4.0 SATURATED ZONE (AQUIFER) MODULE

4.1 PURPOSE OF THE SATURATED-ZONE MODULE

This section of the background document describes the module of EPACMTP used for the simulation of saturated-zone flow and transport of leachate from waste disposal facilities. This module consists of a numerical simulator for three-dimensional steady-state ground-water flow, coupled with both an analytical and a numerical three-dimensional (3D) contaminant transport simulator. Since EPACMTP is intended to be used for Monte-Carlo uncertainty analysis, much emphasis has been placed on numerical robustness and computational efficiency during the development of the saturated-zone module.

The module has three simulation options:

> Option 1: Three-dimensional steady-state ground-water flow and advective-dispersive transport in an aquifer with constant saturated thickness and non-uniform recharge across the upper aquifer boundary;
>
> Option 2: Quasi-three dimensional ground-water flow and advective-dispersive transport, through a combination of 2D areal and cross-sectional solutions; and
>
> Option 3: One-dimensional ground-water flow and pseudo-three-dimensional advective-dispersive transport through a combination of hybrid one-dimensional numerical and two-dimensional analytical solutions.

The three simulation options are listed in descending order of accuracy and in ascending order of computational efficiency. Option 3 is normally preferred because of its acceptable accuracy (see Appendix D) and relatively high computational efficiency. It is several times faster than Options 1 and 2.

4.2 LINKING THE UNSATURATED-ZONE AND SATURATED-ZONE MODULES

The unsaturated-zone and saturated-zone modules of EPACMTP are linked at the water table. The unsaturated-zone module calculates the constituent concentration arriving at the water table as a function of time, that is, the breakthrough curve. This information is stored in an interval table of constituent concentrations versus time. When EPACMTP simulates a decay chain, the concentration values for both the parent constituent and its degradation products are stored. In the subsequent saturated-zone transport simulation, this record of concentration versus time is used to specify the time-varying water table boundary condition. The continuously varying contaminant mass flux entering the saturated zone at the water table is treated as a series of stepwise changes in mass flux. Experience shows that discretizing the time dependent boundary condition into approximately 50 steps yields an accurate approximation. The stepwise treatment of the boundary condition also lends itself readily to incorporation in the Laplace Transform Galerkin (LTG) scheme used in the

saturated-zone transport module. Details of this scheme are provided in Section 4.4.5.2.1. Because linearized sorption isotherms for all constituents, including metals, are used in the saturated zone, the LTG scheme is applicable. The unsaturated-zone simulation is run for a sufficiently long time to ensure that the entire breakthrough curve at the water table is captured. As a practical criterion, the unsaturated-zone transport simulation is terminated when the concentrations of all species in the decay chain arriving at the water table have been reduced to below their respective health-based ground-water concentration limits. The corollary is that for strongly sorbing metals and constituents that degrade via chemical hydrolysis to form non-toxic compounds, when even the maximum concentration at the peak of the water table breakthrough curve remains below the drinking water standard, there is no need to run the saturated transport simulation, because that particular case will not result in an exceedance of the drinking water standard. For constituents with degradation products that may be toxic, the saturated transport simulation is not necessary when the peak concentrations of the parent constituent and its degradation products are below their respective drinking water standards. The drinking water standard for each constituent is an input parameter that must be specified by the user.

4.3 SATURATED-ZONE FLOW SUBMODULE

4.3.1 Description of the Flow Submodule

Ground-water flow in the saturated zone is simulated using a steady-state solution for predicting hydraulic head and Darcy velocities in a uniform ground-water system of constant thickness subject to recharge along the top of the aquifer, and a regional gradient defined by upgradient and downgradient head boundary conditions. A generalized three-dimensional flow system is depicted schematically in Figure 4.1. As shown in this figure, the source is centered about the y-origin. Since the aquifer is taken to be homogeneous, we can therefore take advantage of symmetry and simulate only half of the system along the positive y-axis.

4.3.2 Assumptions Underlying the Flow Submodule

The ground-water flow simulation is based on the following simplifying assumptions:

- The contribution of recharge and infiltration from the unsaturated zone is small relative to the regional flow in the aquifer, and the initial saturated aquifer is large relative to the rise of water table due to recharge and infiltration;
- The aquifer is homogeneous.;
- Ground-water flow is steady-state;
- Flow is single phase, isothermal, and governed by Darcy's Law;
- The fluid is homogeneous and slightly compressible; and

