9.0 Vadose Zone and Aquifer Modules

9.1 Purpose and Scope

The Vadose Zone and Aquifer Modules simulate the subsurface movement of contaminants in leachate from surface impoundments, landfills, land application units (LAUs), and waste piles to downgradient drinking water wells and waterbodies. The modules are not used for aerated tanks, because tanks are assumed not to leak. Detailed information on the Vadose Zone and Aquifer Modules can be found in the technical background document (U.S. EPA, 1999e). Figure 9-1 shows the relationship and information flow between the Vadose Zone and Aquifer Modules and the 3MRA modeling system.

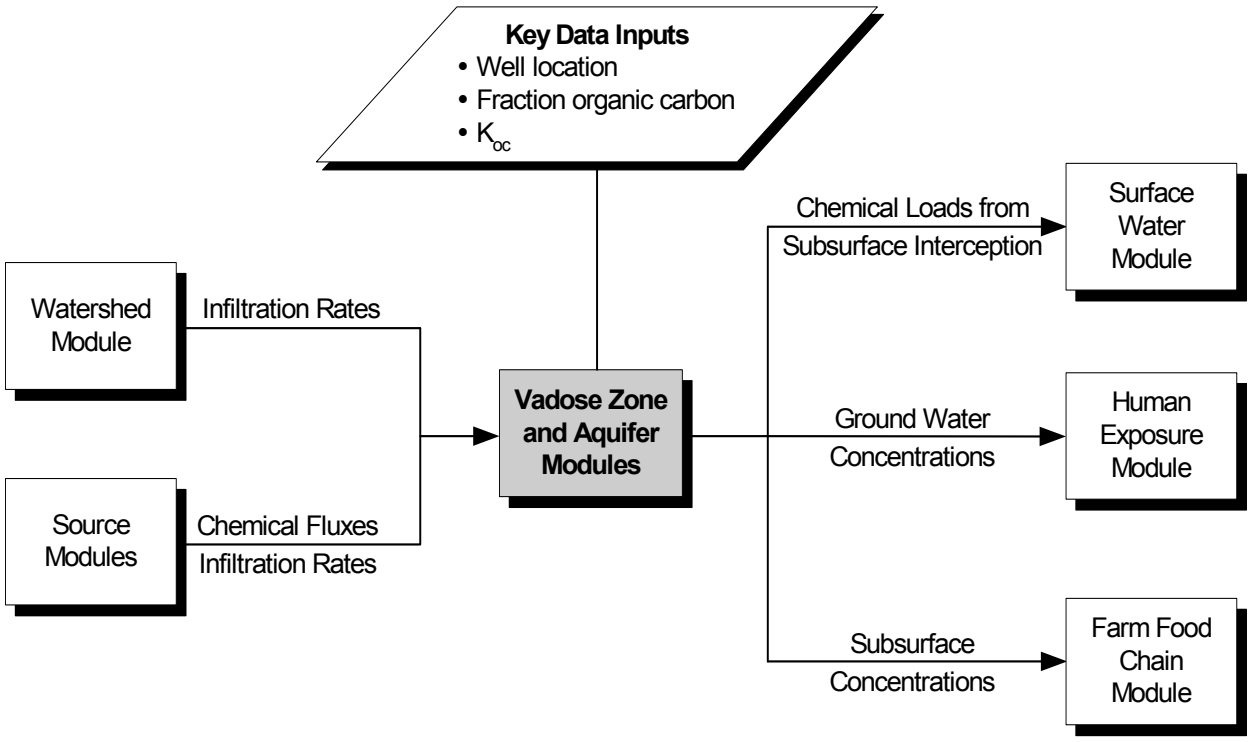

Figure 9-1. Information flow for the Vadose Zone and Aquifer Modules in the 3MRA modeling system.

The Vadose Zone and Aquifer Modules simulate the fate and transport of dissolved contaminants from a point of release at the base of a WMU, through the underlying soil, and through a surficial aquifer (or ground water source). Module outputs include ground water contaminant concentrations in wells, which are used by the Human Exposure Module to estimate

exposures through drinking water and showering, and by the Farm Food Chain Module to estimate contaminant concentrations in beef and milk from farm well use; and contaminant fluxes into waterbodies, which are used by the Surface Water Module, along with contaminant fluxes from atmospheric deposition and overland flow, to estimate contaminant concentrations in streams, lakes, and wetlands.

