Soil Attenuation Model for Derivation of Risk-Based Soil Remediation Standards

J. A. Connor, R. L. Bowers, S. M. Paquette, C. J. Newell
Groundwater Services, Inc., Houston, Texas (713) 522-6300

1.0 Overview of Soil Attenuation Model (SAM)

Under a risk-based corrective action (RBCA) process, soils and groundwater impacted by a chemical release are to be remediated or controlled to concentration levels such that further migration will not expose human or environmental receptors to unsafe levels of hazardous constituents. For this purpose, site-specific target levels (SSTLs) must be established for the affected soil mass such that subsequent soil leachate migration to an underlying water-bearing unit does not cause exceedance of applicable exposure limits for groundwater. To derive such groundwater protection standards, a new Soil Attenuation Model (SAM) has been developed to provide a conservative estimate of soil-to-groundwater contaminant release based on readily available information regarding annual rainfall, soil type, depth to groundwater, and the hydrogeologic properties of the underlying water-bearing unit. Using either site-specific or generic site properties, this analytical model can be used either to i) predict upperbound constituent concentrations in groundwater, based on an observed soil concentration, or ii) back-calculate a lower-bound soil SSTL value, based on the applicable risk-based screening level (RBSL) at the groundwater point of exposure (POE). The model is applicable to analysis of porous media soils impacted by either organic and inorganic constituents, in the absence of mobile non-aqueous phase liquids (NAPLs).

The SAM represents a modification to the soil-leachate equations presented in Appendix X.2 of ASTM E-1739 *Standard Guide for Risk-Based Corrective Action Applied at Petroleum Release Sites* (ASTM, 1995). These modifications are directed toward providing a more rigorous characterization of the soil-to-groundwater leachate process and assisting the user in estimation of critical input parameters. However, to accommodate use in Tiers 1 and 2 of the risk-based site evaluation effort, the SAM retains the format of a simple, screening-level analytical expression requiring limited site-specific data input. The model includes empirical relationships to assist the user in characterization of net infiltration and equilibrium soil moisture content parameters based on annual site rainfall and the predominant soil type overlying the groundwater unit. The soil-to-groundwater leachate process is characterized as a three-step procedure, beginning with i) equilibrium partitioning of soil contaminants from a finite source mass to infiltrating rainwater, followed by ii) sorptive redistribution of contaminants from the leachate onto underlying clean soils, and iii) subsequent leachate dilution within the receiving groundwater flow system. In the base version of this model, contaminant loss through the processes of volatilization and biodegradation are neglected for purpose of conservatism and simplicity.

This paper reviews the principal components of the Soil Attenuation Model (SAM) and presents detailed background information regarding model derivation and key assumptions. The SAM model has recently been specified for incorporation in the proposed Texas Risk Reduction Program (TRRP) (see TNRCC 1996). Sample default values to be used in Tier 1 and Tier 2 of the Texas process are also discussed herein. Summary guidelines regarding calculation procedures and input parameter selection are provided on Figure 2 and Table 4, respectively.

2.0 Model Description

AMENDMENTS TO ASTM RBCA SOIL LEACHATE EQUATION

Appendix X.2 of ASTM E-1739 presents analytical equations for estimation of a soil leachate factor (LF), corresponding to a steady-state ratio between contaminant concentrations in affected soils and the resultant concentrations in an underlying water-bearing unit. Intended as example screening-level models, the ASTM soil leachate equations have been widely adopted for use in calculation of risk-based soil remediation standards under Tiers 1 and 2 of the ASTM RBCA planning process. In the ASTM model, the soil leachate process is characterized as a simple two-step process, involving: i) dissolution of soil contaminants into infiltrating rainwater (estimated using an equilibrium partitioning relationship), followed by ii) leachate dilution within the underlying groundwater (estimated using a simple box model).

The ASTM leachate factor equations meet the Tier 1 and Tier 2 objectives of conservatism, simplicity, and reproducibility; however, practical application of this leachate model has been complicated by difficulties associated with proper estimation of key input parameters and overly conservative characterization of the soil leachate process. Specifically, given the complexity of obtaining site-specific infiltration measurements, upperbound default values have been applied to rainfall infiltration rates (e.g., 30 cm/yr), providing worst-case estimates of soil leachate impacts. Furthermore, a simple two-step characterization of the leachate generation and migration process (ignoring the effect of contaminated soil mass and soil column thickness on leachate mass flux) can prove overly conservative for deep groundwater conditions.

To address these concerns, the SAM augments the existing ASTM soil leachate equation with features intended to assist in characterization of critical input parameters and more accurately simulate rainfall infiltration and leachate migration. A comparison of the SAM and ASTM models with respect to the key elements of the soil-to-groundwater contaminant release process is provided on Table 1. As shown, the SAM differs from the earlier leachate equations published in ASTM E-1739 by addition of the following features:

- *Net Infiltration Estimate*: SAM incorporates an empirical relationship for estimation of net rainfall infiltration based on mean annual rainfall and soil type.
- *Finite Source Mass*: The SAM assumes a finite contaminant source mass based on the mass of affected soil and the representative concentration of each constituent of concern (COC).

- *Sorptive Mass Redistribution*: The SAM incorporates depth effects by accounting for the sorptive redistribution of contaminants from the leachate onto soils underlying the affected soil zone. This sorptive mass loss reduces contaminant concentrations delivered to the underlying groundwater.

- *Default Soil Moisture Parameters*: SAM employs default soil moisture parameters (θ_{as}, θ_{ws}) consistent with the predominant soil type in the surface soil column.

- *Leachate-Groundwater Dilution*: The SAM estimates leachate dilution in the groundwater flow system using the same box model incorporated in the ASTM expression. However, a supplementary algorithm, published as part of the EPA Soil Screening Level Guide (U.S. EPA, 1996), has been added to assist the user in estimation of the groundwater mixing zone depth.

TABLE 1: SUMMARY OF SAM AMENDMENTS TO ASTM SOIL LEACHATE EQUATIONS

		SAM FEATURE	
ELEMENT OF SOIL LEACHING PROCESS	**ASTM LEACHATE MODEL FEATURE**	**REVISED?**	**DESCRIPTION**
1) Net Rainfall Infiltration	Uses upperbound estimate of annual infiltration (e.g., 30 cm/yr).	***Yes***	***Net Infiltration Calculator***: Estimates net infiltration as function of rainfall and soil type.
2) Soil Moisture/Air Contents	Uses conservative default values.	***Yes***	***Soil-Dependent Default Values***: Employs equilibrium soil moisture parameters consistent with soil type.
3) Contaminant Source Mass	Assumes infinite source mass in affected soil zone.	***Yes***	***Finite Source Mass***: Contaminant source mass assumed to be finite (i.e., affected soil mass times representative contaminant concentration). See also "Time Averaging" below.
4) Equilibrium Partitioning: Soil to Leachate	Assumes equilibrium relationship based on soil-water sorption, chemical properties.	No	***Equilibrium Partitioning***: Equilibrium assumption retained as conservative, simplifying measure.
5) Contaminant Loss via Volatilization and Biodegradation	Not considered.	No	***No Biodegradation or Volatilization***: These processes neglected in base model as conservative, simplifying measure. Biodegradation may be applied as optional measure based on site-specific data.
6) Sorptive Redistribution of Contaminant on Underlying Soil (Depth Effect)	Not considered.	***Yes***	*Sorptive Mass Redistribution*: Accounts for mass loss due to redistribution of leachable contaminants onto underlying soils.
7) Leachate Dilution in Groundwater System	Estimated using simple box dilution model.	No/Yes	***Leachate-Groundwater Dilution***: Box model retained as simplifying measure. Supplementary algorithm provided for estimation of mixing zone depth.
8) Time-Averaging of Groundwater Concentrations	Not considered.	No	***No Time Averaging***: Averaging of exposure concentrations over an exposure duration neglected in base model as conservative measure. May be applied as optional measure for carcinogenic constituents under Tier 3 evaluation.

The SAM is consistent with the ASTM model in the use of an equilibrium partitioning relationship for estimation of soil pore water concentrations and in neglecting contaminant loss via volatilization or biodegradation. In addition, neither the SAM nor the ASTM leachate model presently accounts for the gradual loss of source mass to leachate over time and the resultant decrease in contaminant flux to groundwater over a 30-year period of exposure. In each case, these measures represent conservative, simplifying assumptions consistent with the model application as a Tier 1 or Tier 2 screening-level tool. However, as noted on Table 1, biodecay and time averaging may be applied as optional modeling measures based on site-specific considerations under a Tier 2 or Tier 3 evaluation. If such options are to be utilized, biodegradation rates must be based on measured site-specific data. For carcinogenic constituents, time averaging may be applied to consider average chronic effects over the exposure duration.

KEY COMPONENTS OF SAM

The Soil Attenuation Model (SAM) can be used to derive a steady-state soil-to-groundwater contaminant leachate factor (LF) based on available information regarding site soil and groundwater conditions. The model can be used to predict contaminant flux from affected soils to underlying groundwater for either organic or inorganic constituents, in the absence of mobile, free-phase soil contaminants.

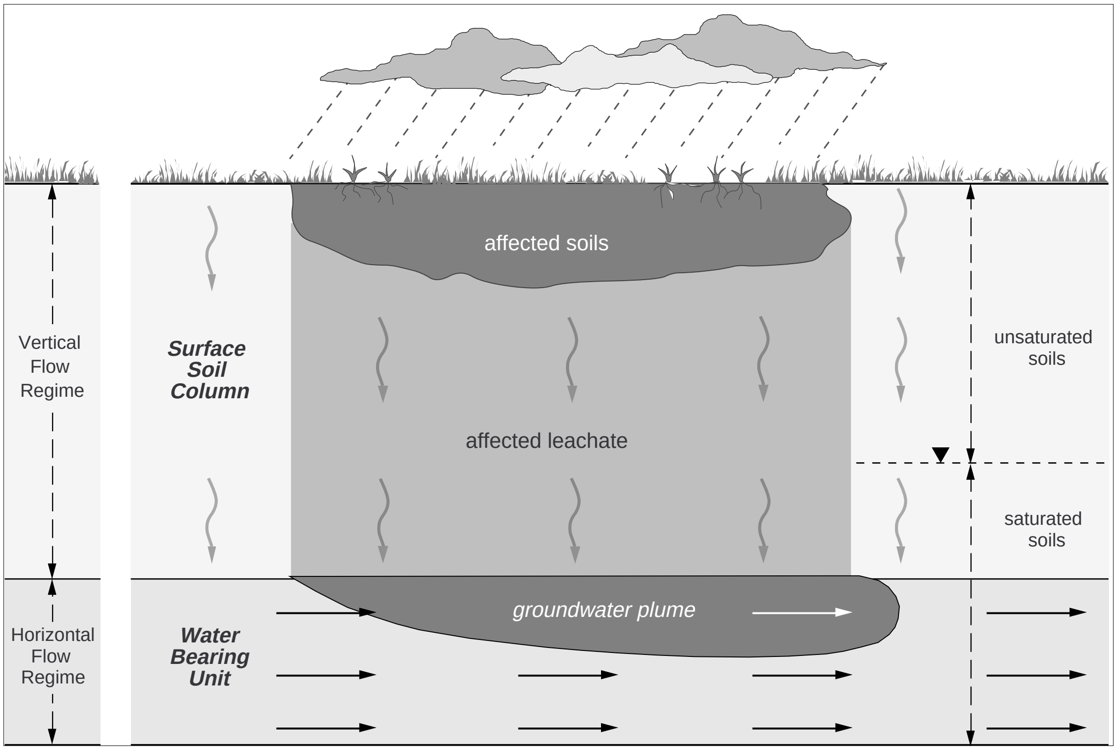
For the purpose of this analysis, shallow site geology is idealized as two principal stratigraphic components: i) a *surface soil column* consisting of unsaturated and saturated soils, wherein pore water flow is primarily vertical (downward), underlain by ii) a saturated, transmissive *water-bearing unit*, wherein pore water flow is principally horizontal (see Figure 1). The boundary of these two flow zones corresponds to the top of the uppermost water-bearing stratum beneath the site. Contaminant transfer from affected soils in the surface soil column to the underlying water-bearing unit occurs via vertical leachate migration. After entering the water-bearing unit, the leachate fluids mix with the lateral groundwater flow stream and spread horizontally from the point of entry in the downgradient direction of shallow groundwater flow (see Figure 1).