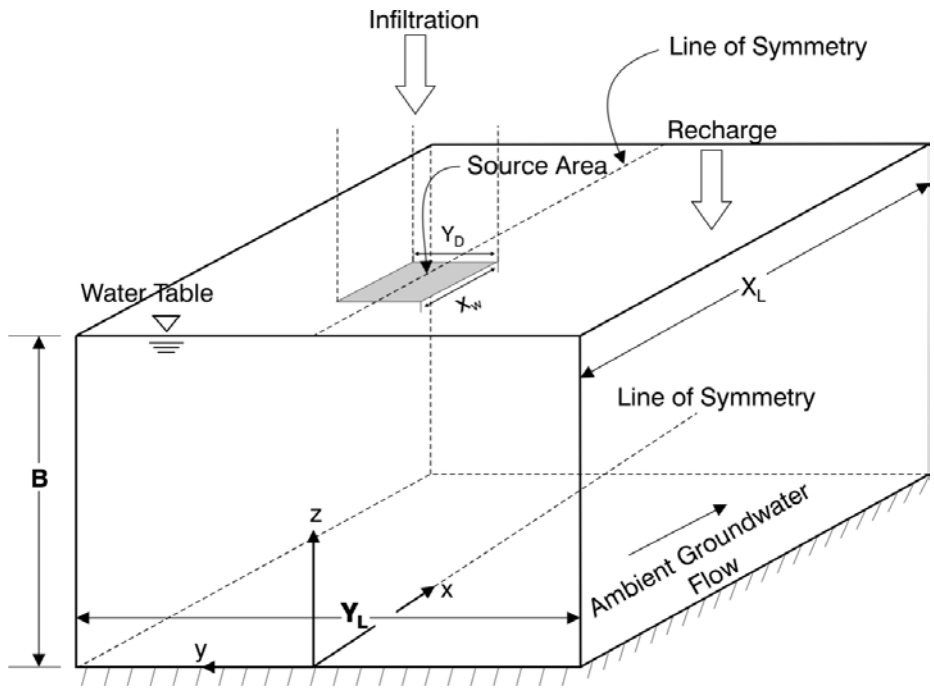

Figure 4.1 Schematic Illustration of the Saturated Three-dimensional Ground-water Flow System Simulated by the Model.

- The principal directions of the hydraulic conductivity tensor are aligned with the Cartesian coordinate system.

The implication of the first assumption is that the saturated zone can be modeled as having a uniform thickness, with mounding underneath the waste source represented by an increased head distribution along the top boundary.

4.3.3 List of Parameters for the Flow Submodule

The aquifer-specific input parameters for the saturated-zone flow submodule include parameters to characterize the ground-water flow regime in the vicinity of the waste management unit. These ground-water flow parameters, together with the transport parameters described in Section 4.4.3, are used to simulate the advective-dispersive transport of dissolved contaminants in a three-dimensional, constant thickness aquifer. The aquifer-specific parameters for the ground-water flow module are presented below and summarized in Table 4.1.

4.3.3.1 <u>Particle Diameter</u>

The particle diameter is a measure of the average grain size of the aquifer material. EPACMTP uses this parameter to determine aquifer porosity and bulk density. As a user, you can either treat the mean particle diameter as an input parameter, or treat

Table 4.1 Aquifer-Specific Variables for the Flow Module

Parameter	Symbol	Units	Section in EPACMTP Parameters/Data Background Document
Particle diameter (input): mean particle diameter of the aquifer material (Section 4.3.3.1)	d	cm	5.3.1
Porosity (derived or input): by default, it is derived and represents the effective porosity of the aquifer material; if input, it may represent the total porosity (Section 4.3.3.2)	ϕ_e (or ϕ)	dimensionless	5.3.2
Bulk Density (derived): bulk density of the aquifer material (Section 4.3.3.3)	ρ_b	g/cm^3	5.3.3
Saturated-zone Thickness (input): saturated thickness of the regional, unconfined aquifer (Section 4.3.3.4)	B	m	5.3.4.3
Hydraulic Conductivity (input): a measure of the ability of the aquifer to transmit water (Section 4.3.3.5)	K	m/y	5.3.4.4
Anisotropy Ratio (input): a factor used to specify the relationship between the horizontal and vertical aquifer hydraulic conductivities (Section 4.3.3.6)	A_r	dimensionless	5.3.6
Hydraulic Gradient (input): regional average hydraulic gradient (Section 4.3.3.7)	r	dimensionless	5.3.4.5
Seepage Velocity (derived): regional average ground-water seepage velocity (Section 4.3.3.8)	V	m/y	5.3.5

it as a derived parameter. In the latter case, EPACMTP will calculate the value for the parameter.

Default data for this parameter are provided in Section 5.3.1 of the *EPACMTP Parameters/Data Background Document* (U.S. EPA, 2003).

