XVI. Figures

Figure 1
Equation for Deriving Site-Specific Cleanup Target Levels for Carcinogens in Groundwater

The formula for calculation is:

$$GCTL(\mu g/L) = \frac{1\times10^{-6}\times BW\times CF}{CSF_o\times WC}$$

Parameter	Definition	Default Value
GCTL	groundwater cleanup target level (µg/L)	-
TR	target cancer risk (unitless)	1×10^{-6}
BW	average body weight (kg)	76.1
CF	conversion factor (µg/mg)	1000
CSF_o	oral cancer slope factor $(mg/kg\text{-}day)^{-1}$	chemical-specific [a]
WC	average water consumption rate (L/day)	2

[a]Toxicity values from IRIS, HEAST or other sources as provided in Table 5a for carcinogens.

Example: hexachloro-1,3-butadiene, $CSF_o = 0.078\ (mg/kg\text{-}day)^{-1}$

$$GCTL(\mu g/L) = \frac{1\times10^{-6}\times70.0\times1000}{0.078\times2} = \frac{0.070}{0.156}$$

GCTL = 0.4 µg/L

Figure 2
Equation for Deriving Site-Specific Cleanup Target Levels for Non-Carcinogens in Groundwater

The formula for calculation is:

$$GCTL(\mu g/L) = \frac{RfD_o \times BW \times RSC \times CF}{WC}$$

Parameter	Definition (units)	Default Value
GCTL	groundwater cleanup target level (µg/L)	-
BW	average body weight (kg)	70
RfD_o	oral reference dose (mg/kg-day)	chemical-specific [a]
RSC	relative source contribution (%)	20
CF	conversion factor (µg/mg)	1000
WC	average water consumption rate (L/day)	2

[a]Toxicity values from IRIS, HEAST, or other sources as provided in Table 5b for non-carcinogens.

Example: 2-chlorophenol, RfD_o = 0.005 mg/kg-day

$$GCTL(\mu g/L) = \frac{0.005 \times 70.0 \times 0.2 \times 1000}{2} = \frac{70.0}{2}$$

GCTL = 35 µg/L

Figure 3A
Equations Used to Calculate Freshwater or Marine Surface Water Cleanup Target Levels Based on Human Health Endpoints[a]

For non-carcinogens:

$$SWCTL\ (\mu g/L) = \frac{(RfD_o \times BW)}{(FI \times BCF)} \times CF$$

For carcinogens:

$$SWCTL(\mu g/L) = \frac{(TR \times BW)}{(CSF_o \times [FI \times BCF])} \times CF$$

Parameter	Definition	Default Value
SWCTL	Surface Water Cleanup Target Level (µg/L)	-
BW	body weight (kg)	70
RfD_o	oral reference dose (mg/kg-day)	chemical-specific [a]
FI	fish ingestion rate (kg/day)	0.0175 [b]
BCF	bioconcentration factor (mg toxicant/kg fish per mg toxicant/L water)	chemical-specific [c]
CF	conversion factor (µg/mg)	1000
TR	target cancer risk (unitless)	1×10^{-6}
CSF_o	oral cancer slope factor $(mg/kg\text{-}day)^{-1}$	chemical-specific [b]

[a]Toxicity values from IRIS, HEAST, or other sources as provided in Tables 5a and 5b.
[b]Equations and default fish consumption from USEPA (2000).
[c]Bioconcentration factors obtained from USEPA sources (USEPA 2000a) or calculated using the EPIWin software package.

Example: dimethylphenol, 3,4-, RfD_o = 0.001 mg/kg-day and BCF = 10.4 L/kg

$$SWCTL(\mu g/L) = \frac{0.001 \times 70}{0.0175 \times 10.4} \times 1000 = 380$$

Example: acrylonitrile, CSF_o = 0.54 $(mg/kg\text{-}day)^{-1}$ and BCF 30 L/kg

$$SWCTL(\mu g/L) = \frac{1 \times 10^{-6} \times 70}{0.54 \times 0.0175 \times 30} \times 1000 = 0.2$$

Figure 3B
Methodology Used to Calculate Freshwater and Marine Surface Water Criteria Based on Chronic Toxicity

Steps:

1. Select data with document codes of "C" or "M" from the USEPA Aquatic Toxicity Information Retrieval (AQUIRE) Database.

2. Take no action for substances for which insufficient data are retrieved to allow a reasonable choice of sensitive organisms.

