Groundwater Services, Inc.

Parameter Estimation Guidelines for Risk-Based Corrective Action (RBCA) Modeling

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Abstract

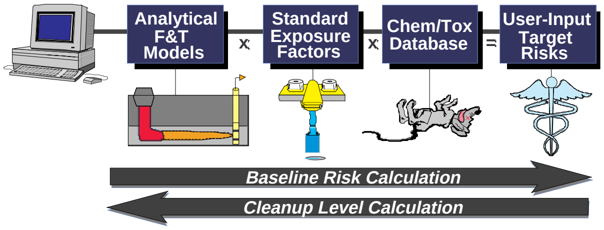
For use in risk-based corrective action (RBCA) analyses, simple analytical fate-and-transport models can provide a cost-effective means of estimating exposure concentrations and developing risk-based soil and groundwater remediation standards. Under ASTM E-1739 "Standard Guide for Risk-Based Corrective Action Applied at Petroleum Release Sites," such models are recommended as a conservative first step under Tiers 1 and 2 of the site evaluation process, prior to use of more complex numerical modeling methods under Tier 3. However, the reliability of an analytical model as a conservative predictor of chronic exposure levels depends upon proper characterization of key physical and chemical parameters.

This paper reviews a system of analytical fate-and-transport models compiled expressly for use with the ASTM RBCA Standard and provides practical guidelines for measurement and/or estimation of key input parameters for each model. Contaminant transport pathways addressed in this paper include soil-to-air volatilization, soil-to-groundwater leaching, lateral air transport, and lateral groundwater transport. Parameter selection guidelines discussed in this paper relate specifically to the analytical expressions listed in Appendix X.2 of ASTM E-1739. However, these guidelines are generally applicable to a broad range of soil, air, and groundwater transport models.

RBCA Spreadsheet System

The RBCA Spreadsheet System, developed by Groundwater Services, Inc. (GSI), is designed to complete all calculations required for Tiers 1 and 2 of the ASTM RBCA planning process (Connor et al, 1995). Based upon site-specific data supplied by the user, the RBCA software combines fate-and-transport modeling and risk characterization functions to complete the following tasks:

- Exposure Concentrations
- Average Daily Intake
- Baseline Risk Levels
- Risk-Based Media Cleanup Levels



Using a system of ten analytical models linked to internal libraries of standard exposure factors and chemical/ toxicological data for 90 compounds, the RBCA Spreadsheet can calculate either baseline risk levels or cleanup standards for each complete exposure pathway identified by the user. Key calculation steps are as follows:

- **Exposure Concentrations:** Based on representative concentrations of constituents of concern (COCs) present in the affected source media, maximum steady-state concentrations likely to occur at the point of exposure (POE) are calculated using the steady-state analytical fate-and-transport models identified in Appendix X.2 of ASTM E-1739. To perform these calculations, the system evaluates cross-media partitioning (e.g., volatilization from soil to air) and lateral transport from the source to the POE (e.g., contaminant transport via air or groundwater flow). The source media and optional exposure pathways included in the software as as follows:

SOURCE MEDIA	EXPOSURE PATHWAYS
Surface Soils	• Inhalation of Volatiles and Particulates • Dermal Contact with Soil • Ingestion of Soil and Dust • Leaching to Groundwater/Ingestion
Subsurface Soils	• Inhalation of Volatiles • Leaching to Groundwater/Ingestion
Groundwater	• Ingestion of Potable Water • Inhalation of Volatiles

- **Average Daily Intake:** Based upon the exposure factors selected by the user, the average daily chemical intake for each receptor along each selected pathway is calculated in accordance with EPA guidelines (see Connor et al, 1995). These values are used in baseline risk calculations for each complete pathway.

- **Baseline Risk Characterization:** Human health risks associated with exposure to COCs are calculated by the spreadsheet on the basis of average daily intake rates and the corresponding toxicological parameters for carcinogenic and non-carcinogenic effects. For each complete pathway, the system output provides both individual and additive constituent results for carcinogens and non-carcinogens.

- **Media Cleanup Values:** The RBCA Spreadsheet System has the ability to i) compare site data to Tier 1 Risk-Based Screening Levels (RBSLs), computed using default parameter values as listed in ASTM E-1739, or ii) calculate Tier 2 Site-Specific Target Levels (SSTLs) based on user-supplied site characterization information. For each source medium (i.e., affected soil and groundwater), the software reports target concentrations for all complete pathways and identifies the applicable (i.e., minimum) value for source remediation.

Fate and Transport Modeling Methods

The RBCA Spreadsheet System contains a series of fate and transport models for predicting COC concentrations at the point of exposure (POE) for each of the optional exposure pathways listed above. Under Tier 2 of the RBCA process, relatively simple analytical models are to be employed for this calculation, representing a minor incremental effort relative to Tier 1. The spreadsheet modeling system is consistent with Appendix X.2 of ASTM E-1739, although selected algorithms and default parameters have been updated to reflect advances in evaluation methods.

The idealized schematic shown on Figure 1 illustrates the steps for predicting transport of contaminants from the source zone to the POE for air and groundwater exposure pathways. Each element in Figure 1 represents a step-specific attenuation factor, corresponding to either a cross-media transfer factor (CM) or a lateral transport factor (LT). The effective natural attenuation factor (NAF) for each COC on each pathway is then calculated as the arithmetic product of the various attenuation factors occurring along the flow path from source to receptor. These steady-state NAF values are then used for calculation of baseline risks and back-calculation of Site-Specific Target Levels (SSTLs), as discussed above. Please note that fate and transport modeling is *not* required for exposure via direct contact with the source medium, such as soil ingestion or dermal contact, where the source and exposure concentrations are equal (i.e., NAF = 1). Analytical models used for conservative estimation of each transport factor per ASTM E-1739 are described below.

