Part 3: MODELS FOR DETAILED ASSESSMENT

The Soil Screening Guidance addresses the inhalation and migration to ground water exposure pathways with simple equations that require a small number of easily obtained soil parameters, meteorologic conditions, and hydrogeologic parameters. These equations incorporate a number of conservative simplifying assumptions—an infinite source, no fractionation between pathways, no biological or chemical degradation, no adsorption—conditions that can be addressed with more complicated models. Applying such models will more accurately define the risk of exposure via the inhalation or the migration to ground water pathway and, depending on site conditions, can lead to higher SSLs that are still protective. However, input data requirements and modeling costs make this option more expensive to implement than the SSL equations.

This part of the Technical Background Document presents information on the selection and use of more complex fate and transport models for calculating SSLs. Generally, the decision to use these models will involve balancing costs: if the models and assumptions used to develop simple site-specific SSLs are overly conservative with respect to site conditions (e.g., a thick unsaturated zone), the additional cost and time required to apply these models may be offset by the potential cost savings associated with higher, but still protective, SSLs.

Sections 3.1 and 3.2 include information on equations and models that can accommodate finite contaminant sources and fractionate contaminants between pathways (e.g., VLEACH and EMSOFT) and predict the subsequent impact on either ambient air or ground water. However, when using a finite source model, the site manager should recognize the uncertainties inherent in site-specific estimates of subsurface contaminant distributions and use conservative estimates of source size and concentrations to allow for such uncertainties. In addition, model predictions should be validated against actual site conditions to the extent possible.

3.1 Inhalation of Volatiles: Detailed Models

Developing SSLs for the inhalation of volatiles involves calculating a site-specific volatilization factor (VF) and dispersion factor (Q/C). This section provides a brief description of finite source volatilization models with potential applicability to SSL development and information on site-specific application of the AREA-ST dispersion model for estimating the Q/C values needed to calculate both VF and PEF. It should not be viewed as an official endorsement of these models (other volatilization models may be available with applicability to SSL development).

3.1.1 Finite Source Volatilization Models. To identify suitable models for addressing a finite contaminant source, EPA contracted Environmental Quality Management, Inc. (EQ), to conduct a preliminary evaluation of a number of soil volatilization models, including volatilization models developed by Hwang and Falco (1986), as modified by EQ (1992), and by Jury et al. (1983, 1984, and 1990) and VLEACH, a multipathway model developed primarily to assess exposure through the ground water pathway. Study results (EQ and Pechan, 1994) show reasonable agreement (within a factor of 2) between emission predictions using the modified Hwang and Falco or Jury models, but consistently lower predictions from VLEACH. However, Shan and Stephens (1995) discovered an error in the VLEACH calculation of the apparent diffusivity, which has been subsequently corrected. The corrected VLEACH model, version 2.2, appears to provide emission estimates similar to the Jury and the modified Hwang and Falco models. The revised VLEACH (v.2.2) program is available from the Center for Subsurface Modeling Support (CSMOS) at EPA's Environmental Research Laboratory in Ada, Oklahoma (WWW.EPA.GOV/ADA/ CSMOS.HTML), and is discussed further in Section 3.2.

For certain contaminant conditions, Jury et al. (1990) present a simplified equation (Jury's Equation B1) for estimating the flux of a contaminant from a finite source of contaminated soil. The following assumptions were used to derive this simplified flux equation:

- Uniform soil properties (e.g., homogeneous average soil water content, bulk density, porosity, and fraction organic carbon)
- Instantaneous linear equilibrium adsorption
- Linear equilibrium liquid-vapor partitioning (Henry's law)
- Uniform initial contaminant incorporation at t=0
- Chemicals in a dissolved form only (i.e., soil contaminant concentrations are below C_{sat})
- No boundary layer thickness at ground level (no stagnant air layer)
- No water evaporation or leaching
- No chemical reactions, biodegradation, or photolysis
- $d_s >> (4D_At)^{1/2}$ (ramifications of this are discussed below).

Under these assumptions, the Jury et al. (1990) simplified finite source model is

$$J_s = C_o(D_A/\pi t)^{1/2}[1-\exp(-d_s^2/4D_At)] \qquad \textbf{(56)}$$

where

J_s = contaminant flux at ground surface (g/cm^2-s)
C_o = uniform contaminant concentration at t=0 (g/cm^3)
D_A = apparent diffusivity (cm^2/s)
π = 3.14
t = time (s)
d_s = depth of uniform soil contamination at t=0 (cm),

and

$$D_A = [(\theta_a^{10/3}\, D_i\, H' + \theta_w^{10/3}\, D_w)/n^2]/(\rho_b\, K_d + \theta_w + \theta_a\, H') \qquad \textbf{(57)}$$

where

θ_a = air-filled soil porosity (L_{air}/L_{soil}) = $n - \theta_w$
n = total soil porosity (L_{pore}/L_{soil}) = $1 - (\rho_b/\rho_s)$
θ_w = water-filled soil porosity (L_{water}/L_{soil}) = $w\rho_b/\rho_w$
ρ_b = soil dry bulk density (g/cm^3)
ρ_s = soil particle density (g/cm^3)
w = average soil moisture content (g/g)

ρ_w = water density (g/cm^3)
D_i = diffusivity in air (cm^2/s)
H' = dimensionless Henry's law constant = 41 × HLC
HLC = Henry's law constant (atm-m^3/mol)
D_w = diffusivity in water (cm^2/s)
K_d = soil-water partition coefficient (cm^3/g) = K_{oc} f_{oc}
K_{oc} = soil organic carbon partition coefficient (cm^3/g)
f_{oc} = organic carbon content of soil (g/g).

