
Soil Attenuation Model (SAM) for Derivation of Risk-Based Soil Remediation Standards

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Abstract

Under sponsorship from the national Partners In RBCA Implementation (PIRI), a new Soil Attenuation Model (SAM) has been developed to provide a conservative estimate of soil-to-groundwater contaminant release based on readily available site data. 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, SAM retains the format of a simple, screening-level analytical expression requiring limited site-specific data input. SAM has recently been specified for use in various state RBCA programs.

This paper provides an overview of SAM, including summary guidelines regarding calculation procedures and input parameter selection, and reviews the key steps of the soil-to-groundwater leachate process. The model is applicable to analysis of porous media soils impacted by either organic or inorganic constituents, in the absence of mobile non-aqueous phase liquids (NAPLs). Using either site-specific or generic site properties, the 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 cleanup level, based on the applicable groundwater standard at the point of exposure. SAM incorporates simplifying assumptions which reduce site-specific data requirements, while retaining the rigor of more complex models.

A case study has been conducted to compare the utility and outcomes of SAM versus three more complex leachate models (SESOIL, VADSAT, and Jury's Model). Results of this case study comparison indicate that SAM is relatively conservative with respect to these other transport models due to its neglect of mass loss via volatilization. Peak leachate concentrations predicted by the four models varied by two orders of magnitude for a given site condition. The predicted leachate concentrations over time exhibited even more significant variability. The observed differences in modeling results relate to differing rates of vertical leachate flow and the associated mass loss via volatilization and biodecay over time. In most cases, SAM provided conservative outcomes relative to the more complex modeling tools.

Overview of Soil Attenuation Model (SAM)

RISK-BASED MODELING REQUIREMENTS

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 Site-Specific Target Levels (SSTLs) derived by SAM represent contaminant concentration limits for an affected soil mass such that subsequent leachate migration to an underlying water-bearing unit will not cause exceedance of applicable groundwater quality standards. Such SSTL values are not *predictive* of groundwater impacts; at many sites, even if these levels are not presently exceeded in the surface soil column, groundwater impacts may have previously occurred via other mechanisms (e.g., product release directly to groundwater). Rather these SSTL levels serve as conservative soil target concentrations designed to prevent any *further* impact on groundwater quality via soil leachate release. Source area soils containing contaminants at concentrations less than or equal to these levels will require no further action to be protective of groundwater.

AMENDMENTS TO ASTM RBCA SOIL LEACHATE EQUATION

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, SAM retains the format of a simple, screening-level analytical expression requiring limited site-specific data input.

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, 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. 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. 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:** 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:** 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 (volumetric water and air contents) consistent with the predominant soil type in the surface soil column.
- **Leachate-Groundwater Dilution:** 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.

In the base version of this model, contaminant loss through the processes of volatilization and biodegradation are neglected for purpose of conservatism and simplicity; however, an option is provided for incorporation of biodegradation effects when appropriate. In addition, SAM can be configured to account for the gradual loss of source mass to leachate over time and the resultant decrease in contaminant flux to groundwater over an extended exposure period (e.g., 30 years). If such options are to be utilized, biodegradation rates should be established on a site-specific basis or matched to conservative default levels. For carcinogenic constituents, time averaging of groundwater exposure concentrations may be applied to consider average chronic effects over the exposure duration.

Key Components of Soil Leachate Modeling

For the purpose of leachate modeling, 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. Contaminant concentrations within leachate flow are a function of the soil contaminant mass and solubility, as well as the effects of sorption, biodegradation, volatilization, and other chemical processes occurring in the surface soil column. 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. Default soil parameters and parameter estimation guidelines for use in SAM are provided in Tables 1 and 2. Background information regarding model derivation is provided in Connor et al (1997).

NET INFILTRATION ESTIMATE

Net infiltration corresponds to total infiltration (precipitation minus runoff) minus the additional loss associated with evapotranspiration. The net infiltration term thereby represents the deep percolation flow 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 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.

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 Connor et al (1997). 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).

EQUILIBRIUM PARTITIONING

The transfer of soil contaminants to infiltrating rainwater is generally characterized on the basis of conventional linear equilibrium partitioning relationships among the sorbed, water, vapor, and immiscible liquid phases present in the surface soil matrix. This approach assumes that i) the rate of mass transport within a given phase is slow with respect to the transfer of mass between phases in contact with one another, ii) the equilibrium between any two phases is independent of the presence of the other phases, and iii) physical contact and mixing among the various phases is 100% efficient, neglecting the effects of soil structure and secondary porosity. In general, this assumption of instantaneous equilibrium partitioning will tend to overestimate the contaminant mass transferred from the affected soil zone to infiltrating rainwater. Nevertheless, equilibrium partitioning is a convenient and common modeling assumption which allows the contaminant concentration in any phase to be expressed as a function of the bulk constituent mass in the soil.