The Vadose Zone and Aquifer Modules are used by the 3MRA modeling system only if there are wells or downgradient streams, lakes, or wetlands at a site. Waterbodies are downgradient if they are in the direction of ground water flow away from the WMU.

The Vadose Zone and Aquifer Modules perform the following functions:

1. **Model vadose zone flow and transport**. The one-dimensional (1-D) Vadose Zone Module simulates infiltration and dissolved contaminant transport, by advection and dispersion, leaching from the bottom of a WMU through the soil above the water table (i.e., the vadose zone) to estimate the contaminant and water flux to the underlying ground water.

2. **Model ground water flow and transport**. The pseudo-3-D Aquifer Module simulates ground water flow and contaminant transport, by advection and dispersion, from the base of the vadose zone to estimate contaminant concentrations in drinking water wells and contaminant discharge fluxes to intercepted waterbodies.

3. **Model subsurface chemical reactions.** Both the Vadose Zone and Aquifer Modules simulate sorption to soil or aquifer materials and biological and chemical degradation, which can reduce contaminant concentrations as they move through soil and ground water. In cases where degradation of a contaminant yields other contaminants that are of concern, the modules can account for the formation and transport of up to six different daughter and granddaughter degradation products. For metals, the modules use sorption isotherms that allow adjustment of sorption behavior to account for varying metal concentrations and geochemical conditions.

The Vadose Zone and Aquifer Modules in the 3MRA modeling system were extracted from EPA's Composite Model for Leachate Migration with Transformation Products (EPACMTP) (U.S. EPA, 1996 a,b,c; 1997). EPACMTP is used in EPA regulatory efforts by OSW and has been subject to extensive peer review and public comment. EPACMTP is a tool used routinely to predict potential ground water pathway exposure at a downstream receptor well for regulatory development purposes.

9.2 Conceptual Approach

Figure 9-2 illustrates how the Vadose Zone and Aquifer Modules work together to calculate receptor well contaminant concentrations and contaminant fluxes to downgradient waterbodies. The Vadose Zone Module and the Aquifer Module are described below, followed by a discussion of the chemical reaction modeling that operates in both modules. Additional