To estimate the average contaminant flux over 30 years, the time-dependent contaminant flux **must be solved for various times and the results averaged**. A simple computer program or spreadsheet can be used to calculate the instantaneous flux of contaminants at set intervals and numerically integrate the results to estimate the average contaminant flux. However, the time-step interval must be small enough (e.g., 1-day intervals) to ensure that the cumulative loss through volatilization is less than the total initial mass. Inadequate time steps can lead to mass-balance violations.

To address this problem, EPA/ORD's National Center for Environmental Assessment has developed a computer modeling program, EMSOFT. The computer program provides an average emission flux over time by using an analytical solution to the integral, thereby eliminating the problem of establishing adequate time steps for numerical integration. In addition, the EMSOFT model can account for water convection (i.e., leaching), and the impact of a soil-air boundary layer on the flux of contaminants with low Henry's law constants. EMSOFT will be available through EPA's National Center for Environmental Assessment (NCEA) in Washington, DC.

Once the average contaminant flux is calculated, VF is calculated as:

$$VF = (Q/C) \times (C_o/\rho_b) \times (1/J_s^{ave}) \times 10^{-4}\ \mathrm{m^2/cm^2} \qquad \textbf{(58)}$$

where

VF = volatilization factor (m^3/kg)
Q/C = inverse concentration factor for air dispersion (g/m^2-s per kg/m^3)
C_o = uniform contaminant concentration at t=0 (g/cm^3)
ρ_b = soil dry bulk density (g/cm^3)
J_s^{ave} = average rate of contaminant flux (g/cm^2-s).

3.1.2 Air Dispersion Models. The inverse concentration factor for air dispersion, Q/C, is used in the determination of both VF and PEF. For a detailed site-specific assessment of the inhalation pathway, a site-specific Q/C can be determined using the Industrial Source Complex Model platform in the short-term mode (ISCST3). Only a very brief overview of the application, assumptions, and input requirements for the model as used to determine Q/C is provided in this section. This model is the final regulatory version of the ISCST3 model.

The ISCST3 model FORTRAN code, executable versions, sample input and output files, description, and documentation can be downloaded from the "Other Models" section of the Office of Air Quality Planning and Standards (OAQPS) Support Center for Regulatory Air Models bulletin board system (SCRAM BBS). To access information, call:

OAQPS SCRAM BBS
(919) 541-5742 (24 hours/day, 7 days/week except Monday AM)
1,200–9,600, 14,400 baud
Line Settings: 8 bits, no parity, 1 stop bit
Terminal Emulation: VT100 or ANSI
System Operator: (919) 541-5384 (normal business hours EST).

The user registers in the first call and then has full access to the BBS.

The ISCST3 model will output an air concentration (in $\mu g/m^3$) when the concentration model option is selected (e.g., CO MODELOPT DFAULT CONC rural/urban). The surface area of the contaminated soil source must be determined. For the ISCST3 model, the source location of an area source is defined by the coordinates of the southwest corner of the square (e.g., SO LOCATION sourcename AREA -$^1/_2$length -$^1/_2$width height=0). For the source parameter input line, the contaminant's area emission rate (in units of g/m^2-s) must be entered. The area emission rate is the site-specific average emission flux rate, as calculated in Equation 56, converted to units of g/m^2-s (i.e., Aremis = $J_s^{ave} \times 10^4\ cm^2/m^2$). Alternatively, an area emission rate of 1 g/m^2-s can be assumed. A grid or circular series of receptor sites should be used in and around the area source to identify the point of maximum contaminant air concentration. Hourly meteorologic data (*.MET files) for the nearest city (i.e., airport) of similar terrain and the preprocessor PCRAMMET also can be downloaded from the SCRAM BBS.

The ISCST3 model output concentration is then used to calculate Q/C as

$$Q/C = (J_s^{ave} \times 10^4\ cm^2/m^2)/(C_{air} \times 10^{-9}\ kg/\mu g) \qquad \textbf{(59)}$$

where

Q/C = inverse concentration factor for air dispersion (g/m^2-s per kg/m^3)
J_s^{ave} = average rate of contaminant flux (g/cm^2-s)
C_{air} = ISC output maximum contaminant air concentration ($\mu g/m^3$).

Note: If an area emission rate of 1 g/m^2-s is assumed, then ($J_s^{ave} \times 10^4\ cm^2/m^2$) = 1, and Equation 59 simplifies to simply the inverse of the maximum contaminant air concentration (in kg/m^3).