The soil leachate partition factor (K_{sw} , see Equation 3b on Figure 2) 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.

MASS TRANSPORT

Soil contaminants dissolved in infiltrating rainwater will be carried downward in leachate flow via the processes of advection, dispersion, and diffusion. Advection refers to the bulk motion of leachate fluid through the soil column toward the underlying water-bearing unit. Actual contaminant transport rates will differ from the rate of advective flow due to *dispersion*, the mechanical mixing and spreading of the leachate front within the soil matrix, and *diffusion*, the movement of individual contaminant molecules toward regions of lower concentration.

In SAM, the rate of advective leachate flow is estimated as the net infiltration rate divided by the equilibrium volumetric moisture content of the surface soil column. Dispersion and diffusion are not considered. For typical soil types, conservative default values for equilibrium soil moisture parameters are provided on Table 1. 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.

The default soil moisture values provided on Table 1 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 $\pm 5\%$ 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 represent a reasonable, simplifying measure in the SAM.

SORPTION

Contaminants dissolved within the advancing leachate front will redistribute onto clean underlying soils due to sorption effects. Such sorptive loss serves to slow the rate of downward contaminant migration and provide additional time for volatilization or biodegradation prior to leachate discharge to underlying groundwater. Sorption effects are typically characterized using the same equilibrium partitioning relationship (soil-leachate partition factor, K_{sw}) used for mass transfer from the affected soils to infiltrating rainwater, except that, for clean underlying soils, the direction of contaminant partitioning is reversed.

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 ratio of the initial equilibrium leachate concentration to the leachate concentration that will reach the water bearing unit will be the initial 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).

VOLATILIZATION

Within unsaturated soils, volatile organic contaminants may partition from the soil, leachate, or NAPL phases into the soil vapor phase and subsequently migrate upward to ground surface via vapor phase diffusion. For shallow affected soils, such volatilization can significantly reduce the contaminant mass moving downward via leachate migration. The rate of subsurface contaminant volatilization is a function of the chemical characteristics of the contaminants of concern (Henry's law constant gaseous diffusion coefficient) and the volumetric air content of the soil. Due to higher equilibrium air contents, volatilization will be more significant in sandy soils than in clayey soils (see Table 1). In SAM, the effect of volatilization is neglected as a simplifying assumption, contributing to an overestimate of soil leachate impacts.

BIODECAY

Natural microbial activity within the surface soil column can serve to destroy organic contaminant mass both in the affected soil zone and in the migrating leachate. Biodecay rates are a function of the degradability of the contaminants of concern, as well as the availability of electron acceptors (oxygen, iron, sulfate, etc.) critical to the reaction pathway. In SAM, the effect of biodegradation on soil leachate concentrations is characterized using a traditional first-order decay equation (see Equation 6c on Figure 2), as an optional modeling feature. Appropriate half-life values for site contaminants must be established on a site-specific basis or matched to conservative values in the research literature.

CHEMICAL PROCESSES

Nonbiological chemical processes commonly transform some chemical species (principally inorganics and heavy metals) during aqueous transport in the subsurface. Among the processes which can result in contaminant mass loss from soil leachate are cation exchange, hydrolysis, metal complexation (or chelation), photolysis, and oxidation-reduction reactions. As a simplifying assumption, the effect of these processes are not considered in SAM, contributing to an overestimate of leachate concentrations for some constituents.

LEACHATE/GROUNDWATER DILUTION

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. To assist in estimation of mixing zone thickness (in the absence of a direct measurement of plume thickness at this point), 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).

SOURCE DEPLETION

Over time, the contaminant mass within the affected soil zone will be reduced due to the continuing effects of leachate dissolution, volatilization, and biodegradation. As a result of this source depletion, the maximum contaminant concentration in soil leachate will similarly diminish over time, resulting in reduced contaminant mass flux to the underlying water-bearing unit. The base version of SAM (see Equation 6a on Figure 2) neglects source depletion as a conservative measure, providing a predicted soil leachate concentration equivalent to the maximum initial leachate front arriving at the depth of groundwater. However, as an optional approach, source removal via the leachate process can be considered, providing a transient prediction of soil leachate concentrations or a time-averaged contaminant concentration in groundwater (see Equation 6d, Figure 2).

Description of Other Leachate Models

To evaluate the performance and utility of SAM, model results have been compared to those of three other unsaturated flow models currently in use for analyses of soil leachate impacts: SESOIL, VADSAT, and Jury's Model. Table 3 compares the key features of these alternate modeling methods and identifies sources of additional information. A brief description of these more complex modeling tools is provided below.