The SAM simulates this soil leachate process from the initial infiltration of rainfall through the affected soil zone to final mixing of the contaminated soil leachate with underlying groundwater. Principal components of this soil leachate model are illustrated on Figure 2 and discussed in further detail below. Background information regarding model derivation is provided in Attachments A through D.

1) Estimation of Net Infiltration

- ***Method Description***: Net infiltration corresponds to total infiltration (precipitation minus runoff) minus the additional loss associated with evapotranspiration. The net infiltration term (I_f) thereby represents the deep percolation flow (cm/year) through the affected soil zone which could result in contaminated leachate release to underlying groundwater. In the SAM, net infiltration is estimated as a function of average annual rainfall (cm/year) and the predominant soil type (sand, silt, or clay) using the empirical relationships plotted on Figure 3 (or using Equations 1a - 1c on Figure 2). Given the predominant soil type in the surface soil column, the curves and accompanying equations can be used to obtain a conservative estimate of net annual infiltration (cm/year), based on a grass ground cover (i.e., no pavement). For highly stratified soil columns composed of multiple soil types (e.g., interbedded sand and clay), the lower permeability soil (i.e., clay) will control vertical infiltration.

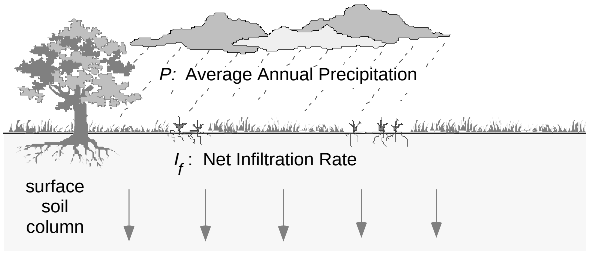
FIGURE 1: IDEALIZED SCHEMATIC OF SOIL LEACHATE MIGRATION



- ***Key Assumptions***: The sand soil curve shown on Figure 3 represents an 80% envelope line for rainfall infiltration data from over 100 sandy soil sites in 18 geographic regions in the United States, as compiled by Stephens & Associates (API, 1996). This curve provides a conservative (upper-range) estimate of deep percolation for over 80% of the sand or gravel soil sites reported in this database. Curves for silty and clayey soils were then derived from the empirical sandy soil curve based on the relative percent infiltration described by Viessman *et al* (1989) for the parameters of the Horton infiltration relationship. Detailed information regarding development of these empirical curves is provided in Attachment A. The net infiltration curves shown on Figure 3 correspond to a grass-covered site and will prove highly conservative for soils overlain by pavement (e.g., 100x overestimate of I_f).

FIGURE 2: SCHEMATIC DIAGRAM OF SOIL ATTENUATION MODEL (SAM)

1. Estimation of the Net Infiltration Rate



Eqn. 1a: For Sand: $I_f\ [cm/yr] = 0.0018 \cdot (P)^2$

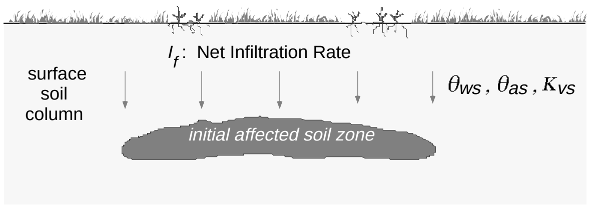
Eqn. 1b: For Silt: $I_f\ [cm/yr] = 0.0009 \cdot (P)^2$

Eqn. 1c: For Clay: $I_f\ [cm/yr] = 0.00018 \cdot (P)^2$

Eqn. 1d: Upperbound net infiltration limit:

$$I_f\ [cm/yr] \le I_{f\,max} = K_{vs} \cdot \left[\frac{3.15x10^7\ sec}{1\ yr}\right]$$

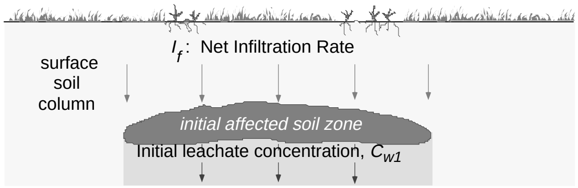
2. Equilibrium Volumetric Water and Air Contents



Option 2a) ***Default Values:*** Select default soil moisture parameters $(\theta_{as}, \theta_{ws})$ and saturated hydraulic conductivity based on soil type (see Table 2).

Option 2b) ***Site Measurements:*** Conduct site-specific measurements of θ_{as}, and θ_{ws} on sufficient number of representative soil samples from surface soil column. Conduct field measurements of K_{vs}.

3. Equilibrium Partitioning: Affected Soil to Leachate



Eqn. 3a: $C_{w1}[mg/L] = K_{sw} \cdot C_T$

where:

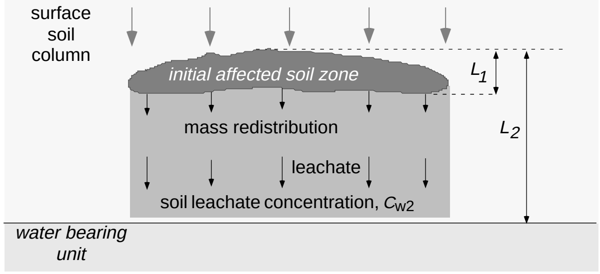
Eqn. 3b: $K_{sw}\left[\frac{mg/L - H_2 0}{mg/Kg - soil}\right] = \frac{\rho_s}{B_w}$

Eqn. 3c: $B_w = \theta_{ws} + k_s \cdot \rho_s + H \cdot \theta_{as}$

Eqn. 3d: $k_s\left[\frac{cm^3 - H_2 0}{g - soil}\right] = k_{oc} \cdot foc$ (Organics)

Eqn. 3e: $k_s\left[\frac{cm^3 - H_2 0}{g - soil}\right] = k_d$ (Inorganics)

4. Sorptive Mass Redistribution: Leachate to Underlying Clean Soil



Eqn. 4a: $C_{w2}[mg/L] = C_{w1} \cdot \frac{L_1}{L_2}$

Eqn. 4b: Upperbound leachate concentration for mass conservation:

$$C_{w2}[mg/L] \le \frac{C_T \cdot \rho_s \cdot L_1}{I_f \cdot ED}$$

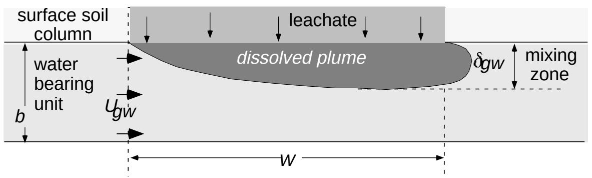
Eqn. 4c: Upperbound leachate concentration for solubility limit:

$$C_{w2}[mg/L] \le X \cdot S$$

Continued

FIGURE 2: SCHEMATIC DIAGRAM OF SOIL ATTENUATION MODEL (SAM) *continued*

5. Leachate/Groundwater Dilution



Eqn. 5a: $$LDF\,[unitless] = 1 + \frac{U_{gw} \cdot \delta_{gw}}{I_f \cdot W}$$

where:

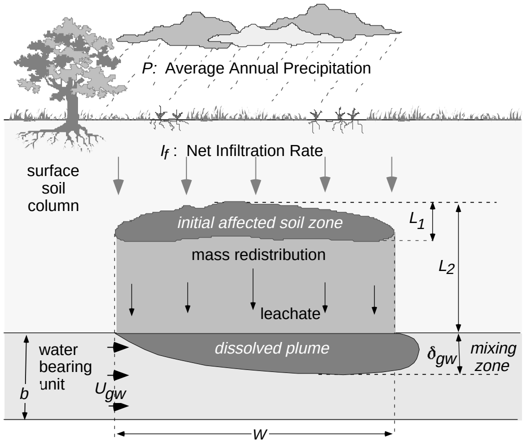
Eqn. 5b: $$U_{gw}[cm/yr] = K \cdot i \cdot \left(\frac{3.15 \times 10^7 \sec}{1yr} \right)$$

Eqn. 5c: $$\alpha_v[cm] = 0.0056 \cdot W$$

Eqn. 5d: $$\delta_{gw}[cm] = \sqrt{2 \cdot a_v \cdot W} + b \cdot \left[1 - \exp\left(\frac{-I_f \cdot W}{U_{gw} \cdot b} \right) \right]$$

Eqn. 5e: **Upperbound mixing zone depth:** $\delta_{gw}[cm] \leq b$

6. Summary Calculations



Eqn. 6a: **Groundwater Exposure Concentration:**

$$C_{gw}[mg/L] = C_{w2} \cdot \frac{1}{LDF} \cdot \left(BDF^* \cdot TAF^* \right)$$

Eqn. 6b: **Soil Target Concentration:**

$${}^{GW}Soil_{Ing.}[mg/Kg] = {}^{GW}RBSL \cdot LDF \cdot \frac{L_2}{L_1} \cdot \frac{1}{K_{sw}} \cdot \left(\frac{1}{BDF^* \cdot TAF^*} \right)$$

where:

*Eqn. 6c: **Optional Biodecay Factor:**

$$BDF[dim] = \exp\left[-\lambda \cdot (L_2 - L_1) \cdot \left(\frac{B_w}{I_f} \right) \right]$$

*Eqn. 6d: **Optional Time Averaging Factor:**

$$TAF[dim] = \frac{L_2 \cdot B_w}{I_f \cdot ED} \cdot \left[1 - \exp\left(\frac{-I_f \cdot ED}{L_2 \cdot B_w} \right) \right]$$

