equations require the dimensionless form of Henry's law constant, or H', which is calculated from HLC (atm-m^3/mol) by multiplying by 41 (U.S. EPA, 1991b). The values taken from SCDM for HLC and the calculated dimensionless values for H' are both presented in Table 36.

5.2 Air ($D_{i,a}$) and Water ($D_{i,w}$) Diffusivities

Few published diffusivities were available for the subject chemicals for air ($D_{i,a}$) and water ($D_{i,w}$). Water and air diffusivities were obtained from the CHEMDAT8 model chemical properties database (DATATWO.WK1). For chemicals not in CHEMDAT8, diffusivities were estimated using the

WATER8 model correlations for air and water diffusivities. Both CHEMDAT8 and WATER8 can be obtained from EPA's SCRAM bulletin board system, as described in Section 3.1.2. Table 37 presents the values used to calculate SSLs.

Table 36. Chemical-Specific Properties Used in SSL Calculations

CAS No.	Compound	S (mg/L)	HLC (atm-m^3/mol)	H' (dimensionless)	log K_{ow}
83-32-9	Acenaphthene	4.24E+00	1.55E-04	6.36E-03	3.92
67-64-1	Acetone	1.00E+06	3.88E-05	1.59E-03	-0.24
309-00-2	Aldrin	1.80E-01	1.70E-04	6.97E-03	6.50
120-12-7	Anthracene	4.34E-02	6.50E-05	2.67E-03	4.55
56-55-3	Benz(*a*)anthracene	9.40E-03	3.35E-06	1.37E-04	5.70
71-43-2	Benzene	1.75E+03	5.55E-03	2.28E-01	2.13
205-99-2	Benzo(*b*)fluoranthene	1.50E-03	1.11E-04	4.55E-03	6.20
207-08-9	Benzo(*k*)fluoranthene	8.00E-04	8.29E-07	3.40E-05	6.20
65-85-0	Benzoic acid	3.50E+03	1.54E-06	6.31E-05	1.86
50-32-8	Benzo(*a*)pyrene	1.62E-03	1.13E-06	4.63E-05	6.11
111-44-4	Bis(2-chloroethyl)ether	1.72E+04	1.80E-05	7.38E-04	1.21
117-81-7	Bis(2-ethylhexyl)phthalate	3.40E-01	1.02E-07	4.18E-06	7.30
75-27-4	Bromodichloromethane	6.74E+03	1.60E-03	6.56E-02	2.10
75-25-2	Bromoform	3.10E+03	5.35E-04	2.19E-02	2.35
71-36-3	Butanol	7.40E+04	8.81E-06	3.61E-04	0.85
85-68-7	Butyl benzyl phthalate	2.69E+00	1.26E-06	5.17E-05	4.84
86-74-8	Carbazole	7.48E+00	1.53E-08 [a]	6.26E-07	3.59
75-15-0	Carbon disulfide	1.19E+03	3.03E-02	1.24E+00	2.00
56-23-5	Carbon tetrachloride	7.93E+02	3.04E-02	1.25E+00	2.73
57-74-9	Chlordane	5.60E-02	4.86E-05	1.99E-03	6.32
106-47-8	*p*-Chloroaniline	5.30E+03	3.31E-07	1.36E-05	1.85
108-90-7	Chlorobenzene	4.72E+02	3.70E-03	1.52E-01	2.86
124-48-1	Chlorodibromomethane	2.60E+03	7.83E-04	3.21E-02	2.17
67-66-3	Chloroform	7.92E+03	3.67E-03	1.50E-01	1.92
95-57-8	2-Chlorophenol	2.20E+04	3.91E-04	1.60E-02	2.15
218-01-9	Chrysene	1.60E-03	9.46E-05	3.88E-03	5.70
72-54-8	DDD	9.00E-02	4.00E-06	1.64E-04	6.10
72-55-9	DDE	1.20E-01	2.10E-05	8.61E-04	6.76
50-29-3	DDT	2.50E-02	8.10E-06	3.32E-04	6.53
53-70-3	Dibenz(*a,h*)anthracene	2.49E-03	1.47E-08	6.03E-07	6.69
84-74-2	Di-*n*-butyl phthalate	1.12E+01	9.38E-10	3.85E-08	4.61
95-50-1	1,2-Dichlorobenzene	1.56E+02	1.90E-03	7.79E-02	3.43
106-46-7	1,4-Dichlorobenzene	7.38E+01	2.43E-03	9.96E-02	3.42
91-94-1	3,3-Dichlorobenzidine	3.11E+00	4.00E-09	1.64E-07	3.51
75-34-3	1,1-Dichloroethane	5.06E+03	5.62E-03	2.30E-01	1.79

Table 36 (continued)

CAS No.	Compound	S (mg/L)	HLC (atm-m^3/mol)	H' (dimensionless)	log K_{ow}
107-06-2	1,2-Dichloroethane	8.52E+03	9.79E-04	4.01E-02	1.47
75-35-4	1,1-Dichloroethylene	2.25E+03	2.61E-02	1.07E+00	2.13
156-59-2	*cis*-1,2-Dichloroethylene	3.50E+03	4.08E-03	1.67E-01	1.86
156-60-5	*trans*-1,2-Dichloroethylene	6.30E+03	9.38E-03	3.85E-01	2.07
120-83-2	2,4-Dichlorophenol	4.50E+03	3.16E-06	1.30E-04	3.08
78-87-5	1,2-Dichloropropane	2.80E+03	2.80E-03	1.15E-01	1.97
542-75-6	1,3-Dichloropropene	2.80E+03	1.77E-02	7.26E-01	2.00
60-57-1	Dieldrin	1.95E-01	1.51E-05	6.19E-04	5.37
84-66-2	Diethylphthalate	1.08E+03	4.50E-07	1.85E-05	2.50
105-67-9	2,4-Dimethylphenol	7.87E+03	2.00E-06	8.20E-05	2.36
51-28-5	2,4-Dinitrophenol	2.79E+03	4.43E-07	1.82E-05	1.55
121-14-2	2,4-Dinitrotoluene	2.70E+02	9.26E-08	3.80E-06	2.01
606-20-2	2,6-Dinitrotoluene	1.82E+02	7.47E-07	3.06E-05	1.87
117-84-0	Di-*n*-octyl phthalate	2.00E-02	6.68E-05	2.74E-03	8.06
115-29-7	Endosulfan	5.10E-01	1.12E-05	4.59E-04	4.10
72-20-8	Endrin	2.50E-01	7.52E-06	3.08E-04	5.06
100-41-4	Ethylbenzene	1.69E+02	7.88E-03	3.23E-01	3.14
206-44-0	Fluoranthene	2.06E-01	1.61E-05	6.60E-04	5.12
86-73-7	Fluorene	1.98E+00	6.36E-05	2.61E-03	4.21
76-44-8	Heptachlor	1.80E-01	1.09E-03	4.47E-02	6.26
1024-57-3	Heptachlor epoxide	2.00E-01	9.50E-06	3.90E-04	5.00
118-74-1	Hexachlorobenzene	6.20E+00	1.32E-03	5.41E-02	5.89
87-68-3	Hexachloro-1,3-butadiene	3.23E+00	8.15E-03	3.34E-01	4.81
319-84-6	α-HCH (α-BHC)	2.00E+00	1.06E-05	4.35E-04	3.80
319-85-7	β-HCH (β-BHC)	2.40E-01	7.43E-07	3.05E-05	3.81
58-89-9	γ-HCH (Lindane)	6.80E+00	1.40E-05	5.74E-04	3.73
77-47-4	Hexachlorocyclopentadiene	1.80E+00	2.70E-02	1.11E+00	5.39
67-72-1	Hexachloroethane	5.00E+01	3.89E-03	1.59E-01	4.00
193-39-5	Indeno(1,2,3-*cd*)pyrene	2.20E-05	1.60E-06	6.56E-05	6.65
78-59-1	Isophorone	1.20E+04	6.64E-06	2.72E-04	1.70
7439-97-6	Mercury	---	1.14E-02[b]	4.67E-01	---
72-43-5	Methoxychlor	4.50E-02	1.58E-05	6.48E-04	5.08
74-83-9	Methyl bromide	1.52E+04	6.24E-03	2.56E-01	1.19
75-09-2	Methylene chloride	1.30E+04	2.19E-03	8.98E-02	1.25
95-48-7	2-Methylphenol	2.60E+04	1.20E-06	4.92E-05	1.99
91-20-3	Naphthalene	3.10E+01	4.83E-04	1.98E-02	3.36
98-95-3	Nitrobenzene	2.09E+03	2.40E-05	9.84E-04	1.84
86-30-6	*N*-Nitrosodiphenylamine	3.51E+01	5.00E-06	2.05E-04	3.16
621-64-7	*N*-Nitrosodi-*n*-propylamine	9.89E+03	2.25E-06	9.23E-05	1.40

Table 36 (continued)

CAS No.	Compound	S (mg/L)	HLC (atm-m^3/mol)	H′ (dimensionless)	log K_{ow}
87-86-5	Pentachlorophenol	1.95E+03	2.44E-08	1.00E-06	5.09
108-95-2	Phenol	8.28E+04	3.97E-07	1.63E-05	1.48
129-00-0	Pyrene	1.35E-01	1.10E-05	4.51E-04	5.11
100-42-5	Styrene	3.10E+02	2.75E-03	1.13E-01	2.94
79-34-5	1,1,2,2-Tetrachloroethane	2.97E+03	3.45E-04	1.41E-02	2.39
127-18-4	Tetrachloroethylene	2.00E+02	1.84E-02	7.54E-01	2.67
108-88-3	Toluene	5.26E+02	6.64E-03	2.72E-01	2.75
8001-35-2	Toxaphene	7.40E-01	6.00E-06	2.46E-04	5.50
120-82-1	1,2,4-Trichlorobenzene	3.00E+02	1.42E-03	5.82E-02	4.01
71-55-6	1,1,1-Trichloroethane	1.33E+03	1.72E-02	7.05E-01	2.48
79-00-5	1,1,2-Trichloroethane	4.42E+03	9.13E-04	3.74E-02	2.05
79-01-6	Trichloroethylene	1.10E+03	1.03E-02	4.22E-01	2.71
95-95-4	2,4,5-Trichlorophenol	1.20E+03	4.33E-06	1.78E-04	3.90
88-06-2	2,4,6-Trichlorophenol	8.00E+02	7.79E-06	3.19E-04	3.70
108-05-4	Vinyl acetate	2.00E+04	5.11E-04	2.10E-02	0.73
75-01-4	Vinyl chloride	2.76E+03	2.70E-02	1.11E+00	1.50
108-38-3	*m*-Xylene	1.61E+02	7.34E-03	3.01E-01	3.20
95-47-6	*o*-Xylene	1.78E+02	5.19E-03	2.13E-01	3.13
106-42-3	*p*-Xylene	1.85E+02	7.66E-03	3.14E-01	3.17

CAS = Chemical Abstracts Service.
S = Solubility in water (20-25 °C).
HLC = Henry's law constant.
H′ = Dimensionless Henry's law constant (HLC [atm-m^3/mol] * 41) (25 °C).
K_{ow} = Octanol/water partition coefficient.