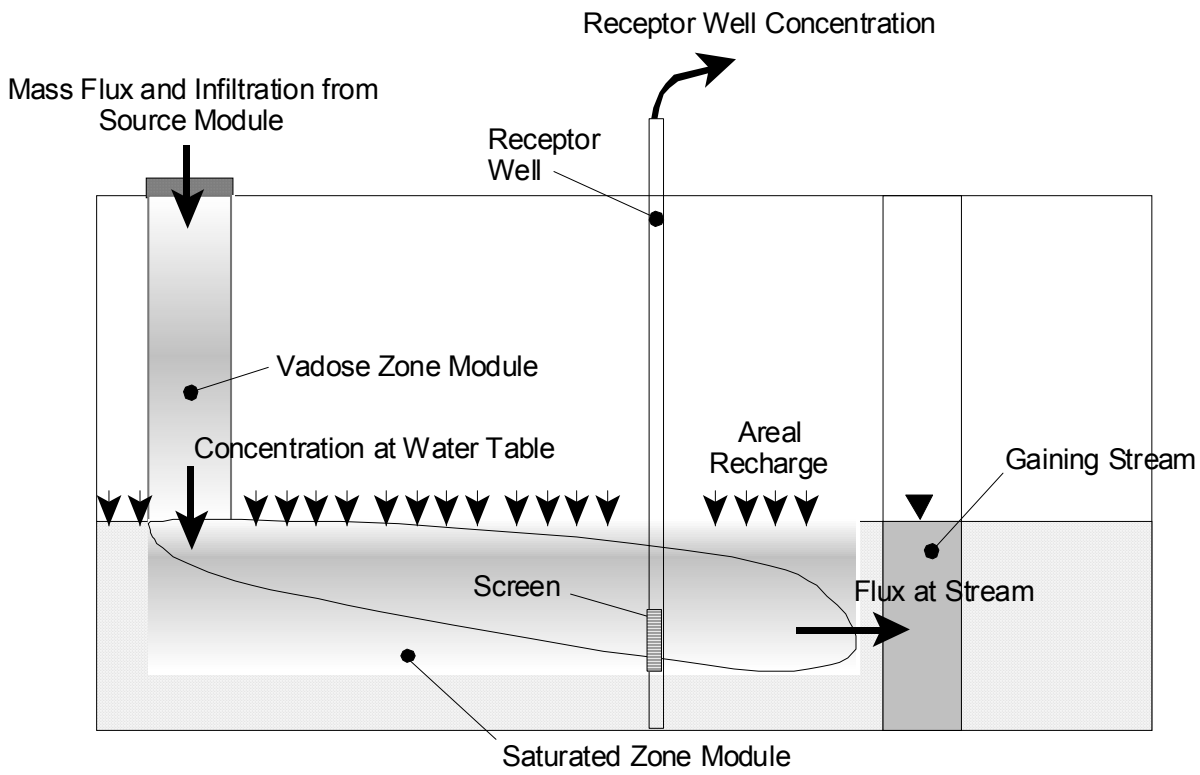

Figure 9-2. Conceptual diagram of Vadose Zone and Aquifer Modules.

details on the Vadose Zone and Aquifer Modules, including governing equations and detailed input/output specifications, can be found in the 3MRA modeling system background documents (U.S. EPA, 1999a-e).

9.2.1 Vadose Zone Module

The Vadose Zone Module simulates the flow and transport of contaminants in leachate from the upper boundary of the vadose zone at the base of the WMU source to the lower vadose zone boundary at the water table. The Vadose Zone Module estimates contaminant flux to the Aquifer Module given leachate flows and fluxes from the 3MRA source modules. Its outputs are the long-term, steady-state infiltration rate and the annual time series of contaminant concentrations that are used as inputs to the Aquifer Module.

Vadose Zone Flow. The Vadose Zone Module performs 1-D analytical and numerical solutions for water flow and contaminant transport in unsaturated soil underlying a WMU source. The model assumes that flow in the vadose zone is at steady-state and flows vertically from underneath the source toward the water table.[1] The Vadose Zone Module receives a time series of annual average infiltration rates and contaminant mass fluxes from the source modules.

[1] Because water flow in the vadose zone is predominantly gravity driven, the vertical flow component accounts for most of the fluid flux between the WMU source and the water table.

Because the Vadose Zone Module assumes steady-state flow, it calculates a long-term average infiltration rate from the full series of annual average infiltration rates. At the same time, the model calculates an annual average time series of leachate concentrations, while conserving contaminant mass with respect to the full series of contaminant mass fluxes output from the source modules.

The vadose zone flow model assumes that the unsaturated soil is a uniform porous medium and that the infiltrating flow rate (*I*) is governed by Darcy's law (Freeze and Cherry, 1979):

$$I = -K_S\, k_{rw}\, (d\psi/dz - 1) \qquad (9\text{-}1)$$

where

ψ	=	pressure head (cm)
z	=	depth in the soil column (positive downward) (cm)
K_S	=	saturated hydraulic conductivity (cm/h)
k_{rw}	=	relative permeability (unitless).

Solution of this equation for unsaturated soil conditions requires stipulation of the relationships between

- The relative permeability and the volumetric water content of the porous medium and
- The volumetric water content and the pressure head.

The Vadose Zone Module assumes that these relationships follow the equations given by Van Genuchten (1980). The governing equations for these relationships are given in U.S. EPA (1999e). Solution methods for these equations can be found in the EPACMTP background document (U.S. EPA, 1996a-c).

Vadose Zone Transport. The Vadose Zone Module simulates transient[2] contaminant transport through the unsaturated zone by advection and dispersion. The model assumes that the unsaturated zone is initially free of contamination and that contaminants migrate downward along with the leachate flow from the WMU. Chemical reactions modeled include single- or multiple-chemical chain decay reactions, and linear or nonlinear sorption. The chemical reaction modeling is described in Section 9.2.3.