SESOIL

The "Seasonal Soil Compartment" (SESOIL) model is a numerical code designed to simulate one-dimensional vertical contaminant fate and transport in the unsaturated zone based on soil, chemical, and meteorological input values (GSC, 1996). SESOIL simulates water transport based on the hydrologic cycle and soil properties of the unsaturated soil column to estimate i) time-varying contaminant concentrations for various depths and ii) the net loss of contaminant mass from the unsaturated zone in terms of percolation to groundwater, surface runoff, biodegradation, and volatilization.

SESOIL characterizes the site hydrology by accounting for rainfall, surface runoff, infiltration, soil moisture content, and evapotranspiration. The climatic data required by the model consist of monthly climatic statistics for a typical year such as average rainfall, temperature, cloud cover, storm duration and frequency, etc. Contaminant fate and transport is based on chemical mass balances, equilibrium partitioning among four phases including a residual NAPL phase, and mass transport of dissolved contaminants via advection and diffusion. SESOIL also accounts for the loss of contaminant mass due to volatilization, biodecay, and other chemical processes. Chemical data input requirements include solubility, diffusion coefficients, sorption constant, biodecay rates, etc. SESOIL does not account for the dilution of leachate in the receiving water-bearing unit.

The unsaturated soil column extends from the ground surface to the groundwater table and is characterized in SESOIL by up to four soil layers which may be further divided into discrete sublayers. Required soil data for each layer consist of soil parameters averaged over the entire layer such as dry bulk density, intrinsic permeability, disconnectedness index, etc. In all, 30 to 40 site-specific and chemical-specific input values are required for leachate modeling using SESOIL.

VADSAT

VADSAT is a semi-analytical code designed to simulate one-dimensional vertical pollutant fate and transport to assess effects of land disposal practices or chemical spills on groundwater quality (API, 1995). This model consists of unsaturated and saturated zone components based on analytical solutions of the flow and transport equations, although for leachate modeling, only the unsaturated portion is needed. VADSAT can produce time-varying pollutant concentrations for various depths based on the release and vertical transport of contaminants in the unsaturated zone.

Vertical unsaturated flow in VADSAT is represented by a steady state net infiltration rate, input by the user. Soil data requirements include soil moisture parameters, bulk density, dispersivity, etc. These properties are averaged over the surface soil zone and assumed constant with depth. Required chemical input parameters include molecular weights, solubility, diffusion coefficients, partitioning parameters, biodecay rates, etc., to account for dissolution from nonaqueous phase liquids, advective and dispersive transport of the dissolved phase, sorption, volatilization, and biodegradation. In all, about 25 site-specific and chemical-specific input values are required for leachate modeling using VADSAT.

JURY'S MODEL

Jury's model, implemented in the American Petroleum Institute Risk/Exposure Assessment Decision Support System (DSS), is an analytical screening-level model that was developed to evaluate the extent of volatilization to the atmosphere from organic contaminants located below the ground surface (API, 1994). It is not, however, intended for use in simulating volatilization for a specific site, but rather, was designed to assess the volatilization potential of a large number of chemicals under various conditions (Jury et al., 1990). While primarily a volatilization model, Jury's model does include an expression for estimating the time-varying concentration profile of a soil contaminant in a homogeneous unsaturated zone. Jury's model does not, however, account for leachate dilution in the receiving water-bearing unit.

Vertical unsaturated flow in Jury's model is represented by a steady state net infiltration rate, input by the user. For the equilibrium partitioning relationship, soil data requirements include soil moisture parameters, bulk density, etc. These properties are averaged over the surface soil zone and assumed constant with depth. Required chemical input parameters include partitioning parameters, molecular weights, solubility, diffusion coefficients, biodecay rates, etc., to account for advective and diffusive transport of the dissolved phase, sorption, volatilization, and biodegradation. A total of 19 site-specific and chemical-specific input values are required in order to predict leachate concentrations using Jury's model.

Case Study Comparison

To assess model consistency and conservatism relative to other common modeling tools, SAM results have been matched against the SESOIL, VADSAT, and Jury's model for a given set of site conditions. Specifically, these various models have been applied to i) predict soil leachate concentrations entering the underlying water-bearing unit over time and ii) back-calculate Site-Specific Target Levels (SSTLs) for the affected soil zone based on non-exceedance of the applicable groundwater quality standard. Procedures and results of this case study analyses are summarized below.

CASE DESCRIPTION

Figure 4 depicts the hypothetical site condition used for this model comparison. As shown, the affected soil zone was assumed to consist of a 15 ft by 15 ft area extending over a depth interval of 0 to 3 ft, with an initial soil benzene concentration of 10 mg/kg. The top of the underlying water-bearing unit occurs at a depth of 13 ft below grade. Two different soil types were considered: a silty sand loam (SM) and a silty clay loam (CL). Rainfall infiltration was estimated on the basis of climatic conditions in Houston, Texas (48 in/yr annual rainfall). For estimation of leachate dilution in groundwater, the underlying water-bearing unit was assumed to have a hydraulic conductivity of 0.001 cm/sec, with a lateral hydraulic flow gradient of 0.001 ft/ft and a mixing zone thickness of 5 ft.