[a] HLC was calculated using the equation: HLC = vapor pressure * molecular wt. / solubility. Vapor pressure is 6.83E-10 atm and molecular weight is 167.21 g/mol for carbazole.

[b] Value from WATER8 model database.

Table 37. Air Diffusivity ($D_{i,a}$) and Water Diffusivity ($D_{i,w}$) Values for SSL Chemicals (25°C)[a]

CAS No.	Compound	$D_{i,a}$ (cm^2/s)	$D_{i,w}$ (cm^2/s)
83-32-9	Acenaphthene	4.21E-02	7.69E-06
67-64-1	Acetone	1.24E-01	1.14E-05
309-00-2	Aldrin	1.32E-02	4.86E-06
120-12-7	Anthracene	3.24E-02	7.74E-06
56-55-3	Benz(*a*)anthracene	5.10E-02	9.00E-06
71-43-2	Benzene	8.80E-02	9.80E-06
205-99-2	Benzo(*b*)fluoranthene	2.26E-02	5.56E-06
207-08-9	Benzo(*k*)fluoranthene	2.26E-02	5.56E-06
65-85-0	Benzoic acid	5.36E-02	7.97E-06
50-32-8	Benzo(*a*)pyrene	4.30E-02	9.00E-06
111-44-4	Bis(2-chloroethyl)ether	6.92E-02	7.53E-06
117-81-7	Bis(2-ethylhexyl)phthalate	3.51E-02	3.66E-06
75-27-4	Bromodichloromethane	2.98E-02	1.06E-05
75-25-2	Bromoform	1.49E-02	1.03E-05
71-36-3	Butanol	8.00E-02	9.30E-06
85-68-7	Butyl benzyl phthalate	1.74E-02 [b]	4.83E-06 [b]
86-74-8	Carbazole	3.90E-02 [b]	7.03E-06 [b]
75-15-0	Carbon disulfide	1.04E-01	1.00E-05
56-23-5	Carbon tetrachloride	7.80E-02	8.80E-06
57-74-9	Chlordane	1.18E-02	4.37E-06
106-47-8	*p*-Chloroaniline	4.83E-02	1.01E-05
108-90-7	Chlorobenzene	7.30E-02	8.70E-06
124-48-1	Chlorodibromomethane	1.96E-02	1.05E-05
67-66-3	Chloroform	1.04E-01	1.00E-05
95-57-8	2-Chlorophenol	5.01E-02	9.46E-06
218-01-9	Chrysene	2.48E-02	6.21E-06
72-54-8	DDD	1.69E-02 [b]	4.76E-06 [b]
72-55-9	DDE	1.44E-02	5.87E-06
50-29-3	DDT	1.37E-02	4.95E-06
53-70-3	Dibenz(*a,h*)anthracene	2.02E-02 [b]	5.18E-06 [b]
84-74-2	Di-*n*-butyl phthalate	4.38E-02	7.86E-06
95-50-1	1,2-Dichlorobenzene	6.90E-02	7.90E-06
106-46-7	1,4-Dichlorobenzene	6.90E-02	7.90E-06
91-94-1	3,3-Dichlorobenzidine	1.94E-02	6.74E-06
75-34-3	1,1-Dichloroethane	7.42E-02	1.05E-05
107-06-2	1,2-Dichloroethane	1.04E-01	9.90E-06
75-35-4	1,1-Dichloroethylene	9.00E-02	1.04E-05
156-59-2	*cis*-1,2-Dichloroethylene	7.36E-02	1.13E-05
156-60-5	*trans*-1,2-Dichloroethylene	7.07E-02	1.19E-05
120-83-2	2,4-Dichlorophenol	3.46E-02	8.77E-06

Table 37 (continued)

CAS No.	Compound	$D_{i,a}$ (cm^2/s)	$D_{i,w}$ (cm^2/s)
78-87-5	1,2-Dichloropropane	7.82E-02	8.73E-06
542-75-6	1,3-Dichloropropene	6.26E-02	1.00E-05
60-57-1	Dieldrin	1.25E-02	4.74E-06
84-66-2	Diethylphthalate	2.56E-02 [b]	6.35E-06 [b]
105-67-9	2,4-Dimethylphenol	5.84E-02	8.69E-06
51-28-5	2,4-Dinitrophenol	2.73E-02	9.06E-06
121-14-2	2,4-Dinitrotoluene	2.03E-01	7.06E-06
606-20-2	2,6-Dinitrotoluene	3.27E-02	7.26E-06
117-84-0	Di-*n*-octyl phthalate	1.51E-02	3.58E-06
115-29-7	Endosulfan	1.15E-02	4.55E-06
72-20-8	Endrin	1.25E-02	4.74E-06
100-41-4	Ethylbenzene	7.50E-02	7.80E-06
206-44-0	Fluoranthene	3.02E-02	6.35E-06
86-73-7	Fluorene	3.63E-02 [b]	7.88E-06 [b]
76-44-8	Heptachlor	1.12E-02	5.69E-06
1024-57-3	Heptachlor epoxide	1.32E-02 [b]	4.23E-06 [b]
118-74-1	Hexachlorobenzene	5.42E-02	5.91E-06
87-68-3	Hexachloro-1,3-butadiene	5.61E-02	6.16E-06
319-84-6	α-HCH (α-BHC)	1.42E-02	7.34E-06
319-85-7	β-HCH (β-BHC)	1.42E-02	7.34E-06
58-89-9	γ-HCH (Lindane)	1.42E-02	7.34E-06
77-47-4	Hexachlorocyclopentadiene	1.61E-02	7.21E-06
67-72-1	Hexachloroethane	2.50E-03	6.80E-06
193-39-5	Indeno(1,2,3-*cd*)pyrene	1.90E-02	5.66E-06
78-59-1	Isophorone	6.23E-02	6.76E-06
7439-97-6	Mercury	3.07E-02 [b]	6.30E-06 [b]
72-43-5	Methoxychlor	1.56E-02	4.46E-06
74-83-9	Methyl bromide	7.28E-02	1.21E-05
75-09-2	Methylene chloride	1.01E-01	1.17E-05
95-48-7	2-Methylphenol	7.40E-02	8.30E-06
91-20-3	Naphthalene	5.90E-02	7.50E-06
98-95-3	Nitrobenzene	7.60E-02	8.60E-06
86-30-6	*N*-Nitrosodiphenylamine	3.12E-02 [b]	6.35E-06 [b]
621-64-7	*N*-Nitrosodi-*n*-propylamine	5.45E-02 [b]	8.17E-06 [b]
87-86-5	Pentachlorophenol	5.60E-02	6.10E-06
108-95-2	Phenol	8.20E-02	9.10E-06
129-00-0	Pyrene	2.72E-02 [b]	7.24E-06 [b]
100-42-5	Styrene	7.10E-02	8.00E-06
79-34-5	1,1,2,2-Tetrachloroethane	7.10E-02	7.90E-06
127-18-4	Tetrachloroethylene	7.20E-02	8.20E-06

Table 37 (continued)

CAS No.	Compound	$D_{i,a}$ (cm^2/s)	$D_{i,w}$ (cm^2/s)
108-88-3	Toluene	8.70E-02	8.60E-06
8001-35-2	Toxaphene	1.16E-02	4.34E-06
120-82-1	1,2,4-Trichlorobenzene	3.00E-02	8.23E-06
71-55-6	1,1,1-Trichloroethane	7.80E-02	8.80E-06
79-00-5	1,1,2-Trichloroethane	7.80E-02	8.80E-06
79-01-6	Trichloroethylene	7.90E-02	9.10E-06
95-95-4	2,4,5-Trichlorophenol	2.91E-02	7.03E-06
88-06-2	2,4,6-Trichlorophenol	3.18E-02	6.25E-06
108-05-4	Vinyl acetate	8.50E-02	9.20E-06
75-01-4	Vinyl chloride	1.06E-01	1.23E-06
108-38-3	*m*-Xylene	7.00E-02	7.80E-06
95-47-6	*o*-Xylene	8.70E-02	1.00E-05
106-42-3	*p*-Xylene	7.69E-02	8.44E-06

CAS = Chemical Abstracts Service.

[a] Value from CHEMDAT8 model database unless indicated otherwise.

[b] Estimated using correlations in WATER8 model.

5.3 Soil Organic Carbon/Water Partition Coefficients (K_{oc})

Application of SSLs for the inhalation and migration to ground water pathways requires K_{oc} values for each organic chemical of concern. K_{oc} values are also needed for site-specific exposure modeling efforts. An initial review of the literature uncovered significant variability in this parameter, with reported measured values for a compound sometimes varying over several orders of magnitude. This variability can be attributed to several factors, including actual variability due to differences in soil or sediment properties, differences in experimental and analytical approaches used to measure the values, and experimental or measurement error. To resolve this difficulty, an extensive literature review was conducted to uncover all available measured values and to identify approaches and information that might be useful in developing valid K_{oc} values.

The soil-water partitioning behavior of nonionizing and ionizing organic compounds differs because the partitioning of ionizing organics can be significantly influenced by soil pH. For this reason, different approaches were required to estimate K_{oc} values for nonionizing and ionizing organic compounds.

5.3.1 K_{oc} for Nonionizing Organic Compounds. As noted earlier, there is significant variability in reported K_{oc} values and an extensive literature search was conducted to collect all available measured K_{oc} values for the nonionizing hydrophobic organic compounds of interest.

In the literature search, misquotation error was minimized by obtaining the original references whenever possible. Values from compilations and secondary references were used only when the original references could not be obtained. Redundancy of values was avoided, although in rare instances it was not possible to determine if compilations included such values, especially when data were reported as "selected" values.