3.2 Migration to Ground Water Pathway

For the migration to ground water pathway, the SSL equations assume an infinite source, contamination extending to the water table, and no attenuation due to degradation or adsorption in the unsaturated zone. At sites with small sources, deep water tables, confining layers in the unsaturated zone that can block contaminant transport, or contaminants that degrade through biological or chemical mechanisms, more complex models that can address such site conditions can be used to calculate higher SSLs that still will be protective of ground water quality. This section provides information on the use of such models in the soil screening process to calculate a dilution-attenuation factor (Section 3.2.1) and to estimate contaminant release in leachate and transport through the unsaturated zone (Section 3.2.2).

3.2.1 Saturated Zone Models. EPA has developed guidance for the selection and application of saturated zone transport and fate models and for interpretation of model applications. The user is referred to *Ground Water Modeling Compendium, Second Edition 1994* (U.S. EPA, 1994b) and *Framework for Assessing Ground Water Modeling Applications* (U.S. EPA, 1994a) for further information.

More complex saturated zone models can be used to calculate a dilution-attenuation factor (DAF) that, unlike the SSL dilution model, can consider attenuation in the aquifer. Some can handle a finite source through a transient mode that requires a time-stepped concentration from a finite-source unsaturated zone model (see Section 3.2.2). In general, to calculate a DAF using such models, the contaminant concentration at the water table under the source (C_w) is set to unity (e.g., 1 mg/L). The DAF is the reciprocal of the predicted concentration at the receptor point (C_{RP}) as follows:

$$DAF = C_w / C_{RP} = 1/C_{RP} \qquad \textbf{(60)}$$

3.2.2 Unsaturated Zone Models. In an effort to provide useful information for model application, EPA's ORD laboratories in Ada, Oklahoma, and Athens, Georgia, conducted an evaluation of nine unsaturated zone fate and transport models (Criscenti et al., 1994; Nofziger et al., 1994). The results of this effort are summarized here. The models reviewed are only a subset of the potentially appropriate models available to the public and are not meant to be construed as having received EPA approval. Other models also may be applicable to SSL development, depending on site-specific circumstances.

Each of the unsaturated zone models selected for evaluation are capable, to varying degrees, of simulating the transport and transformation of chemicals in the subsurface. Even the most unique site conditions can be simulated by either a single model or a combination of models. However, the intended uses and the required input parameters of these models vary. The models evaluated include:

- RITZ (Regulatory and Investigative Treatment Zone model)
- VIP (Vadose zone Interactive Process model)
- CMLS (Chemical Movement in Layered Soils model)
- HYDRUS
- SUMMERS (named after author)
- MULTIMED (MULTIMEDia exposure assessment model)
- VLEACH (Vadose zone LEACHing model)
- SESOIL (SEasonal SOIL compartment model)
- PRZM-2 (Pesticide Root Zone Model).

RITZ, VIP, CMLS, and HYDRUS were evaluated by Nofziger et al. (1994). SUMMERS, MULTIMED, VLEACH, SESOIL, and PRZM-2 were evaluated by Criscenti et al. (1994). These documents should be consulted for further information on model application and use.

The applications, assumptions, and input requirements for the nine models evaluated are described in this section. The model descriptions include model solution method (i.e., analytical, numerical), the purpose of the model, and descriptions of the methods used by the model to simulate water/contaminant transport and contaminant transformation. Each description is accompanied by a table of required input parameters. Input parameters discussed include soil properties, chemical properties, meteorologic data, and other site information. In addition, certain input control parameters may be required such as time stepping, grid discretization information, and output format.

Information on determining general applicability of the models to subsurface conditions is provided, followed by an assessment of each model's potential applicability to the soil screening process.

RITZ. Information on the RITZ model was obtained primarily from Nofziger et al. (1994). RITZ is a steady-state analytical model used to simulate the transport and fate of chemicals mixed with oily wastes (sludge) and disposed of by land treatment. RITZ simulates two layers of the soil column with uniform properties. The soil layers consist of: (1) the upper plow zone where the oily waste is applied and (2) the treatment zone. The bottom of the treatment zone is the water table. It is assumed in the model that the oily waste is completely mixed in and does not migrate out of the plow zone, which represents the contaminant source at an initial time. RITZ also assumes an infinite source (i.e., a continuous flux at constant concentration). The flux of water is assumed to be constant with time and depth and the Clapp-Hornberger constant is used in defining the soil water content resulting from a specified recharge rate. Sorption, vapor transport, volatilization, and biochemical degradation are also considered (van der Heijde, 1994). Partitioning between phases is instantaneous, linear, and reversible. Input parameters required for the RITZ model are presented in Table 10. Biochemical degradation of the oil and contaminant is considered to be a first-order process, and dispersion in the water phase is ignored.

