Default Hydrogeologic Parameter Data For Deriving Soil Concentrations for Groundwater Protection WAC 173-340-747

Please refer to WAC 173-340-747 for a complete explanation of calculations for developing soil cleanup standards that are protective of groundwater. (You must first identify the appropriate groundwater cleanup level at the site). The equations and default values provided in this document are from that section of the regulation. Ecology provides Excel worksheets which use the MTCA equations to calculate soil cleanup levels for protection of groundwater for individual chemicals and for total petroleum hydrocarbon mixtures. The worksheets can be found at http://www.ecy.wa.gov/programs/tcp/tools/toolmain.html. A list of equations used for calculating soil cleanup levels for protection of groundwater is found below.

Summary of Default Values for use in equations and spreadsheets:

- Total Soil Porosity: 0.43
- Volumetric Water Content/Water filled soil porosity: 0.30 ml water/ml soil for unsaturated zone; 0.43 ml water/ml soil for saturated zone
- Volumetric Air Content/Air filled soil porosity : 0.13 ml air/ml soil for unsaturated zone; 0.0 for saturated zone
- Dry Soil Bulk Density: 1.50 kg/l
- Fraction Soil Organic Carbon 0.001 (0.1%); in spreadsheet tool, use "1" for metals
- Dilution Factor: 20 for unsaturated zone soil; 1 for saturated zone soil

Summary of Equations and Tables (refer to WAC 173-340-747):

The equations and default parameter tables shown below are for use in the "fixed parameter" 3 and 4 - phase partitioning models which use default values (i.e. – "fixed parameters"). For information on using site-specific input parameters and related equations for developing site-specific input parameters (i.e. - "variable parameter" partitioning model), refer to 173-340-747 (5).

3 phase partitioning model – fixed parameter (173-340-747 (4) (b):

[Equation 747-1]

$$C_s = C_w(UCF)DF\left[K_d + \frac{(\theta_w + \theta_a H_{cc})}{\rho_b}\right]$$

Where:

C_s = Soil concentration (mg/kg)

C_w = Ground water cleanup level established under WAC 173-340-720 (ug/l)

UCF = Unit conversion factor (1 mg/1,000 ug)

DF = Dilution factor (dimensionless: 20 for unsaturated zone soil; see (e) of this subsection for saturated zone soil)

K_d = Distribution coefficient (L/kg; see (c) of this subsection)

θ_w = Water-filled soil porosity (ml water/ml soil: 0.3 for unsaturated zone soil; see (e) of this subsection for saturated zone soil)

θ_a = Air-filled soil porosity (ml air/ml soil: 0.13 for unsaturated zone soil; see (e) of this subsection for saturated zone soil)

H_{cc} = Henry's law constant (dimensionless; see (d) of this subsection)

ρ_b = Dry soil bulk density (1.5 kg/L)

Distribution Coefficient for Organics (Kd):

[Equation 747-2]

$$K_d = K_{oc} \times f_{oc}$$

Where:

K_d = Distribution coefficient (L/kg)

K_{oc} = Soil organic carbon-water partitioning coefficient (ml/g). See (c)(i) of this subsection.

f_{oc} = Soil fraction of organic carbon (0.1% or 0.001 g/g)

Koc Values:

A) For nonionic organics, use Table 747-1 values

****NOTE**** these Koc Values and values for other organics are also available through the CLARC Chemical Specific Data Search****

Table 747-1
Soil Organic Carbon-Water Partitioning Coefficient (Koc) Values: Nonionizing Organics.

Hazardous Substance	Koc (ml/g)
Acenapthene	4,898
Aldrin	48,685
Anthracene	23,493
Benz(a)anthracene	357,537
Benzene	62
Benzo(a)pyrene	968,774
Bis(2-chloroethyl)ether	76
Bis(2-ethylhexyl)phthalate	111,123
Bromoform	126
Butyl benzyl phthalate	13,746
Carbon tetrachloride	152
Chlordane	51,310
Chlorobenzene	224
Chloroform	53
DDD	45,800
DDE	86,405
DDT	677,934
Dibenzo(a,h)anthracene	1,789,101
1,2-Dichlorobenzene (o)	379
1,4-Dichlorobenzene (p)	616
Dichloroethane-1,1	53
Dichlororthane-1,2	38
Dichloroethylene-1,1	65
Trans-1,2 Dichloroethylene	38
Dichloropropane-1,2	47
Dichloropropene-1,3	27
Dieldrin	25,546
Diethyl phthalate	82
Di-n-butyl phthalate	1,567
EDB	66
Endrin	10,811
Endosulfan	2,040
Ethyl benzene	204
Fluoranthene	49,096
Fluorene	7,707
Heptachlor	9,528
Hexachlorobenzene	80,000
α-HCH (α-BHC)	1,762
β-HCH (β-BHC)	2,139
γ-HCH (Lindane)	1,352
MTBE	11
Methoxychlor	80,000
Methyl bromide	9
Methyl chloride	6
Methylene chloride	10
Naphthalene	1,191