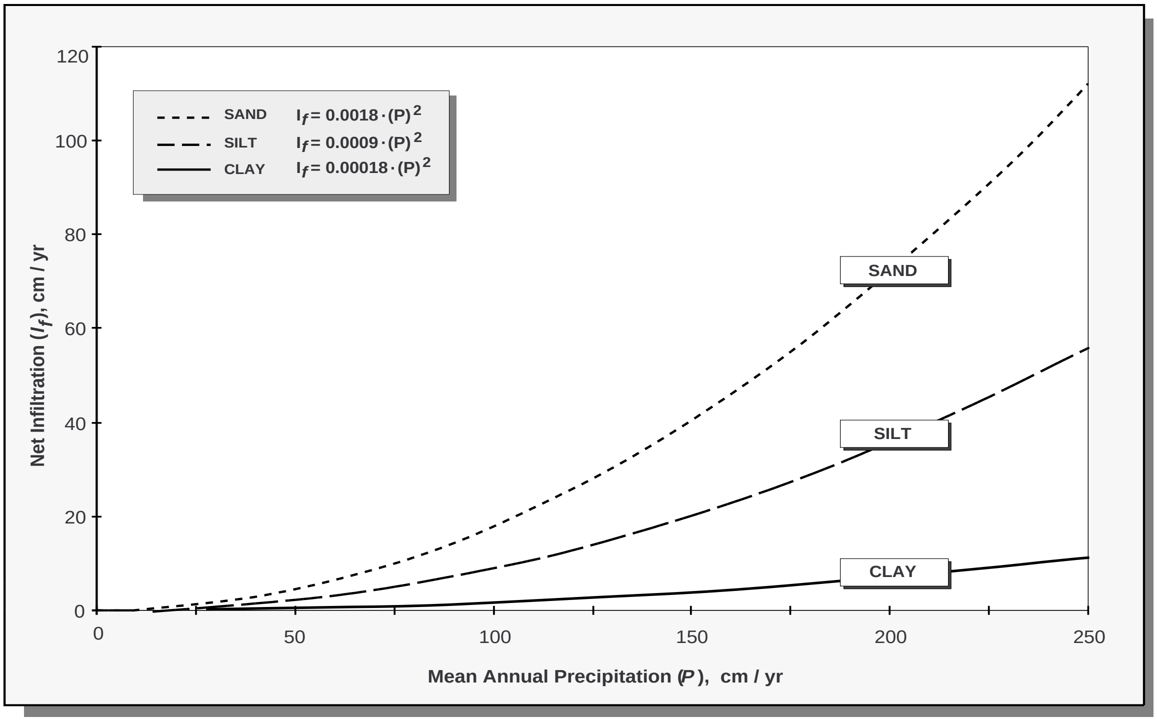
Model Parameters

		TEXAS TIER 1 DEFAULT
b	Saturated thickness of water-bearing unit (cm)	SS
B_w	Bulk water partioning coefficient (unitless)	CS
C_{gw}	Concentration of COC in groundwater (mg/L)	SS
COC	Constituent of Concern	SS
C_T	Bulk COC concentration on the soil mass (mg/Kg)	SS
C_{w1}	Concentration of COC in soil leachate in the initial affected soil zone (mg/L)	SS/CS
C_{w2}	Concentration of COC in soil leachate discharged to underlying water-bearing unit (mg/L)	SS/CS
ED	Exposure duration (yr)	30
foc	Fraction of organic carbon (g-C/g-soil)	0.006
H	Henry's Law constant for COC (cm^3-H_20/cm^3-air)	CS
i	Hydraulic gradient in water-bearing unit (cm/cm)	SS
I_f	Net infiltration (cm/yr)	10
$I_{f\,max}$	Upperbound infiltration limit (cm/yr)	(see above)
K	Hydraulic conductivity of water-bearing unit (cm/sec)	SS
k_d	Inorganic soil-water sorption coefficient for COC (cm^3-H_2O/g-soil)	CS
k_{oc}	Organic carbon partition coefficient for COC (cm^3-H_2O/g-C)	CS
k_s	Soil-water sorption coefficient (cm^3-H_2O/g-soil)	CS
K_{sw}	Soil-leachate partition factor for COC (mg/L-H_2O/mg/Kg-soil)	CS
K_{vs}	Saturated hydraulic conductivity of vadose zone soils (cm/sec)	(see Table 2)
L_1	Thickness of affected soil zone (cm)	60

		TEXAS TIER 1 DEFAULT
L_2	Distance from top of affected soil zone to top of water bearing unit (cm)	60
LDF	Leachate-groundwater dilution factor (unitless)	SS
P	Mean annual precipitation (cm/yr)	SS
^{GW}RBSL	Risk-Based Screening Level in groundwater zone (mg/L)	CS
S	Aqueous solubility of COC (mg/L)	CS
${}^{GW}Soil_{Ing}$	Source Area Concentration Limit for soils (mg/Kg)	CS
U_{gw}	Groundwater Darcy velocity (cm/yr)	2,500
W	Lateral width of affected soil zone in direction of GW flow (cm) • 0.5-acre site • 3.0-acre site	 4,500 34,800
X	Initial mole fraction of COC in source material (unitless)	1.0
α_v	Vertical groundwater dispersivity (cm)	(see above)
δ_{gw}	Groundwater mixing zone thickness (cm)	200
λ	Biodecay rate of COC in vadose zone (yr^{-1})	0
θ_{as}	Volumetric air content of surface soils (cm^3-air/cm^3-soil)	0.13
θ_T	Total porosity of surface soils (cm^3-pore-space/cm^3-soil)	0.43
θ_{ws}	Volumetric water content of surface soils (cm^3-H_2O/cm^3-soil)	0.30
ρ_s	Soil bulk density (g-soil/ cm^3-soil)	1.5

NOTE: SS = Site-specific parameter CS = Chemical-specific parameter

FIGURE 3: ESTIMATION OF NET INFILTRATION BASED ON MEAN ANNUAL RAINFALL & SOIL TYPE



NOTES:

1) Net rainfall infiltration through surface soils estimated based on empirical relationship of mean rainfall and predominant soil type in surface soil column. See Attachment A for derivation of empirical formulas.

2) I_f = Net infiltration (i.e., total infiltration corrected for evapotranspiration loss), cm / yr
P = Mean annual rainfall at site, cm / yr

3) Soil type classified per Unified Soil Classification System (USCS). See Lambe et al., 1969.

2) Volumetric Air and Water Contents

- ***Method Description***: For typical soil types, conservative default values for each of the input parameters required in these equations are provided on Table 2. To employ these defaults, the user must first determine the appropriate soil classification for soils within the surface soil column, using either the Unified Soil Classification System (USCS, Lambe et al, 1969) or USDA textural classification method (Peck et al, 1974), based on the predominant soil type observed in site boring logs. Note that for highly stratified systems composed of multiple soil types of roughly equivalent volumes, the lowest permeability soil will control the rate of infiltration and the resulting average moisture content. If desired, site-specific values for volumetric air and water content and saturated hydraulic conductivity can be developed based on measurements conducted on multiple soil samples spatially distributed throughout the surface soil column. However, as the model is not highly sensitive to these parameters, the expense of site-specific analyses may not be warranted in most cases.

TABLE 2:DEFAULT SOIL PARAMETERS FOR ESTIMATION OF EQUILIBRIUM SOIL MOISTURE CONTENT (USCS SOIL TYPES)

USCS SOIL TYPE		DEFAULT SOIL MOISTURE PARAMETERS			DEFAULT HYDRAULIC CONDUCTIVITY
SYMBOL	DESCRIPTION	θ_T	θ_{ws}	θ_{as}	K_{vs} (cm/s)
SW	SAND, clean, well-graded	0.41	0.08	0.33	10^{-2}
SP	SAND, clean, poorly-graded	0.41	0.08	0.33	10^{-2}
SM	SAND, silty	0.41	0.12	0.29	10^{-3}
SC	SAND, clayey	0.38	0.23	0.15	10^{-5}
ML	SILT, sandy	0.43	0.26	0.17	10^{-5}
ML	SILT	0.46	0.30	0.16	10^{-5}
MH	SILT, clayey	0.36	0.24	0.12	10^{-5}
CL	CLAY, sandy, low plasticity	0.38	0.31	0.07	10^{-6}
CL	CLAY, silty, low plasticity	0.36	0.34	0.02	10^{-7}
CH	CLAY, high-plasticity	0.38	0.38	0	10^{-8}

NOTES:
1) Default values for volumetric water (θ_{ws}) and volumetric air (θ_{as}) contents are to be matched to predominant soil type in surface soil column. See Attachment B for derivation of default values.
2) Typical saturated hydraulic conductivity (K_{vs}) values matched to median values reported by Freeze and Cherry (1979) and Rawls and Brakensiek (1985).
3) Unified Soil Classification System (USCS) described in Lambe et al (1969) and ASTM Standard D-2487.

- ***Model Derivation***: The default soil moisture values shown on Table 2 represent equilibrium levels associated with an annual rainfall of 30 inches (U.S. median), derived using the Brooks-Corey (1964) soil characteristic model and the Burdine (1953) equations for the relative permeability of unsaturated soils. Sensitivity analyses show that use of default soil moisture values based on a median rainfall level provides model results that are on average within ± 5% of those obtained using the site-specific, rainfall-dependent, soil moisture values derived using the Brooks-Corey model. Consequently, use of default soil moisture values represents a reasonable, simplifying measure in the SAM. Attachment B provides detailed information regarding the derivation of these tabulated default values.

Note that the *surface soil column* as defined in this model may consist of an upper unsaturated soil zone as well as a lower saturated soil zone, through which pore water flow is predominantly vertical (downward) toward an underlying water-bearing unit (see Figure 1). In the lower saturated portion of this soil column, the actual volumetric air content (θ_{as}) of the soils will be zero. However, through use of default soil moisture values as listed on Table 2, the SAM characterizes the soil column as a uniform unsaturated soil zone (i.e., $\theta_{as} > 0$). For sites wherein the surface soil column is predominately saturated (e.g., clay stratum overlying confined water-bearing with high confining head), these equilibrium soil moisture values will prove relatively conservative, contributing to an overestimation of soil leachate concentrations (i.e., higher K_{sw} value; see Equation 3b).

3) Equilibrium Partitioning

- ***Method Description***: The transfer of soil contaminants to infiltrating rainwater is characterized on the basis of a conventional equilibrium partitioning relationship among the soil, pore water, and pore vapor phases of the surface soil matrix (see Equations 3a and 3b on Figure 2). Using these equilibrium relationships, the fraction of the soil contaminant mass partitioning to the soil leachate (i.e., soil-leachate partition factor, K_{sw}) is defined on the basis of site soil properties (ρ_s, θ_{ws}, θ_{as}, foc) and the chemical characteristics of the constituent of concern (H, k_{oc}, pH-dependent k_d function). The soil-water sorption coefficient (k_s) for each constituent is calculated using separate functions for organic and inorganic constituents, as indicated on Figure 2. Guidelines for derivation of k_s values are provided in the EPA Soil Screening Level (SSL) Document (U.S. EPA, 1996). Multiplying the representative COC concentration in the affected soil mass (C_T) by the soil-leachate partition factor (K_{sw}) yields an upperbound estimate of the resultant COC concentration in the soil leachate (C_{w1}). Under Tier 1, RBSLs can be derived on the basis of fixed default values for the site soil properties, as specified on Figure 2.

- ***Key Assumptions***: The soil-leachate partition factor (K_{sw}, see Equation 3b) used in the SAM represents the conventional three-phase equilibrium partitioning relationship for affected environmental media, which has been previously incorporated in both the ASTM E-1739 Appendix X.2 examples (ASTM, 1995) and in the EPA Soil Screening Level Document (U.S. EPA, 1996). The equation assumes instantaneous partitioning at equilibrium levels and thereby provides an upperbound estimate of contaminant release from soils to infiltrating rainwater and subsequently to underlying groundwater. The model neglects the effects of immobile residual non-aqueous phase liquids (NAPLs) that may be present within the affected soil mass. If such NAPL materials are present, many organics partition strongly to this fourth phase (i.e., immobile residual NAPL), reducing the mass fraction available for leachate release. (Note the SAM is not applicable to sites where mobile NAPL is actively percolating from the soil column to the underlying water-bearing unit.) In the SAM, such four-way partitioning has been neglected as a conservative, simplifying measure. As shown on Table 3, for BTEX constituents, neglecting such NAPL partitioning effects results in a conservative overprediction of leachate concentrations by a factor of 1.3x to 4.2x, depending on the assumed residual NAPL concentration in the soil pores (see Cases 1 and 2 on Table 3).