In certain references, soil-water partition coefficients (e.g., K_d or K_p) were reported along with the organic carbon content of the soil. In these cases, K_{oc} was computed by dividing K_d by the fractional soil organic carbon content (f_{oc}, g/g). If the partition coefficient was normalized to soil organic matter (i.e., K_{om}), it was converted to K_{oc} as follows (Dragun, 1988):

$$K_{oc} = 1.724\ K_{om} \tag{69}$$

where

1.724 = conversion factor from organic matter to organic carbon ($f_{om} = 1.724\ f_{oc}$)
K_{om} = partition coefficient normalized to organic matter (L/kg)
f_{om} = fraction organic matter (g/g).

Once collected, K_{oc} values were reviewed. It was not possible to systematically evaluate each source for accuracy or consistency or to analyze sources of variability between references because of wide variations in soil and sediment properties, experimental and analytical methods, and the manner in which these were reported in each reference. This, and the limited number of K_{oc} values for many compounds, prevented any meaningful statistical analysis to eliminate outliers.

Collected values were qualitatively reviewed, however, and some values were excluded. Values measured for low-carbon-content sorbents (i.e., $f_{oc} \leq 0.001$) are generally beyond the range of the linear relationship between soil organic carbon and K_d and were rejected in most cases. Some references produced consistently high or low values and, as a result, were eliminated. Values were also eliminated if they fell outside the range of other measured values. The final values used are presented in Appendix K along with their reference sources.

Summary statistics for the measured K_{oc} values are presented in Table 38. The geometric mean of the K_{oc} for each nonionizing organic compound is used as the the central tendency K_{oc} value because it is a more suitable estimate of the central tendency of a distribution of environmental values with wide variability.

The data contained in Table 38 are summarized in Table 39 for each of the nonionizing organic compounds for which measured K_{oc} values were available. As shown, measured values are available for only a subset of the SSL compounds. As a consequence, an alternative methodology was applied to determine K_{oc} values for the entire set of nonionizing hydrophobic organic compounds of interest.

It has long been noted that a strong linear relationship exists between K_{oc} and K_{ow} (octanol/water partition coefficient) (Lyman et al., 1982) and that this relationship can be used to predict K_{oc} in the absence of measured data. One such relationship was reported by Di Toro (1985). This relationship was selected for use in calculating K_{oc} values for most semivolatile nonionizing organic compounds (Group 1 in Table 39) because it considers particle interaction and was shown to be in conformity with observations for a large set of adsorption-desorption data (Di Toro, 1985). Di Toro's equation is as follows:

$$\log K_{oc} = 0.00028 + (0.983 \times \log K_{ow}) \tag{70}$$

For volatile organic compounds (VOCs), Equation 70 consistently overpredicted K_{oc} values when compared to measured data. For this reason, a separate regression equation was developed using log K_{ow} and measured log K_{oc} values for VOCs, chlorinated benzenes, and certain chlorinated pesticides:

$$\log K_{oc} = 0.0784 + (0.7919 \times \log K_{ow}) \tag{71}$$

Equation 71 was developed from a linear regression calculated at the 95 percent confidence level. The correlation coefficient (r) was 0.99 with an r^2 of 0.97. The compounds and data used to develop this equation are provided in Appendix K. Equation 71 was used to calculate K_{oc} values for VOCs, chlorobenzenes, and certain chlorinated pesticides (i.e., Group 2 in Table 39). Log K_{oc} values calculated using Equations 70 and 71 were rounded to two decimal places, and the resulting K_{oc} values were rounded to two decimal places in scientific notation (i.e, as they appear in Table 39) prior to calculating SSLs.

Table 38. Summary Statistics for Measured K_{oc} Values: Nonionizing Organics[a]

	K_{oc} (L/kg)				
Compound	**Geometric Mean**	**Average**	**Minimum**	**Maximum**	**Sample Size**
Acenaphthene	4,898	5,028	3,890	6,166	2
Aldrin	48,685	48,686	48,394	48,978	2
Anthracene	23,493	24,362	14,500	33,884	9
Benz(*a*)anthracene	357,537	459,882	150,000	840,000	4
Benzene	62	66	31	100	13
Benzo(*a*)pyrene	968,774	1,166,733	478,947	2,130,000	3
Bis(2-chloroethyl)ether	76	76	76	76	1
Bis(2-ethylhexyl)phthalate	111,123	114,337	87,420	141,254	2
Bromoform	126	126	126	126	1
Butyl benzyl phthalate	13,746	14,055	11,128	16,981	2
Carbon tetrachloride	152	158	123	224	3
Chlordane	51,310	51,798	44,711	58,884	2
Chlorobenzene	224	260	83	500	9
Chloroform	53	57	28	81	5
DDD	45,800	45,800	45,800	45,800	1
DDE	86,405	86,405	86,405	86,405	1
DDT	677,934	792,158	285,467	1,741,516	6
Dibenz(a,h)anthracene	1,789,101	2,029,435	565,014	3,059,425	14
1,2-Dichlorobenzene (*o*)	379	390	267	529	9
1,4-Dichlorobenzene (*p*)	616	687	273	1,375	16
1,1-Dichloroethane	53	54	46	62	2
1,2-Dichloroethane	38	44	22	76	3
1,1-Dichloroethylene	65	65	65	65	1

Table 38 (continued)

	K_{oc} (L/kg)				
Compound	**Geometric Mean**	**Average**	**Minimum**	**Maximum**	**Sample Size**
trans-1,2-Dichloroethylene	38	38	38	38	1
1,2-Dichloropropane	47	47	47	47	1
1,3-Dichloropropene	27	27	24	32	3
Dieldrin	25,546	25,604	23,308	27,399	3
Diethylphthalate	82	84	69	98	2
Di-*n*-butylphthalate	1,567	1,580	1,384	1,775	2
Endosulfan	2,040	2,040	2,040	2,040	1
Endrin	10,811	11,422	7,724	15,885	4
Ethylbenzene	204	207	165	255	5
Fluoranthene	49,096	49,433	41,687	54,954	3
Fluorene	7,707	8,906	3,989	16,218	6
Heptachlor	9,528	10,070	6,810	13,330	2
Hexachlorobenzene	80,000	80,000	80,000	80,000	1
α-HCH (α-BHC)	1,762	1,835	1,022	2,891	12
β-HCH (β-BHC)	2,139	2,241	1,156	3,563	14
γ-HCH (Lindane)	1,352	1,477	731	3,249	65
Methoxychlor	80,000	80,000	80,000	80,000	1
Methyl bromide	9	9	9	9	1
Methyl chloride	6	6	6	6	1
Methylene chloride	10	10	10	10	1
Naphthalene	1,191	1,231	830	1,950	20
Nitrobenzene	119	141	31	270	10
Pentachlorobenzene	32,148	36,114	11,381	55,176	5
Pyrene	67,992	70,808	43,807	133,590	27
Styrene	912	912	912	912	1
1,1,2,2-Tetrachloroethane	79	79	79	79	1
Tetrachloroethylene	265	272	177	373	15
Toluene	140	145	94	247	12
Toxaphene	95,816	95,816	95,816	95,816	1
1,2,4-Trichlorobenzene	1,659	1,783	864	3,125	17
1,1,1-Trichloroethane	135	139	106	179	5
1,1,2-Trichloroethane	75	77	60	108	4
Trichloroethylene	94	97	57	150	21
o-Xylene	241	241	222	258	4
m-Xylene	196	204	158	289	3
p-Xylene	311	313	260	347	3

[a] See Appendix K for sources of measured values.

Table 39. Comparison of Measured and Calculated K_{oc} Values

CAS No.	Compound	Chemical Group [a]	Log K_{ow}	Log K_{oc} (L/kg)	Calculated K_{oc} (L/kg)	Measured K_{oc} (L/kg)
83-32-9	Acenaphthene	1	3.92	3.85	7.08E+03	4.90E+03
67-64-1	Acetone	1	-0.24	-0.24	5.75E-01	---
309-00-2	Aldrin	1	6.50	6.39	2.45E+06	4.87E+04
120-12-7	Anthracene	1	4.55	4.47	2.95E+04	2.35E+04
56-55-3	Benz(*a*)anthracene	1	5.70	5.60	3.98E+05	3.58E+05
71-43-2	Benzene	2	2.13	1.77	5.89E+01	6.17E+01
205-99-2	Benzo(*b*)fluoranthene	1	6.20	6.09	1.23E+06	---
207-08-9	Benzo(*k*)fluoranthene	1	6.20	6.09	1.23E+06	---
50-32-8	Benzo(*a*)pyrene	1	6.11	6.01	1.02E+06	9.69E+05
111-44-4	Bis(2-chloroethyl)ether	1	1.21	1.19	1.55E+01	7.59E+01
117-81-7	Bis(2-ethylhexyl)phthalate	1	7.30	7.18	1.51E+07	1.11E+05
75-27-4	Bromodichloromethane	2	2.10	1.74	5.50E+01	---
75-25-2	Bromoform	2	2.35	1.94	8.71E+01	1.26E+02
71-36-3	Butanol	1	0.85	0.84	6.92E+00	---
85-68-7	Butyl benzyl phthalate	1	4.84	4.76	5.75E+04	1.37E+04
86-74-8	Carbazole	1	3.59	3.53	3.39E+03	---
75-15-0	Carbon disulfide	2	2.00	1.66	4.57E+01	---
56-23-5	Carbon tetrachloride	2	2.73	2.24	1.74E+02	1.52E+02
57-74-9	Chlordane	2	6.32	5.08	1.20E+05	5.13E+04
106-47-8	*p*-Chloroaniline	1	1.85	1.82	6.61E+01	---
108-90-7	Chlorobenzene	2	2.86	2.34	2.19E+02	2.24E+02
124-48-1	Chlorodibromomethane	2	2.17	1.80	6.31E+01	---
67-66-3	Chloroform	2	1.92	1.60	3.98E+01	5.25E+01
218-01-9	Chrysene	1	5.70	5.60	3.98E+05	---
72-54-8	DDD	1	6.10	6.00	1.00E+06	4.58E+04
72-55-9	DDE	1	6.76	6.65	4.47E+06	8.64E+04
50-29-3	DDT	1	6.53	6.42	2.63E+06	6.78E+05
53-70-3	Dibenz(*a,h*)anthracene	1	6.69	6.58	3.80E+06	1.79E+06
84-74-2	Di-*n*-butyl phthalate	1	4.61	4.53	3.39E+04	1.57E+03
95-50-1	1,2-Dichlorobenzene	2	3.43	2.79	6.17E+02	3.79E+02
106-46-7	1,4-Dichlorobenzene	2	3.42	2.79	6.17E+02	6.16E+02
91-94-1	3,3-Dichlorobenzidine	2	3.51	2.86	7.24E+02	---
75-34-3	1,1-Dichloroethane	2	1.79	1.50	3.16E+01	5.34E+01
107-06-2	1,2-Dichloroethane	2	1.47	1.24	1.74E+01	3.80E+01
75-35-4	1,1-Dichloroethylene	2	2.13	1.77	5.89E+01	6.50E+01
156-59-2	*cis*-1,2-Dichloroethylene	2	1.86	1.55	3.55E+01	---
156-60-5	*trans*-1,2-Dichloroethylene	2	2.07	1.72	5.25E+01	3.80E+01
78-87-5	1,2-Dichloropropane	2	1.97	1.64	4.37E+01	4.70E+01
542-75-6	1,3-Dichloropropene	2	2.00	1.66	4.57E+01	2.71E+01