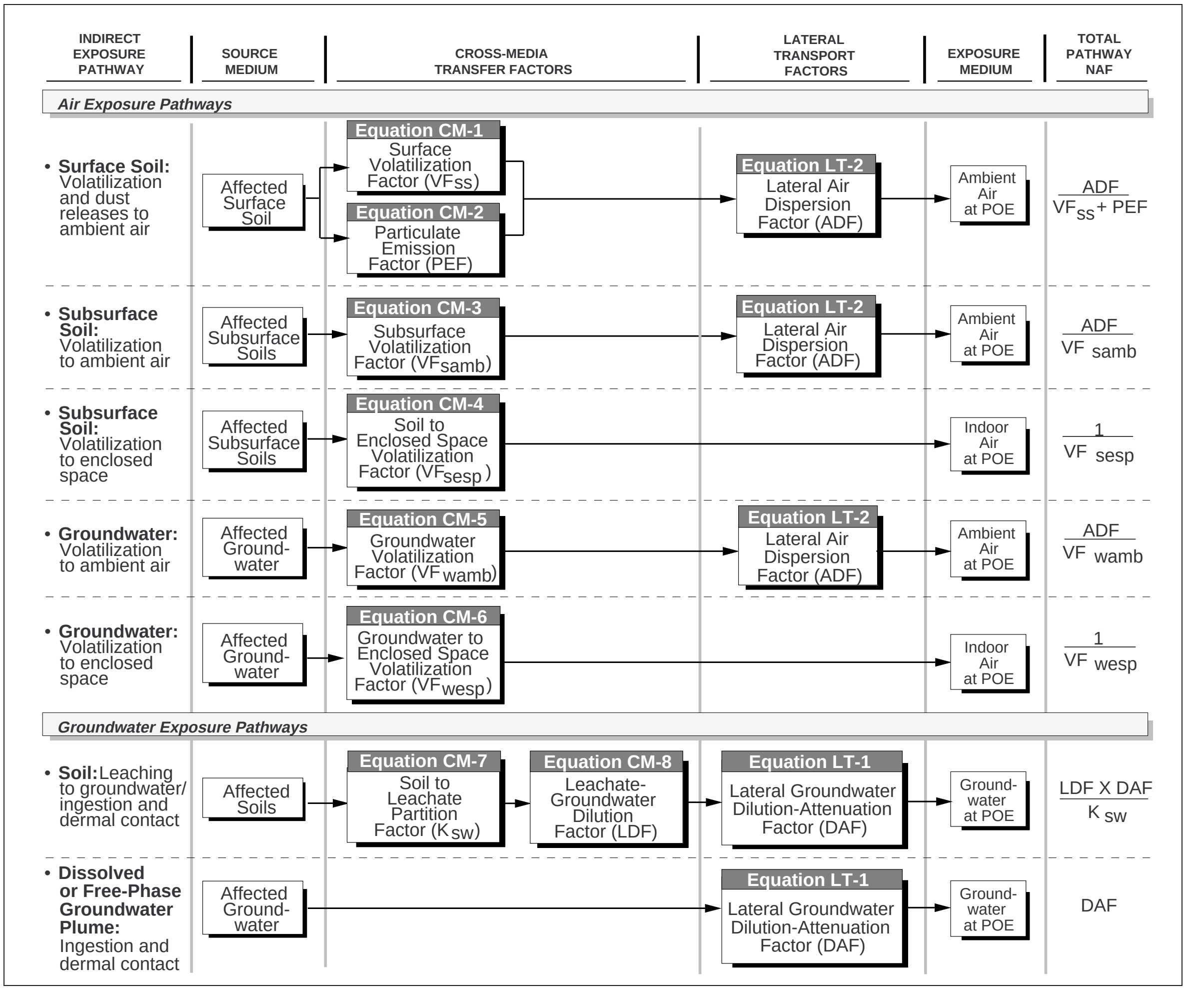
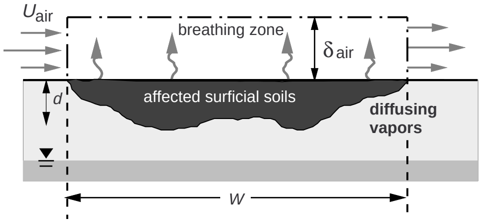


FIGURE 1. NAF CALCULATION SCHEMATIC FOR EXPOSURE PATHWAYS IN RBCA SPREADSHEET SYSTEM

CROSS-MEDIA TRANSFER FACTORS

Exposure pathways involving transport of COCs from one medium to another (e.g., soil-to-air, soil-to-groundwater) require estimation of the corresponding cross-media transfer factor. Various analytical expressions are available for estimating soil-to-air *volatilization factors* as a function of site soil characteristics and the physical/chemical properties of volatile organic COCs. *Leaching factors* for organic and inorganic constituent releases from soil to groundwater can similarly be estimated as a function of COC characteristics, soil conditions, and annual rainfall infiltration. Cross-media transfer equations incorporated in the RBCA Spreadsheet System are presented in Figure 2. Detailed discussion of each of these cross-media factors is provided in the Tier 2 RBCA Guidance Document (Connor et al, 1995).

Equation CM-1: Surface Soil Volatilization Factor (VFss)



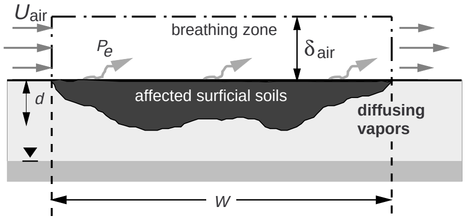
CM-1a:

$$VF_{ss}\left[\frac{(mg/m^3-air)}{(mg/kg-soil)}\right]=\frac{2W\rho_s}{U_{air}\delta_{air}}\sqrt{\frac{D_s^{eff}H}{\pi\tau(\theta_{ws}+k_s\rho_s+H\theta_{as})}}\times 10^3$$

or CM-1b: $$VF_{ss}\left[\frac{(mg/m^3-air)}{(mg/kg-soil)}\right]=\frac{W\rho_s d}{U_{air}\delta_{air}\tau}\times 10^3$$

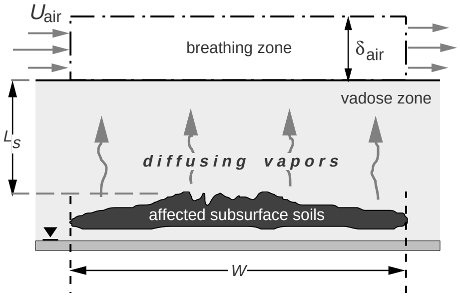
whichever is less

Equation CM-2: Soil Particulate Emission Factor (PEF)



$$PEF\left[\frac{(mg/m^3-air)}{(mg/kg-soil)}\right]=\frac{P_e W}{U_{air}\delta_{air}}\times 10^3$$

Equation CM-3: Subsurface Soil Volatilization Factor (VFsamb)



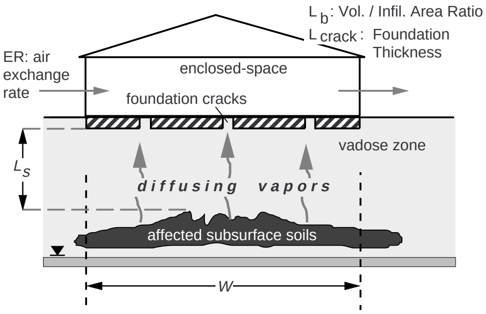
CM-3a:

$$VF_{samb}\left[\frac{(mg/m^3-air)}{(mg/kg-soil)}\right]=\frac{H\rho_s}{[\theta_{ws}+k_s\rho_s+H\theta_{as}]\left[1+\frac{U_{air}\delta_{air}L_s}{D_s^{eff}W}\right]}\text{x}10^3$$

or CM-3b: $$VF_{samb}\left[\frac{(mg/m^3-air)}{(mg/kg-soil)}\right]=\frac{W\rho_s d_s}{U_{air}\delta_{air}\tau}\text{x}10^3$$

whichever is less

Equation CM-4: Subsurface Soil to Enclosed Space Volatilization Factor (VFsesp)



