

Appendix A

Models/Equations for Estimating Tier 3A and Tier 3B Target Levels within the KRBCA Process

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ESTIMATION OF RISK-BASED SCREENING LEVELS

The following equations were used to estimate risk-based levels for carcinogenic and non-carcinogenic effects respectively, for different routes of exposure. For Tier 3A levels, these equations were solved using generic, default, conservative values presented in Tables 3-1 through 3-5. The same equations shall be solved using site-specific data to develop Tier 3B target levels. The use of site-specific data must be justified based on site-specific measurements or other considerations.

By changing the exposure factors these equations can be used for the four receptors of concern; resident child, resident adult, commercial worker, and construction worker.

A.1 INHALATION OF VAPOR EMISSIONS

The screening level concentration in air for this route for carcinogenic effects is estimated using:

$$RBSL_a = \frac{TR * BW * AT_c * 365}{IR_a * ED * EF * SF_i} \quad (A-1)$$

where:

$RBSL_a$	=	Risk-based screening level in air [mg/m^3]
TR	=	Target risk or the increased chance of developing cancer over a lifetime due to exposure to a chemical [--]
BW	=	Body weight [kg]
AT_c	=	Averaging time for carcinogens [years] (Note 365 converts years to days)
IR_a	=	Inhalation rate of air [m^3/day] = IR [m^3/hr]x ET [hr/day]
ET	=	Exposure time [hr/day]
ED	=	Exposure duration [years]
EF	=	Exposure frequency [days/year]
SF_i	=	The chemical-specific slope or potency factor for inhalation [$(\text{mg}/\text{kg}\text{-day})^{-1}$]

The screening level concentration in air for inhalation for noncarcinogenic effects is estimated using the following equation:

$$RBSL_a = \frac{THQ * BW * AT_N * 365 * RfD_i}{IR_a * ED * EF} \quad (A-2)$$

where:

$RBSL_a$	=	Risk-based screening level in air [mg/m^3]
RfD_i	=	The chemical-specific reference dose for inhalation [$(\text{mg}/\text{kg}\text{-day})$]
THQ	=	Target hazard index for individual constituents [--]
AT_N	=	Averaging time for non-carcinogens [years]
IR_a	=	Inhalation rate of air [m^3/day]
	=	$IR [\text{m}^3/\text{hr}] \times ET [\text{hr}/\text{day}]$
ET	=	Exposure time [hr/day]
ED	=	Exposure duration [years]
EF	=	Exposure frequency [days/year]

Note that Equation A-1 and A-2 are used to calculate the air concentration for both indoor and outdoor air, by changing the input parameter.

A.2 ACCIDENTAL INGESTION OF SOIL

The screening level soil concentration protective of a receptor for carcinogenic effects exposed to chemicals by ingestion of soil is estimated using:

$$RBSL_{s\ ing} = \frac{TR * BW * AT_c * 365}{EF * ED [SF_o * 10^{-6} IR_{soil} * RAF_o]} \quad (A-3)$$

where:

$RBSL_{s\ ing}$	=	Risk based screening level in soil for ingestion [mg/kg]
TR	=	Target risk or the increased chance of developing cancer over a lifetime due to exposure to a chemical [--]
BW	=	Body weight [kg]
AT_c	=	Averaging time for carcinogens [years] (Note 365 converts years to days)
SF_o	=	Oral cancer slope factor [$(\text{mg}/\text{kg}\text{-day})^{-1}$]
ED	=	Exposure duration [years]
EF	=	Exposure frequency [days/year]
IR_{soil}	=	Soil ingestion rate [mg/day]
RAF_o	=	Oral relative absorption factor [--]

For non-carcinogenic effects, the screening level concentration in soil protective of a receptor exposed to chemicals from ingestion of soil is estimated using equation A-4.