Table 39 (continued)

CAS No.	Compound	Chemical Group [a]	Log K_{ow}	Log K_{oc} (L/kg)	Calculated K_{oc} (L/kg)	Measured K_{oc} (L/kg)
60-57-1	Dieldrin	2	5.37	4.33	2.14E+04	2.55E+04
84-66-2	Diethylphthalate	1	2.50	2.46	2.88E+02	8.22E+01
105-67-9	2,4-Dimethylphenol	1	2.36	2.32	2.09E+02	---
121-14-2	2,4-Dinitrotoluene	1	2.01	1.98	9.55E+01	---
606-20-2	2,6-Dinitrotoluene	1	1.87	1.84	6.92E+01	---
117-84-0	Di-*n*-octyl phthalate	1	8.06	7.92	8.32E+07	---
115-29-7	Endosulfan	2	4.10	3.33	2.14E+03	2.04E+03
72-20-8	Endrin	2	5.06	4.09	1.23E+04	1.08E+04
100-41-4	Ethylbenzene	2	3.14	2.56	3.63E+02	2.04E+02
206-44-0	Fluoranthene	1	5.12	5.03	1.07E+05	4.91E+04
86-73-7	Fluorene	1	4.21	4.14	1.38E+04	7.71E+03
76-44-8	Heptachlor	1	6.26	6.15	1.41E+06	9.53E+03
1024-57-3	Heptachlor epoxide	1	5.00	4.92	8.32E+04	---
118-74-1	Hexachlorobenzene	2	5.89	4.74	5.50E+04	8.00E+04
87-68-3	Hexachloro-1,3-butadiene	1	4.81	4.73	5.37E+04	---
319-84-6	α-HCH (α-BHC)	2	3.80	3.09	1.23E+03	1.76E+03
319-85-7	β-HCH (β-BHC)	2	3.81	3.10	1.26E+03	2.14E+03
58-89-9	γ-HCH (Lindane)	2	3.73	3.03	1.07E+03	1.35E+03
77-47-4	Hexachlorocyclopentadiene	1	5.39	5.30	2.00E+05	---
67-72-1	Hexachloroethane	2	4.00	3.25	1.78E+03	---
193-39-5	Indeno(1,2,3-*cd*)pyrene	1	6.65	6.54	3.47E+06	---
78-59-1	Isophorone	1	1.70	1.67	4.68E+01	---
72-43-5	Methoxychlor	1	5.08	4.99	9.77E+04	8.00E+04
74-83-9	Methyl bromide	2	1.19	1.02	1.05E+01	9.00E+00
75-09-2	Methylene chloride	2	1.25	1.07	1.17E+01	1.00E+01
95-48-7	2-Methylphenol	1	1.99	1.96	9.12E+01	---
91-20-3	Naphthalene	1	3.36	3.30	2.00E+03	1.19E+03
98-95-3	Nitrobenzene	1	1.84	1.81	6.46E+01	1.19E+02
86-30-6	*N*-Nitrosodiphenylamine	1	3.16	3.11	1.29E+03	---
621-64-7	*N*-Nitrosodi-*n*-propylamine	1	1.40	1.38	2.40E+01	---
1336-36-3	PCBs	1	5.58	5.49	3.09E+05	---
108-95-2	Phenol	1	1.48	1.46	2.88E+01	---
129-00-0	Pyrene	1	5.11	5.02	1.05E+05	6.80E+04
100-42-5	Styrene	1	2.94	2.89	7.76E+02	9.12E+02
79-34-5	1,1,2,2-Tetrachloroethane	2	2.39	1.97	9.33E+01	7.90E+01
127-18-4	Tetrachloroethylene	2	2.67	2.19	1.55E+02	2.65E+02
108-88-3	Toluene	2	2.75	2.26	1.82E+02	1.40E+02
8001-35-2	Toxaphene	1	5.50	5.41	2.57E+05	9.58E+04
120-82-1	1,2,4-Trichlorobenzene	2	4.01	3.25	1.78E+03	1.66E+03

Table 39 (continued)

CAS No.	Compound	Chemical Group [a]	Log K_{ow}	Log K_{oc} (L/kg)	Calculated K_{oc} (L/kg)	Measured K_{oc} (L/kg)
71-55-6	1,1,1-Trichloroethane	2	2.48	2.04	1.10E+02	1.35E+02
79-00-5	1,1,2-Trichloroethane	2	2.05	1.70	5.01E+01	7.50E+01
79-01-6	Trichloroethylene	2	2.71	2.22	1.66E+02	9.43E+01
108-05-4	Vinyl acetate	1	0.73	0.72	5.25E+00	---
75-01-4	Vinyl chloride	2	1.50	1.27	1.86E+01	---
108-38-3	*m*-Xylene	2	3.20	2.61	4.07E+02	1.96E+02
95-47-6	*o*-Xylene	2	3.13	2.56	3.63E+02	2.41E+02
106-42-3	*p*-Xylene	2	3.17	2.59	3.89E+02	3.11E+02

[a] Group 1: log K_{oc} = 0.983 log K_{ow} + 0.00028.

Group 2: (VOCs, chlorobenzenes, and certain chlorinated pesticides) log K_{oc} = 0.7919 log K_{ow} + 0.0784.

Note: Calculated values rounded as shown for subsequent SSL calculations.

5.3.2 K_{oc} for Ionizing Organic Compounds.

Sorption models used to describe the behavior of nonionizing hydrophobic organic compounds in the natural environment are not appropriate for predicting the partitioning of ionizable organic compounds. Certain organic compounds such as amines, carboxylic acids, and phenols contain functional groups that ionize under subsurface pH conditions (Schellenberg et al., 1984). Because the ionized and the neutral species of such compounds have different sorption coefficients, sorption models based solely on the partitioning of the neutral species may not accurately predict soil sorption under different pH conditions.

To address this problem, a technique was employed to predict K_{oc} values for the 15 ionizing SSL organic compounds over the pH range of the subsurface environment. These compounds include:

Organic Acids

- Benzoic acid
- 2-Chlorophenol
- 2,4-Dichlorophenol
- 2,4-Dimethylphenol
- 2,4-Dinitrophenol
- 2-Methylphenol
- Pentachlorophenol
- Phenol
- 2,3,4,5-Tetrachlorophenol
- 2,3,4,6-Tetrachlorophenol
- 2,4,5-Trichlorophenol
- 2,4,6-Trichlorophenol

Organic Bases

- *p*-Chloroaniline
- *N*-Nitrosodiphenylamine
- *N*-Nitrosodi-*n*-propylamine

Estimation of K_{oc} values for these chemicals involves two analyses. First, the extent to which the compound ionizes under subsurface conditions must be determined to estimate the relative proportion of neutral and ionized species under the conditions of concern. Second, the K_{oc} values for the neutral and ionized forms ($K_{oc,n}$ and $K_{oc,i}$) must be determined and weighted according to the extent of ionization at a particular pH to estimate a pH-specific K_{oc} value. For organic acids, the ionized species is an anion (A^-) with a lower tendency to sorb to subsurface materials than the neutral species. Therefore, $K_{oc,i}$ for organic acids is likely to be less than $K_{oc,n}$. In the case of organic bases, the ionized species is positively charged (HB^+) so that $K_{oc,i}$ is likely to be greater than $K_{oc,n}$.

It should be noted that this approach is based on the assumption that the sorption of ionizing organic compounds to soil is similar to hydrophobic organic sorption in that the dominant sorbent is soil organic carbon. Shimizu et al. (1993) demonstrated that, for several "natural solids," pentachlorophenol sorption correlates more strongly with cation exchange capacity and clay content than with organic carbon content. This suggests that this organic acid interacts more strongly with soil mineral constituents than organic carbon. The estimates of K_{oc} developed here may overpredict contaminant mobility because they ignore potential sorption to soil components other than organic carbon.

Extent of Ionization. The sorption potential of ionized and neutral species differs because most subsurface solids (i.e., soil and aquifer materials) have a negative net surface charge. Therefore, positively charged chemicals have a greater tendency to sorb than neutral forms, and neutral species sorb more readily than negatively charged forms. Thus, predictions for the total sorption of any ionizable organic compound must consider the extent to which it ionizes over the range of subsurface pH conditions of interest. Consistent with the EPA/Office of Solid Waste (EPA/OSW) Hazardous Waste Identification Rule (HWIR) proposal (U.S. EPA, 1992a), the 7.5th, 50th, and 92.5th percentiles (i.e., pH values of 4.9, 6.8, and 8.0) for 24,921 field-measured ground water pH values in the U.S. EPA STORET database are defined as the pH conditions of interest for SSL development.

The extent of ionization can be viewed as the fraction of neutral species present that, for organic acids, can be determined from the following pH-dependent relationship (Lee et al., 1990):

$$\Phi_{n,\,acid} = \frac{[HA]}{[HA] + [A^-]} = \left(1 + 10^{\,pH - pKa}\right)^{-1} \tag{72}$$

where

$\Phi_{n,acid}$ = fraction of neutral species present for organic acids (unitless)
[HA] = equilibrium concentration of organic acid (mol/L)
$[A^-]$ = equilibrium concentration of anion (mol/L)
pKa = acid dissociation constant (unitless).