Nitrobenzene	119
PCB-Arochlor 1016	107,285
PCB-Arochlor 1260	822,422
Pentachlorbenzene	32,148
Pyrene	67,992
Styrene	912
1,1,2,2,-Tetrachloroethane	79
Tetrachloroethylene	265
Toluene	140
Toxaphene	95,816
1,2,4-Trichlorobenzene	1,659
Trichloroethane-1,1,1	135
Trichloroethane-1,1,2	75
Trichloroethylene	94
o-Xylene	241
m-Xylene	196
p-Xylene	311

Sources: Except as noted below, the source of the Koc values is the 1996 *EPA Soil Screening Guidance: Technical Background Document.* The values obtained from this document represent the geometric mean of a survey of values published in the scientific literature. Sample populations ranged from 1-65. EDB value from *ATSDR Toxicological Profile* (TP 91/13). MTBE value from *USGS Final Draft Report on Fuel Oxygenates* (March 1996). PCB-Arochlor values from 1994 *EPA Draft Soil Screening Guidance.*

B) For Ionizing Organics, use Table 747-2 Values:
****NOTE**** these Koc Values (pH 6.8) and values for other organics are also available through the CLARC Chemical Specific Data Search****

Table 747-2
Predicted Soil Organic Carbon-Water Partitioning Coefficient (Koc) as a Function of pH: Ionizing Organics.

Hazardous Substance	Koc Value (ml/g)		
	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	2,385	1,597	298
2,4,6-Trichlorophenol	1,040	381	131

Source: 1996 *EPA Soil Screening Guidance: Technical Background Document.* The predicted Koc values in this table were derived using 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.

Distribution Coefficient for Metals:
****NOTE**** these Kd values and values for other metals are also available through the CLARC Chemical Specific Data Search****

Table 747-3
Metals Distribution Coefficients (Kd).

Hazardous Substance	Kd (L/kg)
Arsenic	29
Cadmium	6.7

Total Chromium	1,000
Chromium VI	19
Copper	22
Mercury	52
Nickel	65
Lead	10,000
Selenium	5
Zinc	62

Source: Multiple sources compiled by the Department of Ecology

4 phase partitioning model – (173-340-747(6):

[Equation 747-7]

$$\frac{M_T^i}{m_{soil}} = \frac{x_i S_i}{\rho_b}\left[\theta_w + K_{oc}^i f_{oc} \rho_b + H_{cc}^i \theta_a + \frac{GFW_i}{S_i}\rho_{NAPL}\theta_{NAPL}\right]$$

Where:

M^i_T = Total mass of each component in the system (mg). This value is derived from site-specific measurements.

m_{soil} = Total soil mass (kg).

x_i = Mole fraction (at equilibrium) of each component (dimensionless). This value is unknown and must be solved for.

S_i = Solubility of each component (mg/l). See Table 747-4 for petroleum hydrocarbons; see the scientific literature for other hazardous substances.

ρ_b = Dry soil bulk density (1.5 kg/l).

K^i_{oc} = Soil organic carbon-water partitioning coefficient for each component (l/kg). See Table 747-4 for petroleum hydrocarbons; see subsection (4)(b) of this section for other hazardous substances.

f_{oc} = Mass fraction of soil natural organic carbon (0.001 g soil organic/g soil).

H^i_{cc} = Henry's law constant for each component (dimensionless). See Table 747-4 for petroleum hydrocarbons; see subsection (4)(c) of this section for other hazardous substances.

GFW_i = Gram formula weight, or molecular weight of each component (mg/mol). See Table 747-4 for petroleum hydrocarbons; see the scientific literature for other hazardous substances.

θ_{NAPL} = Molar density of the mixture (mol/l). See Equation 747-8.

Component = For petroleum mixtures, this means the petroleum fractions, and organic hazardous substances with a reference dose; for other hazardous substances, this means each organic hazardous substance that is found in the NAPL.

Molar Density Equation - [Equation 747-8]

$$\rho_{NAPL} = \frac{\left[\sum x_i GFW_i \Big/ \left(\sum x_i GFW_i / \rho_i\right)\right]}{\sum x_i GFW_i} = \frac{1}{\sum (x_i GFW_i / \rho_i)}$$

Where:

GFW_i = Gram formula weight, or molecular weight of each component (mg/mol). See Table 747-4 for petroleum hydrocarbons; see the scientific literature for other hazardous substances.

x_i = Mole fraction (at equilibrium) of each component (dimensionless). This value is unknown and must be solved for.

ρ_i = Density of each component (mg/l). See Table 747-4 for petroleum hydrocarbons; see the scientific literature for other hazardous substances.

Component = For petroleum mixtures, this means the petroleum fractions plus organic hazardous substances with a reference dose; for other hazardous substances, this means each organic hazardous substance that is found in the NAPL.

Table 747-4
Petroleum EC Fraction Physical / Chemical Values.