MODELING PROCEDURES

Each of the four models were matched to the input conditions indicated on Figure 4 and run to i) predict benzene concentrations in soil leachate entering the groundwater over time (based on an initial affected soil concentration of 10 mg/kg benzene) and ii) back-calculate soil SSTL values based on a groundwater quality standard of 0.005 mg/L for benzene. For model inputs not specified on Figure 4, model parameters were matched to interval default values for the specified soil type (e.g., SESOIL and VADSAT soil profiles). For SESOIL, the net rainfall infiltration was using the model's interval climatic database for Houston, Texas. Net infiltration values for VADSAT, Jury's and SAM were determined using the empirical estimation method provided in SAM (see Figure 3). For back-calculation of SSTL values, the same groundwater-leachate dilution factor (LDF) was used for all four models based on the LDF expression used in SAM (see Equation 5a, Figure 2).

RESULTS AND CONCLUSIONS

Results of the case study comparison are summarized on Table 4. Figures 5a and 5b show predicted time-concentration plots for the sandy loam and silty clay soils, respectively. These results support the following general observations:

- **Model Variability:** Predicted soil leachate concentrations and back-calculated soil SSTL values exhibit significant variability among the four models. For the sandy loam soil, initial peak leachate concentrations range over 6 orders of magnitude, with somewhat less scatter observed in concentrations predicted after 10 years (see Table 4). Soil leachate values and SSTL values determined from the silty clay soil are in somewhat better agreement, ranging over 2 to 3 orders of magnitude. The significant difference between the SAM results and those of the other three models (particularly for the sandy soil case) is principally due to effect of mass loss via volatilization, which is neglected in SAM. Differences among SESOIL, VADSAT, and Jury's relate to their differing rates of vertical leachate flow and the consequent variation in mass lost due to volatilization and biodecay during the leachate travel time through the surface soil column. In all cases, soil SSTL values are less variable than the predicted soil leachate concentrations, with less scatter observed for the clay than for the sandy soil.
- **Model Conservatism:** As evidenced by the predicted time-concentration plots on Figures 5a and 5b, SAM generally provides a more conservative estimate of leachate concentrations entering the underlying water unit than the other three models. For the silty clay soil case, SAM is roughly in agreement with SESOIL results

(see Figure 5a). The degree of conservatism in SAM results is significantly greater for the sandy soil case, most likely due to the neglect of mass loss via loss via volatilization.

- **Model Reliability:** This case study evaluation is not indicative of the relative accuracy of these four models in simulating actual leachate migration process. No comparison of model results to observed field measurements has been conducted. Rather, this case study compares only the relative consistency and conservatism of the four models for use in risk-based site evaluation. The results discussed above show that model selection can significantly impact risk-based cleanup standard calculations for the two cases considered. However, in all cases, SAM provided either conservative or consistent outcomes relative to the more complex modeling methods. SAM involves considerably fewer parameter inputs and operating expertise than either SESOIL, VADSAT, or Jury's. Based on these findings, SAM should prove a reliable screening-level model for use in development of Tier 1 or Tier 2 soil-to-groundwater protection standards.

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Tables

Table I: Default Moisture Soil Parameters and Saturated Hydraulic Conductivity Values Based on USCS Soil Type

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.
- 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.

Table 2: SAM Model Calculation Steps and Input Data Requirements

SAM Model Eqn. No.	Model Input Requirements			
	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_{sa}, θ_{ss}	Eqns. 2a and 2b	soil type	Use default θ_{sa} and θ_{ss} values from Table 1 based on predominant USCS soil type. Define I_1 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_1	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 1 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_s , W, I_1 , 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_s (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.
<p>Parameter Definitions:</p> <ul style="list-style-type: none"> 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 [cm³-H₂O / cm³-air] i Lateral groundwater flow gradient in water-bearing unit (cm/cm) I_1 Net rainfall infiltration through affected soil zone (cm/yr) k_s Carbon-water sorption coefficient for constituent [g-H₂O / g-C] K Hydraulic conductivity of underlying water-bearing unit (cm/sec) K_{sw} Soil-leachate partition coefficient [(mg/L-H₂O) / (mg/Kg-soil)] K_s 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/cm³] SS Site-specific measure U_{gw} Darcy velocity (cm/sec) ($U_{gw} = K \cdot i$) W Width of affected soil zone parallel to groundwater flow direction (cm) θ_{sa} Volumetric air content of surface soils [cm³ - air/cm³ - soil] δ_{gw} Leachate-groundwater mixing zone thickness (cm) θ_s Total soil porosity [cm³-pore space / cm³-soil] θ_{sw} Volumetric water content of surface soils [cm³-water / cm³-soil] 				