3. Select only animal LC_{50} data, except that plant data should be selected in the case of substances in which plant EC_{50} values for growth or photosynthesis, or LC_{50} values for biomass, are several orders of magnitude lower than animal LC_{50} values.

4. Ignore data from salmonid fishes (salmon and freshwater trout).

5. Select the test and organism showing the greatest sensitivity to the toxicant. Extreme outliers should be ignored during this procedure, and several other types of data (such as data in which the endpoint or concentration had to be recalculated by the USEPA for entry into the database, and data based only on active ingredients) should also be removed from consideration if more clearly applicable data are available for sensitive organisms.

6. A factor of 5% (1/20) should be applied to the animal LC_{50} data to generate a surface water cleanup target level. If a plant LC_{50} or EC_{50} value was chosen, then that value becomes the guideline, without the use of a factor.

Figure 4

Model Equation for Developing Acceptable Risk-Based Concentrations in Soil.

Acceptable Soil Cleanup Target Levels for Carcinogens

$$SCTL = \frac{TR \times BW \times AT}{EF \times ED \times FC \times \left[\left(CSF_o \times IR_o \times RBA \times 10^{-6} kg/mg \right) + \left(CSF_d \times SA \times AF \times DA \times 10^{-6} kg/mg \right) + \left(CSF_i \times IR_i \times \left(\frac{1}{VF} + \frac{1}{PEF} \right) \right) \right]}$$

SCTL = Soil Cleanup Target Level
TR = target cancer risk (unitless)
BW = body weight (kg)
AT = averaging time (days)
EF = exposure frequency (days/yr)
ED = exposure duration (years)
RBA = relative bioavailability factor (unitless)
FC = fraction from contaminated source (unitless)
IR_o = ingestion rate, oral (mg/day)
SA = surface area of skin exposed (cm^2/day)
AF = adherence factor (mg/cm^2)
DA = dermal absorption (unitless)
IR_i = inhalation rate (m^3/day)
VF = volatilization factor (m^3/kg)
PEF = particulate emission factor (m^3/kg)
CSF = cancer slope factor $(mg/kg\text{-}day)^{-1}$
CSF_o = oral
CSF_d = dermal
CSF_i = inhalation

Sample SCTL Calculation for Direct Exposure (Aggregate Resident): benzene

$$SCTL = \frac{0.000001 \times 51.9 \times 25500}{350 \times 30 \times 1.0 \times \left[\left(0.055 \times 120 \times 1 \times 10^{-6} \right) + \left(\begin{matrix} 0.0611 \\ \times 4810 \times 0.1 \times 0.01 \times 10^{-6} \end{matrix} \right) + \left(0.0273 \times 12.2 \times \left(\frac{1}{3.3572 \times 10^3} + \frac{1}{1.24 \times 10^9} \right) \right) \right]}$$

$$\text{SCTL} = \frac{1.323}{10500 \times \left[\left(6.6 \times 10^{-6} \right) + \left(2.94 \times 10^{-7} \right) + \left(9.9210 \times 10^{-5} \right) \right]} = \frac{1.323}{10500 \times 1.061 \times 10^{-4}} = \frac{1.323}{1.11405} = 1.2 mg/kg$$

Given:

TR = 0.000001 (unitless)
BW = 51.9 kg
AT = 25500 days
RBA = 1.0
CSF_o = 0.055 $(mg/kg\text{-}day)^{-1}$
CSF_d = 0.0611 $(mg/kg\text{-}day)^{-1}$
CSF_i = 0.0273 $(mg/kg\text{-}day)^{-1}$
EF = 350 days/year
ED = 30 years
FC = 1.0 (unitless)
IRo = 120 mg/day
SA = 4810 cm^2
AF = 0.1 mg/cm^2
DA = 0.01 (unitless)
IRi = 12.2 m^3/day
VF = 3.3572 x 10^3 m^3/kg
PEF = 1.24 x 10^9 m^3/kg

Note: All calculations carried out to 18 decimal places. For simplicity of demonstration, the calculated values above are not shown to the same precision. Final SCTL value is rounded to two significant figures if >1 and to one significant figure if <1.

Figure 5

Model Equation for Developing Acceptable Risk-Based Concentrations in Soil.