The vadose zone transport model simulates the 1-D transport of contaminants through the soil column using the advection-dispersion equation of Huyakorn and Pinder (1983). This equation estimates contaminant degradation using a first-order decay constant that calculates mass fractions of both parent and daughter compounds. The effect of equilibrium sorption of a species is expressed by a retardation coefficient that can simulate sorption using either linear or nonlinear (Freundlich) sorption isotherms. The governing equations for the vadose zone

[2] Contaminant transport can vary year to year as leachate concentration changes.

transport model can be found in U.S. EPA (1999e). Solution methods for these equations, which are semianalytical for organic chemicals and analytical for nonlinear metals, are described in detail in the EPACMTP background documents (U.S.EPA, 1996a-c).

Key assumptions of the Vadose Zone Module

- Contaminants are released from a square WMU source; there is no contaminant flux outside the WMU
- Flow and transport are steady-state and are 1-D, with year-to-year changes in leachate concentration from the source.
- Flow is vertical with no horizontal component.
- The soil is initially free of contamination.
- Soil is a uniform porous medium with uniform properties; there are no soil layers or preferential pathways such as fractures or soil macropores.
- Contaminant transport is by advection and dispersion only; there is no facilitated transport by colloids or nonaqueous-phase liquid (NAPL).
- Contaminants are in the aqueous and sorbed phases only; there are no mass transfer processes between phases other than adsorption onto soil particles.
- There is no volatilization from the unsaturated zone (i.e., no gas-phase release or transport).
- NAPLs (e.g., oil) are not present.

Vadose Zone Module Assumptions, Inputs, and Outputs. Key assumptions for the Vadose Zone Module are summarized in the text box. Vadose Zone Module inputs include

- Contaminant fluxes and infiltration rates from the 3MRA source modules;
- Soil hydrologic properties (saturated hydraulic conductivity, total porosity, residual water content, and Van Genuchten water-retention parameters);
- Soil bulk density, pH, temperature, and organic matter content;
- Vadose zone thickness (depth to ground water); and
- Contaminant-specific degradation and sorption variables (see Section 9.2.3).

The module produces a time series of contaminant concentrations in the infiltrate passed to the aquifer, a long-term average infiltration rate, and the duration of the WMU source of contamination, all of which are used as input to the Aquifer Module. Detailed specifications of these inputs and outputs can be found in U.S. EPA (1999e).

9.2.2 Aquifer Module

The Aquifer Module simulates 1-D ground water flow and pseudo-3-D contaminant transport to calculate ground water contaminant concentrations at downgradient[3] drinking water wells and intercepting surface waterbodies (i.e., streams, rivers, lakes, and wetlands). The Aquifer Module estimates these concentrations and fluxes given infiltration flow rate and contaminant concentrations from the Vadose Zone Module. Its primary outputs include time series of annual average contaminant concentrations at each downgradient receptor well (used by

[3] "Downgradient" refers to features (wells, waterbodies) that are downstream from the WMU with respect to the ground water flowpath.

the Human Exposure and Farm Food Chain Modules) and a time series of contaminant fluxes at any downgradient intercepting waterbody (used by the Surface Water Module).

Ground Water Flow. The Aquifer Module simulates ground water flow in a surficial (unconfined) aquifer of constant thickness using a 1-D ground water flow submodel and a pseudo-3-D transport submodel. The model accounts for the effects of infiltration from the WMU and regional recharge downgradient of the WMU on the magnitude and direction of ground water flow.[4] The concept accounts for regional flow in the horizontal direction driven by a regional hydrologic gradient, along with vertical disturbance of this regional flow by water infiltrating to the surficial aquifer from the overlying vadose zone and WMU.

The Aquifer Module uses a 1-D, steady-state solution for predicting hydraulic head and Darcy velocities that assumes that the aquifer is composed of a uniform porous media, and that ground water flow is governed by Darcy's law (Bear, 1972). This solution begins with the classic 3-D governing equation for ground water flow that is used in EPACMTP:

$$K_x\,(\partial^2 H/\partial x^2) + K_y\,(\partial^2 H/\partial y^2) + K_z(\partial^2 H/\partial z^2) = 0 \qquad (9\text{-}2)$$

where

H = hydraulic head (cm)
K_x = hydraulic conductivity in the longitudinal direction (cm/hr)
K_y = hydraulic conductivity in the horizontal-transverse direction (cm/hr)
K_z = hydraulic conductivity in the vertical direction (cm/hr).