Table 3: Comparison of Various Soil Leachate Models

MODEL FEATURES	SESOIL	VADSAT	JURY'S	SAM
Net Infiltration Estimate	√			√
Equilibrium Partitioning				
• Source Zone		√		
- NAPL-to-Leachate	√		√	√
- Soil-to-Leachate	√			
Mass Transport				
• Advection	√	√	√	√
• Dispersion		√		
• Diffusion	√	√	√	
• Sublayer Discretization	√			
Sorption	√	√	√	√
Volatilization	√	√	√	
Biodecay	√	√	√	√
Chemical Processes				
• Cation Exchange, Hydrolysis, Metal Complexation	√			
Leachate-Groundwater Dilution		√		√
Source Depletion	√	√	√	√
MODEL INFORMATION/REFERENCES				
SESOIL: Scientific Software Group, (703) 620-9214				
VADSAT: ES&T, (540) 552-0685				
JURY'S: in API DSS: Geraghty & Miller, (410) 987-0032				
SAM: Groundwater Services, Inc., (713) 522-6300				

Table 4: Comparison of Case Study Modeling Results

Leachate Model	Predicted Benzene Conc. in Leachate Entering GW (mg/L)		Applicable Soil SSTL Value for Benzene (mg/kg)	
	@ Peak	@ t = 10 years	@ Peak	@ t = 10 years
Sandy Loam Soil				
• SESOIL	1.8 E-6	4.0 E-8	1.5 E+3	>1.5 E+4
• VADSAT	1.6 E-2	1.4 E-11	9.0 E+0	8.1 E+1
• JURY'S	1.0 E-1	<1.0 E-8	8.0 E-1	5.0 E+2
• SAM	4.0 E+0	9.3 E-2	2.1 E-2	9.1 E-1
Silty Clay Soil				
• SESOIL	2.1 E+0	5.8 E-1	6.5 E-2	2.5 E-1
• VADSAT	9.8 E-3	8.5 E-3	1.4 E+1	1.7 E+1
• JURY'S	5.0 E-1	9.2 E-3	1.8 E-1	1.1 E+1
• SAM	5.2 E-1	2.9 E-1	1.9 E-1	3.5 E-1
NOTE:				
1) Modeling Methods: Modeling results for four optional soil leachate models were compared for two soil types (sandy loam soil and silty clay soil), based on site configuration shown on Figure 4.				
2) Predicted Leachate Concentrations: Benzene concentration in leachate entering underlying water-bearing unit (prior to dilution in groundwater flow) based on initial source concentration of 10 mg/kg in affected soil zone. Values reported correspond to initial peak concentration level (@ peak) and concentration after 10 years (@ t = 10 yr). See Figure 4 for predicted time-concentration plots.				
3) Applicable Soil SSTL: Site-Specific Target Level for affected soil zone was back calculated based on groundwater quality standard of 0.005 mg/L for benzene. Assumed leachate-groundwater dilution factor matched to value determined by SAM for all cases (see Equation 5a on Figure 2).				