Table 10. Input Parameters Required for RITZ Model

Soil properties	Site characteristics	Pollutant properties	Oil properties
Percent organic carbon	Plow zone depth	Concentration in sludge	Concentration of oil in sludge
Bulk density	Treatment zone depth	K_{oc}	Density of oil
Saturated water content	Recharge rate (constant)	K_{ow}	Degradation half-life of oil
Saturated hydraulic conductivity	Evaporation rate (constant)	Henry's law constant	---
Clapp-Hornberger constant	Air temperature (constant)	Degradation half-life (constant)	---
---	Relative humidity (constant)	Diffusion coefficient (in air)	---
---	Sludge application rate	---	---
---	Diffusion coefficient (water vapor in oil)	---	---

VIP. Information on the VIP model was obtained from Nofziger et al. (1994). The VIP model is a one-dimensional, numerical (finite-difference) fate and transport model also designed for simulating the movement of compounds in the unsaturated zone resulting from land application of oily wastes. Like the RITZ model, VIP considers dual soil zones (a plow zone and a treatment zone) and considers the source to be infinite. VIP differs from RITZ in that it solves the governing differential equations numerically, which allows variability in the flux of water and chemicals over time. Advection and hydrodynamic dispersion are the primary transport mechanisms for the contaminant in water (van der Heijde, 1994). Instead of assuming instantaneous, linear equilibrium between all phases, VIP considers the partitioning rates between the air, oil, soil, water, and vapor-phase transport. Contaminant transformation processes include hydrolysis, volatilization, and sorption. Oxygen-limited degradation and diffusion of the contaminant in the air phases are also considered. Sorption is instantaneous as described for the RITZ model. The input parameters required for the VIP model are presented in Table 11.

Table 11. Input Parameters Required for VIP Model

Soil properties	Site characteristics	Pollutant properties	Oxygen properties	Oil properties
Porosity	Plow zone depth	Concentration in sludge	Oil-air partition coefficient[a]	Density of oil
Bulk density	Treatment zone depth	Oil-water partition coefficient[a]	Water-air partition coefficient[a]	Degradation rate constant of oil
Saturated hydraulic conductivity	Mean daily recharge rate	Air-water partition coefficient[a]	Oxygen half-saturation constant in air phase [a]	---
Clapp-Hornberger constant	Temperature (each layer)	Soil-water partition coefficient[a]	Oxygen half-saturation constant in oil phase [a]	---
---	Sludge application rate	Degradation constant in oil[a]	Oxygen half-saturation constant in water phase[a]	---
---	Sludge density	Degradation constant in water[a]	Oxygen half-saturation constant (oil degradation)	---
---	Application period and frequency in period	Dispersion coefficient	Stoichiometric ratio of oxygen to pollutant consumed	---
---	Weight fraction water in sludge	Adsorption-desorption rate constant (water/oil)	Stoichiometric ratio of oxygen to oil consumed	---
---	Weight fraction oil in waste	Adsorption-desorption rate constant (water/soil)	Oxygen transfer rate coefficient between oil and air phases	---
---	---	Adsorption-desorption rate constant (water/air)	Oxygen transfer rate coefficient between water and air phases	---

[a] Parameters required for plow zone and treatment zone.

CMLS. Information on CMLS was obtained from Nofziger et al. (1994). CMLS is an analytical model developed as a management tool to describe the fate and transport of pesticides in layered soils and to estimate the amount of chemical at a certain position at a certain time. The model allows designation of up to 20 soil layers with uniform soil and chemical properties defined for each layer.

Water in the soil system is "pushed ahead" of new water (recharge) entering the system. The water content is reduced to the field capacity after each infiltration event, and water is removed from the root zone in proportion to the available water stored in that layer (Nofziger et al., 1994). CMLS assumes movement of the chemical in liquid phase only and allows a finite source. Chemical partitioning between the soil and the water is assumed to be linear, instantaneous, and reversible. Volatilization is not considered. Dispersion and diffusion of the chemical is ignored and degradation is defined as a first-order process. The input parameters required for the CMLS model are presented in Table 12.

Table 12. Input Parameters Required for CMLS

Soil properties	Site characteristics	Chemical properties
Depth of bottom of soil layers	Daily infiltration or precipitation	Degradation half-life (each soil layer)
Organic carbon content	Daily evapotranspiration	Amount applied
Bulk density	---	Depth of application
Saturated water content	---	Date of application
Field capacity	---	K_{oc}
Permanent wilting point	---	---

HYDRUS. Information on the HYDRUS model was obtained from Nofziger et al. (1994). HYDRUS is a finite-element model for one-dimensional solute fate and transport simulations. The boundary conditions for flow, as well as soil and chemical properties, can therefore vary with time. A finite source also can be modeled. Soil parameters are described by the van Genuchten parameters. The model also considers root uptake and hysteresis in the water movement properties. Solute transport and transformation incorporates molecular diffusion, hydrodynamic dispersion, linear or nonlinear equilibrium partitioning (sorption), and first-order decay (van der Heijde, 1994). Volatilization is not considered. The input parameters required by HYDRUS are presented in Table 13.

SUMMERS. Information on the SUMMERS model was obtained from Criscenti et al. (1994). SUMMERS is a one-dimensional analytical model that simulates one-dimensional, nondispersive transport in a single layer of soil from an infinite source. It was developed to determine the contaminant concentrations in soil that would result in ground water contamination above specified levels for evaluating geothermal energy sites. The model is similar to the SSL equations in that it assumes steady-state water movement and equilibrium partitioning of the contaminant in the unsaturated zone and performs a mass-balance calculation of mixing in an underlying aquifer. For the saturated zone, the model assumes a constant flux from the surface source and instantaneous, complete mixing in the aquifer. The mixing depth is therefore defined by the thickness of the aquifer. The model does not account for volatilization. The input parameters required for SUMMERS are listed in Table 14.