$$RBSL_{s\ ing} = \frac{THQ * BW * AT_N * 365}{EF * ED \left[\frac{10^{-6} * (IR_{soil} * RAF_o)}{RfD_o} \right]} \quad (A-4)$$

Where:

$RBSL_{sing}$	=	Risk based screening level in soil for ingestion [mg/kg]
RfD_o	=	The chemical-specific reference dose for ingestion [(mg/kg-day)]
THQ	=	Target hazard index for individual constituents [--]
BW	=	Body weight [kg]
AT_N	=	Averaging time for non-carcinogens [years]
ED	=	Exposure duration [years]
EF	=	Exposure frequency [days/year]
IR_{soil}	=	Soil ingestion rate [mg/day]
RAF_o	=	Oral relative absorption factor [--]

A3. DERMAL CONTACT WITH SOIL

The screening level soil concentration protective of a receptor for carcinogenic effects exposed to chemicals by dermal contact with soil is estimated using:

$$RBSL_{s_{der}} = \frac{TR * BW * AT_c * 365}{EF * ED [SF_o * 10^{-6} SA * M * RAF_d]} \quad (A-5)$$

where:

$RBSL_{s_{der}}$	=	Risk based screening level for soil for dermal contact [mg/kg]
TR	=	Target risk or the increased chance of developing cancer over a lifetime due to exposure to a chemical [--]
BW	=	Body weight [kg]
AT_c	=	Averaging time for carcinogens [years] (Note 365 converts years to days)
SF_o	=	Oral cancer slope factor [(mg/kg-day) ⁻¹]
SA	=	Skin surface area exposed to soil [cm ² /day]
RAF_d	=	Dermal relative absorption factor [--]
M	=	Soil to skin adherence factor, soil specific factor [mg/cm ²]
ED	=	Exposure duration [years]
EF	=	Exposure frequency [days/year]

For non-carcinogenic effects, the screening level concentration in soil protective of a receptor exposed to chemicals from dermal contact with soil is estimated using equation A-6.

$$RBSL_{s_{der}} = \frac{THQ * BW * AT_N * 365 * RfD_o}{EF * ED * 10^{-6} * SA * M * RAF_d} \quad (A-6)$$

where:

$RBSL_{s_{der}}$	=	Risk based screening level for soil for dermal contact [mg/kg]
RfD_o	=	The chemical-specific reference dose for ingestion [(mg/kg-day)]
THQ	=	Target hazard index for individual constituents [--]
BW	=	Body weight [kg]

AT_N	=	Averaging time for non-carcinogens [years]
ED	=	Exposure duration [years]
EF	=	Exposure frequency [days/year]
SA	=	Skin surface area exposed to soil [cm ² /day]
RAF_d	=	Dermal relative absorption factor [--]
M	=	Soil to skin adherence factor, soil specific factor [mg/cm ²]

A.4 SOIL CONCENTRATIONS PROTECTIVE OF GROUNDWATER

The soil concentration protective of an exposure well is:

$$RBSL_{sgw} = \frac{RBSL_w * DAF}{LF_{sw}} \quad (A-7)$$

where:

$RBSL_{sgw}$	=	Risk-based screening level in soil protective of groundwater [mg/kg-soil]
$RBSL_w$	=	Risk-based screening level of water at the point of exposure calculated using equation A-8 or A-9 [mg/l]
LF_{sw}	=	Leaching factor which accounts for (i) the equilibrium conversion factor to convert the soil concentration to leachate concentration and (ii) the mixing of the leachate with the groundwater directly beneath the site [(mg/l)/(mg/kg)]
DAF	=	The dilution attenuation factor for the migration of the dissolved phase from directly beneath the source to the exposure point

Note the screening level concentration in water at the POE is either the MCL or if an MCL does not exist is the value calculated using equation A-8.

$$RBSL_w = \frac{TR * BW * AT_c * 365}{IR_w * ED * EF * SF_o} \quad (A-8)$$

where:

$RBSL_w$	=	Risk-based screening level of water at the point of exposure [mg/l]
IR_w	=	Ingestion rate of water [l/day]
TR	=	Target risk or the increased chance of developing cancer over a lifetime due to exposure to a chemical [--]
BW	=	Body weight [kg]
AT_c	=	Averaging time for carcinogens [years] (Note 365 converts years to days)
SF_o	=	Oral cancer slope factor [(mg/kg-day) ⁻¹]
ED	=	Exposure duration [years]

EF = Exposure frequency [days/year]

In Equation A-7, $RBSL_w$ for non-carcinogenic effects is calculated as:

$$RBSL_w = \frac{THQ * BW * AT_N * 365 * RfD_o}{IR_w * ED * EF} \quad (A-9)$$

where:

$RBSL_w$ = Risk-based screening level of water at the point of exposure [mg/l]
 IR_w = Ingestion rate of water [l/day]
 THQ = Target hazard index for individual constituents [--]
 BW = Body weight [kg]
 AT_N = Averaging time for non-carcinogens [years]
 RfD_o = The chemical-specific reference dose for ingestion [(mg/kg-day)]
 ED = Exposure duration [years]
 EF = Exposure frequency [days/year]

In Equation A-7, LF_{SW} is calculated as:

$$LF_{SW} = \frac{\rho_s}{(\theta_{ws} + K_s * \rho_s + H * \theta_{as}) * \left(1 + \frac{U_{gw} * \delta_{gw}}{I * L_{mz}} \right)} \quad (A-10)$$

where:

LF_{SW} = Leaching factor which accounts for (i) the equilibrium conversion factor to convert the soil concentration to leachate concentration and (ii) the mixing of the leachate with the groundwater directly beneath the site [(mg/l)/(mg/kg)]
 ρ_s = Soil bulk density [g-soil/cm³-soil]
 θ_{ws} = Volumetric water content of soil in the impacted zone [cm³-H₂O/cm³-soil]
 K_s = Chemical specific soil-water partition coefficient [g-H₂O/g-soil]
 H = Dimensionless form of the Henry's Law Constant [(cm³-H₂O)/(cm³-air)]
 θ_{as} = Volumetric air content in the impacted zone soil [cm³-air/cm³-soil]
 U_{gw} = Groundwater Darcy velocity [cm/s]
 δ_{gw} = Groundwater mixing zone thickness [cm]
 I = Infiltration rate of water through soil [cm/yr]
 L_{mz} = Length of source area parallel to the groundwater flow direction (groundwater mixing zone length) [cm]

In equation A-7, DAF is estimated using Domenico's steady-state model along the centerline of the plume:

$$DAF^{-1} = \frac{C_x}{C_{source}} = \exp\left[\frac{x}{2\alpha_x}\left(1 - \sqrt{1 + \frac{4\lambda\alpha_x}{v}}\right)\right] \times \operatorname{erf}\left(\frac{W_g}{4\sqrt{\alpha_y x}}\right) \times \operatorname{erf}\left(\frac{\delta_{gw}}{2\sqrt{\alpha_z x}}\right) \quad (A-11)$$

where:

- C_x = Concentration at distance "x" feet along the centerline of the plume [mg/L]
- C_{source} = Concentration at the downgradient edge of the impacted zone [mg/L]
- W_g = Source width perpendicular to the flow in the horizontal direction (groundwater mixing zone width) [feet]
- δ_{gw} = Groundwater mixing zone thickness [feet]
- erf = The error function
- v = Retarded seepage velocity [feet/day]
- λ = First order bio-decay rate [day^{-1}]
- x = Distance to the exposure point from the source [feet]
- α_x = Longitudinal dispersivity [feet] ($= x/10$)
- α_y = Transverse dispersivity [feet] ($= \alpha_x/3$)
- α_z = Vertical dispersivity [feet] ($= \alpha_x/20$)