4) Sorptive Mass Redistribution

- ***Method Description***: The SAM corrects the equilibrium soil leachate concentration for the effect of sorptive mass loss as the leachate percolates downward toward the underlying water-bearing unit. This adjustment can prove significant in deep groundwater systems, wherein a significant thickness of unaffected soils underlies the affected soil zone. For the SAM, the affected soil zone is characterized as a finite source mass equivalent to the affected soil mass times the representative constituent concentration. Prior to reaching groundwater, percolating rainwater serves to redistribute this finite source mass among soil, air, and pore fluids throughout the full thickness of the surface soil column.

As a result of this sorptive redistribution of contaminant mass onto intervening soils, the initial equilibrium leachate concentration (C_{w1}, as defined by Equation 3a) will be reduced by the ratio of the affected soil zone thickness (L_1), divided by the total soil column thickness from the top of the affected soils to the top of the saturated water-bearing unit (L_2). These depth parameters can be determined on a site-specific basis from soil boring logs and soil test results. The adjusted leachate concentration (C_{w2}) calculated using Equation 4a (see Figure 2) represents the maximum dissolved contaminant concentration in leachate entering the groundwater at any time (i.e., initial leachate front). This maximum leachate concentration can be expected to diminish over time, as the leachate process continually removes source mass from the affected soil zone. However, as a conservative measure, the SAM assumes this initial leachate concentration to remain constant for the full duration of the groundwater exposure period. Note that this upperbound leachate concentration (C_{w2}) must be adjusted for mass conservation considerations (Equation 4b) and effective solubility limits (Equation 4c). In each case, the lowest concentration determined by Equations 4a, 4b, and 4c will apply. For derivation of Tier 1 RBSL values, the affected soil unit can be assumed to be in contact with the water-bearing unit (i.e., $L_2/L_1 = 1$) thereby neglecting sorptive redistribution effects. Alternatively, Tier 1 soil RBSL charts can be provided for various ratios of L_1/L_2.

- ***Key Assumptions***: Attachment C details the derivation of the sorptive redistribution expression (Equation 4). The equation is based upon an assumption of COC mass conservation as the leachate front moves downward through the surface soil column, with the equilibrium partitioning of contaminants from the leachate to the encountered soil, vapor, and pore liquid phases characterized per Equation 3b. This model corresponds to movement of dissolved constituents through porous media and does not apply to cases involving downward migration of mobile NAPL materials. The equation determines the maximum leachate concentration reaching the depth of groundwater, neglecting the effects of the diminishing source concentration (C_T) over time as the leachate process continues. As shown on Table 3 (see Cases 7 and 8), using this maximum leachate concentration rather than a time-averaged value results in a conservative overprediction of chronic groundwater exposure concentrations by a factor of 1.1x to 1.4x, depending on soil column thickness.

TABLE 3: EFFECT OF KEY ASSUMPTION ON SAM RESULTS

SAM MODEL ASSUMPTION	CALCULATED SOIL BENZENE LIMIT (mg/Kg)		EFFECT OF BASE CASE ASSUMPTION ON CALCULATED SOIL LIMIT	
	SENSIVITY RUN RESULTS	BASE CASE RESULT	BASE CASE	SOIL LIMIT MULTIPLIER
No NAPL Partitioning Effect				
• **Case 1: Four-way Partitioning:** Benzene θ_{or} = 0.01	1.94	0.46	Conservative	4.2x
• **Case 2: Four-way Partitioning:** Benzene θ_{or} = 0.001	0.60	0.46	Conservative	1.3x
No Biodegradation				
• **Case 3: First-Order Decay:** Benzene Half-Life = 160 days; depth to GW: 5 ft	644	0.46	Conservative	1400x
• **Case 4: First-Order Decay:** Benzene Half-Life = 1600 days; depth to GW: 5 ft	0.92	0.46	Conservative	2x
No Competitive Sorption Effects				
• **Case 5: Competitive Sorption:** Equal BTEX concentrations	0.16	0.46	Non-Conservative	2.8x
• **Case 6: Competitive Sorption:** Benzene concentration = 10% of TEX	0.11	0.46	Non-Conservative	4.1x
No Time-Averaging of Groundwater Exposure Levels				
• **Case 7: Time Averaging** ED = 30 yrs; depth to GW: 0 ft	0.62	0.46	Conservative	1.4x
• **Case 8: Time Averaging:** ED = 30 yrs; depth to GW: 5 ft	1.38	1.23	Conservative	1.1x

NOTES:

1) To evaluate impact of simplifying assumptions on SAM results, sensitivity runs were conducted for the various cases identified above. Sensitivity run results compared to standard model output (base case) to determine net effect (increase/decrease) on calculated soil cleanup standard.

2) **Base Case Input Parameters:**
Thickness of affected soil = 3 ft
Width of affected soil = 15 ft
Lateral Darcy velocity = 0.25 ft/day
Saturated thickness of water-bearing unit = 10 ft
Surface Soil Type: Silty Sand (SM)
Base Case Decay Rate: 0
Soil bulk density = 1.65 kg/L
Organic carbon partition coefficient = 83 L/kg (benzene)
Henry's Law coefficient = 0.23 (benzene)
Fraction organic carbon = 0.005
Soil Moisture Parameters: See SM, Table 2

3) θ_{or} = Residual saturation of NAPL in soil pores
Depth to GW = Distance from base of affected soils to top of water-bearing unit

The equilibrium partitioning relationship incorporated in the SAM (Equation 3b) also neglects the effects of competitive sorption of dissolved organic constituents onto the free organic carbon (foc) fraction of the soil matrix. In the derivation of the soil-leachate partition factor (K_{SW}) for each COC, the full foc mass is assumed to be available for sorption of each constituent. In reality, in the presence of multiple dissolved constituents, the soil-water sorption coefficient (k_S) for each COC will be a function of the relative concentration of that COC in the dissolved phase and its binding energy to the soil carbon sorbate. Such competitive sorption relationships have been characterized using Langmuir-type isotherms for filtration design, but are not well understood at the field level. Therefore, for purpose of simplicity, competitive sorption processes have been neglected in the SAM. This measure can prove unconservative by overestimating soil sorption and consequently underestimating leachate concentrations. As shown on Table 3 (Cases 5 and 6), the degree of error involved depends upon the relative concentrations of the dissolved COCs. For BTEX mixtures, given equal source concentrations of each compound, leachate concentrations are underestimated by a factor of 2.8x to 4.1x. However, in conjunction with the other conservative elements of this model, this simplifying measure does not compromise the conservative nature of the SAM equation (see Item 6 below).

5) Leachate/Groundwater Dilution

- ***Model Description***: The SAM incorporates a leachate dilution factor (LDF) to account for dilution of dissolved COC concentrations as leachate mixes with lateral groundwater flow in the underlying water-bearing unit (see Equation 5a on Figure 2). This dilution factor is based upon a simple box model used to estimate mass dilution within a *mixing zone* located in the water-bearing unit directly beneath the affected soil mass (see Figure 2). Dividing the incoming leachate concentration (C_{w2}) by the LDF value yields a steady-state groundwater concentration within the mixing zone area.

  The infiltration rate I_f used in Equation 5a can be estimated using the empirical relationships of Equations 1a - 1c or determined from direct site measurements. The lateral groundwater Darcy velocity within the water-bearing unit (U_{gw}) can be based on default values (Tier 1) or on site-specific measurements of the hydraulic conductivity and lateral flow gradient of the water-bearing unit (Tier 2). To assist in estimation of mixing zone thickness, the SAM incorporates an equation relating mixing zone dimensions to the saturated thickness of the water-bearing unit and the relative magnitudes of the leachate infiltration and lateral groundwater flowrates (Equations 5b and 5c). This expression can be used to obtain a reasonable estimate of mixing zone thickness in the absence of a measured vertical plume dimension. Alternatively, for an unconfined water-bearing unit, the estimated plume thickness may be matched to the range of water table fluctuation observed at the site. Under Tier 1, the LDF can be derived on the basis of the fixed default plume thickness and groundwater flow parameters, per the example Texas values specified on Figure 2.

- ***Key Assumptions***: The LDF equation used in the SAM (Equation 5a) assumes uniform mixing of groundwater and soil leachate within the area of the mixing zone, estimated to extend over only the upper portion of the water-bearing unit. Given that the screened interval of a water supply well would typically extend below this mixing zone depth, this dilution equation will provide a conservative (upper-range) estimate of potential COC concentrations in groundwater produced from a well drilled in the immediate vicinity of the affected soil zone. The LDF expression and the associated mixing zone equations shown on Figure 2 (Equations 5a - 5c) are the same as those used for development of EPA Soil Screening Level (SSL) values. Detailed discussion of these calculation methods can be found in the SSL Technical Background Document (U.S. EPA, 1996).

6) Summary Calculations

- ***Method Description***: Equations 6a and 6b on Figure 2 summarize the calculation methods for i) a groundwater exposure concentration (C_{gw}), associated with a given affected soil concentration and ii) a soil target concentration (SSTL value), associated with a given groundwater risk-based exposure limit. These expressions incorporate each of the SAM components described above. Under Tier 2, site-specific input parameters are to be employed as outlined on Table 4. Tier 1 RBSL values can be based on the fixed default parameters specified on Figure 2.

- ***Key Assumptions***: The net effects of the various modeling assumptions noted above on the calculated soil PCL value are indicated on Table 3. As noted previously, neglecting the effects of NAPL-phase partitioning and time-averaged exposure concentrations introduces a conservative factor of roughly 1.5x - 4x into the model results, reducing the calculated soil SSTL value in each case (see Cases 1, 2, 7, and 8). For constituent mixtures, ignoring competitive sorption may contribute a non-conservative factor of 3x - 4x to the model (see Cases 5 and 6). The absence of biodegradation effects may represent the most conservative assumption in the SAM. As shown on Table 3 (Cases 3 and 4), use of first-order decay half-lives of 160 days or 1600 days for benzene (equivalent to 10x and 100x slower decay rates than the published half-life for benzene in soils; see Howard et al, 1991) would increase the allowable soil SSTL value by factors of 1200x and 2x, respectively, above the no-biodegradation case assumed in the SAM.

  As noted previously, the various modeling assumptions itemized on Table 3 have been incorporated in the SAM for purpose of simplicity. Their sum effect is a likely under-estimate of allowable soil SSTL levels and an over-estimate of potential groundwater impacts associated with soil leachate release. Consequently, this modeling approach should prove appropriate for use as a screening-level model under Tiers 1 and 2 of the site evaluation process.

3.0 Application of SAM

SELECTION OF INPUT PARAMETERS FOR TIERS 1 AND 2

The SAM may be employed for either i) prediction of groundwater exposure concentrations associated with a given affected soil concentration (Equation 6a) or ii) calculation of a soil SSTL value associated with a given groundwater exposure limit (Equation 6b). Applicable input parameters for each component of the SAM are identified on Figure 2. General guidelines for selection of the model input values required for each step of the calculation process are provided on Table 4.

Under Tier 1 of the site evaluation process, soil concentration limits for each COC can be defined on the basis of default values for all model input parameters, including a default soil type (sand) and a fixed or variable ratio of L_2/L_1. Example Tier 1 default values for all SAM input parameters proposed for use in the Texas Risk Reduction Program are shown on Figure 2.