Fuel Fraction	Equivalent Carbon Number[1]	Water Solubility[2] (mg/L)	Molecular Weight[3] (g/mol)	Henry's Constant[4] (cc/cc)	Gram Formula Weight[5] (mg/mol)	Density[6] (mg/l)	Soil Organic Carbon-Water Partitioning Coefficient Koc[7] (L/kg)
ALIPHATICS							
EC 5 – 6	5.5	36.0	81.0	33.0	81,000	670,000	800
EC > 6 – 8	7.0	5.4	100.0	50.0	100,000	700,000	3,800
EC > 8 – 10	9.0	0.43	130.0	80.0	130,000	730,000	30,200
EC > 10 – 12	11.0	0.034	160.0	120.0	160,000	750,000	234,000
EC > 12 – 16	14.0	7.6E-04	200.0	520.0	200,000	770,000	5.37E+06
EC > 16 – 21	19.0	1.3 E-06	270.0	4,900	270,000	780,000	9.55E+09
EC > 21 – 34	28.0	1.5E-11	400.0	100,000	400,000	790,000	1.07E+10
AROMATICS							
EC > 8 – 10	9.0	65.0	120.0	0.48	120,000	870,000	1,580
EC > 10 – 12	11.0	25.0	130.0	0.14	130,000	900,000	2,510
EC > 12 – 16	14.0	5.8	150.0	0.053	150,000	1,000,000	5,010
EC > 16 – 21	19.0	0.51	190.0	0.013	190,000	1,160,000	15,800
EC > 21 – 34	28.0	6.6E-03	240.0	6.7E-04	240,000	1,300,000	126,000
TPH COMPONENTS							
Benzene	6.5	1,750	78.0	0.228	78,000	876,500	62.0
Toluene	7.6	526.0	92.0	0.272	92,000	866,900	140.0

Ethylbenzene	8.5	169.0	106.0	0.323	106,000	867,000	204.0
Total Xylenes[8] (average of 3)	8.67	171.0	106.0	0.279	106,000	875,170	233.0
n-Hexane[9]	6.0	9.5	86.0	74.0	86,000	659,370	3,410
MTBE[10]		50,000	88.0	0.018	88,000	744,000	10.9
Naphthalenes	11.69	31.0	128.0	0.0198	128,000	1,145,000	1,191

Sources:

1 **Equivalent Carbon Number.** Gustafson, J.B. et al., *Selection of Representative TPH Fractions Based on Fate and Transport Considerations. Total Petroleum Hydrocarbon Criteria Working Group Series*, Volume 3 (1997) [hereinafter *Criteria Working Group*].
2 **Water Solubility.** For aliphatics and aromatics EC groups, *Criteria Working Group.* For TPH components except n-hexane and MTBE, *1996 EPA Soil Screening Guidance: Technical Background Document.*
3 **Molecular Weight.** *Criteria Working Group.*
4 **Henry's Constant.** For aliphatics and aromatics EC groups, *Criteria Working Group.* For TPH components except n-hexane and MTBE, *1996 EPA Soil Screening Guidance: Technical Background Document.*
5 **Gram Formula Weight (GFW).** Based on 1000 x Molecular Weight.
6 **Density.** For aliphatics and aromatics EC groups, based on correlation between equivalent carbon number and data on densities of individual hazardous substances provided in *Criteria Working Group.* For TPH components except n-hexane and MTBE, *1996 EPA Soil Screening Guidance: Technical Background Document.*
7 **Soil Organic Carbon-Water Partitioning Coefficient.** For aliphatics and aromatics EC groups, *Criteria Working Group.* For TPH components except n-hexane and MTBE, *1996 EPA Soil Screening Guidance: Technical Background Document.*
8 **Total Xylenes.** Values for total xylenes are a weighted average of m, o and p xylene based on gasoline composition data from the *Criteria Working Group* (m= 51% of total xylene; o = 28% of total xylene; and p = 21% of total xylene).
9 **n-Hexane.** For values other than density, *Criteria Working Group.* For the density value, *Hawley's Condensed Chemical Dictionary,* 11th ed., revised by N. Irving Sax and Richard J. Lewis (1987).
10 **MTBE.** *USGS Final Report on Fuel Oxygenates* (March 1996).

Table 747-5
Residual Saturation Screening Levels for TPH.

Fuel	Screening Level (mg/kg)
Weathered Gasoline	1,000
Middle Distillates (e.g., Diesel No. 2 Fuel Oil)	2,000
Heavy Fuel Oils (e.g., No. 6 Fuel Oil)	2,000
Mineral Oil	4,000
Unknown Composition or Type	1,000

Note: The residual saturation screening levels for petroleum hydrocarbons specified in Table 747-5 are based on coarse sand and gravelly soils; however, they may be used for any soil type. Screening levels are based on the presumption that there are no preferential pathways for NAPL to flow downward to ground water. If such pathways exist, more stringent residual saturation screening levels may need to be established.