CM-4a:

$$VF_{sesp}\left[\frac{(mg/m^3-air)}{(mg/kg-soil)}\right]=\frac{\frac{H\rho_s}{[\theta_{ws}+k_s\rho_s+H\theta_{as}]}\left[\frac{D_s^{eff}\ /\ L_s}{ER\ \ L_B}\right]}{1+\left[\frac{D_s^{eff}\ /\ L_s}{ER\ \ L_B}\right]+\left[\frac{D_s^{eff}\ /\ L_s}{\left(D_{crack}^{eff}\ /\ L_{crack}\right)\eta}\right]}\text{x}10^3$$

or CM-4b: $$VF_{sesp}\left[\frac{(mg/m^3-air)}{(mg/kg-soil)}\right]=\frac{\rho_s d_s}{L_B ER\tau}\text{x}10^3$$

whichever is less

FIGURE 2. CROSS-MEDIA PARTITIONING EQUATIONS IN THE RBCA SPREADSHEET SYSTEM ***Continued***

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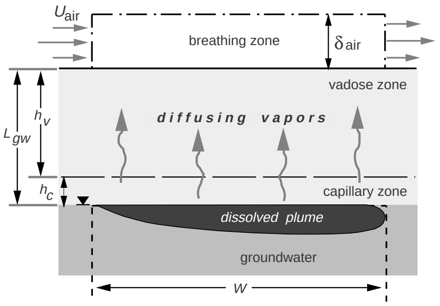
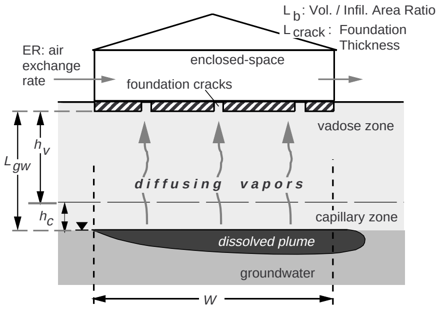
Equation CM-5: Groundwater Volatilization Factor (VFwamb)



$$VF_{wamb}\left[\frac{\left(mg/m^3-air\right)}{\left(mg/L-H_2O\right)}\right]=\frac{H}{1+\left[\frac{U_{air}\delta_{air}L_{GW}}{WD_{ws}^{eff}}\right]}\text{x}10^3$$

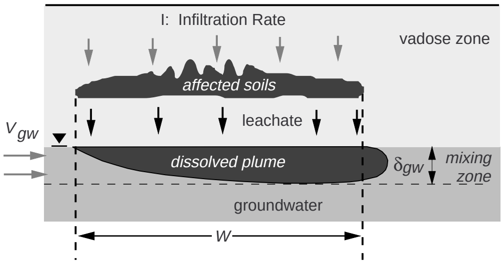
Equation CM-6: Groundwater to Enclosed Space Volatilization Factor (VFwesp)



$$VF_{wesp}\left[\frac{\left(mg/m^3-air\right)}{\left(mg/L-H_2O\right)}\right]=\frac{H\left[\frac{D_{ws}^{eff}/L_{GW}}{ER\ \ L_B}\right]}{1+\left[\frac{D_{ws}^{eff}/L_{GW}}{ER\ \ L_B}\right]+\left[\frac{D_{ws}^{eff}/L_{GW}}{\left(D_{crack}^{eff}/L_{crack}\right)\eta}\right]}\text{x}10^3$$

Equation CM-7: Soil Leachate Partition Factor (Ksw)

Equation CM-8: Leachate-Groundwater Dilution Factor (LDF)



$$K_{sw}\left[\frac{\left(mg/L-H_2O\right)}{\left(mg/kg-soil\right)}\right]=\frac{\rho_s}{\theta_{ws}+k_s\rho_s+H\theta_{as}}$$

$$LDF\left[dimensionless\right]=1+\frac{V_{gw}\delta_{gw}}{IW}$$

FIGURE 2. CROSS-MEDIA PARTITIONING EQUATIONS IN THE RBCA SPREADSHEET SYSTEM ***Continued***

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Definitions for Cross-Media Transfer Equations

D_s^{eff} Effective diffusivity in vadose zone soils:

$$D_s^{eff}\left[\frac{cm^2}{s}\right] = D^{air}\frac{\theta_{as}^{3.33}}{\theta_T^2} + \left[\frac{D^{wat}}{H}\right]\left[\frac{\theta_{ws}^{3.33}}{\theta_T^2}\right]$$

D_{ws}^{eff} Effective diffusivity above the water table:

$$D_{ws}^{eff}\left[\frac{cm^2}{s}\right] = \left(h_{cap} + h_v\right)\left[\frac{h_{cap}}{D_{cap}^{eff}} + \frac{h_v}{D_s^{eff}}\right]^{-1}$$

d	Lower depth of surficial soil zone (cm)
d_s	Thickness of affected subsurface soils
D^{air}	Diffusion coefficient in air (cm^2/s)
D^{wat}	Diffusion coefficient in water (cm^2/s)
ER	Enclosed-space air exchange rate (l/s)
f_{oc}	Fraction of organic carbon in soil (g-C/g-soil)
H	Henry's law constant (cm^3-H_2O)/(cm^3-air)
h_{cap}	Thickness of capillary fringe (cm)
h_v	Thickness of vadose zone (cm)
I	Infiltration rate of water through soil (cm/year)
k_{oc}	Carbon-water sorption coefficient (g-H_2O/g-C)
k_s	Soil-water sorption coefficient (g-H_2O/g-soil)
L_B	Enclosed space volume/infiltration area ratio (cm)
L_{crack}	Enclosed space foundation or wall thickness (cm)
L_{GW}	Depth to groundwater = $h_{cap} + h_v$ (cm)
L_s	Depth to subsurface soil sources (cm)
P_e	Particulate emission rate (g/cm^2-s)
U_{air}	Wind speed above ground surface in ambient mixing zone (cm/s)
V_{gw}	Groundwater Darcy velocity (cm/s)

D_{crack}^{eff} Effective diffusivity through foundation cracks:

$$D_{crack}^{eff}\left[\frac{cm^2}{s}\right] = D^{air}\frac{\theta_{acrack}^{3.33}}{\theta_T^2} + \left[\frac{D^{wat}}{H}\right]\left[\frac{\theta_{wcrack}^{3.33}}{\theta_T^2}\right]$$

D_{cap}^{eff} Effective diffusivity in the capillary zone:

$$D_{cap}^{eff}\left[\frac{cm^2}{s}\right] = D^{air}\frac{\theta_{acap}^{3.33}}{\theta_T^2} + \left[\frac{D^{wat}}{H}\right]\left[\frac{\theta_{wcap}^{3.33}}{\theta_T^2}\right]$$

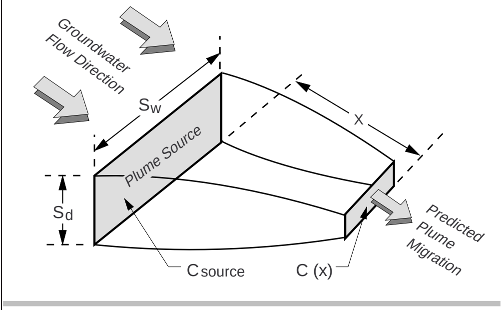
W	Width of source area parallel to wind, or groundwater flow direction (cm)
δ_{air}	Ambient air mixing zone height (cm)
δ_{gw}	Groundwater mixing zone thickness (cm)
η	Areal fraction of cracks in foundations/walls (cm^2-cracks/cm^2-total area)
θ_{acap}	Volumetric air content in capillary fringe soils (cm^3-air/cm^3-soil)
θ_{acrack}	Volumetric air content in foundation/wall cracks (cm^3-air/cm^3 total volume)
θ_{as}	Volumetric air content in vadose zone soils (cm^3-air/cm^3-soil)
θ_T	Total soil porosity (cm^3-pore-space/ cm^3-soil)
θ_{wcap}	Volumetric water content in capillary fringe soils (cm^3-H_2O/cm^3-soil)
θ_{wcrack}	Volumetric water content in foundation/wall cracks (cm^3-H_2O)/cm^3 total volume)
θ_{ws}	Volumetric water content in vadose zone soils (cm^3-H_2O/cm^3-soil)
ρ_s	Soil bulk density (g-soil/cm^3-soil)
τ	Averaging time for vapor flux (s)