Table 13. Input Parameters Required for HYDRUS

Soil properties	Site characteristics	Pollutant properties	Root uptake parameters
Depth of soil layers	Uniform or stepwise rainfall intensity	Molecular diffusion coefficient	Power function in stress-response function
Saturated water content	Contaminant concentrations in soil	Dispersivity	Pressure head where transpiration is reduced by 50%
Saturated hydraulic conductivity	---	Decay coefficient (dissolved)	Root density as a function of depth
Bulk density	---	Decay coefficient (adsorbed)	---
Retention parameters	---	Freundlich isotherm coefficients	---
Residual water content	---	---	---

Table 14. Input Parameters Required for SUMMERS

Parameters required	
Target concentration in ground water	Thickness of aquifer
Volumetric infiltration rate into aquifer	Width of pond/spill perpendicular to flow
Downward porewater velocity	Initial (background) concentration
Ground water seepage velocity	Equilibrium partition coefficient
Void fraction	Darcy velocity in aquifer
Horizontal area of pond or spill	Volumetric ground water flow rate

MULTIMED. Information on the MULTIMED model was obtained from Criscenti et al. (1994) and Salhotra et al. (1990). MULTIMED was developed as a multimedia fate and transport model to simulate contaminant migration from a waste disposal unit. For this review, only the fate and transport of pollutants from the soil to migration to ground water pathway was considered in detail.

In MULTIMED, infiltration of waste into the unsaturated or saturated zones can be simulated using a landfill module or by direct infiltration to the unsaturated or saturated zones. Flow in the unsaturated zone and for the landfill module is simulated by a one-dimensional, semianalytical module. Transport in the unsaturated zone considers the effects of dispersion, sorption, volatilization, biodegradation, and first-order chemical decay. The saturated transport module is also one-dimensional, but considers three-dimensional dispersion, linear adsorption, first-order decay, and dilution due to recharge. Mixing in the underlying saturated zone is based on the vertical dispersivity specified, the length of the disposal facility parallel to the flow direction, the thickness of the saturated zone, the ground water velocity, and the infiltration rate. The saturated zone module can simulate steady-state and transient ground water flow and thus can consider a finite source assumption through a leachate "pulse duration." The parameters required for the unsaturated and saturated zone transport in MULTIMED are presented in Table 15.

Table 15. Input Parameters Required for MULTIMED

Unsaturated zone parameters		
Saturated hydraulic conductivity	Thickness of each layer	Reference temperature for air diffusion
Porosity	Longitudinal dispersivity	Molecular weight
Air entry pressure head	Percent organic matter	Infiltration rate
Depth of unsaturated zone	Soil bulk density	Area of waste disposal unit
Residual water content	Biological decay coefficient	Duration of pulse
Number of porous materials	Acid, base, and neutral hydrolysis rates	Source decay constant
Number of layers	Reference temperature	Initial concentration at landfill
Alpha coefficient	Normalized distribution coefficient	Particle diameter
van Genuchten exponent	Air diffusion coefficient	---
Saturated zone parameters		
Recharge rate	Longitudinal dispersivity	Organic carbon content
First-order decay coefficient	Transverse dispersivity	Well distance from site
Biodegradation coefficient	Vertical dispersivity	Angle off-center of well
Aquifer thickness	Temperature of aquifer	Well vertical distance
Hydraulic gradient	pH	---

VLEACH. Information on the VLEACH model was obtained from Criscenti et al. (1994). VLEACH is a one-dimensional, finite difference model developed to simulate the transport of contaminants displaying linear partitioning behavior through the vadose zone to the water table by aqueous advection and diffusion. Multiple layers can be modeled and are expressed as polygons with different soil properties and recharge rates. Water flow is assumed to be steady state. Linear equilibrium partitioning is used to determine chemical concentrations between the aqueous, gaseous, and adsorbed phases (sorption and volatilization), and a finite source can be considered. Chemical or biological degradation is not considered. The input parameters required for VLEACH are presented in Table 16.

Table 16. Input Parameters Required for VLEACH

Soil properties	Chemical characteristics	Site properties
Dry bulk density	K_{oc}	Recharge rate
Total porosity	Henry's law constant	Contaminant concentrations in recharge
Volumetric water content	Aqueous solubility	Depth to ground water
Fractional organic carbon	Free air diffusion coefficient	Dimensions of "polygons"

SESOIL. Information on the SESOIL model was obtained from Criscenti et al. (1994). SESOIL is a one-dimensional, finite difference flow and transport model developed for evaluating the movement of contaminants through the vadose zone. The model contains three components: (1) hydrologic cycle, (2) sediment cycle, and (3) pollutant fate cycle. The model estimates the rate of vertical solute transport and transformation from the land surface to the water table. Up to four layers can be simulated by the model and each layer can be subdivided into 10 compartments with uniform soil characteristics. Hydrologic data can be included using either monthly or annual data options. Solute transport is simulated for ground water and surface runoff including eroded sediment. Pollutant fate considers equilibrium partitioning to soil and air phases (sorption and diffusion), volatilization from the surface layer, first-order chemical degradation, biodegradation, cation exchange, hydrolysis, and metal complexation and allows for a stationary free phase. The required input parameters for SESOIL are presented in Table 17 for the monthly option.