Retarded seepage velocity, $v = \frac{K \times i}{R \times \theta_T}$

where:

- K = Hydraulic conductivity [cm/year]
- i = Hydraulic gradient [--]
- R = Retardation factor [--]
- θ_T = Total porosity [cm^3 voids/ cm^3 soil]

Retardation factor, $R = 1 + \frac{\rho_s \times K_s}{\theta_T}$

where:

- ρ_s = Dry bulk density of soil [g/cm^3]
- K_s = Chemical specific soil-water partition coefficient [$\text{g-H}_2\text{O}/\text{g-soil}$]
- = $f_{oc} \times K_{oc}$
- f_{oc} = Fractional organic carbon content [$\text{g C}/\text{g soil}$]
- K_{oc} = Carbon-water partition coefficient [$\text{cm}^3\text{-water}/\text{g-C}$]
- θ_T = Total porosity [cm^3 voids/ cm^3 soil]

Under steady-state conditions without bio-decay, Equation A-11 reduces to:

$$DAF^{-1} = \frac{C_x}{C_{source}} = \left(\operatorname{erf} \left[\frac{W_g}{4\sqrt{\alpha_{yx}}} \right] \right) \left(\operatorname{erf} \left[\frac{\delta_{gw}}{2\sqrt{\alpha_{zx}}} \right] \right) \quad (A-12)$$

A.5 OUTDOOR INHALATION OF VAPORS AND PARTICULATES, DERMAL CONTACT AND INGESTION OF CHEMICALS IN SURFICIAL SOIL

Note this equation is also used for the construction worker where the surficial soil depth is equivalent to the depth of construction.

The screening level soil concentration protective of a receptor simultaneously exposed to chemicals from these three routes of exposure for carcinogenic effects is estimated using:

$$RBSL_s = \frac{TR * BW * AT_c * 365}{EF * ED [(SF_o * 10^{-6} (IR_{soil} + SA * M * RAF_d)) + (SF_i * IR_a (1/VF_s + 1/PEF))]} \quad (A-13)$$

where:

$RBSL_s$	=	Risk-based screening level of soil for the combined soil pathway [mg/kg]
TR	=	Target risk or the increased chance of developing cancer over a lifetime due to exposure to a chemical [--]
BW	=	Body weight [kg]
AT_c	=	Averaging time for carcinogens [years] (Note 365 converts years to days)
ED	=	Exposure duration [years]
EF	=	Exposure frequency [days/year]
SF_o	=	Oral cancer slope factor [(mg/kg-day) ⁻¹]
SF_i	=	Inhalation cancer slope factor [(mg/kg-day) ⁻¹]
IR_{soil}	=	Soil ingestion rate [mg/day]
IR_a	=	Inhalation rate of air [m ³ /day]
SA	=	Skin surface area [cm ² /day]
RAF_d	=	Dermal relative absorption factor [--]
M	=	Soil to skin adherence factor [mg/cm ²]
PEF	=	Particulate emission factor [m ³ /kg]
VF_s	=	Volatilization factor for vapor emissions from surficial soil to ambient air [m ³ /kg]

In Equation A-13, the VF_s factor accounts for the volatilization of vapors from soil to ambient air and is calculated using Equation A-14 (below).

$$VF_s = \frac{Q}{C} \frac{\sqrt{3.14 * D_A * \tau}}{2 * \rho_s * D_A} * 10^{-4} \quad (A-14)$$

where:

- VF_s = Volatilization factor for vapor emissions from surficial soil to ambient air [m^3/kg]
- Q/C = Inverse of the mean concentration at the center of square source [$(\text{g}/\text{m}^2\text{-s}) / (\text{kg}/\text{m}^3)$]
- D_A = Apparent diffusivity [cm^2/s]
- τ = Averaging time for vapor flux [s]
- ρ_s = Soil bulk density [$\text{g-soil}/\text{cm}^3\text{-soil}$]