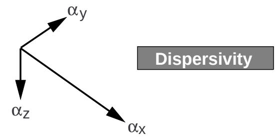
FIGURE 2. CROSS-MEDIA PARTITIONING EQUATIONS IN THE RBCA SPREADSHEET SYSTEM

LATERAL TRANSPORT FACTORS

During lateral transport within air or groundwater, COC concentrations in the flow stream will be diminished due to mixing and attenuation effects (see Figure 1). Site-specific attenuation factors characterizing COC mass dilution or loss during lateral transport can be estimated using the air dispersion and groundwater transport models provided in the RBCA Spreadsheet System. Equations for the steady-state analytical transport models incorporated in the RBCA spreadsheet are shown on Figure 3. Equations LT-1 and LT-2 correspond to the Domenico 3-D groundwater solute transport model and the standard gaussian air dispersion model, respectively. The user must provide information regarding COC properties and transport parameters (flow velocities, dispersion coefficients, retardation factors, decay factors, etc.), as required for the selected contaminant transport model. Procedures for definition of the contaminant source term for the groundwater solute model (Equation LT-1) are illustrated on Figure 4. Key assumptions of these lateral transport models are detailed in the Tier 2 RBCA Guidance Manual (Connor et al, 1995).

Equation LT- 1: Lateral Groundwater Dilution Attenuation Factor





LT-1a: Solute Transport with First-Order Decay:

$$\frac{C(x)_i}{Csi} = \exp\left(\frac{x}{2\alpha_x}\left[1-\sqrt{1+\frac{4\lambda_i\alpha_x R_i}{v}}\right]\right) erf\left(\frac{S_w}{4\sqrt{\alpha_y x}}\right) erf\left(\frac{S_d}{4\sqrt{\alpha_z x}}\right)$$

where: $$v = \frac{K\cdot i}{\theta_e}$$

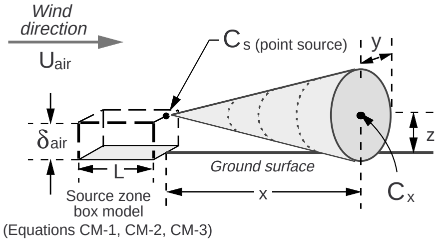
LT-1b: Solute Transport with Biodegradation by Electron-Acceptor Superposition Method:

$$C(x)_i = \left[\left(C_{si}+BC_i\right) erf\left(\frac{S_w}{4\sqrt{\alpha_y x}}\right) erf\left(\frac{S_d}{4\sqrt{\alpha_z x}}\right)\right] - BC_i$$

where: $BC_i = BC_T \text{ x } \frac{C_{si}}{\sum C_{si}}$ *and* $BC_T = \Sigma \frac{C(ea)_n}{UF_n}$

[Note: For Equations LT-1a and LT-1b, NAF = $Cs_i / C(x)_i$]

Equation LT-2: Lateral Air Dispersion Factor



$$\frac{C(x)_i}{C_{si}} = \frac{Q}{2\pi U_{air}\sigma_y\sigma_z} \text{ x } \exp\left(-\frac{y^2}{2\sigma_y^2}\right)\left(\exp\left(-\frac{\left(z-\delta_{air}\right)^2}{2\sigma_z^2}\right)+\exp\left(-\frac{\left(z+\delta_{air}\right)^2}{2\sigma_z^2}\right)\right)$$

where: $$Q = \frac{U_{air}\left(\delta_{air}\right)(A)}{L}$$

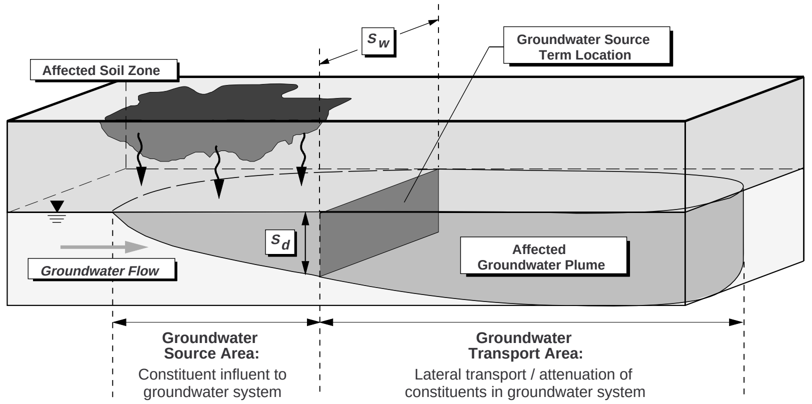
[Note: For Equation LT-2, NAF = $Cs_i / C(x)_i$]

Definitions for Lateral Transport Equations

$C(x)_i$	Concentration of constituent *i* at distance x downstream of source (mg/L) or (mg/m^3)
C_{si}	Concentration of constituent *i* in Source Zone (mg/L) or (mg/m^3)
BC_i	Biodegradation capacity available for constituent *i*
BC_T	Total biodegradation capacity of all electron acceptors in groundwater
$C(ea)_n$	Concentration of electron acceptor *n* in groundwater
UF_n	Utilization factor for electron acceptor *n* (i.e., mass ratio of electron acceptor to hydrocarbon consumed in biodegradation reaction)
x	Distance downgradient of source (cm)
α_x	Longitudinal groundwater dispersivity (cm)
α_y	Transverse groundwater dispersivity (cm)
α_z	Vertical groundwater dispersivity (cm)
θ_e	Effective Soil Porosity

λ_i	First-Order Degradation Rate (day^{-1}) for constituent *i*
υ	Groundwater Seepage Velocity (cm/day)
K	Hydraulic Conductivity (cm/day)
R_i	Constituent retardation factor
i	Hydraulic Gradient (cm/cm)
S_w	Source Width (cm)
S_d	Source Depth (cm)
δ_{air}	Ambient air mixing zone height (cm)
Q	Air volumetric flow rate through mixing zone (cm^3/s)
U_{air}	Wind Speed (cm/sec)
σ_y	Transverse air dispersion coefficient (cm)
σ_z	Vertical air dispersion coefficient (cm)
y	Lateral Distance From source zone (cm)
z	Height of Breathing Zone (assumed equal to δ_{air}) (cm)
A	Cross Sectional Area of Air Emissions Source (cm^2)
L	Length of Air Emissions source (cm) parallel to wind direction

FIGURE 3. LATERAL TRANSPORT EQUATIONS IN THE RBCA SPREADSHEET SYSTEM



SELECTION OF GROUNDWATER MODEL INPUT PARAMETERS

For use of Domenico groundwater solute transport model (see Equations LT-1a and LT-1b, Figure 3), select source term location, dimensions, and concentration as follows:

1) Groundwater Source Term Location

The source term corresponds to a vertical source plane, normal to the direction of groundwater flow, located at the downgradient limit of the area serving as the principal source of constituent release to groundwater (e.g., affected unsaturated zone soils, NAPL plume, land disposal unit, spill area, etc.). In the absence of such data, the source term should be located at the point of the maximum measured plume concentration(s). Distances to downgradient points of exposure (POEs) should then be measure from this location along the principal direction of groundwater flow.