Figures

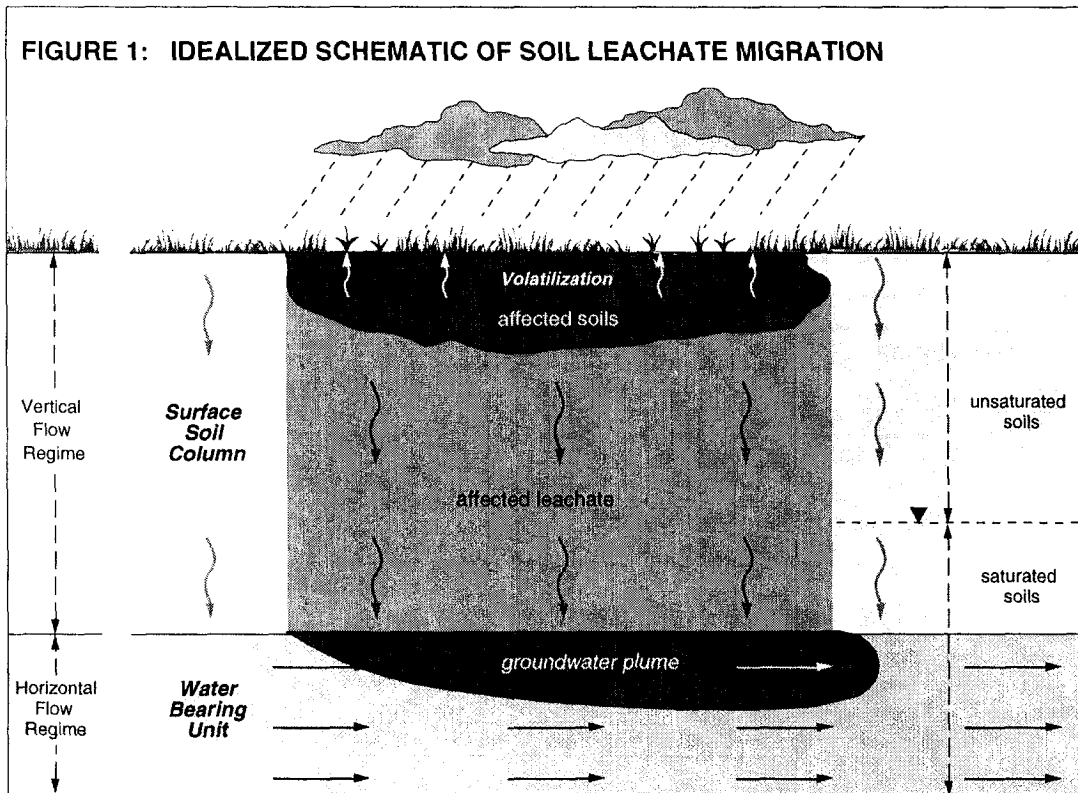


FIGURE 2: SCHEMATIC DIAGRAM OF SOIL ATTENUATION MODEL (SAM)

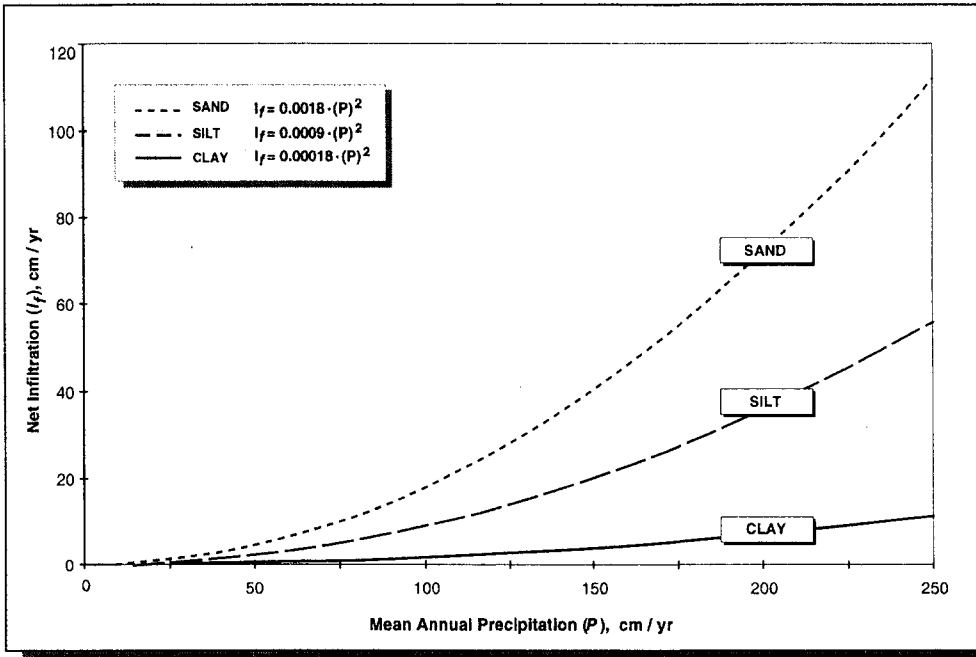
1. Estimation of the Net Infiltration Rate	
	<p>Eqn. 1a: For Sand: $I_f [cm/yr] = 0.0018 \cdot (P)^2$</p> <p>Eqn. 1b: For Silt: $I_f [cm/yr] = 0.0009 \cdot (P)^2$</p> <p>Eqn. 1c: For Clay: $I_f [cm/yr] = 0.00018 \cdot (P)^2$</p> <p>Eqn. 1d: Upperbound net infiltration limit: $I_f [cm/yr] \leq I_{fmax} = K_{vs} \cdot \left[\frac{3.15 \times 10^7 sec}{1 yr} \right]$</p>
2. Equilibrium Volumetric Water and Air Contents	
	<p>Option 2a) Default Values: Select default soil moisture parameters (θ_{as}, θ_{ws}) and saturated hydraulic conductivity based on soil type (see Table 1).</p> <p>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}.</p>
3. Equilibrium Partitioning: Affected Soil to Leachate	
	<p>Eqn. 3a: $C_{w1} [mg/L] = K_{sw} \cdot C_T$ where:</p> <p>Eqn. 3b: $K_{sw} \left[\frac{mg/L - H_2O}{mg/Kg - soil} \right] = \frac{\rho_s}{B_w}$</p> <p>Eqn. 3c: $B_w = \theta_{ws} + k_s \cdot \rho_s + H \cdot \theta_{as}$</p> <p>Eqn. 3d: $k_s \left[\frac{cm^3 - H_2O}{g - soil} \right] = k_{oc} \cdot foc \text{ (Organics)}$</p> <p>Eqn. 3e: $k_s \left[\frac{cm^3 - H_2O}{g - soil} \right] = k_d \text{ (Inorganics)}$</p>
4. Sorptive Mass Redistribution: Leachate to Underlying Clean Soil	
	<p>Eqn. 4a: $C_{w2} [mg/L] = C_{w1} \cdot \frac{L_1}{L_2}$</p> <p>Eqn. 4b: Upperbound leachate concentration for mass conservation: $C_{w2} [mg/L] \leq \frac{C_T \cdot \rho_s \cdot L_1}{I_f \cdot ED}$</p> <p>Eqn. 4c: Upperbound leachate concentration for solubility limit: $C_{w2} [mg/L] \leq X \cdot S$</p>