Using Equation 68, one can show that, in ground water systems with pH values exceeding the pKa by 1.5 pH units, the ionizing species predominates, and, in ground water systems with pH values that are 1.5 pH units less than the pKa, the neutral species predominates. At pH values approximately equal to the pKa, a mixed system of both neutral and ionizing components occurs.

The fraction of neutral species for organic bases is defined by:

$$\Phi_{n\,,base} = \frac{[B^\circ]}{[B^\circ] + [HB^+]} = \left(1 + 10^{\,pKa - pH}\right)^{-1} \tag{73}$$

where

$\Phi_{n,base}$ = fraction of neutral species present for organic bases (unitless)
$[B^\circ]$ = equilibrium concentration of neutral organic base (mol/L)
$[HB^+]$ = equilibrium concentration of ionized species (mol/L).

As with organic acids, pH conditions determine the relative concentrations of neutral and ionized species in the system. However, unlike organic acids, the neutral species predominates at pH values that exceed the pKa, and the ionized species predominates at pH values less than the pKa. For the SSL organic bases, *N*-nitrosodi-*n*-propylamine and *N*-nitrosodiphenylamine have very low pKa values and the neutral species are expected to prevail under environmental pH conditions. The pKa for *p*-chloroaniline, however, is 4.0 and, at low subsurface pH conditions (i.e., pH = 4.9), roughly 10 percent of the compound will be present as the less mobile ionized species.

Table 40 presents pKa values and fraction neutral species present over the ground water pH range for the SSL ionizing organic compounds. This table shows that ionized species are significant for only some of the constituents under normal subsurface pH conditions. The pKa values for phenol, 2-methylphenol, and 2,4-dimethylphenol are 9.8 or greater. Hence, the neutral species of these compounds predominates under typical subsurface conditions (i.e., pH = 4.9 to 8), and these compounds will be treated as nonionizing organic compounds (see Section 5.3.1). The pKa value for 2,4-dinitrophenol is less than 4 and the ionized species of this compound predominates under subsurface conditions. However, the pKas for 2-chlorophenol, 2,4-dichlorophenol, 2,4,5-trichlorophenol, 2,4,6-trichlorophenol, 2,3,4,5-tetrachlorophenol, 2,3,4,6-tetrachlorophenol, pentachlorophenol, and benzoic acid fall within the range of environmentally significant pH conditions. Mixed systems consisting of both the neutral and the ionized species will prevail under such conditions with both species contributing to total sorption.

Table 40. Degree of Ionization (Fraction of Neutral Species, Φ) as a Function of pH

Compound	pKa[a]	pH = 4.9	pH = 6.8	pH = 8.0
Benzoic acid	4.18	0.1600	0.0024	0.0002
p-Chloroaniline[b]	4.0	0.8882	0.9984	0.9999
2-Chlorophenol	8.40	0.9997	0.9755	0.7153
2,4-Dichlorophenol	7.90	0.9990	0.9264	0.4427
2,4-Dimethylphenol	10.10	1.0000	0.9995	0.9921
2,4-Dinitrophenol	3.30	0.0245	0.0003	0.00002
2-Methylphenol	9.80	1.0000	0.9990	0.9844
N-Nitrosodiphenylamine[b]	< 0	1.0000	1.0000	1.0000
N-Nitrosodi-*n*-propylamine[b]	< 1	0.9999	1.0000	1.0000
Pentachlorophenol	4.80	0.4427	0.0099	0.0006
Phenol	10.0	1.0000	0.9994	0.9901
2,3,4,5-Tetrachlorophenol	6.35[c]	0.9657	0.2619	0.0219
2,3,4,6-Tetrachlorophenol	5.30	0.7153	0.0307	0.0020
2,4,5-Trichlorophenol	7.10	0.9937	0.6661	0.1118
2,4,6-Trichlorophenol	6.40	0.9693	0.2847	0.0245

[a] Kollig et al. (1993).

[b] Denotes that the compound is an organic base.

[c] Lee et al. (1991).

Prediction of Soil-Water Partition Coefficients. Lee et al. (1990) developed a relationship from thermodynamic equilibrium considerations to predict the total sorption of an ionizable organic compound from the partitioning of its ionized and neutral forms:

$$K_{oc} = K_{oc,n}\Phi_n + K_{oc,i}\,(1 - \Phi_n) \qquad \textbf{(74)}$$

where

K_{oc} = soil organic carbon/water partition coefficient (L/kg)
$K_{oc,n}$ = partition coefficient for the neutral species (L/kg)
Φ_n = fraction of neutral species present for acids or bases
$K_{oc,i}$ = partition coefficient for the ionized species (L/kg).

This relationship defines the total sorption coefficient for any ionizing compound as the sum of the weighted individual sorption coefficients for the ionized and neutral species at a given pH. Lee et al. (1990) verified that this relationship adequately predicts laboratory-measured K_{oc} values for pentachlorophenol.

A literature review was conducted to compile the pKa and the laboratory-measured values of $K_{oc,n}$ and $K_{oc,i}$ shown in Table 41. Data collected during this review are presented in RTI (1994), along with the references reviewed. Sorption coefficients for both neutral and ionized species were reported for only four of the nine ionizable organic compounds of interest. Sorption coefficients reported for the remaining compounds were generally $K_{oc,n}$, and estimates of $K_{oc,i}$ were necessary to predict the compound's total sorption. The methods for estimating $K_{oc,i}$ for organic acids and organic bases are discussed separately in the following subsections.

Organic Acids. Sorption coefficients for both the neutral and ionized species have been reported for two chlorophenolic compounds: 2,4,6-trichlorophenol and pentachlorophenol. For 2,4,5-trichlorophenol and 2,3,4,5-tetrachlorophenol, soil-water partitioning coefficient (K_p) data in the literature were adequate to allow calculation of $K_{oc,i}$ from K_p and soil f_{oc} (Lee et al., 1991). From these measured values, the ratios of $K_{oc,i}$ to $K_{oc,n}$ are: 0.1 (2,4,6-trichlorophenol), 0.02 (pentachlorophenol), 0.015 (2,4,5-trichlorophenol), and 0.051 (2,3,4,5-tetrachlorophenol). A ratio of 0.015 (1.5 percent) was selected as a conservative value to estimate $K_{oc,i}$ for the remaining phenolic compounds, benzoic acid, and vinyl acetate.

Organic Bases. No measured sorption coefficients for either the neutral or the ionized species were found for the three organic bases of interest (*N*-nitrosodi-*n*-propylamine, *N*-nitrosodiphenylamine, and *p*-chloroaniline). Generally, the sorption of ionizable organic bases has not been as well investigated as that of the organic acids, and there has been no relationship developed between the sorption coefficients of the neutral and ionized species. EPA is currently initiating research on models for predicting the sorption of organic bases in the subsurface.

As noted earlier, the neutral species of the organic base predominates at pH values exceeding the pKa. For *N*-nitrosodi-*n*-propylamine (pKa < 1) and *N*-nitrosodiphenylamine (pKa < 0), the neutral species is present under environmentally significant conditions. The neutral species constitutes approximately 90 percent of the system for *p*-chloroaniline (Table 40).

Table 41. Soil Organic Carbon/Water Partition Coefficients and pKa Values for Ionizing Organic Compounds

Compound	$K_{oc,n}$ (L/kg)	$K_{oc,i}$ (L/kg)	pKa[a]
Benzoic acid	32[b]	0.5[c]	4.18
2-Chlorophenol	398[b]	6.0[c]	8.40
2,4-Dichlorophenol	159[d]	2.4[c]	7.90
2,4-Dinitrophenol	0.8[a]	0.01[c]	3.30
Pentachlorophenol	19,953[e]	398[e]	4.80
2,3,4,5-Tetrachlorophenol	17,916[f]	67[g]	6.35[h]
2,3,4,6-Tetrachlorophenol	6,190[i]	93[c]	5.30
2,4,5-Trichlorophenol	2,380[i]	36[j]	7.10
2,4,6-Trichlorophenol	1,070[i]	107[k]	6.40

[a] Kollig et al. (1993).

[b] Meylan et al. (1992).

[c] Estimate based on the ratio of $K_{oc,i}/K_{oc,n}$ for compounds for which data exist; $K_{oc,i}$ was estimated to be 0.015 × $K_{oc,n}$.

[d] Calculated using data ($K_p = 0.62$, $f_{oc} = 0.0039$) contained in Lee et al. (1991); agrees well with Boyd (1982) reporting measured $K_{oc} = 126$ L/kg.

[e] Lee et al. (1990).

[f] Average of values reported for two aquifer materials from Schellenberg et al. (1984).

[g] Calculated using data ($K_p = 0.26$, $f_{oc} = 0.0039$) contained in Lee et al. (1991).

[h] Lee et al. (1991).

[i] Schellenberg et al. (1984).

[j] Calculated using data ($K_p = 0.14$, $f_{oc} = 0.0039$) contained in Lee et al. (1991).

[k] Kukowski (1989).

The neutral species has a lower tendency to sorb to subsurface materials than the positively charged ionized species. As a consequence, the determination of overall sorption potential based solely on the neutral species for *N*-nitrosodi-*n*-propylamine, *N*-nitrosodiphenylamine, and *p*-chloroaniline is conservative, and these three organic bases will be treated as nonionizing organic compounds (see Section 5.3.1).

Soil-Water Partition Coefficients for Ionizing Organic Compounds. Partition coefficients for the neutral and ionized species ($K_{oc,n}$ and $K_{oc,i}$, respectively) and pKa values for nine ionizable organic compounds are provided in Table 41. These parameters can be used in Equation 74 to compute K_{oc} values for organic acids at any given pH. K_{oc} values for each of the ionizable compounds of interest are presented in Table 42 for pHs of 4.9, 6.8, and 8.0. Appendix L contains pH-specific K_{oc} values for ionizable organics over this entire range.

5.4 Soil-Water Distribution Coefficients (K_d) for Inorganic Constituents

As with organic chemicals, development of SSLs for inorganic chemicals (i.e., toxic metals) requires a soil-water partition coefficient (K_d) for each constituent. However, the simple relationship between soil organic carbon content and sorption observed for organic chemicals does not apply to inorganic constituents. The soil-water distribution coefficient (K_d) for metals and other inorganic compounds is affected by numerous geochemical parameters and processes, including pH; sorption to clays, organic matter, iron oxides, and other soil constituents; oxidation/reduction conditions; major ion chemistry; and the chemical form of the metal. The number of significant influencing parameters, their variability in the field, and differences in experimental methods result in as much as seven orders of magnitude variability in measured metal K_d values reported in the literature (Table 43). This variability makes it much more difficult to derive generic K_d values for metals than for organics.