The 1-D flow equation used in the Aquifer Module is derived by setting the transverse hydraulic conductivity, K_y, equal to zero and invoking the Dupuit- Forchheimer assumption (Bear, 1972), in conjunction with vertical boundary conditions to account for infiltration and recharge. Details on this flow equation, its derivation, and its solution can be found in U.S. EPA (1999e).

The ground water flow model accounts for ground water mounding beneath the WMU by allowing different recharge rates underneath and outside the source area. Within the model, ground water mounding beneath the source is represented in the flow system by increased hydraulic head values at the top of the aquifer. This approach is reasonable so long as the height of the mound is small relative to the thickness of the saturated zone.

Ground Water Transport. The Aquifer Module simulates contaminant transport through ground water by use of a pseudo-3-D advection and dispersion submodel. The model assumes that ground water is initially free of contamination; that is, initial aquifer contaminant concentration and concentration gradients along the downstream and upstream boundaries are set to zero. Contaminants enter the aquifer only from the vadose zone immediately underneath the

[4] Recharge is provided by the 3MRA Watershed Module as a time series of annual average recharge rates with units of m/d. Because the aquifer model requires a steady-state recharge rate with units of m/yr, the model calculates an effective long-term recharge rate as the average of the time series recharge rates received from the Watershed Module.

WMU, which is modeled as a square, horizontal plane source. Chemical reactions modeled include single- or multiple-chemical chain decay reactions, and linear or nonlinear sorption. The chemical reaction modeling is described in Section 9.2.3.

The Aquifer Module simulates the advective-dispersive transport of dissolved contaminants in one dimension with dispersion in the other two dimensions added analytically (pseudo-3-D). The model is based on the 3-D advection-dispersion governing equation from Huyakorn and Pinder (1983), with a simplified solution to model advection in one dimension (horizontally) and dispersion in three dimensions. Although this may not be as accurate as a fully 3-D solution, it is much more computationally efficient and therefore more suitable for the large-scale Monte Carlo simulations for which the 3MRA modeling system was designed.

The ground water transport equation estimates contaminant degradation using a first-order decay constant that calculates mass fractions of both parent and daughter compounds. The effect of equilibrium sorption of a species is expressed by a retardation coefficient, R, that can simulate sorption using linear sorption isotherms.[5] Governing equations for the ground water transport equation can be found in U.S. EPA (1999e), which also describes the solution methods applied to develop the Aquifer Module.

Aquifer Fractures and Heterogeneity. The basic Aquifer Module described above assumes that aquifers are homogeneous and isotropic, and it therefore does not simulate flow and transport under the fractured or heterogenous subsurface conditions that are common across the United States. Because modeling fractures and heterogeneity is complex, EPA developed an indirect approach to address fracture flow, which tends to increase the rate of migration compared to nonfractured settings, and heterogeneity, which can cause a plume to break into fingers of higher concentration ground water that can increase the concentration at a well.

To address fracture flow conditions, the Aquifer Module uses an equivalent porous media (EPM) approach, which applies uniform porous media analogues to a fractured aquifer flow field. The approach involves developing "fracture multiplier" distributions for several classes of fractured hydrogeologic settings. For a particular Monte Carlo realization at a fractured site, the 3MRA modeling system selects a multiplier from the appropriate distribution and applies it to increase the porous media hydraulic conductivity selected for the site. Additional details on the development and implementation of this approach can be found in U.S. EPA (1999d,e).

To incorporate effects of heterogeneity in aquifers, EPA first assessed the effects of heterogeneity on receptor well concentrations (U.S. EPA, 1999b). Based on this study, EPA developed an algorithm and database to estimate the effects of heterogeneity on well concentrations output by the Aquifer Module. For a particular Monte Carlo realization, the 3MRA modeling system selects input values from the database and applies the algorithm to adjust the well concentration outputs. Additional details on the development and application of this method can be found in U.S. EPA (1999b,e).

[5] The aquifer model differs from the vadose zone model in that it does not allow the use of nonlinear Freundlich sorption isotherms.