Continued

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

5. Leachate/Groundwater Dilution	
	<p>Eqn. 5a: $LDF [unitless] = 1 + \frac{U_{gw} \cdot \delta_{gw}}{I_f \cdot W}$</p> <p>where:</p> <p>Eqn. 5b: $U_{gw} [cm/yr] = K \cdot i \cdot \left(\frac{3.15 \times 10^7 \text{ sec}}{\text{lyr}} \right)$</p> <p>Eqn. 5c: $\alpha_v [cm] = 0.0056 \cdot W$</p> <p>Eqn. 5d: $\delta_{gw} [cm] = \sqrt{2\alpha_v W} + b \left[1 - \exp\left(\frac{-I_f W}{U_{gw} \cdot b}\right) \right]$</p> <p>Eqn. 5e: Upperbound mixing zone depth: $\delta_{gw} [cm] \leq b$</p>
6. Summary Calculations	
	<p>Eqn. 6a: Groundwater Exposure Concentration:</p> $C_{gw} [mg/L] = C_{w2} \cdot \frac{1}{LDF} \cdot (BDF^* \cdot TAF^*)$ <p>Eqn. 6b: Soil Target Concentration:</p> $^{GW}Soil_{mg} [mg/Kg] = ^{CW}RBSL \cdot LDF \cdot \frac{L_2}{L_1} \cdot \frac{1}{K_{sw}} \cdot \left(\frac{1}{BDF^* \cdot TAF^*} \right)$ <p>where:</p> <p>*Eqn. 6c: Optional Biodecay Factor:</p> $BDF [dim] = \exp \left[-\lambda \cdot (L_2 - L_1) \cdot \left(\frac{B_w}{I_f} \right) \right]$ <p>*Eqn. 6d: Optional Time Averaging Factor:</p> $TAF [dim] = \frac{L_2 \cdot B_w}{I_f \cdot ED} \cdot \left[1 - \exp \left(\frac{-I_f \cdot ED}{L_2 \cdot B_w} \right) \right]$
Model Parameters	
<p>b Saturated thickness of water-bearing unit (cm)</p> <p>B_w Bulk water partitioning coefficient (unitless)</p> <p>C_{gw} Concentration of COC in groundwater (mg/L)</p> <p>COC Constituent of Concern</p> <p>C_T Bulk COC concentration on the soil mass (mg/Kg)</p> <p>C_{w1} Concentration of COC in soil leachate in the initial affected soil zone (mg/L)</p> <p>C_{w2} Concentration of COC in soil leachate discharged to underlying water-bearing unit (mg/L)</p> <p>ED Exposure duration (yr)</p> <p>foc Fraction of organic carbon (g-C/g-soil)</p> <p>H Henry's Law constant for COC ($cm^3 \cdot H_2O/cm^3 \cdot air$)</p> <p>i Hydraulic gradient in water-bearing unit (cm/cm)</p> <p>I_f Net infiltration (cm/yr)</p> <p>$I_{f \max}$ Upperbound infiltration limit (cm/yr)</p> <p>K Hydraulic conductivity of water-bearing unit (cm/sec)</p> <p>k_d Inorganic soil-water sorption coefficient for COC ($cm^3 \cdot H_2O/g \cdot soil$)</p> <p>$k_{oc}$ Organic carbon partition coefficient for COC ($cm^3 \cdot H_2O/g \cdot C$)</p> <p>$k_s$ Soil-water sorption coefficient ($cm^3 \cdot H_2O/g \cdot soil$)</p> <p>$K_{sw}$ Soil-leachate partition factor for COC (mg/L-$H_2O/mg/Kg \cdot soil$)</p> <p>K_{vs} Saturated hydraulic conductivity of vadose zone soils (cm/sec)</p>	<p>L_1 Thickness of affected soil zone (cm)</p> <p>L_2 Distance from top of affected soil zone to top of water-bearing unit (cm)</p> <p>LDF Leachate-groundwater dilution factor (unitless)</p> <p>P Mean annual precipitation (cm/yr)</p> <p>$^{GW}RBSL$ Risk-Based Screening Level in groundwater zone (mg/L)</p> <p>S Aqueous solubility of COC (mg/L)</p> <p>S Source Area Concentration Limit for soils (mg/Kg)</p> <p>$^{GW}Soil_{mg}$ Groundwater Darcy velocity (cm/yr)</p> <p>U_{gw} Lateral width of affected soil zone in direction of GW flow (cm)</p> <p>W Initial mole fraction of COC in source material (unitless)</p> <p>X Vertical groundwater dispersivity (cm)</p> <p>α_v Groundwater mixing zone thickness (cm)</p> <p>δ_{gw} Biodecay rate of COC in vadose zone (yr^{-1})</p> <p>λ Volumetric air content of surface soils ($cm^3 \cdot air/cm^3 \cdot soil$)</p> <p>$\theta_{as}$ Total porosity of surface soils ($cm^3 \cdot pore-space/cm^3 \cdot soil$)</p> <p>$\theta_T$ Volumetric water content of surface soils ($cm^3 \cdot H_2O/cm^3 \cdot soil$)</p> <p>$\theta_{ws}$ Soil bulk density (g-soil/$cm^3 \cdot soil$)</p> <p>ρ_s</p>