Table 42. Predicted Soil Organic Carbon/Water Partition Coefficients (K_{oc},L/kg) as a Function of pH: Ionizing Organics

Compound	pH = 4.9	pH = 6.8	pH = 8.0
Benzoic acid	5.5	0.6	0.5
2-Chlorophenol	398	388	286
2,4-Dichlorophenol	159	147	72
2,4-Dinitrophenol	0.03	0.01	0.01
Pentachlorophenol	9,055	592	410
2,3,4,5-Tetrachlorophenol	17,304	4,742	458
2,3,4,6-Tetrachlorophenol	4,454	280	105
2,4,5-Trichlorophenol	2,365	1,597	298
2,4,6-Trichlorophenol	1,040	381	131

Because of their great variability and a limited number of data points, no meaningful estimate of central tendency K_d values for metals could be derived from available measured values. For this reason, an equilibrium geochemical speciation model (MINTEQ) was selected as the best approach for estimating K_d values for the variety of environmental conditions expected to be present at Superfund sites.

This approach and model were also used by OSW to estimate generic K_d values for metals proposed for use in the HWIR proposal (U.S. EPA, 1992a). The HWIR MINTEQA2 analyses were conducted under a variety of geochemical conditions and metal concentrations representative of solid waste landfills across the Nation. The metal K_d values developed for this effort were reviewed for SSL application and were used as preliminary values to develop the September 1993 draft SSLs.

Upon further review of the HWIR MINTEQ modeling effort, EPA decided it was necessary to conduct a separate MINTEQ modeling effort to develop metal K_d values for SSL application. Reasons for this decision include the following:

- It was necessary to expand the modeling effort to include other metal contaminants likely to be encountered at Superfund sites (i.e., beryllium, copper, and zinc).
- HWIR work incorporated low, medium, and high concentrations of dissolved organic acids that are present in municipal solid waste (MSW) leachate. These organic acids are not expected to exist in high concentrations in pore waters underlying Superfund sites; therefore, their inclusion in the Superfund contaminated soil scenario is not warranted.
- The HWIR modeling simulations for chromium (+3) were found to be in error. This error has been corrected in subsequent HWIR modeling work but corrected results were not available at the time of preliminary SSL development.

Table 43. Summary of Collected K_d Values Reported in Literature

	AECL (1990)[a]	Baes and Sharp (1983) or Baes et al. (1984)[b]			Coughtrey et al. (1985)[c]	Battelle (1989)[d]
Metal	**Range**	**Geometric Mean[e]**	**Range**	**No. Values**	**Range**	**Range**
Antimony	45-550	45[f]	--	--	--	2.0-15.9
Arsenic[e]	--	200[f]	--	--	--	5.86-19.4
Arsenic (+3)	--	3.3[g]	1.0-8.3	19	--	--
Arsenic (+5)	--	6.7[g]	1.9-18	37	--	--
Barium	--	60[f]	--	--	--	530-16,000
Beryllium	250-3,000	650[f]	--	--	--	70-8,000
Cadmium	2.7-17,000	6.4[h]	1.26-26.8	28	32-50	14.9-567
Chromium	1.7-2,517	850[f]	--	--	--	--
Chromium (+2)	--	2,200[g]	470-150,000	15	--	--
Chromium (+3)	--	--	--	--	--	168-3,600
Chromium (+6)	--	37[g]	1.2-1,800	18	--	16.8-360
Mercury[e]	--	10[f]	--	--	--	322-5,280
Nickel	60-4,700	150[f]	--	--	~20	12.2-650
Selenium	150-1,800	300[f]	--	--	< 9	5.9-14.9
Silver	2.7-33,000	46[h]	10-1,000	16	50	0.4-40.0
Thallium	--	1,500[f]	--	--	--	0.0-0.8
Vanadium	--	1,000[f]	--	--	--	50-100.0
Zinc	0.1-100,000	38[h]	0.1-8,000	146	≥ 20	--

[a] The Atomic Energy of Canada, Limited (AECL, 1990) presents the distribution of K_d values according to four major soil types—sand, silt, clay, and organic material. Their data were obtained from available literature.

[b] Baes et al. (1984) present K_d values for approximately 220 agricultural soils in the pH range of 4.5 to 9. Their data were derived from available literature and represent a diverse mixture of soils, extracting solutions, and laboratory techniques.

[c] Coughtrey et al. (1985) report best estimates and ranges of measured soil K_d values for a limited number of metals.

[d] Battelle Memorial Institute (Battelle, 1989) reports a range in K_d values as a function of pH (5 to 9) and sorbent content (a combination of clay, aluminum and iron oxyhydroxides, and organic matter content). The sorbent content ranges were <10 percent, 10 to 30 percent, and >30 percent sorbent. Their data were based on available literature.

[e] The valence of these metals is not reported in the documents.

[f] Estimated based on the correlation between K_d and soil-to-plant concentration factor (B_v).

[g] Average value reported by Baes and Sharp (1983).

[h] Represents the median of the logarithms of the observed values.

For these reasons, a MINTEQ modeling effort was expanded to develop a series of metal-specific isotherms for several of the metals expected to be present in soils underlying Superfund sites. The model used was an updated version of MINTEQA2 obtained from Allison Geoscience Consultants, Inc. Model results are reported in the December 1994 draft Technical Background Document (U.S. EPA, 1994i) and were used to calculate the SSLs presented in the December 1994 draft Soil Screening Guidance (U.S. EPA, 1994h).

The MINTEQA2 model was further updated by Allison Geoscience Consultants, Inc., in 1995 to include thermodynamic data for silver, an improved estimate of water saturation in the vadose zone (i.e., water saturation is assumed to be 77.7 percent saturated as opposed to 100 percent), and revised estimates of sorbent mass (i.e., organic matter content, iron oxide content).

This updated model, which is expected to be made public through EPA's Environmental Research Laboratory in Athens, Georgia, was used to revise the generic K_d values for the EPA/OSW HWIR modeling effort. The metal K_d values for SSL application were also revised. Model results are contained in this document. The following section describes the important assumptions and limitations of this modeling effort.

5.4.1 Modeling Scope and Approach. New MINTEQA2 modeling runs were conducted to develop sorption isotherms for barium, beryllium, cadmium, chromium (+3), copper, mercury (+2), nickel, silver, and zinc. The general approach and input values used for pH, iron oxide (FeOx) concentration, and background chemistry were unchanged from the HWIR modeling effort.

The HWIR MINTEQA2 analyses were conducted under a variety of geochemical conditions and metal concentrations. Three types of parameters were identified as part of the chemical speciation modeling effort: (1) parameters that have a direct first-order impact on metal speciation and are characterized by a wide range in environmental variability; (2) parameters that have an indirect, generally less pronounced effect on metal speciation and are characterized by a relatively small or insignificant environmental variability; and (3) parameters that may have a direct first-order impact on metal speciation but neither the natural variability nor its significance is known.

In the HWIR modeling effort, parameters of the first type ("master variables") were limited to those having a significant effect on model results, including pH, concentration of available amorphous iron oxide adsorption sites (i.e., FeOx content), concentration of solid organic matter adsorption sites (with a dependent concentration of dissolved natural organic matter), and concentration of leachate organic acids expected to be present in MSW leachate. High, medium, and low values were assigned to each of the master variables to account for their natural environmental variability. The SSL modeling effort used this same approach and inputs except that anthropogenic organic acids were not included in the model simulations. Furthermore, the SSL modeling effort incorporated a medium fraction of organic carbon (f_{oc}) that correlated to the HWIR high concentration.

Parameters of the second type constitute the background pore-water chemistry, which consists of chemical constituents commonly occurring in ground water at concentrations great enough to affect metal speciation. These constituents were treated as constants in both the SSL and HWIR effort. The third type of parameter was entirely omitted from consideration in both modeling efforts due to poorly understood geochemistry and the lack of reliable thermodynamic data. The most important of these parameters is the oxidation-reduction (redox) potential. To compensate, both modeling efforts incorporated an approach that was most protective of the environment with respect to the impact of redox potential on the partitioning of redox-sensitive metals (i.e., each metal was modeled in the oxidation state that most enhances metal mobility).

For the HWIR modeling effort, metal concentrations were varied from the maximum contaminant level (MCL) to 1,000 times the MCL for each individual metal. This same approach was taken for SSL modeling, although for certain metals the concentration range was extended to determine the metal concentration at which the sorption isotherm departed from linearity.

Sorption isotherms for arsenic (+3), chromium (+6), selenium, and thallium are unchanged from the previous efforts and are based on laboratory-derived pH-dependent sorption relationships developed for HWIR. Using these relationships, the K_d distribution as a function of pH is presented for each of these four metals in Figure 10.

Sorption isotherms for antimony and vanadium could not be estimated using MINTEQA2 because the thermodynamic databases do not contain the required reactions and associated equilibrium constants. Sufficient experimental research has not been conducted to develop pH-dependent relationships for these two metals. As a consequence, K_d values for antimony and vanadium were obtained from Baes et al. (1984) (Table 43). These K_d values are not pH-dependent.

5.4.2 Input Parameters. Table 44 lists high, medium, and low values for pH and iron oxide used for both the HWIR and SSL MINTEQ modeling efforts. Sources for these values are as follows (U.S. EPA, 1992a):

- Values for pH were obtained from analysis of 24,921 field-measured pH values contained in the EPA STORET database. The pH values of 4.9, 6.8, and 8.0 correspond to the 7.5th, 50th, and 92.5th percentiles of the distribution.
- Iron oxide contents were based on analysis of six aquifer samples collected over a wide geographic area, including Florida, New Jersey, Oregon, Texas, Utah, and Wisconsin. The lowest of the six analyses was taken to be the low value, the average of the six was used as the medium value, and the highest was taken as the high value.

The development of the values presented in Table 44 is described in more detail in U.S. EPA (1992a).

Thirteen chemical constituents commonly occurring in ground water were used to define the background pore-water chemistry for HWIR and SSL modeling efforts (Table 45). Because these constituents were treated as constants, a single total ion concentration, corresponding to the median total metal concentration from a probability distribution obtained from the STORET database, was assigned to each of the background pore-water constituents (U.S. EPA, 1992a).