Under Tier 2, site-specific values may be employed for the various site parameters used in the SAM. Each of these inputs may be characterized on the basis of actual site measurements, given adequate field and laboratory data. However, given the difficulty of obtaining representative measurements of certain site parameters (e.g., I_f, θ_{ws}, etc.), a combination of parameter estimates and direct site measurements may be applied as described below.

Reasonable Parameter Estimates Under Tier 2

Under Tier 2, reasonable estimates for the following model input parameters can be derived on the basis of general site information or published references, as follows:

- ***Net Infiltration (I_f)***: Estimate using Equations 1a - 1c based on i) predominant soil type in surface soil column and ii) mean annual rainfall in site vicinity.
- ***Estimated Soil Properties (θ_{as}, θ_{ws}, ρ_s, foc)***: Volumetric air and water contents (θ_{as}, θ_{ws}) in the surface soil column may be obtained from Table 2 based on the relevant soil type. Soil bulk density (ρ_s) and free organic carbon (foc) can be matched to default values (e.g., 1.5 g/cm^3 and 0.006, respectively) or measured on a site-specific basis.
- ***Chemical Reference Properties (K_{oc}, H)***: Use the chemical property values provided by the regulatory agency or other relevant source (e.g. RBCA Toolkit Software).
- ***Estimated Mixing Zone Thickness (δ_{gw})***: In lieu of directly measuring the groundwater plume thickness beneath the affected soil zone, Equations 5b and 5c can be used to establish a reasonable estimate of the groundwater-leachate mixing zone thickness. If the saturated thickness (b) of the water-bearing unit has not been determined to date, the user may estimate saturated thickness as the maximum measured vertical extent of the water-bearing unit (i.e., from top of water-bearing unit to base of deepest well or boring) plus some fixed distance. All other parameters required for Equations 5b and 5c should be determined from site-specific measurements under Tier 2. Alternatively, the groundwater-leachate mixing zone thickness may be estimated as the maximum rage of documented annual water table fluctuations within an unsaturated water-bearing unit.

Direct Site Parameter Measurements Under Tier 2

For a Tier 2 evaluation, the following site parameters will typically require direct measurement to ensure accurate model results:

- ***Soil Properties (W, L_1, L_2, C_s)***: The lateral (W) and vertical (L_1) dimensions of the affected soil zone should be delineated on the basis of soil sampling and testing. For use in the SAM, L_1 for each COC should be matched to the maximum thickness of the affected soils containing the COC at levels in excess of Tier 1 limits. To provide a reasonable prediction of potential groundwater impacts, the COC concentration in the affected soil zone (C_s) should then be matched to the *average* value measured within soil samples from locations evenly distributed over the depth interval L_1.The distance from the top of the

TABLE 4: SAM MODEL CALCULATION STEPS AND INPUT DATA REQUIREMENTS

	MODEL INPUT REQUIREMENTS			
SAM MODEL EQN. NO.	EQUATION PARAMETER	ESTIMATION METHOD	REQUIRED INPUT DATA	TIER 2 MEASUREMENT OR ESTIMATION GUIDELINES
Step 1: Soil-Leachate Partition Coefficient (K_{sw})				
Eqn. 3b	p_s	D or SS	soil type	Use default value (e.g., 1.5 g/cm^3) or measure average value directly.
	θ_{ws}, θ_{as}	Eqns. 2a and 2b	soil type	Use default θ_{as} and θ_{ws} values from Table 2 based on predominant USCS soil type. Define I_f per Step 3 below.
	k_s	Eqns. 3c and 3d	foc, pH, k_{oc}, K_d-metals	Measure foc or use default value (e.g., 0.006) for vadose zone. Determine k_{oc} for each COC from chemical reference. For metals, measure soil pH and determine K_d-pH function from reference literature.
Step 2: Sorptive Redistribution Factor (L_2/L_1)				
----	L_1	SS	L_1	Define maximum vertical thickness of affected soil zone exceeding Tier 1 limits based on field or laboratory analyses of soil cores
	L_2	SS	L_2	Define vertical distance from top of affected soil zone to top of water-bearing unit based on soil boring logs and soil test results. If depth to groundwater is unknown, either set L_2 equal to L_1 or estimate L_2 based on depth to same water-bearing unit at another site in the immediate vicinity.
Step 3: Leachate-Groundwater Dilution Factor (LDF)				
Eqn. 5a	I_f	Eqns. 1a - 1c	P, soil type	Measure directly or estimate using Equations 1a, 1b, or 1c per relevant soil type. For estimation, base P on local climatic records. Match soil type to site boring logs.
	U_{gw}	Eqn. 5b	K, i	Measure i for groundwater using appropriate field methods. Based on soil classification tests (ASTM D-422 and D-2487), use default K value from Table 2 for corresponding USCS classification or conduct field measurement of K.
	W	SS	W	Parallel to groundwater flow, measure width of soil zone exceeding Tier 1 limit.
	δ_{gw}	Eqn. 5c	b, α_v, W, I_f, U_{gw}	Measure plume thickness beneath source or use Eqn. 5c. For Eqn. 5c, determine b from boring logs or estimate as maximum known thickness plus fixed distance (e.g., 10 ft). Use default value for α_v (see Eqn. 5c). Alternatively, estimate δ_{gw} as maximum range of documented annual water table fluctuation. Define all other input parameters as above.
Step 4: Summary Calculations				
Eqn. 6a	C_s	SS	C_s	From field and lab test data, determine average COC concentration (mg/kg) within full affected soil zone corresponds to depth interval L_1.
Groundwater Exposure Concentration	K_{sw}, LDF, L_1, L_2	----	----	Define per Steps 1 - 3 above.
Eqn. 6b	$^{GW}RBSL_{Ing.}$	----	----	Identify applicable groundwater exposure limit (mg/L), for relevant exposure pathway (e.g., groundwater ingestion or dermal contact).
Soil Site-Specific Target Level (SSTL)	K_{sw} LDF, L_1, L_2	----	----	Define per Steps 1 - 3 above.

Parameter Definitions:

b	Saturated thickness of water-bearing unit (cm)
D	Default value
E	Exponent from Burdine relative permeability model (unitless)
foc	Free organic carbon content of surface soils [g-C / g-soil]
H	Henry's Law constant for constituent [cm^3-H_2O / cm^3-air]
i	Lateral groundwater flow gradient in water-bearing unit (cm/cm)
I_f	Net rainfall infiltration through affected soil zone (cm/yr)
k_{oc}	Carbon-water sorption coefficient for constituent [g-H_2O / g-C]
K	Hydraulic conductivity of underlying water-bearing unit (cm/sec)
K_{sw}	Soil-leachate partition coefficient [(mg/L-H_2O) / (mg/Kg-soil)]
K_{vs}	Saturated hydraulic conductivity of surface soils (cm/sec)
L_1	Thickness of affected soil zone (cm)
L_2	Thickness of soil column from top of affected soil zone to top of water-bearing unit (cm)
P	Average annual rainfall precipitation (cm/yr)
p_s	Soil bulk density [g/cm^3]
SS	Site-specific measure
U_{gw}	Darcy velocity (cm/sec) (U_{gw} = K•I)
W	Width of affected soil zone parallel to groundwater flow direction (cm)
θ_{as}	Volumetric air content of surface soils [cm^3 - air/cm^3 - soil]
δ_{gw}	Leachate-groundwater mixing zone thickness (cm)
θ_T	Total soil porosity [cm^3-pore space / cm^3-soil]
θ_{ws}	Volumetric water content of surface soils [cm^3-water / cm^3-soil]

affected soil zone to the top of the underlying water-bearing unit (L_2) can be determined from on-site boring logs or from data obtained from a separate location in close proximity to the site under evaluation.

- ***Groundwater Flow Properties (U_{gw}, K, i)***: For estimation of the leachate-dilution factor (LDF) and mixing zone depth (δ_{gw}), the groundwater Darcy velocity within the underlying water-bearing unit (U_{gw}) should be calculated on the basis of site-specific lateral hydraulic flow gradient (i) value and an estimated or measured hydraulic conductivity (K) value. Determination of the lateral hydraulic flow gradient within the water-bearing unit involves triangulation among static water levels measured in at least 3 site wells or piezometers, per standard guidelines. If the soil type of the water-bearing unit has been classified in the laboratory in accordance with ASTM Standards D-422 and D-2487 (ASTM), the hydraulic conductivity of the unit may be estimated using the default values listed on Table 2. Alternatively, K can be directly measured in the field by means of rising-head slug tests or constant-rate pumping tests conducted on properly completed wells or piezometers.

EXAMPLE APPLICATION OF SAM

Table 5 presents example soil cleanup standards calculated using the SAM for a range of soil types, depths, and annual rainfall levels. Assumed site conditions are illustrated on Figure 4. In each case, the source area SSTL for the affected soil zone was back-calculated using Equation 6b, based on a 0.005 mg/L benzene exposure limit in the underlying water-bearing unit. For purpose of comparison, benzene soil limits calculated using the soil leachate equations and default infiltration rate (30 cm/yr) listed in ASTM E-1739 are also shown on Table 5.

For the cases analyzed, the ASTM soil concentration limit is a constant (i.e., 0.069 mg/kg benzene on soil). However, the SAM results vary according to annual rainfall, soil type, and thickness of the underlying soils. As shown on Table 5, allowable benzene soil concentrations vary by roughly one order of magnitude between an arid climate condition (e.g., Albuquerque, New Mexico) and a high rainfall area (e.g., Houston, Texas) for a given soil type. For a given rainfall and soil thickness, the allowable benzene level in sand versus clay soils also differs by roughly 10-fold. For each site and each soil type, the soil benzene limit increases with increasing thickness of underlying soils (at a rate that is linear with respect to the ratio L_2/L_1, as defined in Equation 6b). Please note that the soil concentration limits listed on Table 5 are example model results for a given set of site conditions and **do not** represent generic cleanup values. Site-specific soil SSTL values must be derived using appropriate model input parameters, per the procedures outlined on Table 4.