In Equation A-13, the PEF factor accounts for the emission of particulates from soil to ambient air and is calculated using Equation A-15 (below).

$$PEF = \frac{Q}{C} \times \frac{3600}{0.036 \times (1-V) \times \left(\frac{U_m}{U_t}\right)^3 \times F(x)} \quad (A-15)$$

where:

- Q/C = Inverse of the mean concentration at the center of square source [$(\text{g}/\text{m}^2\text{-s}) / (\text{kg}/\text{m}^3)$]
- V = Fraction of vegetative cover [--]
- U_m = Mean annual wind speed [m/s]
- U_t = Equivalent threshold value of wind speed at 7 m [m/s]
- $F(x)$ = Function dependent on U_m/U_t derived using Cowherd (1985) [--]
- 3600 = seconds/hour

In Equation A-14, the apparent diffusion coefficient D_A is calculated as:

$$D_A = \frac{[\theta_{as}^{3.33} * D^a * H + \theta_{ws}^{3.33} * D^w]}{(\rho_s * K_s + \theta_{ws} + \theta_{as} * H) \theta_T^2} \quad (A-16)$$

- D_A = Apparent diffusivity [cm^2/s]
- D^a = Diffusivity in air [cm^2/s]

D^w	=	Diffusivity in water [cm^2/s]
H	=	Chemical-specific Henry's Law constant [$(\text{cm}^3\text{-H}_2\text{O})/(\text{cm}^3\text{-air})$]
θ_{ws}	=	Volumetric water content in vadose zone soils [$\text{cm}^3\text{-H}_2\text{O}/\text{cm}^3\text{-soil}$]
K_s	=	Solid-water sorption coefficient [$\text{g-H}_2\text{O}/\text{g-soil}$]
ρ_s	=	Soil bulk density [$\text{g-soil}/\text{cm}^3\text{-soil}$]
θ_{as}	=	Volumetric air content in the vadose zone soils [$\text{cm}^3\text{-air}/\text{cm}^3\text{-soil}$]
θ_T	=	Total soil porosity [$\text{cm}^3\text{-air}/\text{cm}^3\text{-soil}$]

The screening level concentration in soil protective of a receptor simultaneously exposed to chemicals from these routes of exposure for noncarcinogenic effects is estimated using:

$$RBSL_s = \frac{THQ * BW * AT_N * 365}{EF * ED * \left[\frac{10^{-6} * (IR_{soil} + SA * M * RAF_d)}{RfD_o} + \frac{(IR_a * (1/VF_s + 1 / PEF))}{RfD_i} \right]} \quad (A-17)$$

where:

$RBSL_s$	=	Risk-based screening level of soil for the combined soil pathway [mg/kg]
THQ	=	Target hazard index for individual constituents [--]
BW	=	Body weight [kg]
AT_N	=	Averaging time for non-carcinogens [years]
ED	=	Exposure duration [years]
EF	=	Exposure frequency [days/year]
RfD_o	=	The chemical-specific reference dose for ingestion [(mg/kg-day)]
RfD_i	=	The chemical-specific reference dose for inhalation [(mg/kg-day)]
IR_{soil}	=	Soil ingestion rate [mg/day]
IR_a	=	Inhalation rate of air [m^3/day]
SA	=	Skin surface area [cm^2/day]
RAF_d	=	Dermal relative absorption factor [--]
M	=	Soil to skin adherence factor [mg/cm^2]
PEF	=	Particulate emission factor [m^3/kg]
VF_s	=	Volatilization factor for vapor emissions from surficial soil to ambient air [m^3/kg]

Note that the factors VF_s and PEF are estimated using Equations A-14 and A-15.