Table 17. Input Parameters Required for SESOIL (Monthly Option)

Climate data	Soil data	Chemical data	Application data
Mean air temperature[a]	Number of layers and sublayers	Solubility in water	Application area
Mean cloud cover fraction[a]	Thickness of layers	Air diffusion coefficient	Site latitude
Mean relative humidity[a]	pH of each layer	Henry's law constant	Spill index
Short wave albedo fraction[a]	Bulk density	Organic carbon adsorption ratio	Pollutant load
Total precipitation	Intrinsic permeability	Soil adsorption coefficient	Mass removed or transformed
Mean storm duration	Pore disconnectedness index	Molecular weight	Index of volatile diffusion
Number of storm events	Effective porosity	Valence	Index of transport in surface runoff
---	Organic carbon content	Hydrolysis constants (acid, base, neutral)	Ratio pollutant conc. in rain to solubility
---	Cation exchange capacity	Biodegradation rates (liquid, solid)	Washload area
---	Freundlich exponent	Ligand stability constant	Average slope and slope length
---	Silt, sand, and clay fractions	Moles ligand per mole compound	Erodibility factor
---	Soil loss ratio	Molecular weight of ligand	Practice factor
---	---	Ligand mass	Manning coefficient

[a] SESOIL uses these parameters to calculate evapotranspiration if an evapotranspiration value is not specified.

PRZM-2. Information on PRZM-2 was obtained from Criscenti et al. (1994). PRZM-2 is a combination of two models developed to simulate the one-dimensional movement of chemicals in the unsaturated and saturated zones. The first model, PRZM, is a finite difference model that simulates water flow and detailed pesticide fate and transformation in the unsaturated zone. The second model, VADOFT, is a one-dimensional finite element model with more detailed water movement simulation capabilities. The coupling of these models results in a detailed representation of contaminant transport and transformation in the unsaturated zone.

PRZM has been used predominantly for evaluation of pesticide leaching in the root zone. PRZM uses detailed meteorologic and surface hydrology data for the hydrologic simulations. Runoff, erosion, plant uptake, leaching, decay, foliar washoff, and volatilization are considered in the surface hydrologic and chemical transport components. Chemical transport and fate in the subsurface is simulated by advection, dispersion, molecular diffusion, first-order chemical decay, biodegradation, daughter compound progeny, and soil sorption. The input parameters required for PRZM are presented in Table 18.

VADOFT can be run independently of PRZM and output from the PRZM model can be used to set the boundary conditions for VADOFT. The lower boundaries could also be specified as a constant pressure head or zero velocity. Transport simulations consider advection and diffusion with sorption and first-order decay. The input requirements for VADOFT are presented in Table 19.

Considerations for Unsaturated Zone Model Selection. The accuracy of a model in a site-specific application depends on simplifications and assumptions implicit in the model and their relationship to site-specific conditions. Additional error may be introduced from assumptions made when deriving input parameters. Although each of the nine models evaluated has been tested and validated for simulation of water and contaminant movement in the unsaturated zone, they are different in purpose and complexity, with certain models designed to simulate very specific scenarios.

A model should be selected to accommodate a site-specific scenario as closely as possible. For example, if contaminant volatilization is of concern, the model should consider volatilization and vapor phase transport. After a model is determined to be appropriate for a site, contaminant(s), and conditions to be modeled, the site-specific information available (or potentially available) should be compared to the input requirements for the model to ensure that adequate inputs can be developed.

The unsaturated zone models addressed in this study use either analytical, semianalytical, or numerical solution methods. Analytical models represent the simplest models, requiring the least number of input parameters. They use a closed-form solution for the pertinent equations. In analytical models, certain assumptions have to be made with respect to the geometry of the system and external stresses. For this reason, there are few analytical flow models (van der Heijde, 1994). Analytical solutions are common, however, for fate and transport problems by solution of convection-dispersion equations. Analytical models require the assumption of uniform flow conditions, both spatially and temporally.

Semianalytical models approximate complex analytical solutions using numerical techniques (van der Heijde, 1994). Transient or steady-state conditions can be approximated using a semianalytical model. However, spatial variability in soil or aquifer conditions cannot be accommodated.

Numerical models use approximations of pertinent partial differential equations usually by finite-difference or finite-element methods. The resolution of the area and time of simulation is defined by the modeler. Numerical models may be used when simulating time-dependent scenarios, spatially variable soil conditions, and unsteady flow (van der Heijde, 1994).