Although the HWIR and the SSL MINTEQ modeling efforts were consistent in the majority of the assumptions and input parameters used, the fraction of organic carbon (f_{oc}) used for the SSL modeling effort was slightly different than that used for the HWIR modeling effort. The f_{oc} used for the SSL effort was equal to 0.002 g/g, which better reflected average subsurface conditions at Superfund sites. This value is approximately equal to the high value of organic carbon used in the HWIR modeling effort.

Table 44. Summary of Geochemical Parameters Used in SSL MINTEQ Modeling Effort

Value	pH	Iron oxide content (weight percent)
Low	4.9	0.01
Medium	6.8	0.31
High	8.0	1.11

Source: U.S. EPA (1992a)

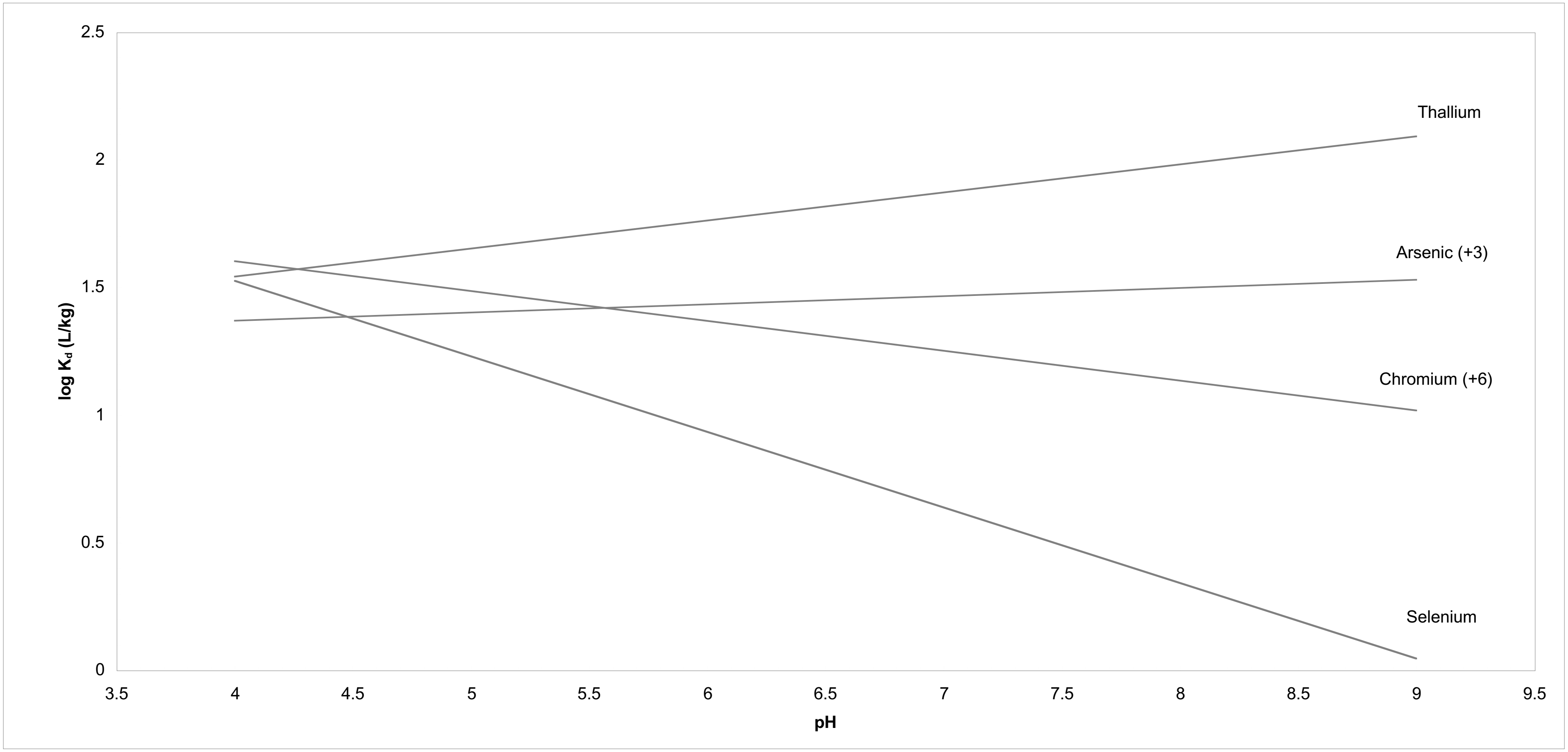


Figure 10. Empirical pH-dependent adsorption relationship: arsenic (+3), chromium

Table 45. Background Pore-Water Chemistry Assumed for SSL MINTEQ Modeling Effort[a]

Parameter	Concentration (mg/L)
Aluminum	0.2
Bromine	0.3
Calcium	48
Carbonate	187
Chlorine	15
Iron (+3)	0.2
Magnesium	14
Manganese (+2)	0.04
Nitrate	1
Phosphate	0.09
Potassium	2.9[b]
Sodium	22
Sulfate	25

[a] Median values from STORET database as reported in U.S. EPA (1992a).

[b] Median values from STORET database; personal communication from J. Allison, Allison Geosciences.

5.4.3. Assumptions and Limitations. The SSL MINTEQ modeling effort incorporates several basic simplifying assumptions. In addition, the applicability and accuracy of the model results are subject to limitations. Some of the more significant assumptions and limitations are described below.

- **The system is assumed to be at equilibrium.** This assumption is inherent in geochemical aqueous speciation models because the fundamental equations of mass action and mass balance are equilibrium based. Therefore, any possible influence of adsorption (or desorption) rate limits is not considered.

  This assumption is **conservative**. Because the model is being used to simulate metal desorption from the solid substrate, if equilibrium conditions are not met, the desorption reaction will be incomplete and the metal concentration in pore water will be less than predicted by the model.

- **Redox potential is not considered.** The redox potential of the system is not considered due to the difficulty in obtaining reliable field measurements of oxidation reduction potential (Eh), which are needed to determine a realistic frequency distribution of this parameter. Furthermore, the geochemistry of redox-sensitive species is poorly understood. Reactions involving redox species are often biologically mediated and the concentrations of redox species are not as likely to reflect thermodynamic equilibrium as other inorganic constituents.

  To provide a **conservative** estimate of metal mobility, all environmentally viable oxidation states are modeled separately for the redox-sensitive metals; the most conservative was selected for defining SSL metal K_d values. The redox-sensitive constituents that make up the background chemistry are represented only by the oxidation state that most enhances metal mobility (U.S. EPA, 1992a).

- **Potential sorbent surfaces are limited.** Only metal adsorption to FeOx and solid organic matter is considered in the system. It is recognized that numerous other natural sorbents exist (e.g., clay and carbonate minerals); however, thermodynamic databases describing metal adsorption to these surfaces are not available and the potential for adsorption to such surfaces is not considered. This assumption is **conservative** and will underpredict sorption for soils with significant amounts of such sorption sites.

- **The available thermodynamic database is limiting.** As metal behavior increases in complexity, thermodynamic data become more rare. The lack of complete thermodynamic data requires simplification to the defined system. This simplification may be **conservative** or **nonconservative** in terms of metal mobility.

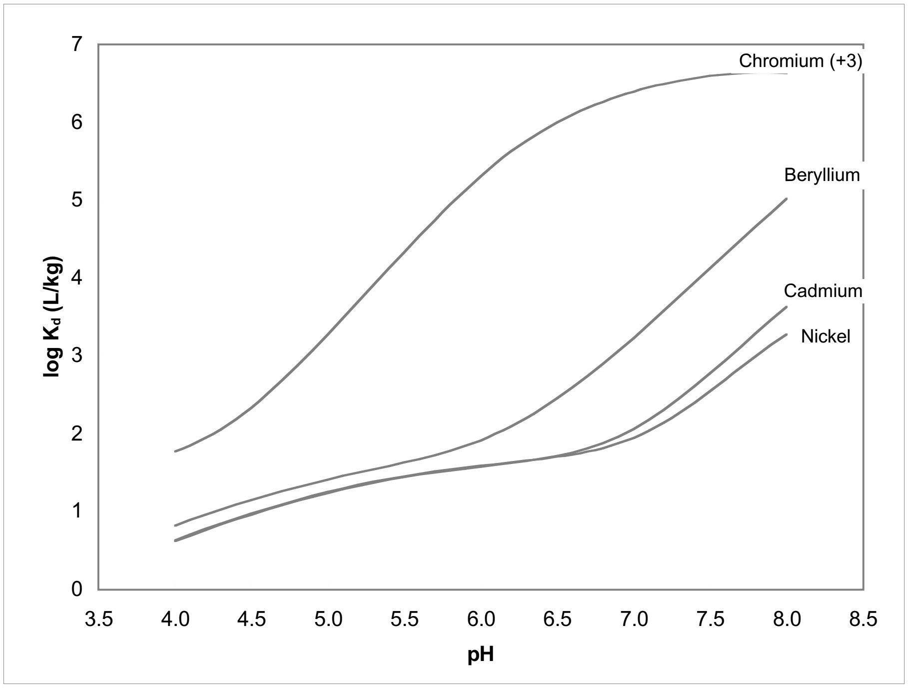
- **Metal competition is not considered.** Model simulations were performed for systems comprised of only one metal (i.e., the potential for competition between multiple metals for available sorbent surface sites was not considered). Generally, the competition of multiple metals for available sorption sites results in higher dissolved metal concentrations than would exist in the absence of competition. Consequently, this assumption is **nonconservative** but is significant only at metal concentrations much higher than the SSLs.

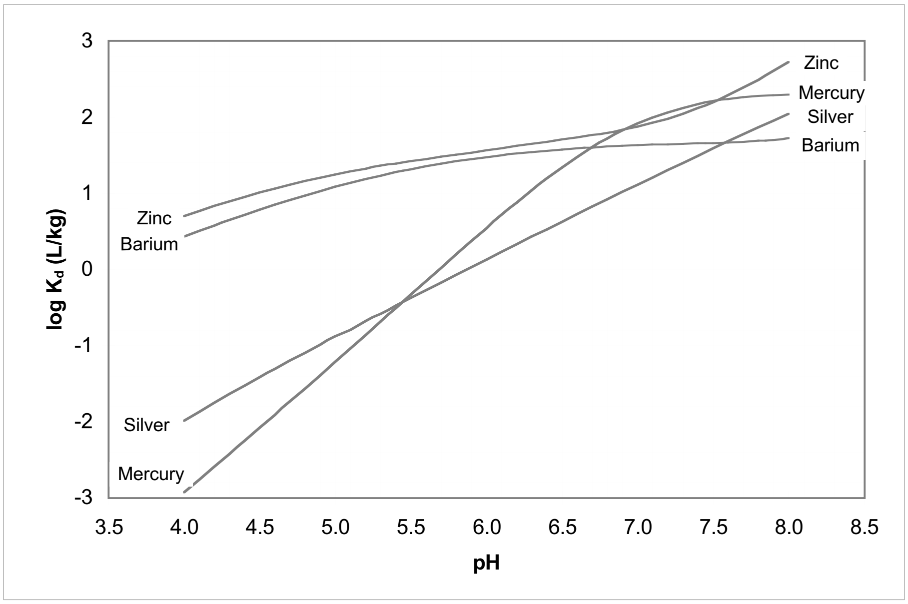
Other assumptions and limitations associated with this modeling effort are discussed in RTI (1994).