Acceptable Soil Cleanup Target Levels for Non-Carcinogens

$$SCTL = \frac{THI \times BW \times AT}{EF \times ED \times FC \times \left[\left(\frac{1}{RfD_o} \times IR_o \times RBA \times 10^{-6}\,kg/mg\right) + \left(\frac{1}{RfD_d} \times SA \times AF \times DA \times 10^{-6}\,kg/mg\right) + \left(\frac{1}{RfD_i} \times IR_i \times \left(\frac{1}{VF} + \frac{1}{PEF}\right)\right)\right]}$$

SCTL = Soil Cleanup Target Level
THI = target hazard index (unitless)
BW = body weight (kg)
AT = averaging time (days)
EF = exposure frequency (days/yr)
ED = exposure duration (years)
RBA = relative bioavailability factor (unitless)
FC = fraction from contaminated source (unitless)
IR_o = ingestion rate, oral (mg/day)
SA = surface area of skin exposed (cm^2/day)
AF = adherence factor (mg/cm^2)
DA = dermal absorption (unitless)
IR_i = inhalation rate (m^3/day)
VF = volatilization factor (m^3/kg)
PEF = particulate emission factor (m^3/kg)
RfD = reference dose (mg/kg-day)
RfD_o = oral
RfD_d = dermal
RfD_i = inhalation

Sample SCTL Calculation for Direct Exposure (Child Resident): fluorene

$$SCTL = \frac{1.0 \times 16.8 \times 2190}{350 \times 6 \times 1.0 \times \left[\left(\frac{1}{0.04} \times 200 \times 1 \times 10^{-6}\,kg/mg\right) + \left(\frac{1}{0.02} \times 2960 \times 0.2 \times 0.01 \times 10^{-6}\,kg/mg\right) + \left(\frac{1}{0.02} \times 8.1 \times \left(\frac{1}{2.80802 \times 10^{5}} + \frac{1}{1.24 \times 10^{9}}\right)\right)\right]}$$

$$SCTL = \frac{36792}{2100 \times \left[\left(5.00 \times 10^{-3}\right) + \left(2.96 \times 10^{-4}\right) + \left(1.4426 \times 10^{-3}\right)\right]} = \frac{36792}{2100 \times 6.7386 \times 10^{-3}} = \frac{36792}{14.151} = 2600\ mg/kg\ \ddagger$$

Given:

THI = 1.0 (unitless)
BW = 16.8 kg
AT = 2190 days
RBA = 1.0
RfD_o = 0.04 mg/kg-day
RfD_d = 0.02 mg/kg-day
RfD_i = 0.02 mg/kg-day
EF = 350 days/year
ED = 6 years
FC = 1.0 (unitless)
IRo = 200 mg/day
SA = 2960 cm^2
AF = 0.2 mg/cm^2
DA = 0.01 (unitless)
IRi = 8.1 m^3/day
VF = 2.80802 x 10^5 m^3/kg
PEF = 1.24 x 10^9 m^3/kg

Note: All calculations carried out to 18 decimal places. For simplicity of demonstration, the calculated values above are not shown to the same precision. Final SCTL value is rounded to two significant figures if >1 and to one significant figure if <1.

Figure 6
Derivation of the Particulate Emission Factor [a]

$$PEF(m^3/kg) = Q/C \times \frac{3600(s/h)}{0.036 \times (1-V) \times (U_m/U_t)^3 \times F(x)}$$

Parameter	Definition (units)	Default
PEF	particulate emission factor (m^3/kg)	1.241005×10^9
Q/C	inverse of mean conc. at center of a 0.5-acre-square source (g/m^2-s per kg/m^3)	85.61 [b]
V	fraction of vegetative cover (unitless)	0.5 (50%) [c]
U_m	mean annual windspeed (m/s)	4.69 [c]
U_t	equivalent threshold value of windspeed at 7 m (m/s)	11.32
F(x)	function dependent on U_m/U_t, (unitless) [d]	0.194

[a] Equation taken from USEPA (1996b).
[b] Based on Q/C Value for Zone IX (Miami, FL) as listed in USEPA (1996b). The default is for 0.5 acre sites with undisturbed soil. Site-specific PEFs must be calculated for sites with contaminated areas which are significantly larger in size or if warranted based on site-specific conditions.
[c] Value may be substituted with documented, DERM accepted site-specific information.
[d] USEPA (1985).

Note: All calculations carried out to 18 decimal places. For simplicity of demonstration, the calculated values below are not shown to the same precision.