A.6 SUBSURFACE SOIL CONCENTRATIONS PROTECTIVE OF INDOOR AIR VAPOR INHALATION

Consider vapor emissions from subsurface soils to enclosed air space. The screening level for indoor inhalation of subsurface soil emissions is estimated using:

$$RBTL_{si} = \frac{RBTL_a}{VF_{seep}} \quad (A-18)$$

where:

- $RBTL_{si}$ = Risk-based target level for indoor inhalation of vapors from subsurface soils [mg/kg-soil]
 $RBTL_a$ = Risk-based target level for indoor inhalation of air [mg/m³-air]
 VF_{seep} = Volatilization factor from subsurface soil to indoor (enclosed space) air [(mg/m³-air)/(mg/kg-soil)]

$RBTL_a$ varies depending upon whether the chemical is a carcinogen, or a non-carcinogen, as calculated by Equations A-1 or A-2.

VF_{seep} is calculated as:

$$VF_{seep} = \frac{\frac{H \times \rho_s}{[\theta_{ws} + K_s \times \rho_s + H \times \theta_{as}]} \times \left[\frac{D_s^{eff} / L_s}{ER \times L_b} \right]}{1 + \left[\frac{D_s^{eff} / L_s}{ER \times L_b} \right] + \left[\frac{D_s^{eff} / L_s}{(D_{crack}^{eff} / L_{crack}) \times \eta} \right]} \times 10^3 \quad (A-19)$$

where:

- VF_{seep} = Volatilization factor from subsurface soil to indoor (enclosed space) air [(mg/m³-air)/(mg/kg-soil)]
 H = Chemical-specific Henry's Law constant [(cm³-H₂O)/(cm³-air)]
 θ_{ws} = Volumetric water content in vadose zone soils [cm³-H₂O/cm³-soil]
 K_s = Solid-water sorption coefficient [g-H₂O/g-soil]
 ρ_s = Soil bulk density [g-soil/cm³-soil]
 θ_{as} = Volumetric air content in the vadose zone soils [cm³-air/cm³-soil]
 L_s = Depth to subsurface soil sources [cm]
 L_b = Enclosed space volume/infiltration area ratio [cm]
 L_{crack} = Enclosed space foundation or wall thickness [cm]
 ER = Enclosed space air exchange rate [1/s]
 D_s^{eff} = Effective diffusion coefficient in soil based on vapor-phase concentration [cm²/s]
 D_{crack}^{eff} = Effective diffusion coefficient through foundation cracks [cm²/s]
 η = Areal fraction of cracks in foundation and/or walls [cm²-cracks/ cm²-total area]
 10^3 = Conversion factor [(cm³-kg)/(m³-g)]

D_s^{eff} and D_{crack}^{eff} may be calculated using equations A-20 and A-21.

$$D_s^{eff} = D^a \times \frac{\theta_{as}^{3.33}}{\theta_T^{2.0}} + D^w \times \frac{1}{H} \times \frac{\theta_{ws}^{3.33}}{\theta_T^{2.0}} \quad (A-20)$$

$$D_{crack}^{eff} = D^a \times \frac{\theta_{acrack}^{3.33}}{\theta_T^{2.0}} + D^w \times \frac{1}{H} \times \frac{\theta_{wcrack}^{3.33}}{\theta_T^{2.0}} \quad (A-21)$$

where:

D_s^{eff}	=	Effective diffusion coefficient in soil based on vapor-phase concentration [cm ² /s]
D_{crack}^{eff}	=	Effective diffusion coefficient through foundation cracks [cm ² /s]
θ_{acrack}	=	Volumetric air content in foundation/wall cracks [cm ³ -air/cm ³ -total volume]
θ_{wcrack}	=	Volumetric water content in foundation/wall cracks [cm ³ -H ₂ O/cm ³ -total volume]
θ_T	=	Total soil porosity [cm ³ -air/cm ³ -soil]
D^a	=	Diffusivity in air [cm ² /s]
D^w	=	Diffusivity in water [cm ² /s]
H	=	Chemical-specific Henry's Law constant [(cm ³ -H ₂ O)/(cm ³ -air)]