Table 18. Input Parameters Required for PRZM

Daily climate data			
Pan evaporation and pan factor	Precipitation	Windspeed	Snowmelt factor
Temperature	Monthly daylight hours	Solar radiation	Minimum evaporation extraction depth
Erosion data			
Topographic factor/soil erodibility	Average duration of rainfall	Field area	Practice factor
Crop data			
Surface condition of crop	Maximum interception storage	Maximum rooting depth	Maximum canopy coverage
Maximum dry weight of crop after harvest	---	Emergence, maturation, and harvest dates	---
Pesticide data			
Application quantity	Number of applications (50 maximum)	Number of chemicals (3 maximum)	Application dates
Foliar extraction coefficient	Incorporation depth	Plant uptake factor	Foliar decay rates
Diffusion coefficient in air	Enthalpy of vaporization	K_d and K_{oc}	Henry's law constant
Initial concentration levels	Parent/daughter transform rates	Aqueous, sorbed, vapor decay rates	
Soil data			
Compartment thicknesses	Runoff curve numbers	Core depth	Number and thickness of horizons
Soil drainage parameter	Hydrodynamic dispersion	Bulk density	Initial soil water content
Wilting point	Percent organic carbon	Field capacity	---
Soil temperature			
Heat capacity per unit volume	Albedo	Reflectivity of soil surface	Height of windspeed measurement
Thermal conductivity of horizon	Avgerage monthly bottom boundary temperature	Initial horizon temperature	Sand and clay content
Biodegradation and irrigation parameters (not presented)			

Table 19. Input Parameters Required for VADOFT

Pesticide data	Soil data	
Number of chemicals	Number of soil horizons	Relative permeability vs. saturation
Aqueous decay rate	Horizon thicknesses	Pressure head vs. saturation
Initial concentration	Saturated hydraulic conductivity	Residual water phase saturation
Longitudinal dispersivity	Effective porosity	Brooks and Corey n
Retardation coefficient	Air entry pressure head	van Genuchten alpha
Molecular diffusion	---	---
Conc. flux at first node (if independent of PRZM)	Input flux or head at first node (if independent of PRZM)	

In certain cases, input parameters to be used in a model are not definitively known. Some models allow some input parameters to be expressed as probability distributions rather than a single value, referred to as Monte Carlo simulations. This method can provide an estimate of the uncertainty of the model output (i.e., percent probability that a contaminant will be greater than a certain concentration at a depth), but requires knowledge of the parameter distributions. Alternatively, a bounding approach can be used to estimate the effects of likely parameter ranges on model results where there is uncertainty in input parameter values.

Model Applicability to SSLs. The unsaturated models evaluated herein can provide inputs necessary for soil screening by calculating leachate concentrations at the water table or by calculating infiltration rates. In the former application, they produce results comparable to the leach test option. As with the leach test, the leachate concentration from the model is **divided** by the dilution factor to obtain an estimated ground water concentration at the receptor well. This receptor point concentration is then compared with the acceptable ground water concentration to determine if a site's soils exceed SSLs.

Table 20 summarizes characteristics and capabilities of the models evaluated for this study. All nine of the models can calculate contaminant concentrations in leachate that has infiltrated down to the water table from the vadose zone, although CMLS requires a separate calculation to estimate leachate concentration. If there is reliable site data indicating significant degradation in soil, several of the models can consider biological and/or chemical degradation processes. The models also can address contaminant adsorption; those that can model layered soils can be especially useful in settings where low-permeability clay layers may attenuate contaminants through adsorption. Finally, several of the models can address a finite source if the size of the source is accurately known.

The average annual infiltration rate at a site is difficult to measure in the field yet is required for estimating a dilution factor or DAF. Four of the models evaluated, CMLS, HYDRUS, SESOIL, and PRZM, can calculate infiltration rates given either daily or monthly rainfall data.

Two models, VLEACH and SESOIL, address volatilization from the soil surface along with leachate emissions and therefore may be useful for SSL development for the volatilization and migration to ground water pathways. The volatile emission portion of VLEACH is discussed in Section 3.1.

Table 20. Characteristics of Unsaturated Zone Models Evaluated

	Type			Fate and Transport Processes Considered														Other		
Model	Analytical	Semianalytical	Numerical	Finite source	Partitioning with oil phase	Volatilization	Vapor phase transport	Hydrodynamic dispersion	Diffusion	Sorption	Nonequilibrium partitioning	Hydrolysis (1st-order decay)	Biodegradation	Layered soils	Root zone uptake	Runoff	Erosion	Saturated zone included	Monte Carlo analysis	Water balance calculations
RITZ	•				•	•			•	•		•	•							
VIP			•		•	•	•	•		•	•	•								
CMLS	•			•						•		•		•						•
HYDRUS			•	•				•	•	•		•		•	•					•
MULTIMED		•				•		•		•	•	•	•	•				•	•	
SUMMERS	•									•								•		
PRZM-2			•	•		•		•	•	•		•	•	•	•	•	•		•	•
SESOIL			•	•		•		•	•	•	•	•	•	•		•	•			•
VLEACH			•	•		•	•		•	•	•			•						

Table 20 addresses only unsaturated zone fate and transport model components, although two models (MULTIMED and SUMMERS) have saturated zone flow and transport capabilities. The following text highlights some of the differences between the models, outlines their advantages and disadvantages, and describes appropriate scenarios for model application.