2) Groundwater Source Term Width, S_W

The width of the source term should be matched to the **greater** of the following dimensions:

i) the measured groundwater plume width, (as defined by Tier 1 limits) normal to the principal direction of groundwater flow at the designated source term location.

ii) the maximum width of the affected soil zone, normal to the principal groundwater flow direction.

3) Groundwater Source Term Thickness, S_d

The thickness of the source term should be matched to **either**:

i) the measured vertical extent of the affected groundwater plume, at the designated source term location.

ii) in the absence of actual site measurements establishing the vertical extent of the affected groundwater plume, the full saturated thickness of the water-bearing unit at this location.

4) Groundwater Source Term Concentration, C_S

To calculate baseline risk levels, the user must also provide a groundwater source concentration for each constituent of concern (COC). The vertical plane source functions as a constant source term, applying these input concentrations to all groundwater flowing through the source location. Under a Tier 2 evaluation, the source concentration of each COC may be defined as follows:

i) use the maximum concentration of each COC detected at the source location or
ii) if multiple sampling locations are available to characterize plume concentrations across the source term width Sw, calculate a weighted average source concentration for each constituent across this plume transect based on time-consistent measurements.

FIGURE 4. DEFINITION OF SOURCE TERM FOR USE IN DOMENICO SOLUTE TRANSPORT MODEL

Parameters Selection Guidelines

For purpose of parameter value selection, the input parameters required for each of the fate-and-transport models identified above can be grouped in the following categories:

- **Site-Specific Parameter Measurements**: Required for parameters which i) exhibit a wide range of site-specific variability (e.g., orders of magnitude) that may significantly impact model predictions and ii) are amenable to characterization based upon limited site-specific measurements. Examples include hydraulic conductivity, flow gradient, source dimensions, etc.
- **Reasonable Parameter Estimates**: Suitable for parameters which i) exhibit a moderate degree of site-specific variability (e.g., less than 1X) and ii) may be characterized on the basis of generic estimates without significantly impacting model predictions. Examples include soil porosity, soil unit weight, and volumetric air and water content, etc.
- **Chemical-Specific Parameter Values**: Physical properties of chemical constituents which must be characterized on the basis of published laboratory values. Examples include Henry's Law constant, air and water diffusion coefficients, and carbon-water sorption coefficients, etc.

For each of the analytical fate-and-transport models identified in Appendix X.2 of ASTM E-1739 and incorporated in the RBCA Spreadsheet System, practical guidelines for appropriate selection of input parameters per these general categories are outlined below. Please note that, although these recommendations relate to the modeling equations listed on Figures 1-3, these guidelines are generally applicable to various analytical models used for characterization of chronic exposure conditions.

VOLATILIZATION MODELS: Equations CM-1 through CM-6

The volatilization models provided in Equations CM-1 thorugh CM-6 (see Figure 2) define the steady-state ratio of the concentration in air at the POE to the source concentration in the underlying soil (Equations CM-1 through CM-4) or groundwater (Equations CM-5 and CM-6). Guidelines for selection of input parameters, grouped according to the three categories noted above, are summarized on Table 1.

SOIL-TO-GROUNDWATER LEACHING MODELS: Equations CM-7 and CM-8

Per the approach outlined in Appendix X.2 of ASTM E-1739, a soil-to-groundwater DAF value can be calculated as the product of: i) a leachate-groundwater dilution factor (Equation CM-8), divided by ii) a soil-leachate partition factor (Equation CM-7), providing a steady-state ratio between the concentration of a constituent on the affected soil mass to the resultant concentration in the underlying groundwater mixing zone. The model is applicable to both organic and inorganic constituents; however, as noted on Table 2, care must be taken to employ the appropriate equation for estimation of the soil-water sorption coefficient (k_s). Guidelines for selection of each input parameter required for Equations CM-7 and CM-8 are summarized on Table 2.

LATERAL GROUNDWATER TRANSPORT MODEL: Equation LT-1

To account for attenuation of affected groundwater concentrations between the source and POE, the Domenico analytical solute transport model has been incorporated into the RBCA software. This model uses a partially or completely penetrating vertical plane source, perpendicular to groundwater flow, to simulate the release of organics from the mixing zone to the moving groundwater (see Figure 4). Within the groundwater flow regime, the model accounts for the effects of advection, dispersion, sorption, and biodegradation. Given a representative source zone concentration for each COC, the model can predict steady-state plume concentrations at any point (x, y, z) in the downgradient flow system. In Equation LT-1 (see Figure 3), the model is set to predict centerline plume concentrations at any downgradient distance x, based on 1-D advective flow and 3-D dispersion. The receptor well is assumed to be located on the plume centerline, directly downgradient of the source zone at a location specified by the user. Note that the model incorporates biodegradation of organic constituents, based on use of a first-order decay function (LT-1a) or an electron-acceptor superposition algorithm (LT-1b). Inorganic constituents are assumed to be conservative ($\lambda = 0$), with no resultant sorption or bioattenuation under steady-state conditions. Guidelines for selection of key input parameters are outlined on Table 3.

LATERAL AIR TRANSPORT MODEL: EQUATION LT-2

The RBCA software includes a 3-dimensional gaussian dispersion model to account for transport of air-borne contaminants from the source area to a downwind POE (see Equation LT-2 on Figure 3). The model incorporates two conservative assumptions: i) a source zone height equivalent to the breathing zone and ii) a receptor located directly downwind of the source at all times. As indicated on Figure 3, an effective pathway NAF value is calculated as the steady-state ratio between the source concentration in the on-site affected soil zone and the ambient organic vapor or particulate concentration at the downwind POE. The model requires input data for the affected soil zone dimensions and concentrations, wind speed, and horizontal and vertical air dispersion coefficients to compute the resulting COC concentrations in ambient air at the POE. Guidelines for defining key input parameters are provided on Table 4.

Summary

As demonstrated by the RBCA Spreadsheet System, a system of simple analytical fate-and-transport models can be used for comprehensive evaluation of chronic exposure levels associated with potential soil, air, and groundwater exposure pathways. However, as with all predictive modeling efforts, reliable results require proper characterization of the input parameters, particularly those requiring site-specific measurement as noted on Tables 1-4. In all cases, model predictions must be shown to be consistent with the actual constituent distributions observed at the site. Use of the Tier 1 and Tier 2 calculation methods discussed in ASTM E-1739 and incorporated in the RBCA Spreadsheet System can significantly reduce the time and effort required for estimation of baseline risk levels or calculation of site-specific, risk-based soil and groundwater remediation goals. However, proper scientific and/or engineering expertise is required for both characterization of input parameters and assessment of model results.