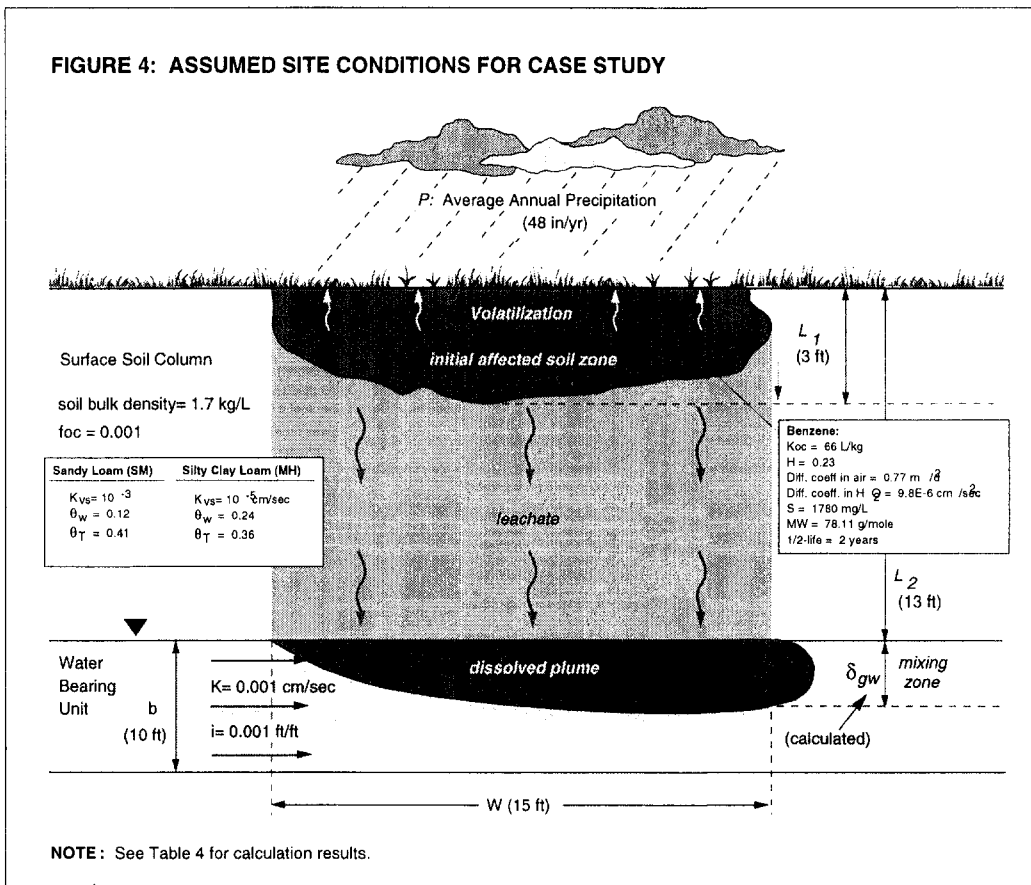
FIGURE 3: ESTIMATION OF NET INFILTRATION BASED ON MEAN ANNUAL RAINFALL & SOIL TYPE



NOTES:

- 1) Net rainfall infiltration through surface soils estimated based on empirical relationship of mean rainfall and predominant soil type in surface soil column.
- 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.

FIGURE 4: ASSUMED SITE CONDITIONS FOR CASE STUDY



NOTE: See Table 4 for calculation results.

FIGURE 5: COMPARISON OF MODEL RESULTS: PREDICTED LEACHATE CONCENTRATION RELEASED TO GROUNDWATER VS. TIME