Aquifer Module Assumptions, Inputs, and Outputs. Key assumptions for the Aquifer Module are summarized in the text box. Aquifer Module inputs include

- WMU length, width, and location;
- A steady-state, long-term annual infiltration rate and a time series of annual average contaminant concentrations from the Vadose Zone Module;
- A time series of annual-average recharge rates from the Watershed Module;
- Aquifer properties, including saturated hydraulic conductivity, regional gradient, thickness, pH, organic carbon content, and temperature;
- The ratio of horizontal to vertical hydraulic conductivity;
- Longitudinal, horizontal-transverse, and vertical dispersivities;
- Receptor well locations and screen depths below the water table surface;
- Location coordinates for downgradient intercepting waterbodies;
- Direction of regional ground water flow, measured clockwise from due north;
- Contaminant-specific degradation and sorption variables (see Section 9.2.3); and
- Termination criteria for ending the model simulation, including the maximum simulation time.

Key assumptions of the Aquifer Module

- The aquifer is unconfined and subject to recharge from the ground surface.
- The upper aquifer boundary is the water table; the lower aquifer boundary is an impermeable confining layer.
- The aquifer has a uniform (regional) hydraulic gradient and a constant saturated thickness.
- Aquifer materials are uniform porous media that are isotropic except for hydraulic conductivity, which can vary between the vertical and horizontal directions.
- The downgradient intercepting waterbody does not fully alter the ground water flow pattern.
- The ground water is initially free of contamination.
- Contaminants are released from a square WMU source; there is no contaminant flux outside the WMU.
- Recharge of contaminant-free water occurs from the watershed outside of the WMU.
- Ground water flow is steady-state, but contaminant concentrations can vary year to year.
- Preferential flow through fractures and aquifer heterogeneities is addressed by adjusting aquifer hydraulic conductivity or well concentrations.
- The model does not apply to solution openings in karst limestone.
- Contaminants are transported by advection and dispersion only; there is no facilitated transport by colloids or NAPL.
- Contaminants are in the aqueous and sorbed phases only; there are no mass transfer processes between phases other than adsorption onto soil particles.
- There is no volatilization from the water table (i.e., no gas-phase release or transport).
- NAPLs (e.g., oil, halogenated solvents) are not present.

The Aquifer Module outputs time series of annual average ground water contaminant concentrations at downgradient receptor wells within the ground water plume, which are used by the Human Exposure and Farm Food Chain Modules. It also outputs a time series of contaminant fluxes into a downgradient intercepting waterbody that is read by the Surface Water Module. Detailed specifications of aquifer model inputs and outputs can be found in U.S. EPA (1999e).

9.2.3 Chemical Reaction Modeling

The Vadose Zone and Aquifer Modules include code to simulate sorption to soil or aquifer materials and biological and chemical degradation, processes that can reduce contaminant concentrations as they move through soil and ground water. The Vadose Zone and Aquifer Modules use very similar methods to model these processes. The modeling approach differs between organic chemicals, which can degrade but follow simple sorption relationships, and metals, which do not degrade but require a more complicated approach to model sorption.

Organic Chemical Reactions. For organic chemicals, the Vadose Zone and Aquifer Modules simulate decay reactions for single compounds or multiple-compound chains, along with sorption to solid soil and aquifer components. Degradation reactions addressed include both chemical and biological transformation processes, with all transformation reactions represented by first-order decay processes. The models account for chemical and biological transformations by combining first-order degradation rates derived for chemical hydrolysis and biological degradation.

The transport of organic chemicals is influenced in part by hydrolysis. Chemical hydrolysis is modeled using acid-catalyzed, base-catalyzed, and neutral contaminant-specific hydrolysis rates (i.e., the Arrhenius equation). These rate constants are all influenced by ground water temperature, while the acid- and base-catalyzed rate constants are also influenced by pH. If chemical degradation by-products are hazardous and their contaminant-specific parameters are known, they can also be modeled in the simulation as part of a decay chain.

To model biological degradation, the Vadose Zone Module uses aerobic biodegradation rates and the Aquifer Module uses anaerobic rates. Both modules combine biological and chemical degradation rates to determine an overall decay rate. As a result, the modules cannot explicitly consider the separate effects of hydrolysis and biodegradation.