TABLE 5: EXAMPLE SOIL CLEANUP LEVELS CALCULATED USING SAM AND ASTM SOIL LEACHING MODELS

SOIL ZONE DIMENSIONS			SOIL CONCENTRATION LIMIT FOR BENZENE (MG/KG)					
DEPTH TO GROUNDWATER	L_1	L_2	ALBUQUERQUE, NM (P=12 IN/YR)		KANSAS CITY, KS (P=32 IN/YR)		HOUSTON, TX (P=48 IN/YR)	
(ft)	(ft)	(ft)	SAM	ASTM	SAM	ASTM	SAM	ASTM
SAND (SW-SP)								
0	3	3	0.283	0.069	0.043	0.069	0.021	0.069
5	3	8	0.756	0.069	0.114	0.069	0.055	0.069
10	3	13	1.23	0.069	0.185	0.069	0.090	0.069
20	3	23	2.17	0.069	0.326	0.069	0.159	0.069
50	3	53	5.01	0.069	0.752	0.069	0.365	0.069
SILT (ML)								
0	3	3	0.756	0.069	0.110	0.069	0.051	0.069
5	3	8	2.01	0.069	0.293	0.069	0.137	0.069
10	3	13	3.27	0.069	0.476	0.069	0.222	0.069
20	3	23	5.79	0.069	0.843	0.069	0.393	0.069
50	3	53	13.3	0.069	1.94	0.069	0.905	0.069
CLAY (CH)								
0	3	3	3.98	0.069	2.12	0.069	2.12	0.069
5	3	8	10.6	0.069	5.65	0.069	5.65	0.069
10	3	13	17.3	0.069	9.18	0.069	9.18	0.069
20	3	23	30.5	0.069	16.2	0.069	16.2	0.069
50	3	53	70.4	0.069	37.4	0.069	37.4	0.069

NOTES:

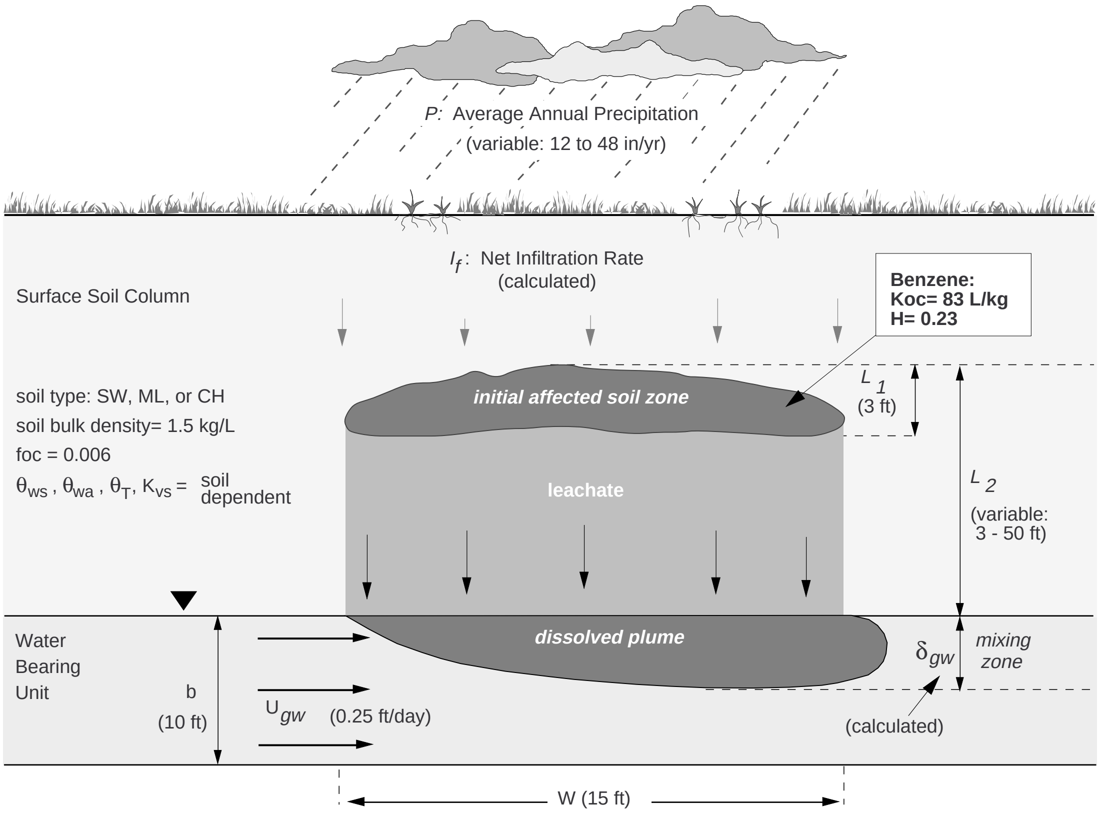
1) Soil concentration limits protective of 0.005 mg/L benzene exposure level in underlying groundwater were calculated using both the SAM (Equation 6b) and the ASTM E-1739 soil leaching equation (ASTM, 1995). ASTM value (0.069 mg/Kg) was based on default infiltration rate listed in Appendix X.2 of ASTM E-1739 (i.e., 30 cm/yr). SAM input varied according to soil type, annual rainfall, and depth of underlying soil. See Figure 4 for case study illustration.

2) Input Parameters:

Thickness of affected soil = 3 ft	Soil bulk density = 1.7 kg/L
Width of affected soil = 15 ft	Organic carbon partition coefficient =38 L/kg (benzene)
Lateral Darcy's velocity = 0.25 ft/day	Henry's Law coefficient = 0.23 (benzene)
Saturated thickness of water-bearing unit = 10 ft	Fraction organic carbon = 0.006

3) P = Mean annual precipitation
Depth to Groundwater = Distance from base of affected soils to top of water-bearing unit (L_2 - L_1).
L1 = Thickness of affected soils exceeding Tier 1 limits.
L2 = Distance from top of affected soils to top of water-bearing unit.

FIGURE 4: ASSUMED SITE CONDITIONS FOR EXAMPLE SAM MODEL CALCULATION



NOTES: See Table 5 for calculation results.
See Attachment B for soil-dependent parameter values.

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ATTACHMENT A
ESTIMATION OF ANNUAL NET INFILTRATION AS A FUNCTION OF MEAN ANNUAL PRECIPITATION AND SOIL TYPE

Overview of Estimation Method

Net infiltration corresponds to total rainfall infiltration minus the loss associated with evapotranspiration. The net infiltration term (I_f) thereby represents the deep percolation flow (in cm/year) through the affected soil zone which could result in leachate release to underlying groundwater. In the SAM, net infiltration is estimated as a function of average annual rainfall (cm/year) and the predominant soil type in the vadose zone (sand, silt, or clay) using the empirical relationships plotted on Figure 2. Derivation of these empirical relationships is detailed below.

The sand soil curve shown on Figure 2 represents an 80% envelope based on rainfall infiltration data for over 100 sandy soil sites in 18 geographic regions in the United States, as compiled by Stephens & Associates (API, 1996). This regression curve provides a conservative (upper-range) estimate of deep percolation for over 80% of the sand or gravel soil sites reported in this database. Curves for silty and clayey soils were derived from this empirical sandy soil curve based on the relative percent infiltration occurring in a 2-hour storm event, as characterized using the Horton infiltration relationship (Viessman et al., 1989). Derivation procedures are detailed below.

Net Infiltration as a Function of Precipitation for a Sandy Soil

The empirical relationship between net infiltration and annual rainfall in sandy soils was based upon a database of 140 sites from 18 different geographic regions compiled by Stephens & Associates (API, 1996). Among these, 101 sites consisting of sandy or gravelly soils were selected for characterization of sand infiltration rates. Many of the data points included in this subset contain soils much more permeable than sand, such as glacial outwash and other soils containing high percentages of gravel. Consequently, the dataset likely represents a high-range estimate for infiltration through sand.

A plot of percent annual net infiltration vs. mean annual precipitation for these 101 selected data points (see FigureA-1) indicates considerable scatter, but confirms a general trend of increasing percent infiltration with increased annual rainfall. The purpose of this net infiltration model is to provide a reasonable high-range estimate of infiltration rates. Therefore, as shown on FigureA-1, an envelope line for sandy soil infiltration exceeding actual reported infiltration rates for 80% of the site population has been selected as the characteristic curve for net infiltration. This relationship is conservative in that: i) approximately 80% of the representative data fall below the line, and ii) a majority of the data points plotted pertain to soil types more permeable than a sandy soil. Consequently, this curve can be relied upon to provide a conservative over-estimate of infiltration rates and leachate impacts in most sandy soil conditions.

The 80% envelope line for a sandy soil yields the following relationship between percent annual net infiltration and mean annual precipitation (see Figure 1.1):

A) $I_f\,[\text{as }\%\,P] = 0.018 \bullet (P)$

where: I_f = mean annual net infiltration as a percentage of precipitation
P = mean annual precipitation, mm/yr

Converting this formula to determine net infiltration in cm/year for an input of annual precipitation in cm/year for a sandy soil yields:

B) I_f [cm/year]= $0.0018 \bullet (P)^2$

where: I_f = mean annual net infiltration in cm/year
P = mean annual precipitation in cm/year

Estimation of the Net Infiltration Relationships for Clay and Silt Soils

In order to establish infiltration vs. rainfall relationships for clay and silt soils comparable to that shown on Figure A-1, Horton's infiltration method can be used to estimate infiltration into clay and silt soils as a percentage of infiltration into sandy soils. These infiltration ratios may then be applied to Equation B above to derive clay and silt soil infiltration curves.

Horton's equation:

C) $f_p = f_c + (f_o - f_c) \bullet e^{-kt}$

where: f_p = the infiltration capacity (depth/time) at some time (t), in/hr
k = a constant representing the rate of decrease in f capacity, 1/hr
f_c = a final or equilibrium capacity, in/hr
f_o = the initial infiltration capacity, in/hr

The Horton infiltration method is a three-parameter model relating the infiltration capacity at any time (f_p) during a storm event to the initial infiltration rate (f_o), the final or equilibrium infiltration rate (f_c), and an exponential constant representing the decrease in infiltration capacity over time (k) (see Maidment, 1993). The model indicates that in a storm event, as rainfall intensity exceeds infiltration capacity, infiltration tends to decrease in an exponential manner. Based on the use of typical default parameters for various soil types, this model can be used to define infiltration rates in clay and silt soils as a percentage of the rate in sand for a given rainfall. Viessman *et al.* (1989) present typical infiltration curves and Horton parameter values for infiltration through sands, silts, and clays. Maximum parameter values for each given range are shown on Table A-1.

Table A-1: Typical Parameters for Horton's Method

	Infiltration Rate (in/hr)		
Soil Group	**f_o @ t=0**	**f_1 @ t=1**	**f_c @ t=∞**
High (Sandy Soils)	5.0	1.0	0.85
Intermediate (Silty Soils)	2.5	0.5	0.425
Low (Clayey Soils)	0.5	0.1	0.085

From: Viessman et al., 1989

Note that the ratios among sand, silt, and clay are the same (100%, 50%, 10%) for any time. Therefore, the empirical relationship of net infiltration vs. annual rainfall for a sandy soil (Figure A-1) may simply be adjusted by the relative infiltration ratios used for the Horton infiltration method. This yields:

D) i) For **Sand**:

$$\boxed{I_f = (0.0018) \bullet (P)^2}$$

ii) For **Silt**:

$$I_f = (50\%) \bullet (0.0018) \bullet (P)^2$$

$$\boxed{I_f = (0.0009) \bullet (P)^2}$$

iii) For **Clay**:

$$I_f = (10\%) \bullet (0.0018) \bullet (P)^2$$

$$\boxed{I_f = (0.00018) \bullet (P)^2}$$

where: I_f = mean annual net infiltration, cm/year
P = mean annual precipitation, cm/year

References

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ATTACHMENT B
DERIVATION OF DEFAULT SOIL MOISTURE PARAMETERS

Overview of Methodology

The Brooks and Corey relationship (1964) combined with the Burdine equations (1959) can be used to derive volumetric air and water content values for vadose zone soils that are in equilibrium with the net annual rainfall infiltration rate. For use in the Soil Attenuation Model (SAM), these relationships have been used to establish default soil moisture volumes for various soil types, based on a median annual rainfall. Model sensitivity runs indicate that use of these median values in place of site-specific equilibrium moisture levels does not significantly affect model results. On this basis, these default values have been incorporated in SAM as a simplifying measure.