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TABLE 1. PARAMETER SELECTION GUIDELINES: VOLATILIZATION MODELS

Input Parameter				
Symbol	**Description**	**Typical Range**	**Parameter Measurement or Estimation Guidelines**	**Reference**
SITE-SPECIFIC PARAMETER MEASUREMENTS				
W	Soil source zone dimension parallel to wind direction (cm)	Site-specific	Measure lateral extent of soil zone serving as source of vapor release (e.g., zone exceeding Tier 1 limits). For on-site POE, use maximum lateral source dimension. For off-site POE, use dimension measured along line passing from source zone to nearest downwind off-site POE location.	Connor et al, 1995
L_{GW}	Depth to groundwater	Site-specific	For unconfined unit, measure depth to static water level. For confined unit, measure depth to top of water-bearing stratum.	Connor et al, 1995
L_s	Depth to subsurface soil source (cm)	Site-specific	Measure depth from ground surface to top of affected source zone.	Connor et al, 1995
d or d_s	Thickness of affected soil zone	Site-specific	Measure average vertical dimension from top to base of affected soil zone over lateral area corresponding to W.	Connor et al, 1995
h_v	Thickness of vadose zone (cm)	Site-specific	Measure from ground surface to depth of static water level in unconfined unit. In confined unit, measure from ground surface to depth of soil saturation (often corresponding to potentiometric surface elevation).	Connor et al, 1995
f_{oc}	Fraction of organic carbon in soil (g-C/g-soil)	0.001 - 0.03	Conduct lab analyses on representative unaffected soil samples over depth interval of vertical vapor migration or use generic value of 0.01 for vadose zone.	LaGrega, 1994
REASONABLE PARAMETER ESTIMATES				
U_{air}	Windspeed above ground surface in ambient mixing zone (cm/s)	45 - 450 cm/sec	Match to average annual windspeed for site area, based on published climatic data.	Connor et al, 1995
δ_{air}	Ambient air mixing zone height (cm/s)	200 cm	Match to typical height of human breathing zone (6 ft or 2m).	Connor et al, 1995
k_s	Soil-water sorption coefficient (g-H_2O/g-soil)	-----	For organics, estimate as: $k_s = k_{oc} \times f_{oc}$. For ionizing organics (e.g., chlorophenols), estimate k_s based on published pH-dependent partitioning coefficients for ionized and neutral forms. For inorganics, estimate k_s per published pH-dependent isotherms, based on measured groundwater pH. Detailed guidelines provided in U.S. EPA SSL Background Document (1996).	U.S. EPA, 1996
ρ_s	Soil bulk density (g-soil/cm^3-soil)	1.6 - 1.75	Use median soil value of 1.7 g/cm^3.	ASTM, 1995
Θ_T	Total soil porosity (cm^3-pore space/cm^3-soil)	35 - 55%	Estimate based on predominant soil type as follows: Uniform Sand: 40% Soft Clay: 55% Mixed-Grain-Sand: 35% Stiff Clay: 37% Silt: 50%	Peck et al, 1974
Θ_{ws}	Volumetric water content in vadose zone soils (cm3-H_2O/cm^3-soil)	13 - 52%	Estimate based on predominant soil type as follows: Uniform Sand: 13% Soft Clay: 52% Mixed-Grain-Sand: 16% Stiff Clay: 34% Silt: 42% NOTE: Typical Θ_{ws} values approximated as saturated water content minus specific yield of soil.	Peck et al, 1974 Todd, 1980
Θ_{as}	Volumetric air content in vadose zone soils (cm^3-air/cm^3-soil)	3-27%	Calculate as $\Theta_{as} = \Theta_T - \Theta_{ws}$, where Θ_{ws} and Θ_T estimated per predominant soil type as above.	Peck et al, 1974 Todd, 1980

NOTE: See Equation CM 1 through CM 6 on Figure 2 regarding use of the above parameters for estimation of steady-state volatilization factors for affected soils. Detailed discussion of these volatilization models is provided in the Tier 2 RBCA Guidance Manual (see Connor et al, 1995).

continued

TABLE 1. PARAMETER SELECTION GUIDELINES: VOLATILIZATION MODELS

continued

Input Parameter				
Symbol	**Description**	**Typical Range**	**Parameter Measurement or Estimation Guidelines**	**Reference**
REASONABLE PARAMETER ESTIMATES (CONT'D)				
h_{cap}	Thickness of capillary fringe (cm)	2 - 200 cm	Estimate based on predominant soil type, as follows: Medium Samd: 25 cm Clayey Silt: 200 cm Fine Sand: 43 cm Silt: 105 cm	Todd, 1980
P_e	Particulate emission rate (g/cm^2-s)	-----	Use generic upperbound value (e.g., 6.9 x 10^{-14} g/cm^2-sec)) or estimate reasonable site-specific value using method outlined in U.S. EPA SSL guide.	ASTM, 1995 EPA, 1996
z	Averaging time for vapor flux (s)	-----	Match to assumed exposure duration (in seconds).	ASTM, 1995
ER	Enclosed space air-exchange rate (L/s)	-----	Use generic lowerbound value (e.g., 0.00014 L/s for residential, 0.00023 L/s commercial) or match to minimum allowable indoor air ventilation rate per local building code.	ASTM, 1995
L_B	Ratio of enclosed space volume to infiltration area (cm)	-----	Use generic lowerbound value (e.g., 200 cm) or develop reasonable estimates based on size (no. of floors) and area (foundation outline) of typical residential or commercial structures in site area.	ASTM, 1995
L_{crack}	Enclosed space foundation or wall thickness (cm)	-----	Use generic upperbound value (e.g., 15 cm) or match to local building code specifications for residential or commercial structures.	ASTM, 1995
Z	Areal fraction of cracks in foundations /walls (cm^2-cracks/cm^2-total area)	-----	Use generic upperbound value (e.g., 1%) or estimate based on observed site conditions.	ASTM, 1995
CHEMICAL-SPECIFIC PARAMETER VALUES				
H	Henry's Law Constant (cm3-H_2O/cm^3-air)	-----	Use median value reported for each constituent of concern in published chemical reference.	Connor et al, 1995 a
k_{oc}	Carbon-water sorption coefficient (g-H_2O/g-C)	-----	Use median value reported for each constituent of concern in published chemical reference.	Connor et al, 1995 a
D^{air}	Diffusion coefficient in air (cm^2/s)	-----	Use median value reported for each constituent of concern in published chemical reference.	Connor et al, 1995 a
D^{wat}	Diffusion coefficient in water (cm^2/s)	-----	Use median value reported for each constituent of concern in published chemical reference.	Connor et al, 1995 a
D_s^{eff}	Effective diffusivity in vadose zone soils (cm^2/s)	-----	Estimate as shown on Figure 2.	-----
D_{ws}^{eff}	Effective diffusivity above the water table (cm^2/s)	-----	Estimate as shown on Figure 2.	-----

NOTE: See Equation CM 1 through CM 6 on Figure 2 regarding use of the above parameters for estimation of steady-state volatilization factors for affected soils. Detailed discussion of these volatilization models is provided in the Tier 2 RBCA Guidance Manual (see Connor et al, 1995).

TABLE 2. PARAMETER SELECTION GUIDELINES: SOIL-TO-GROUNDWATER LEACHATE MODELS (EQUATIONS CM-7 AND CM-8)