RITZ. RITZ was designed to model land treatment units and is appropriate for sites where oily wastes are present (it includes sorption on an immobile oil phase as well as onto soil particles). Sorption, degradation, volatilization, and first-order decay processes are considered in the subsurface simulations. The most significant drawback for the model is the limit on the number of soil layers. Optimally, RITZ would be recommended for modeling chemical migration in a uniform unsaturated zone as a result of land application. Although the oil phase can be omitted for simulations of scenarios without oily materials, the RITZ model's focus on oily waste degradation in land treatment units limits its utility for soil screening (SSLs are not applicable when soils contain a separate oil phase).

VIP. VIP also is appropriate for sites where release of oily wastes has occurred. Some of the limitations described in RITZ also apply to the VIP model. VIP could be used as a followup model to RITZ since variable chemical and water fluxes can be simulated. In this case, significant additional input parameters are required to simulate transient partitioning between the air, soil, water, and oil phases. Like RITZ, VIP's focus on land treatment of oily waste limits its application to SSLs.

CMLS. CMLS differs from RITZ and VIP in that it allows designation of up to 20 soil layers with different properties. It does not consider nonaqueous phase liquids, dispersion, diffusion, or vapor phase transport, but a finite source can be modeled. CMLS estimates the location of the peak concentration of contaminants through a layered soil system. A limitation of the CMLS model for SSL application is that it does not calculate leachate concentrations. Instead, it calculates the amount of chemical at a certain depth at a certain time. The user must estimate the concentration based on the amount of chemical present and the total flux of water in the system (Nofziger et al., 1994). The model is typically used to estimate the time for a chemical entering the unsaturated zone to reach a certain depth.

HYDRUS. Like CMLS, the HYDRUS model can also simulate chemical movement in layered soils and can consider a finite source, but also includes dispersion and diffusion as well as sorption and first-order decay. In addition, HYDRUS outputs the chemical concentration in the soil water as a function of time and depth along with the amount of chemical remaining in the soil. The model considers root zone uptake, but other models such as PRZM should be used if the comprehensive effects of plant uptake are to be considered in the simulations. Because it can estimate infiltration from rainfall contaminant concentrations, HYDRUS may be useful in SSL applications.

SUMMERS. The SUMMERS model is a relatively simple model designed to simulate leaching in the unsaturated zone and is essentially identical to the SSL migration to ground water equations in assumptions and limitations. It is appropriate for use as an initial screening model where site data are limited and where volatilization is not of concern. However, since attenuation processes such as biodegradation, first-order decay, volatilization, or other attenuation processes (other than sorption) are not considered, it is a quite conservative model. Since volatilization is not considered, it cannot be used to simulate migration of volatile compounds to the atmosphere. Because of its similarities to the SSL migration to ground water equations, the SUMMERS model is not suitable for a more detailed assessment of site conditions.

MULTIMED. MULTIMED simulates simple vertical water movement in the unsaturated zone. Since an initial soil concentration cannot be specified, either the soil/water partition equation or a leaching test (SPLP) must be used to estimate soil leachate contaminant concentrations. MULTIMED is appropriate for simulating contaminant migration in soil and can be used to model vadose zone attenuation of leachate concentrations derived from a partition equation (see Section 2.5.1). In addition, since it links the output from the unsaturated zone transport module with a saturated zone module, it can be used to determine the concentration of a contaminant in a well located downgradient from a contaminant source. MULTIMED is appropriate for early-stage site simulations because the input parameters required are typically available and uncertainty analyses can be performed using Monte Carlo simulations for those parameters for which reliable values are not known.

VLEACH. In VLEACH, biological or chemical degradation is not considered. It therefore provides conservative estimates of contaminant migration in soil. This model may be appropriate as an initial screening tool for sites for which there is little information available. VLEACH can estimate volatile emissions (see Section 3.1) and can consider a finite source. It is therefore potentially applicable to both subsurface pathways addressed by the soil screening process.

SESOIL. SESOIL was designed as a screening tool, but it is actually more complex than some of the models described. Some of the input data would be cumbersome to obtain, especially for use as an initial screening tool. It is applicable for simulating spill sites since it allows consideration of surface transport by erosion and runoff and can utilize detailed meteorologic information to estimate infiltration. In the soil zone, several fate and transport options are available such as metal complexation, hydrolysis, cation exchange, and degradation. This model is especially applicable to sites where significant subsurface and meteorologic information is available. Although the model does consider volatilization from surface soils, the available documentation (Criscenti et al., 1994) is not clear as to whether it produces an output of volatile flux to the atmosphere.

PRZM-2. PRZM-2 is a relatively detailed model as a result of the coupling of the two models PRZM and VADOFT. Although PRZM is predominantly used as a pesticide leaching model, it could also be used for simulation of transport of other chemicals. Because detailed meteorology and surface application parameters can be included, it is appropriate for simulation of surface spills or land disposal scenarios. In addition, uncertainty analyses can be performed based on Monte Carlo simulations. Numerous subsurface fate and transport options exist in PRZM. Water movement is somewhat simplified in PRZM, and it may not be applicable for low-permeability soils (Criscenti et al., 1994). However, water flow simulation is more detailed in the VADOFT module of the PRZM-2 program. The combination of these programs makes PRZM-2 a relatively complex model. This model is especially applicable to sites for which significant site and meteorologic data are available.