The Vadose Zone and Aquifer Modules take into account adsorption behavior of organic chemicals by calculating a retardation factor based on a contaminant-specific partition coefficient (K_d). To develop K_d, the modules apply a distribution coefficient normalized for organic carbon (K_{oc}), in conjunction with a media-specific fractional organic carbon content to obtain the soil (or aquifer material)/water partition coefficient (K_d). The use of K_{oc} to estimate sorption is appropriate for organic compounds that tend to sorb preferentially on the natural organic matter in the soil or aquifer. Although the Aquifer Module is limited to using linear K_d values, the Vadose Zone Module can use nonlinear Freundlich sorption coefficients if these are available for the organic compounds being modeled.

Additional details on modeling organic chemical reactions within the Vadose Zone and Aquifer Modules can be found in U.S. EPA (1996a,b; 1999e).

Organic Chemical Reaction Model Assumptions and Inputs. Key assumptions for the organic chemical reaction models used in the Vadose Zone and Aquifer Modules are summarized in the text box. Chemical-specific inputs include

- Acid-catalyzed, base-catalyzed, and neutral hydrolysis rates, specified for a default constant reference temperature of 25°C;
- First-order aerobic (vadose zone) and anaerobic (aquifer) biodegradation rates; and
- Partition coefficient normalized for soil organic carbon (K_{oc}).

Key assumptions and limitations of vadose zone and aquifer organic chemical reaction models

- The sorption of contaminants onto soil or aquifer solids occurs instantaneously and is entirely reversible.
- Sorption of organic compounds is linear in the saturated zone but can be nonlinear in the vadose zone.
- The model cannot explicitly consider the separate effects of multiple degradation processes.
- Biodegradation is aerobic in the unsaturated zone and anaerobic in the saturated zone.
- All transformation reactions are adequately represented by first-order decay processes.

When a multichemical simulation is desired for parent and daughter compounds, the necessary chemical-specific parameters must be repeated for all species in the decay chain.

Metal Sorption Processes. Site geochemistry and metal concentration are important determinants of the fate and transport of metals in the subsurface. Varying geochemical conditions result in the large variability in metal sorption behavior observed from site to site. Metals that sorb readily at low concentrations usually show much lower sorption at higher concentrations. To help capture this effect, the Vadose Zone and Aquifer Modules use sorption isotherms generated by the MINTEQA2 metal speciation model (Allison et al., 1991) that are nonlinear with respect to metal concentration. To represent nationwide variability in geochemistry, these concentration-dependent partition coefficients have been developed for various combinations of key geochemical parameters (MINTEQA2 master variables) known to affect metal sorption, including the pH, iron oxide content, and organic matter content of the subsurface environment, and the leachate organic matter content.

MINTEQA2 generates concentration-dependent effective partition coefficients (K_d values) for various combinations of the key geochemical parameters that are sampled during the Monte Carlo runs. Based on the selection of these parameters for each Monte Carlo realization, the Vadose Zone and Aquifer Modules call the appropriate sorption isotherm for use during transport modeling. The set of sorption isotherms included in the 3MRA modeling system has two subsets of isotherms for each metal: one representing vadose zone conditions and the other representing aquifer conditions.

In the Vadose Zone Module, metal partition coefficients are adjusted using these isotherms to represent the general increase in K_d that is expected to occur as contaminant

concentrations decrease along the transport path. This procedure is described in the background document for the modeling of metals transport (U.S. EPA, 1996c). Because it is limited to linear sorption processes, the Aquifer Module selects a single K_d value from the isotherm that corresponds to the maximum ground water concentration under the source. This is appropriate because by the time the contamination reaches the Aquifer, metal concentration is usually low enough that a linear isotherm (i.e., a single K_d value not dependent on metal concentration) is appropriate.

The MINTEQA2 sorption isotherms implemented in the Vadose Zone and Aquifer Modules are a significant improvement over those used in previous EPACMTP versions in that they address a greater number of metals, including antimony, arsenic (+3 and +5 species), barium, beryllium, cadmium, chromium (+3 and +6), copper, lead, mercury, nickel, selenium, silver, thallium, vanadium, and zinc. This was made possible by improvements in MINTEQA2's thermodynamic, iron oxide sorption, and organic matter sorption databases (U.S. EPA, 1999a).