Input Parameter				
Symbol	**Description**	**Typical Range**	**Parameter Measurement or Estimation Guidelines**	**Reference**
SITE-SPECIFIC PARAMETER MEASUREMENTS				
W	Soil source zone dimension parallel to groundwater flow direction (cm)	Site-specific	Measure lateral extent of soil zone serving as source of leachate release to underlying groundwater (e.g., exceeding Tier 1 limits) along line parallel to natural groundwater flow.	Connor et al, 1995
f_{oc}	Fraction of organic carbon in soil (g-C/g-soil)	0.001 - 0.03	Measure on representative unaffected soil samples over vertical depth interval of vapor migration or use generic lowerbound value of 0.01 for vadose zone.	La Grega, 1994
V_{gw}	Groundwater Darcy velocity (cm/w)	Site-specific	Estimate as follows: $V_{gw} = K \bullet i$ where K and i are defined as noted below.	Bedient et al, 1994
K	Hydraulic conductivity of water-bearing unit (cm/sec)	Site-specific	Measure K values vased upon either i) rising-head slug tests or ii) constant-rate aquifer pumping tests conducted on wells properly installed and developed in water-bearing unit. Re-evaluate test results if measured values fall outside typical range for predominant soil type, as follows: Clays: $<1x10^{-6}$ cm/s Silts: $1x10^{-6}$ - $1x10^{-3}$ cm/s Silty Sands: $1x10^{-4}$ - $1x10^{-2}$ cm/s Clean Sands: $1x10^{-1}$ - 1 cm/s Gravels: >1 cm.s	Bedient et al, 1994
i	Lateral hydraulic flow gradient of water-bearing unit (cm/cm)	0.001 - 0.1	Measure lateral flow gradient in area beneath soil source zone based on triangulation among 3 or more monitoring wells or piezometers screened within water-bearing unit.	Newell et al, 1996
δ_{gw}	Groundwater mixing zone thickness (cm)	Site-specific	Measure vertical extent of affected groundwater zone within water-bearing unit in area underlying soil source zone. If vertical plume extent undetermined at this location, use lowerbound estimate (e.g., 200 cm).	ASTM, 1995
REASONABLE PARAMETER ESTIMATES				
I	Infiltration rate of water through soil (cm/year)	------	Estimate I as function of annual rainfall (P) in site area, depending on predominant surface soil type, as follows: Clayey Soils: I = (1 - 2%) x P Sandy Soils: I = (5 - 10%) x P Paved Site: I = (0.1 - 1%) x P	(NOTE: Values are preliminary. Supporting guidelines under development.)
P_s	Soil bulk density (g-soil/cm^3-soil)		Use median soil value of 1.7 g/cm^3.	ASTM, 1995
Θ_{ws}	Volumetric water content in vadose zone soils (cm3-H_2O/cm^3-soil)		Estimate based on predominant soil type as follows: Uniform Sand: 13% Soft Clay: 52% Mixed-Grain-Sand: 16% Stiff Clay: 34% Silt: 42% NOTE: Typical Θ_{ws} values approximated as saturated water content minus specific yield of soil.	Peck et al, 1974 Todd, 1980
Θ_{as}	Volumetric air content in vadose zone soils (cm^3-air/cm^3-soil)		Calculate as $\Theta_{as} = \Theta_T - \Theta_{ws}$, where Θ_{ws} and Θ_T estimated per predominant soil type as above. NOTE: Values correspond to drained conditions. Dry weather may increase Θ_{as} in near-surface silts and clays (< 6 ft depth).	Peck et al, 1974 Todd, 1980
NOTE:	See Equations CM-7 and CM-8 on Figure 2 regarding use of the above parameters for estimation of soil-to-groundwater leaching factor for affected soils. Detailed discussion of this soil leachate model is provided in the Tier 2 RBCA Guidance Manual (Connor et al, 1995).			

continued

TABLE 2. PARAMETER SELECTION GUIDELINES: SOIL-TO-GROUNDWATER LEACHATE MODELS (EQUATIONS CM-7 AND CM-8) *continued*

Input Parameter		Typical Range	Parameter Measurement or Estimation Guidelines	Reference
Symbol	**Description**			
REASONABLE PARAMETER ESTIMATES (CONT'D)				
$\mathbf{k_s}$	Soil-water sorption coefficient (g-H_2O/g-soil)	-----	For organics, estimate as: k_s =k_{oc} x f_{oc}. For ionizing organics (e.g., chlorophenols), estimate k_s based on published pH dependent partitioning coefficients for ionized and neutral forms. For inorganics, estimate k_s as published pH-dependent isotherms, based on measured groundwater pH.	U.S. EPA, 1996
CHEMICAL-SPECIFIC PARAMETERS				
H	Henry's Law Constant (cm3-H_2O/cm^3-air)	-----	Use median value reported for each constituent of concern in published chemical reference.	Connor et al, 1995a
$\mathbf{k_{oc}}$	Carbon-water sorption coefficient (g-H_2O/g-c)	-----	Use median value reported for each constituent of concern in published chemical reference.	Connor et al, 1995a
NOTE: See Equations CM-7 and CM-8 on Figure 2 regarding use of the above parameters for estimation of soil-to-groundwater leaching factor for affected soils. Detailed discussion of this soil leachate model is provided in the Tier 2 RBCA Guidance Manual (Connor et al, 1995).				

TABLE 3. PARAMETER SELECTION GUIDELINES: LATERAL GROUNDWATER TRANSPORT MODEL (EQUATION LT-1)

Input Parameter		Typical Range	Parameter Measurement or Estimation Guidelines	Reference
Symbol	**Description**			
SITE-SPECIFIC PARAMETER MEASUREMENTS				
υ	Groundwater seepage velocity (cm./sec)	Site-specific	Calculate site-specific value based on the following equation: $\upsilon=\frac{K\bullet i}{\theta_e}$ where K, i, and θ_e are determined as specified below..	Bedient et al, 1994
K	Hydraulic conductivity of water-bearing unit (cm/sec)	Site-specific	Measure K values based upon either i) rising-head slug tests or ii) constant-rate aquifer pumping tests conducted on wells properly installed and developed in water-bearing unit. Re-evaluate test results if measured values fall outside typical range for predominant soil type, as follows: Clays: <1x10^{-6} cm/s Silts: 1x10^{-6} - 1x10^{-3} cm/s Silty Sands: 1x10^{-4} - 1x10^{-2} cm/s Clean Sands: 1x10^{-1} - 1 cm/s Gravels: >1 cm.s	Bedient et al, 1994
i	Lateral hydraulic flow gradient of water-bearing unit (cm/cm)	0.001 - 0.1	Measure lateral flow gradient in area beneath soil source zone based on triangulation among 3 or more monitoring wells or piezometers screened within water-bearing unit.	Newell et al, 1996
$\mathbf{R_i}$	Constituent retardation factor	Site-specific	Calculate site-specific values based on the following equation: $R=1+\frac{k_s\bullet\rho_s}{\theta_e}$ where k_s, ρ_s, and θ_e are determined as specified below.	Newell et al, 1996