Relationships of Soil Moisture to Rainfall Infiltration

Vertical infiltration under equilibrium conditions is related to the vertical hydraulic gradient and the unsaturated hydraulic conductivity at the ambient water content of the vadose zone soil. Unsaturated hydraulic conductivity is commonly expressed as the product of saturated hydraulic conductivity and the relative permeability, yielding the following vertical flow equation:

A) $I_f = i \bullet K_{vs} \bullet k_{rw}$

where:
I_f = net infiltration
i = hydraulic gradient
k_{rw} = relative permeability of the soil, unitless
K_{vs} = saturated hydraulic conductivity of vadose zone soils

By assuming that infiltration occurs under an average unit hydraulic gradient and solving for the relative permeability, this relationship converts to:

B) $$k_{rw} = \frac{I_f}{K_{vs}}$$

Studies have shown that the relative permeability is a function of the volumetric water content. Using the Brooks and Corey (1964) soil characteristic model combined with the Burdine equations (1959), the relative permeability function is given by:

C) $$k_{rw} = \left[\frac{\theta_{ws} - \theta_{wr}}{\theta_T - \theta_{wr}}\right]^{\varepsilon}$$

where:
k_{rw} = relative permeability of the soil, unitless
θ_{ws} = volumetric water content soil
θ_T = total soil porosity
θ_{wr} = irreducible soil water content
ε = $3 + 2/\lambda_{BC}$
λ_{BC} = pore size distribution index, unitless (Brooks and Corey, 1964)

Substituting Equation B into Equation C yields the following equation for volumetric water content as a function of annual rainfall infiltration, I_f:

$$\text{D)}\quad \theta_{ws} = \theta_{wr} + \left[\theta_T - \theta_{wr}\right] \bullet \left[\frac{I_f}{K_{vs}}\right]^{\frac{1}{\varepsilon}}$$

The volumetric air content of the soil can then be derived as:

$$\text{E)}\quad \theta_{as} = \theta_T - \theta_{ws}$$

Derivation of Default Values for Volumetric Water and Air Content

Default Brooks-Corey Parameters

Equations D and E can be used to estimate equilibrium soil moisture parameters (θ_{ws}, θ_{as}) for a given soil type based on default values of θ_T, θ_{wr}, and K_{vs} for that soil type. For USDA soil types, default values for θ_T and θ_{wr} have been established by Carsel and Parrish (1988) using the multiple regression method of Rawls and Brakensiek (1985). Results of the Carsel and Parrish analyses are provided on Table B-1. To develop comparable values for Unified Soil Classification System (USCS) soils, USCS soil types were first correlated to USDA textural classifications as shown on Figure B-1. In most cases, the USCS soil type was found to overlap multiple USDA classifications. Therefore, to establish conservative values for USCS soils, the most conservative value (with respect to leachate concentration) among the overlapped USDA classifications was selected to represent the USCS soil type. For each USCS soil type, Table B-2 provides the resulting θ_T and θ_{wr} values. The saturated hydraulic conductivity (K_{vs}) of the surface soil column can also be characterized based on predominant soil type. Representative default values obtained from research literature are listed on Table B-3.

Table B-1: Default Brooks-Corey Parameter Values for USDA Textural Classifications

USDA Textural Classification	θ_T	θ_{wr}	λ_{BC}
Clay	0.38	0.068	0.09
Clay loam	0.41	0.095	0.31
Loam	0.43	0.078	0.56
Loamy sand	0.41	0.057	1.28
Silt	0.46	0.034	0.37
Silt loam	0.45	0.067	0.41
Silt clay	0.36	0.070	0.09
Silty clay loam	0.43	0.089	0.23
Sand	0.43	0.045	1.68
Sandy clay	0.38	0.100	0.23
Sandy clay loam	0.39	0.100	0.48
Sandy loam	0.41	0.065	0.89

Source: Carsel and Parrish, 1988 See Peck et al., 1974 for USDA soil classification.

Parameters as defined under Equation C above.

Table B-2: Default Brooks-Corey Parameter Values for USCS Soil Types

USCS Soil Classification	θ_T	θ_{wr}	λ_{BC}
SW/SP: Clean Sand	0.41	0.045	1.68
SM: Silty Sand	0.41	0.057	1.28
SC: Clayey Sand	0.38	0.065	0.89
ML: Sandy Silt	0.43	0.067	0.56
ML: Silt	0.46	0.034	0.37
MH: Clayey Silt	0.36	0.067	0.41
CL: Sandy Clay	0.38	0.1	0.23
CL: Silty Clay	0.36	0.07	0.09
CH: Clay	0.38	0.068	0.09

Note: Derived based on correlation to USDA default values, see Figure B-1 See Lambe et al., 1969, for USCS soil classification. Parameters as defined under Equation C above.

Table B-3: Typical Hydraulic Conductivity Values for Various Soil Types

USCS Soil Classification	Typical Hydraulic Conductivity Values (K_{vs}) (cm/s)
SW/SP: Clean Sand	10^{-2}
SM: Silty Sand	10^{-3}
SC: Clayey Sand	10^{-5}
ML: Sandy Silt	10^{-5}
ML: Silt	10^{-5}
MH: Clayey Silt	10^{-5}
CL: Sandy Clay	10^{-6}
CL: Silty Clay	10^{-7}
CH: Clay	10^{-8}

Note: Typical saturated hydraulic conductivity values represent median values reported by Freeze and Cherry (1979), Rawls and Brakensiek (1985).

Derivation of Default Volumetric Air and Water Content Values

Using Equations D and E in combination with the default parameters on Tables B-1 through B-3, equilibrium soil moisture values (θ_{ws}, θ_{as}) can be derived as a function of soil type and annual rainfall infiltration (I_f). To evaluate the sensitivity of the SAM equation to the use of rainfall-dependent soil moisture values, soil leachate concentrations have been calculated for each soil type to compare the use of i) site-specific, rainfall-dependent, soil moisture values (derived using Equations D and E for site-specific rainfall level) and ii) default soil moisture values, derived using

Equations D an E for a fixed rainfall level matched to the U.S. Median level of 30 in/yr (Geraghty-Miller, 1973). Table B-4 summarizes the results of this analysis. As shown, the use of default values instead of site-specific soil moisture values at these rainfall levels produces an average variation of only 5% in the soil leachate concentration predicted by SAM. Consequently, fixed default soil moisture values based upon a median rainfall (i.e., 30 in/yr) can be used in place of the rainfall-dependent values (Equations D and E) with very little error. Default values for volumetric water content (θ_{ws}) and volumetric air content (θ_{as}) for each USCS soil type are provided on Table B-5.

Table B-4: Comparison of Soil Leachate Concentrations Calculated Using Both Site Specific and Default Soil Moisture Values (θ_{ws}, θ_{as}) for Two Different Rainfall Levels

USCS Soil Classification	**Predicted Leachate Concentration (mg/L-Benzene)**						
	Low Rainfall (P = 9 in/yr)			High Rainfall (P = 55 in/yr)			Maximum Difference
	Site-Specific θ_{ws} and θ_{as}	Default θ_{ws} and θ_{as}	Percent Difference	Site-Specific θ_{ws} and θ_{as}	Default θ_{ws} and θ_{as}	Percent Difference	
SW/SP: Clean Sand	0.715	0.695	3%	0.130*	0.130*	0%	3%
SM: Silty Sand	0.682	0.655	4%	0.130*	0.130*	0%	4%
SC: Clayey Sand	0.618	0.571	8%	0.130*	0.130*	0%	8%
ML: Sandy Silt	0.579	0.540	7%	0.260*	0.260*	0%	7%
ML: Silt	0.555	0.510	8%	0.260*	0.260*	0%	8%
MH: Clayey Silt	0.604	0.568	6%	0.260*	0.260*	0%	6%
CL: Sandy Clay	0.546	0.518	5%	0.507	0.518	2%	5%
CL: Silty Clay	0.515	0.504	2%	0.493	0.504	2%	2%
CH: Clay	0.487	0.479	2%	0.479	0.479	0%	2%
						AVERAGE:	**5%**

Notes:

1) *Table compares SAM results for soil leachate concentrations as calculated using either i) rainfall-dependent soil moisture values, calculated per Equations D and E or ii) default soil moisture values, derived using Equations D and E for assumed rainfall of 30 in/yr (U.S. Median).*

2) *Leachate concentrations calculated for 2 rainfall levels corresponding to lowest (9 in/yr) and highest (55 in/yr) average annual rainfall levels reported for U.S. States (Geraghty-Miller, 1973). Net infiltration estimated for each soil type using Equations 1a - 1d of Figure 2. Soil leachate concentrations calculated using Equation 4a of Figure 2.*

3) *Concentrations based on a benzene source concentration of 1.0 mg/L, source thickness of 3 ft, source width of 15 ft, and no biodegradation. The distance from the bottom of the affected soil zone to the to the top table of the water (L_2) was assumed to be 10 ft; however, relative leachate concentrations for different rainfalls are independent of this distance.*

4) ** = Value corresponds to upperbound leachate concentration for mass conservation (see Equation 4b of Figure 2).*

Table B-5: Default Volumetric Water and Air Contents for USCS Soil Types

USCS Soil Classification	θ_T	θ_{ws}	θ_{as}
SW/SP: Clean Sand	0.41	0.076	0.334
SM: Silty Sand	0.41	0.12	0.29
SC: Clayey Sand	0.38	0.23	0.15
ML: Sandy Silt	0.43	0.26	0.17
ML: Silt	0.46	0.3	0.16
MH: Clayey Silt	0.36	0.24	0.12
CL: Sandy Clay	0.38	0.31	0.07
CL: Silty Clay	0.36	0.34	0.02
CH: Clay	0.38	0.38	0

Note:

θ_T = *Total soil porosity* (cm^3*-voids/*cm^3*-soil)*

θ_{ws} = *Volumetric water content* (cm^3*-water/*cm^3*-soil)*

θ_{as} = *Volumetric air content* (cm^3*-air/*cm^3*-soil)*

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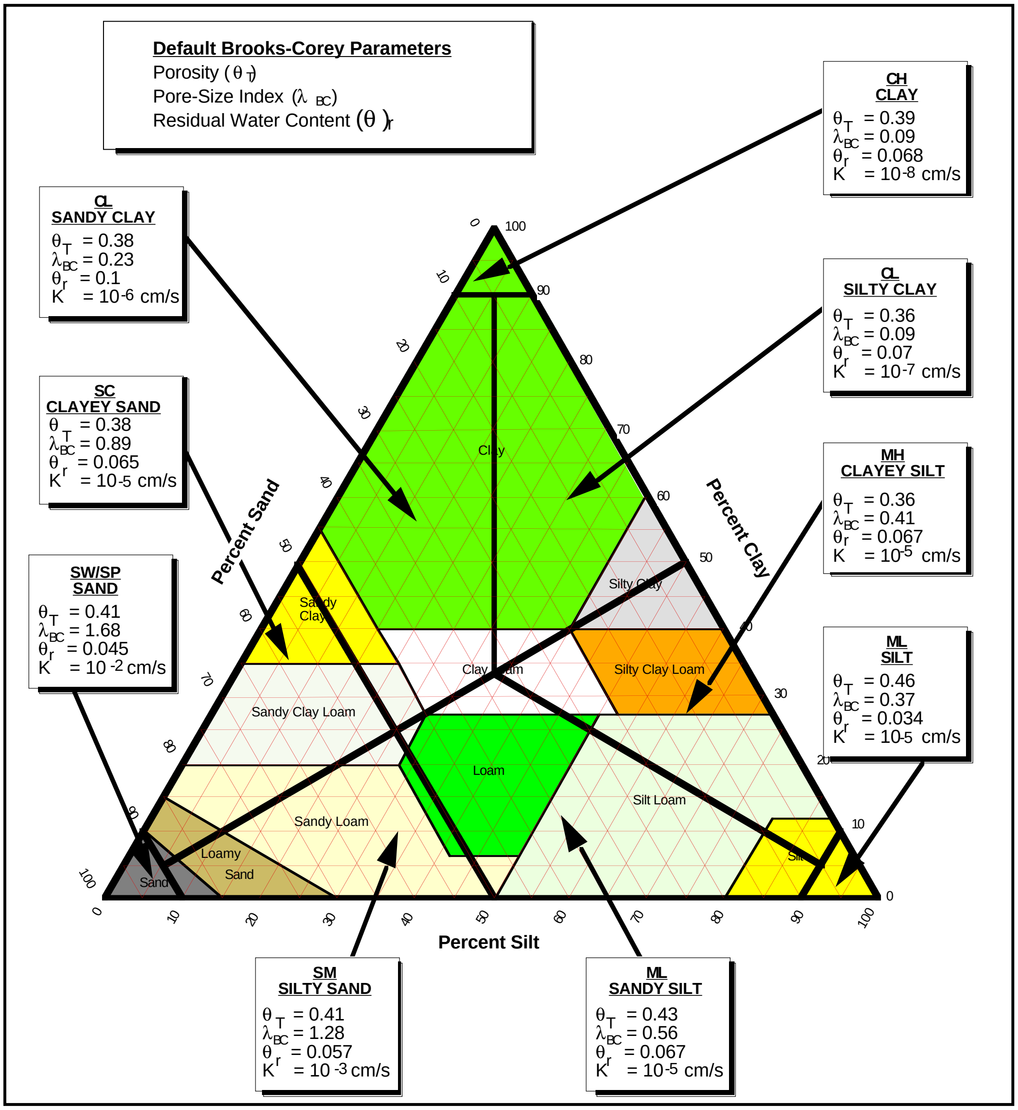
FIGURE B-1: GENERALIZED CORRELATION OF USCS AND USDA SOIL TYPES AND DEFAULT BROOKS-COREY PARAMETERS



Notes:

1) Correlations between USDA and USCS soil classification categories are approximate, based on the general range of soil grain size. Parameter values for USCS Classification were chosen as the most conservative values from corresponding USDA estimates (Carsel and Parrish, 1988; Rawls & Brakensiek, 1985). See Table B-1 for parameter values corresponding to USDA soil types.
2) See Peck et al., 1974 for USDA soil classifications. See Lambe et al., 1969 or USCS soil classifications.

ATTACHMENT C
SORPTIVE MASS REDISTRIBUTION: LEACHATE TO UNDERLYING CLEAN SOIL

Overview

In the SAM model, contaminant transfer from the affected soil to the infiltrating porewater is characterized on the basis of a conventional equilibrium partitioning relationship (see Equations 3b and 3c on Figure 2). The model then corrects this initial leachate concentration for the effect of sorptive mass loss as the leachate percolates downward through the soil column toward the underlying groundwater zone. As a result of sorptive redistribution of contaminant mass from the leachate onto intervening soils, the initial equilibrium leachate concentration will be reduced prior to reaching the depth of the water-bearing unit. This adjustment can prove significant in deep groundwater systems, wherein a significant thickness of unaffected soils may underlie the affected soil zone.

This Attachment derives a simple expression for this sorptive redistribution effect, based on a finite source mass and equilibrium partitioning of leachate onto underlying soils.

Sorptive Mass Redistribution

As indicated on Figure C-1, the source zone for contaminated leachate release to groundwater can be characterized as a discrete area (A) and thickness (L_1) of affected soils within the surface soil column overlying the uppermost water-bearing unit beneath the site. This source zone represents a finite source mass (equivalent to the bulk mass of affected soil times the representative COC concentration) that is spread downward through the soil column via leachate percolation. If, as a conservative measure, the processes of contaminant biodegradation and volatilization are neglected, the total mass of contaminants in the soil column remains constant as the leachate front moves toward the underlying water-bearing unit.

Assuming equilibrium partitioning among the soil solid, pore liquid, and vapor phases as the contaminants spread over a soil depth (L) yields the following expression:

A) $$A \bullet B_w \bullet C_w \bullet L = \text{Constant}$$

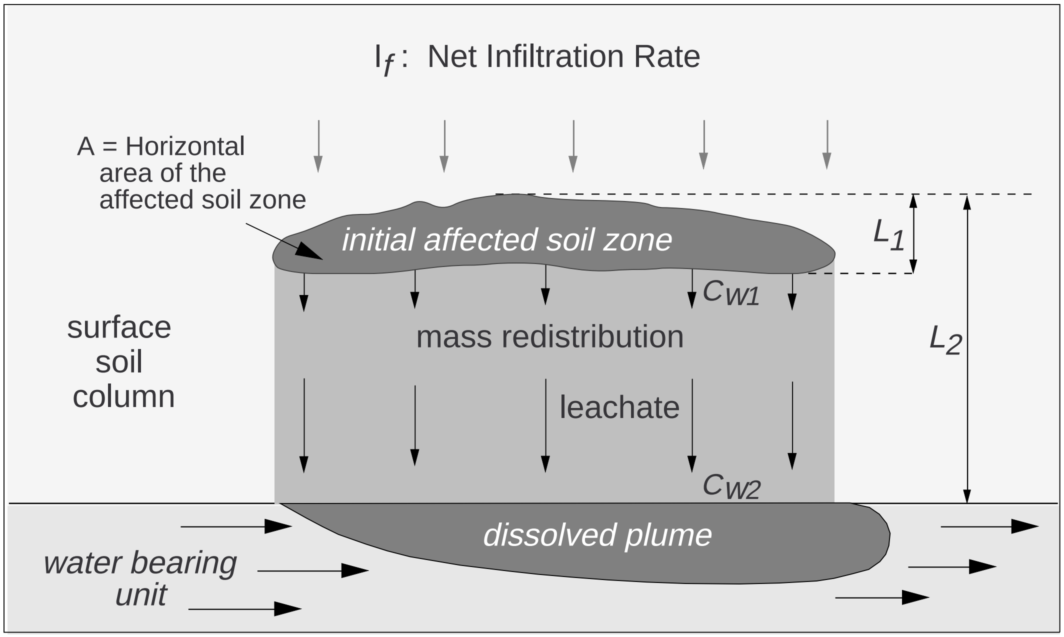
where: A = area of affected soil zone
B_w = bulk water partitioning coefficient
C_w = COC concentration in the soil pore water
L = distance from the top of the affected soil zone to depth of leachate front

Given equilibrium partitioning, the bulk water partitioning coefficient (B_w) is expressed as:

B) $$B_w = \theta_{ws} + H \bullet \theta_{as} + \rho_s \bullet k_s$$

where: θ_{ws} = volumetric water content of soil column
θ_{as} = volumetric air content of soil column
H = Henry's law constant for COC
p_s = bulk soil density

FIGURE C-1: MASS REDISTRIBUTION PARAMETERS



The affected soil area *(A)* and the bulk partitioning coefficient *(B_w)* remain constant as the finite contaminant mass is redistributed to soils below the initial source zone. Prior to leachate release into the underlying water-bearing unit, the total contaminant mass is a constant for any soil depth *L*. Therefore:

Mass in the redistributed source zone can be expressed as a function of its length and concentration and is equal the original source zone mass:

C) $A \bullet B_w \bullet C_{w_1} \bullet L_1 = A \bullet B_w \bullet C_{w2} \bullet L_2$, or

D) $C_{w2} \bullet L_2 = C_{w1} \bullet L_1$

Solving for the leachate concentration (C_{w2}) immediately prior to leachate release to the water-bearing unit yields:

E) $C_{w2} = C_{w1} \bullet \frac{L_1}{L_2}$

where: C_{w2} = COC concentration in the leachate at the depth of the water-bearing unit
C_{w1} = COC concentration in the leachate at the base of the initial affected soil zone
L_1 = thickness of the original source zone
L_2 = distance from the top of the affected soil zone to the top of the saturated water-bearing unit

As the leachate process continues, contaminant mass will be released to underlying lateral groundwater flow, resulting in a net reduction in contaminant mass in the soil column and a consequent reduction in the soil leachate concentration (C_{w2}) entering the groundwater unit over time. In the SAM model, this diminishing source concentration is neglected as a conservative measure. The influent soil leachate concentration is assumed to remain constant over time, equal to the initial concentration in the leachate front (i.e., C_{w2} as calculated per Equation E above).

ATTACHMENT D
TIME AVERAGING FACTOR: DIMINISHING LEACHATE SOURCE TO GROUNDWATER

Overview of Source Depletion Process

In the SAM, a constant finite contaminant mass is redistibuted downward through the vertical soil column via equilibrium partitioning between the advancing leachate and the clean underlying soils. Upon reaching the water-bearing unit, the contaminant mass in the vertical soil column will decrease with time as the leachate process continually removes mass from the affected soil. However, as a conservative measure, the SAM assumes this initial leachate concentration to remain constant for the full duration of the groundwater exposure period. This assumption may prove to be overly conservative for carcinogenic compounds, where chronic effects are dependant on average COC concentrations over a particular exposure duration (e.g., typically 25 or 30 years for residential and industrial exposure scenarios, respectively). As an optional meaure for use with the SAM, a time averaging factor (TAF) has been derived to account for the diminishing leachate source to groundwater for a Tier 3 evaluation of carcinogenic COCs.

This Attachment derives a simple expression for a 30-year time averaging factor starting with the time the leachate first reaches the water bearing zone at an initial concentration (C_{w0}). This derivation is based on a mass balance of the vertical soil column between the top of the affected soil zone and the water table. The control volume has a discrete cross-sectional area (A) and thickness (L)

Time Averaging Factor (TAF) Derivation

C(t) is the leachate concentration in the control volume at any time, t. Assuming equilibrium partitioning, the total contaminant mass is given by

A) $M(t) = A \bullet L \bullet B_w \bullet C(t)$ and

B) $B_w = \theta_{ws} + H \bullet \theta_{as} + \rho_s \bullet k_s$

where: B_w = bulk water partitioning coefficient
θ_{ws} = volumetric water content of soil column
θ_{as} = volumetric air content of soil column
H = Henry's law constant for COC
p_s = bulk soil density
k_s = soil-water sorption coefficient for COC

The time rate of change of contaminant mass in the control volume is equivalent to the advective contaminant flux via leachate to the groundwater. This is expressed as:

C) $\frac{dM}{dt} = A \bullet L \bullet B_w \bullet \frac{dC}{dt} = -A \bullet I_f \bullet C(t)$

where: I_f = net infiltration rate

and rearranging yields:

D) $$\frac{dC}{C(t)} = \frac{-I_f}{L \bullet B_w} dt$$

For $C(t)=C_{w0}$ at $t=0$, this expression is integrated to yield:

E) $$C(t) = C_{w0} \bullet \exp\left[\frac{-I_f \bullet t}{L \bullet B_w}\right]$$

The TAF is the normalized average concentration C_{avg}/C_{w0} over the exposure duration (ED) from $t=0$ to $t= ED$. This is expressed by:

F)

$$TAF = \frac{C_{avg}}{C_{w0}} = \frac{1}{ED} \bullet \int_0^{ED} \exp\left[\frac{-I_f \bullet t}{L \bullet B_w}\right] dt = \frac{L \bullet B_w}{I_f \bullet ED} \bullet \left[1 - \exp\left[\frac{-I_f \bullet ED}{L \bullet B_w}\right]\right]$$