5.4.4 Results and Discussion. MINTEQ model results indicate that metal mobility is most affected by changes in pH. Based on this observation and because iron oxide content is not routinely measured in site characterization efforts, pH-dependent K_ds for metals were developed for SSL application by fixing iron oxide at its medium value and fraction organic carbon at 0.002. For arsenic (+3), chromium (+6), selenium, and thallium, the empirical pH-dependent K_ds were used.

Table 46 shows the SSL K_d values at high, medium, and low subsurface pH conditions. Figure 11 plots MINTEQ-derived metal K_d values over this pH range. Figure 10 shows the same for the empirically derived metal K_ds. These results are discussed below by metal and compared with measured values. See RTI (1994) for more information. pH-dependent values are not available for antimony, cyanide, and vanadium. The estimated K_d values shown in Table 46 for antimony and vanadium are reported by Baes et al. (1984) and the K_d value for cyanide is obtained from SCDM.

Arsenic. K_d values developed using the empirical equation for arsenic (+3) range from 25 to 31 L/kg for pH values of 4.9 to 8.0, respectively. These values correlate fairly well with the range of measured values reported by Battelle (1989)—5.86 to 19.4 L/kg. They are slightly above the range reported by Baes and Sharp (1983) for arsenic (+3) (1.0-8.3). The estimated K_d values for arsenic (+3) do not correlate well with the value of 200 L/kg presented by Baes et al. (1984). Oxidation state is not specified in Baes et al. (1984), and the difference between the empirical-derived K_d values presented here and the value presented by Baes et al. (1984) may reflect differences in oxidation states (arsenic (+3) is the most mobile species).





Note: Conditions depicted are medium iron oxide content (0.31 wt %) and organic matter of 0.2 wt %.

Figure 11. Metal Kd as a function of pH.

Table 46. Estimated Inorganic K_d Values for SSL Application

		Estimated K_d (L/kg)	
Metal	**pH = 4.9**	**pH = 6.8**	**pH = 8.0**
Antimony[a]		4.5E+01	
Arsenic (+3)[b]	2.5E+01	2.9E+01	3.1E+01
Barium	1.1E+01	4.1E+01	5.2E+01
Beryllium	2.3E+01	7.9E+02	1.0E+05
Cadmium	1.5E+01	7.5E+01	4.3E+03
Chromium (+3)	1.2E+03	1.8E+06	4.3E+06
Chromium (+6)[b]	3.1E+01	1.9E+01	1.4E+01
Cyanide[c]		9.9E+00	
Mercury (+2)	4.0E-02	5.2E+01	2.0E+02
Nickel	1.6E+01	6.5E+01	1.9E+03
Selenium[b]	1.8E+01	5.0E+00	2.2E+00
Silver	1.0E-01	8.3E+00	1.1E+02
Thallium[b]	4.4E+01	7.1E+01	9.6E+01
Vanadium[a]		1.0E+03	
Zinc	1.6E+01	6.2E+01	5.3E+02

[a] Geometric mean measured value from Baes et al., 1984 (pH-dependent values not available).
[b] Determined using an empirical pH-dependent relationship (Figure 10).
[c] SCDM = Superfund Chemical Data Matrix (pH-dependent values not available).

Barium. For ground water pH conditions, MINTEQ-estimated K_d values for barium range from 11 to 52 L/kg. This range correlates well with the value of 60 L/kg reported by Baes et al. (1984). Battelle (1989) reports a range in K_d values from 530 to 16,000 L/kg for a pH range of 5 to 9. The model-predicted K_d values for barium are several orders of magnitude less than the measured values, possibly due to the lower sorptive potential of iron oxide, used as the modeled sorbent, relative to clay, a sorbent present in the experimental systems reported by Battelle (1989).

Beryllium. The K_d values estimated for beryllium range from 23 to 100,000 L/kg for the conditions studied. AECL (1990) reports medians of observed values for K_d ranging from 250 L/kg for sand to 3,000 L/kg for organic matter. Baes et al. (1984) report a value of 650 L/kg. Battelle (1989) reports a range of K_d values from 70 L/kg for sand to 8,000 L/kg for clay. MINTEQ results for medium ground water pH (i.e., a value of 6.8) yields a K_d value of 790 L/kg. Hence, there is reasonable agreement between the MINTEQ-predicted K_d values and values reported in the literature.

Cadmium. For the three pH conditions, MINTEQ K_d values for cadmium range from 15 to 4,300 L/kg, with a value of 75 at a pH of 6.8. The range in experimentally determined K_d values for cadmium is as follows: 1.26 to 26.8 L/kg (Baes et al., 1983), 32 to 50 L/kg (Coughtrey et al., 1985), 14.9 to 567 L/kg (Battelle, 1989), and 2.7 to 17,000 L/kg (AECL, 1990). Thus the MINTEQ estimates are generally within the range of measured values.

Chromium (+3). MINTEQ-estimated K_d values for chromium (+3) range from 1,200 to 4,300,000 L/kg. Battelle (1989) reports a range of K_d values of 168 to 3,600 L/kg, orders of magnitude lower than the MINTEQ values. This difference may reflect the measurements of mixed systems comprised of both chromium (+3) and (+6). The incorporation of chromium (+6) would tend to lower the K_d. Because the model-predicted values may overpredict sorption, the user should exercise care in the use of these values. Values for chromium (+6) should be used where speciation is mixed or uncertain.

Chromium (+6). Chromium (+6) K_d values estimated using the empirical pH-dependent adsorption relationship range from 31 to 14 L/kg for pH values of 4.9 to 8.0. Battelle (1989) reports a range of 16.8 to 360 L/kg for chromium (+6) and Baes and Sharp (1983) report a range of 1.2 to 1,800. The predicted chromium (+6) K_d values thus generally agree with the lower end of the range of measured values and the average measured values (37) reported by Baes and Sharp (1983). These values represent conservative estimates of mobility the more toxic of the chromium species.

Mercury (+2). MINTEQ-estimated K_d values for mercury (+2) range from 0.04 to 200 L/kg. These model-predicted estimates are less than the measured range of 322 to 5,280 L/kg reported by Battelle (1989). This difference may reflect the limited thermodynamic database with respect to mercury and/or that only the divalent oxidation state is considered in the simulation. Allison (1993) reviewed the model results in comparison to the measured values reported by Battelle (1989) and found reasonable agreement between the two sets of data, given the uncertainty associated with laboratory measurements and model precision.

Nickel. MINTEQ-estimated K_d values for nickel range from 16 to 1,900 L/kg. These values agree well with measured values of approximately 20 L/kg (mean) and 12.2 to 650 L/kg, reported by Coughtrey et al. (1985) and Battelle (1989), respectively. These values also agree well with the value of 150 L/kg reported by Baes et al. (1984). However, the predicted values are at the low end of the range reported by the AECL (1990)—60 to 4,700 L/kg.

Selenium. Empirically derived K_d values for selenium range from 2.2 to 18 L/kg for pH values of 8.0 to 4.9. The range in experimentally determined K_d values for selenium is as follows: less than 9 L/kg (Coughtrey et al., 1985), 5.9 to 14.9 L/kg (Battelle, 1989), and 150 to 1,800 L/kg (AECL, 1990). Baes et al. (1984) reported a value of 300 L/kg. Although they are significantly below the values presented by the AECL (1990) and Baes et al. (1984), the MINTEQ-predicted K_d values correlate well with the values reported by Coughtrey et al. (1985) and Battelle (1989).

Silver. The K_d values estimated for silver range from 0.10 to 110 L/kg for the conditions studied. The range in experimentally determined K_d values for silver is as follows: 2.7 to 33,000 L/kg (AECL, 1990), 10 to 1,000 L/kg (Baes et al., 1984), 50 L/kg (Coughtrey et al., 1985), and 0.4 to 40 L/kg (Battelle, 1989). The model-predicted K_d values agree well with the values reported by Coughtrey et al. (1985) and Battelle (1989) but are at the lower end of the ranges reported by AECL (1990) and Baes et al. (1984).

Thallium. Empirically derived K_d values for thallium range from 44 to 96 L/kg for pH values of 4.9 to 8.0. Generally, these values are about an order of magnitude greater than those reported by Battelle (1989)—0.0 to 0.8 L/kg - but are well below the value predicted by Baes et al. (1984).

Zinc. MINTEQ-estimated K_d values for zinc range from 16 to 530 L/kg. These estimated K_d values are within the range of measured K_d values reported by the AECL (1990) (0.1 to 100,000 L/kg) and Baes et al. (1984) (0.1 to 8,000 L/kg). Coughtrey et al. (1985) reported a K_d value for zinc of greater than or equal to 20 L/kg.

5.4.5 Analysis of Peer-Review Comments. A peer review was conducted of the model assumptions and inputs used to estimate K_d values for SSL application. This review identified several issues of concern, including:

- The charge balance exceeds an acceptable margin of difference (5 percent) in most of the simulations. A variance in excess of 5 percent may indicate that the model problem is not correctly chemically poised and therefore the results may not be chemically meaningful.
- The model should not allow sulfate to adsorb to the iron oxide. Sulfate is a weakly outer-sphere adsorbing species and, by including the adsorption reaction, sulfate is removed from the aqueous phase at pH values less than 7 and is prevented from participating in precipitation reaction at these pH values.
- Modeled K_d values for barium and zinc could not be reproduced for all studied conditions.

A technical analysis of these concerns indicated that, although these comments were based on true observations about the model results, these factors do not compromise the validity of the MINTEQ results in this application. This technical analysis is provided in Appendix M.