Additional details on the MINTEQA2 modeling approach, including model formulation, assumptions, and limitations, can be found in Allison et al. (1991) and U.S. EPA (1996c, 1999a, e).

9.3 Module Discussion

9.3.1 Strengths and Advantages

The Vadose Zone Module simulates the migration of constituents from the bottom of land-based WMUs to the water table, and the Aquifer Module simulates the migration of constituents in the saturated zone from the water table immediately below the WMU to the downgradient receptor wells. Both modules have been used in regulations and have been thoroughly tested and verified and validated as part of the integrated groundwater model EPACMTP. Strengths of the two modules include the following:

Strengths and advantages for the Vadose Zone Module are listed below:

- **Widely used, verified, validated, state-of-the-science approach.** The Vadose Zone Module is based on a state-of-the-science approach and is part of EPACMTP, which has been tested, verified, and validated. EPACMTP has been used to support regulations and has undergone various peer and public reviews, including reviews by the SAB.

- **Computational efficiency.** The solution procedure used in the Vadose Zone Module is computationally very efficient and stable and, therefore, ideally suited for use in Monte Carlo frameworks.

- **Use of nonlinear metal isotherms.** The module can handle nonlinear metal isotherms while maintaining computationally efficiency because of the solution technique used in the module.

- **Simulation of multiple transformation products.** The module can simulate the transformation of waste constituents into multiple transformation products (up to seven chain members).

Strengths and advantages for the Aquifer Module are listed below:

- **Widely used, verified, validated, state-of-the-science approach.** The Aquifer Module is based on a state-of-the-science approach and is part of EPACMTP, which has been tested, verified, and validated. EPACMTP has been used to support regulations and underwent various peer and public reviews, including reviews by the SAB.

- **Computational efficiency.** The module uses a special solution technique for the boundary value problem that makes it computationally very efficient and stable. The module is ideally suited for use in Monte Carlo framework in which numerous simulations are required using a minimum amount of computational time.

- **Complete transient response at multiple well locations.** The module provides complete transient response at multiple receptor well locations.

- **Simulation of multiple transformation products.** The module can simulate the transformation of waste constituents into multiple transformation products (up to seven chain members).

9.3.2 Uncertainty and Limitations

Limitations and uncertainties for the Vadose Zone Module are listed below:

- Transient effects of the flow are not considered (i.e., year-to-year variability in infiltration is not considered).

- Multiphase flow and transport are not modeled; NAPL flow and transport are not modeled.

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- Volatilization and vapor-phase diffusion are not modeled.

- Preferential flow due to fractures or heterogeneity in the vadose zone is not considered.

- Clay lenses or other potential flow and transport barriers in the vadose zone are not considered.

- Decay is limited to first-order reactions; lag time for decay is not considered.

- The transport domain in the saturated zone is kept constant. Effects due to mounding caused by infiltration from WMUs are not considered. These effects would decrease the depth of the flow and transport domain in the vadose zone.

Limitations and uncertainties for the Aquifer Module are listed below:

- Transient effects of ground water flow, recharge, and infiltration are not considered.
- Spatially varied recharge is not considered.
- Source geometry is limited to an idealized square, with two opposite sides parallel to the flow direction.
- Multiphase flow and transport are not modeled. NAPL flow and transport are not modeled.
- Contaminant contribution to the saturated zone via vapor-phase diffusion above the water table is not modeled.
- Karst conditions are not modeled.
- Decay is limited to first order. Lag time for decay is not considered.
- The presence of different hydrogeologic zones in the flow and transport domain is not considered.
- The transport domain in the saturated zone is kept constant. Effects due to significant mounding caused by infiltration from WMUs are not considered.
- Domain geometry is limited to the idealized rectangular shape. Other geometries are not considered.
- Only gaining streams, with axes normal to the ground water flow direction, are permitted. Effects of streams on the flow field are not considered.
- Only receptor wells with small extraction rates are considered. Effects of well extraction on the ground water flow field are not considered.
- There are many sources of uncertainty associated with the distribution coefficients generated by the metal speciation model. These can be categorized as uncertainty arising from model input parameters, uncertainty in database equilibrium constants, and uncertainty due to application of the model. Additional details can be found in the MINTEQA2 background documents (Allison et al., 1991; U.S. EPA, 1991a, c).

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