Calculation of PEF based on Zone IX Q/C Value:

$$PEF(m^3/kg) = 85.61 \times \frac{3600(s/h)}{0.036 \times (1-0.5) \times (4.69/11.32)^3 \times 0.194)}$$

Figure 7
Equation Used for the Determination of the Volatilization Factor [a]

$$VF = Q/C \times CF \times \frac{(3.14 \times D_A \times T)^{1/2}}{2 \times \rho_b \times D_A}$$

$$D_A = \frac{\left[\left(\theta_a^{10/3} D_i H' + \theta_w^{10/3} D_w\right) / n^2\right]}{\rho_b K_d + \theta_w + \theta_a H'}$$

Where:

Model Parameters (Units)		Default Value
VF	volatilization factor (m^3/kg)	-
D_A	apparent diffusivity (cm^2/s)	-
CF	conversion factor (m^2/cm^2)	10^{-4}
Q/C	inverse of the mean concentration (g/m^2-s per kg/m^3)	85.61[b]
T	exposure interval (s)	ED x 3.1536×10^7 s/yr
ED	exposure duration (years)	Exposure-specific [d]
η	total soil porosity (L_{pore}/L_{soil})	1- (ρ_b/ρ_s) [e]
ω	average soil moisture content (g_{water}/g_{soil})	0.1 (10%) [c]
ρ_b	dry soil bulk density (g/cm^3)	1.5 [e]
ρ_s	soil particle density (g/cm^3)	2.65
θ_a	air-filled soil porosity (L_{air}/L_{soil})	$\eta - \theta_w$
θ_w	water-filled soil porosity (L_{water}/L_{soil})	$\omega\rho_b$
K_d	soil-water partition coefficient L/kg)	$K_{oc} \times f_{oc}$
D_i	diffusivity in air (cm^2/s)	Chemical-specific [c]
D_w	diffusivity in water (cm^2/s)	Chemical-specific [c]
H	Henry's Law constant (atm-m^3/mol)	Chemical-specific [c]
H'	Henry's Law constant (unitless)	H x 41
K_{oc}	soil-organic carbon partition coefficient (L/kg)	Chemical-specific [c]
f_{oc}	organic carbon content of soil (g/g)	0.006 (0.6%)‡

[a] Model equation taken from USEPA (1996b).
[b] Value derived for an undisturbed 0.5-acre site in Miami, FL (USEPA 1996b). Site-specific PEFs must be calculated for disturbed sites, or sites significantly larger than 0.5 acres.
[c] Listed in Table 4.
[d] See Table 3 for exposure durations for the child, aggregate resident, and worker exposure scenarios.
[e] Value may be substituted with appropriate site-specific information upon approval by the DERM.

Sample VF Calculation for Benzene Aggregate Resident Exposure

Note: All calculations carried out to 18 decimal places. For simplicity of demonstration, the calculated values below are not shown to the same precision.

Given: $D_i = 0.088$ cm^2/s
$D_w = 1.02 \times 10^{-5}$ cm^2/s
H' = 0.22755000
T = 9.460800×10^8 s
K_{oc} = 59 L/kg
K_d = 0.35400 L/kg

Then:

$$D_A = \frac{\left[\left(1.504996 \times 10^{-2} \times 0.088 \times 2.27550 \times 10^{-1}\right) + \left(1.793236 \times 10^{-3} \times 9.80 \times 10^{-6}\right)\right] / 1.883232 \times 10^{-1}}{\left(1.5 \times 3.3540 \times 10^{-1}\right) + \left(0.15\right) + \left(0.2839362 \times 0.2755\right)}$$

$$= \frac{1.6 \times 10^{-3}}{7.59244 \times 10^{-1}} \text{cm}^2/\text{s} = 2.146 \times 10^{-3} \text{cm}^2/\text{s}$$

And:

$$VF = 85.61 \times 10^{-4} \times \frac{\left(3.14 \times 2.1462 \times 10^{-3} \times 9.46080 \times 10^{8}\right)^{0.5}}{2 \times 1.5 \times 2.1462 \times 10^{-3}}$$

$$= \frac{2.1617 \times 10^{1}}{6.4390 \times 10^{-3}} = 3.3572 \times 10^{3} \left(\frac{\text{m}^3}{\text{kg}}\right)$$

Figure 8
Equation for the Determination of Soil Cleanup Target Levels (SCTLs)
Based on Leachability

$$SCTL(mg/kg) = GCTL(\mu g/L) \times CF(mg/\mu g) \times DF \times \left[K_{oc}(L/kg) \times f_{oc}(g/g) + \frac{\theta_w (L_{water}/L_{soil}) + \theta_a (L_{air}/L_{soil}) \times H'}{\rho_b (g/cm^3)} \right]$$