continued

TABLE 3. PARAMETER SELECTION GUIDELINES: LATERAL GROUNDWATER TRANSPORT MODEL (EQUATION LT-1) *continued*

Input Parameter				
Symbol	**Description**	**Typical Range**	**Parameter Measurement or Estimation Guidelines**	**Reference**
SITE-SPECIFIC PARAMETER MEASUREMENTS (CONT'D)				
$\mathbf{k_s}$	Soil-water sorption coefficient (g-H_2O/g-soil)		For organics, estimate as: $k_s = k_{oc} \times f_{oc}$. For ionizing organics (e.g., chlorophenols), estimate k_s based on published pH dependent partitioning coefficients for ionized and neutral forms. For inorganics, estimate k_s as published pH-dependent isotherms, based on measured groundwater pH. See EPA SSL Guidance for detailed information.	U.S. EPA, 1996
$\mathbf{f_{oc}}$	Fraction of organic carbon in soil (g-C/g-soil)	0.001 - 0.03	Measure depth from ground surface to top of affected source zone. Measure average vertical dimension from top to base of affected soil zone over area corresponding to W. Generic lowerbound value of 0.001.	La Grega, 1994
$\mathbf{BC_i}$	Biodegradation capacity for constituent i	Site-specific	If using electron-acceptor superposition form of Domenico model (Equation LT-1b), calculate $\mathbf{BC_i}$ value as indicated on Figure 3. Detailed instructions for $\mathbf{BC_i}$and BC_T estimation are provided in BIOSCREEN user's manual (Newell et al, 1996). Calculation must be based on site-specific measurement of principal electron acceptor concentrations in site groundwater.	Newell et al, 1996 Connor et al, 1995
X	Distance from source to downgradient POE (cm)	Site-specific	Measure from source term location to downgradient POE location along line of groundwater flow.	Connor et al, 1995
$\mathbf{S_w}$	Groundwater source term width (cm)	Site-specific	See Figure 4 for guidelines regarding site-specific determination of source width of water-bearing unit.	Connor et al, 1995
$\mathbf{S_d}$	Groundwater source term thickness (cm)	Site-specific	See Figure 4 for guidelines regarding site-specific determination of source thickness in water-bearing unit.	Connor et al, 1995
REASONABLE PARAMETER ESTIMATES				
θ_e	Effective porosity of water-bearing unit (cm^3-pore/cm^3-soil)	0.001 - 0.1	Match to representative value for predominant soil type in water-bearing unit, as follows: Clay = 0.01 - 0.20 Silt = 0.01 - 0.30 Fine Sand = 0.10 - 0.30 Med. Sand = 0.15 - .30 Coarse Sand = 0.20 - 0.33 Gravel = 0.10 - 0.35	Domenico et al, 1990 Walton, 1988

TABLE 3. PARAMETER SELECTION GUIDELINES: LATERAL GROUNDWATER TRANSPORT MODEL (EQUATION LT-1) *continued*

Input Parameter		Typical Range	Parameter Measurement or Estimation Guidelines	Reference
Symbol	**Description**			
REASONABLE PARAMETER ESTIMATES (CONT'D)				
α_x α_y α_z	Groundwater dispersivity coefficients in longitudinal (x), transverse (y), and vertical (z) dimensions	-----	For use with biodegradation functions in Domenico model (LT-1a or LT-1b), reasonable dispersivity estimates may be derived as follows: **Longitudinal Dispersivity**: $\alpha_x = 3.28 \bullet 0.83 \bullet \left[\log_{10}\left(\frac{X}{3.28}\right)\right]^{-2.414}$ **Transverse Dispersivity**: α_y = 0.10 alpha x (*based on high reliability points from Geihar et al, 1992*) **Vertical Dispersivity**: α_z = very low (i.e., 1 x 10^{-99} ft) (*based on conservative estimate*)	Xu and Eckstein, 1995 Gelhar et al, 1992 Newell et al, 1996
			Other commonly used relationships include: $\alpha_x = 0.1 \bullet X$ $\alpha_y = 0.33 \bullet \alpha_x$ $\alpha_z = 0.025$ to $0.1 \bullet \alpha_x$ [Note: If used with electron-acceptor superposition version of Domenico model (Equation LT-1b), these later relationshipos may result in overestimation of biodegradation effects.]	Pickens and Grisak, 1981 ASTM, 1995 EPA, 1986
λ_e	First-order degradation rate for constituent i (sec^{-1})	------	Optional methods for selection of appropriate decay coefficients for each constituent of concern are as follows: **Calibrate to Existing Plume Data**: If the plume is in a steady-state or diminishing condition, the BIOSCREEN or FATE II models can be used to determine first-order decay coefficients that best match the observed site concentrations. This site-specific calibration effort will require representative measurements of each constituent along the centerline of the groundwater plume. Detailed instructions are provided in the BIOSCREEN and FATE II User's Guides. **Literature Values**: If the plume is in an expanding condition or if a preliminary estimate of biodegradation effects is desired, decay half-life values for hydrolysis and biodegradation from published references (e.g., see Howard et al, 1991). Note that many references report the half-lives; these values can be converted to the first-order decay coefficients using $k = 0.693/t_{1/2}$ (see dissolved plume half-life). In the absence of site-specific calibration data, minimum values (maximum half-life values) should be used. The selected values should correspond to the half-life for full constituent decay to non-hazardous progeney. For inorganics, $\lambda = 0$.	Newell et al, 1996 Connor et al, 1995 Connor et al, 1994

NOTE: See Equation LT-1 on Figure 3 regarding use of the above parameters for estimation of steady-state groundwater dilution attenuation factor for dissolved groundwater plume. Detailed discussion of this groundwater solute transport model is provided in the Tier 2 RBCA Guidance Manual (see Connor et al, 1995).

TABLE 4. PARAMETER SELECTION GUIDELINES: LATERAL AIR TRANSPORT MODEL (EQUATION LT-2)

Input Parameter				
Symbol	**Description**	**Typical Range**	**Parameter Measurement or Estimation Guidelines**	**Reference**
SITE-SPECIFIC PARAMETER MEASUREMENTS				
L	Length of affected soil zone parallel to wind direction (cm)	Site-specific	Determine lateral extent of affected soil zone serving as source of vapor release (e.g., zone exceeding Tier 1 limits) measured along line passing from source zone to downwind off-site POE.	Connor et al, 1995
A	Lateral area of affected soil zone (cm^2)	Site-specific	Measure areal extent of affected soils serving as source of vapor release (e.g., zone exceeding Tier 1 limits).	Connor et al, 1995
X	Lateral distance downwind of source zone (cm)	Site-specific	For most conservative evaluation, measure as distance from edge of affected soil zone to nearest off-site POE location (in some direction as L above). For typical case, measure this distance along line of predominant annual wind direction.	Connor et al, 1995
REASONABLE PARAMETER ESTIMATES				
U_{air}	Windspeed above ground surface in ambient mixing zone (cm/s)	45 - 450 cm/sec	Match to average annual windspeed for site area, based on published climatic data.	Connor et al, 1995
δ_{air}	Ambient air mixing zone height (cm/s)	200 cm	Match to typical height of human breathing zone (6 ft or 2m).	ASTM, 1995
y	Transverse distance off air plume centerline (cm)	-----	To evaluate exposure concentrations along plume centerline, y is set equal to zero.	Connor et al, 1995
z	height of breathing zone (cm)	-----	Assume equal to δ_{air} above.	Connor et al, 1995
σ_y, σ_z	Air dispersion coefficients (cm) in the transverse (y) and vertical (z) directions	-----	For average annual climatic conditions, characterize σ_y, σ_z based on Stability Class C (slightly unstable) using the following relationships: $\sigma_y = 10^{(\text{Log}(x) \bullet 0.941 - 0.861)}$ $\sigma_z = 10^{(\text{Log}(x) \bullet 0.927 - 1.01)}$ If Stability Class C determined to be inapplicable, estimate air dispersion coefficient values using Pasquill-Gifford system as discussed in DeVaull et al, 1994.	Connor et al, 1995 Devaull et al, 1994 U.S. EPA, 1988
C_{si}	Concentration of constituent i in ambient air at point source	-----	Estimate based on appropriate soil-to-air volatilization model (see Equations CM-1 through CM-3 on Figure 2) or conduct site-specific measurements in breathing zone air overlying affected soil source area.	Connor et al, 1995
NOTE: See Equation LT-2 on Figure 3 regarding use of the above parameters for estimation of lateral air dispersion factor for wind-borne contaminant transport to downwind receptor. Detailed discussion of this air dispersion model is provided in the Tier 2 RBCA Guidance Manual (see Connor et al, 1995).				