A.7 GROUNDWATER CONCENTRATIONS PROTECTIVE INDOOR AIR VAPOR INHALATION

Consider vapor emissions from impacted groundwater to enclosed air space. The screening level concentration in water for this route is estimated using:

$$RBTL_{wi} = \frac{RBTL_a}{VF_{wesp}} \quad (A-22)$$

$RBTL_{wi}$	=	Risk-based target level for indoor inhalation of vapors from groundwater [mg/L-H ₂ O]
$RBTL_a$	=	Risk-based target level for indoor inhalation of air [mg/m ³ -air]
VF_{wesp}	=	Volatilization factor from groundwater to indoor (enclosed space) air [(mg/m ³ -air)/(mg/L-H ₂ O)]

$RBTL_a$ is calculated as described in equation A-1 or A-2, depending upon whether the chemical of concern is a carcinogen or a non-carcinogen.

VF_{wesp} accounts for volatilization from groundwater to enclosed space air and is calculated as:

$$VF_{wesp} = \frac{H \times \left[\frac{D_{ws}^{eff} / L_{gw}}{ER \times L_b} \right]}{1 + \left[\frac{D_{ws}^{eff} / L_{gw}}{ER \times L_b} \right] + \left[\frac{D_{ws}^{eff} / L_{gw}}{(D_{crack}^{eff} / L_{crack}) \times \eta} \right]} \times 10^3 \quad (A-23)$$

where:

L_{gw}	=	Depth to groundwater [cm]
D_{ws}^{eff}	=	Effective diffusion coefficient between groundwater and soil surface [cm ² /s]

D_{crack}^{eff}	=	Effective diffusion coefficient through foundation cracks [cm ² /s]
L_b	=	Enclosed space volume/infiltration area ratio [cm]
L_{crack}	=	Enclosed space foundation or wall thickness [cm]
H	=	Chemical-specific Henry's Law constant [(cm ³ -H ₂ O)/(cm ³ -air)]
ER	=	Enclosed space air exchange rate [1/s]
η	=	Areal fraction of cracks in foundation and/or walls [cm ² -cracks/ cm ² -total area]
10^3	=	Conversion factor [(cm ³ -kg)/(m ³ -g)]

D_w^{eff} is calculated as:

$$D_{ws}^{eff} = (h_{cap} + h_v) \times \left[\frac{h_{cap}}{D_{cap}^{eff}} + \frac{h_v}{D_s^{eff}} \right]^{-1} \quad (A-24)$$

where:

h_{cap}	=	Thickness of capillary fringe [cm]
h_v	=	Thickness of vadose zone [cm]
D_{cap}^{eff}	=	Effective diffusion coefficient through capillary fringe [cm ² /s]
D_s^{eff}	=	Effective diffusion coefficient in soil based on vapor-phase concentration [cm ² /s]

D_{cap}^{eff} is calculated as:

$$D_{cap}^{eff} = D^a \times \frac{\theta_{acap}^{3.33}}{\theta_T^{2.0}} + D^w \times \frac{I}{H} \times \frac{\theta_{wcap}^{3.33}}{\theta_T^{2.0}} \quad (A-25)$$

where:

D_{cap}^{eff}	=	Effective diffusion coefficient through capillary fringe [cm ² /s]
θ_{acap}	=	Volumetric air content in capillary fringe soils [cm ³ -air/cm ³ -soil]
θ_{wcap}	=	Volumetric water content in capillary fringe soils [cm ³ -H ₂ O/cm ³ -soil]
θ_T	=	Total soil porosity [cm ³ -air/cm ³ -soil]
D^a	=	Diffusivity in air [cm ² /s]
D^w	=	Diffusivity in water [cm ² /s]
H	=	Chemical-specific Henry's Law constant [(cm ³ -H ₂ O)/(cm ³ -air)]