Parameter	Definition (units)	Variables and Default
GCTL	groundwater cleanup target level (µg/L)	table-specific value [1]
CF	conversion factor (mg/µg)	0.001
DAF	dilution attenuation factor (unitless)	20 [2]
K_{oc}	soil-organic carbon partition coefficient (L/kg)	chemical-specific value [3]
f_{oc}	fraction organic carbon in soil (g/g)	0.002 [4]
θ_w	water-filled soil porosity (L_{water}/L_{soil})	$\omega\rho_b$
θ_a	air-filled soil porosity (L_{air}/L_{soil})	$\eta - \theta_w$
H	Henry's Law constant (atm-m^3/mol)	chemical-specific value [3]
H'	Henry's Law constant (unitless)	H × 41
ρ_b	dry soil bulk density (g/cm^3)	1.5 [4]
ω	average soil moisture content (g_{water}/g_{soil})	0.2 (20%) [4]
η	total soil porosity (L_{pore}/L_{soil})	$1-(\rho_b/\rho_s)$
ρ_s	soil particle density (g/cm^3)	2.65

[1] Groundwater Cleanup Target Levels (see Table 1).

[2] If the site is significantly larger than 0.5 acres or if warranted by site-specific conditions (such as a shallow water table), a lower DAF may be required.

[3] Listed in Table 4.

[4] Value may be substituted with appropriate site-specific information upon approval by the DERM. It should be noted that the default values for f_{oc}, ω, and θ_w in the calculation of leachability-based SCTLs differ from those used to calculate the VF and C_{sat} as per guidance in USEPA (1996b).

Note: All calculations carried out to 18 decimal places. For simplicity of demonstration, the calculated values below are not shown to the same precision. Final SCTL is rounded to two significant figures if >1 and to one significant figure if <1.

Sample SCTL calculation for benzene migration into groundwater:

Given: GCTL = 1 µg/L
K_{oc} = 59 L/kg
H' = 0.227550

Then:

$$SCTL = 1.0 \times 0.001 \times 20 \times \left[59 \times 0.002 + \frac{0.3 + (0.13396 \times 0.22755)}{1.5} \right] =$$

$$SCTL = 0.007 \text{ mg/kg}$$

Figure 9
Equation[a] Used for the Determination of C_{sat}

$$C_{sat} = \frac{S}{\rho_b}\left(K_d \rho_b + \theta_w + H' \theta_a\right)$$

Parameter	Definition (Units)	Default Value
C_{sat}	soil saturation concentration (mg/kg)	-
S	solubility in water (mg/L)	chemical-specific [b]
ρ_s	soil particle density (g/cm^3)	2.65
ρ_b	dry soil bulk density(g/cm^3)	1.5 [c]
η	total soil porosity (L_{pore}/L_{soil})	$1 - (\rho_b/\rho_s)$
θ_a	air-filled soil porosity (L_{air}/L_{soil})	$\eta - \theta_w$
θ_w	water-filled soil porosity (L_{water}/L_{soil})	$\omega\rho_b$
K_d	soil-water partition coefficient (cm^3/g)	$K_{oc} \times f_{oc}$
ω	average soil moisture content (kg_{water}/kg_{soil})	0.1 (10%) [c]
H	Henry's Law constant (atm-m^3/mol)	chemical-specific [b]
H'	Henry's Law constant (unitless)	H × 41
K_{oc}	soil-organic carbon partition coefficient (L/kg)	chemical-specific [b]
f_{oc}	fraction organic carbon in soil (g/g)	0.006 (0.6%) [c]

[a] Model equation taken from USEPA (1996b).
[b] Listed in Table 4.
[c] Value may be substituted with appropriate site-specific information upon approval by the DERM.

Note: All calculations carried out to 18 decimal places. For simplicity of demonstration, the calculated values below are not shown to the same precision. C_{sat} values used as SCTLs are rounded to two significant figures if > 1 and to one significant figure if < 1.

Sample C_{sat} Calculation for ethylbenzene

Given:
$S = 169$ mg/L
$K_d = 2.178$ L/kg
$K_{oc} = 363$ L/kg
$H' = 0.32308$

Then:

$$C_{sat} = \frac{169}{1.5}\left((2.178 \times 1.5) + (0.15) + (0.32308 \times 0.2839362)\right)$$
$$C_{sat} = 112.6667 \times 3.5087$$
$$C_{sat} = 400 \text{ mg/kg}$$

XVII. Principal Table