Alternatively, if the particle diameter is treated as a derived parameter, then its value is calculated using the value of porosity (which may be constant or randomly generated from a probability distribution) using an empirical relationship based on data reported by Davis (1969):

$$d = \exp\,[(0.261 - \phi)/0.0385] \tag{4.1}$$

where

d	=	mean particle diameter (cm)
exp (·)	=	exponential operator
ϕ	=	total porosity (dimensionless)

4.3.3.2 Porosity

In the absence of a user-specified distribution for porosity, it can be calculated from the particle diameter by rewriting the equation above as:

$$\phi = 0.261 - 0.0385 \ln(d) \tag{4.2a}$$

where

ϕ	=	total porosity (dimensionless)
d	=	mean particle diameter (cm)

This approximation yields the total porosity of the aquifer. For contaminant transport assessments, it is generally more appropriate to use effective porosity, ϕ_e, than total porosity. The effective porosity can be significantly smaller than the total porosity, although an exact relationship cannot be established. McWorter and Sunada (1977) present data on total and effective porosity for a range of aquifer materials. EPA used their data to establish ranges for the ratio between effective and total porosity as a function of grain size (see Table 4.2). For Monte-Carlo assessments, EPACMTP assumes that the actual ratio varies uniformly between the upper and lower value for ϕ_e/ϕ in each particle-size class for a given value of the mean aquifer grain size class. For a given value of the mean aquifer grain size, that total porosity can thus be converted into effective porosity using the following relationship:

$$\phi_e = r_\phi \, \phi \tag{4.2b}$$

where

ϕ_e	=	effective porosity (dimensionless)
r_ϕ	=	radio between effective and total porosities (dimensionless) given in Table 4.2
ϕ	=	total porosity (dimensionless)

It should be noted that the default setting for this parameter in EPACMTP is as a derived parameter (calculated from grain size); only in this case will the model automatically make the conversion from total to effective porosity. In all other cases, no conversion is performed, and the user must specify the actual porosity data to be used by the model by specifying a constant value or a distribution of values for either total porosity or effective porosity in the EPACMTP input file.

Table 4.2 Ratio Between Effective and Total Porosities as a Function of Particle Diameter (after McWorter and Sunada, 1977)

Mean Particle Diameter (cm)	Range of Ratio ϕ_e/ϕ
$\leq 6.25 \times 10^{-3}$	0.03 to 0.77
6.25×10^{-3} to 2.5×10^{-2}	0.04 to 0.87
2.5×10^{-2} to 5.0×10^{-2}	0.31 to 0.91
5.0×10^{-2} to 1.0×10^{-1}	0.58 to 0.94
$> 1.0 \times 10^{-1}$	0.52 to 0.95

4.3.3.3 Bulk Density

Bulk density is defined as the mass of aquifer solid material per unit volume of the aquifer, in g/cm^3 or mg/L. Bulk density takes into account the fraction of the volume that is taken up by pore space.

The aquifer bulk density directly influences the retardation of solutes and is related to aquifer porosity. An exact relationship between porosity, particle density, and the bulk density can be derived (Freeze and Cherry, 1979). Assuming the particle density to be 2.65 g/cm^3, this relationship can be expressed as:

$$\rho_b = 2.65\ (1 - \phi) \tag{4.3}$$

where

ρ_b = bulk density of the soil (g/cm^3)
ϕ = total porosity of the aquifer material (dimensionless)

The bulk density is one of several parameters used to calculate the degree to which contaminant velocities are retarded (that is, the retardation factor for the given chemical species).

4.3.3.4 Saturated-zone Thickness

Saturated-zone thickness is the vertical distance from the water table to the base of the saturated zone.

In a typical Monte-Carlo analysis using EPACMTP, the aquifer saturated thickness is assigned as a regional site-based parameter. Information about the regional, site-based methodology is provided in Section 5.5. The aquifer thickness impacts the dilution rates in the saturated zone.

4.3.3.5 Hydraulic Conductivity

Hydraulic conductivity (*K*) is a measure of the ability to transmit water.

By default, the aquifer hydraulic conductivity is assigned as a regional site-based parameter using the procedure detailed in Section 5.5.2.

Alternatively, the hydraulic conductivity can be specified as a derived parameter. In this case, K is calculated directly from the particle diameter using the Kozeny-Carman (Bear, 1979) equation

$$K = \frac{\rho g}{\mu} \frac{\phi^3}{(1-\phi)^2} \frac{d^2}{1.8} \tag{4.4}$$

where

K = hydraulic conductivity (cm/s)
ρ = density of water (kg/m^3)
g = acceleration due to gravity (m/s^2)
μ = dynamic viscosity of water (N-s/m^2)
ϕ = total porosity of the aquifer material (dimensionless)
d = mean particle diameter (m)

In Equation (4.4) shown above, the constant 1.8 is a unit conversion factor to yield K in units of cm/s. Both the density and the dynamic viscosity of water are functions of temperature and are computed using the regression equations presented in *The Handbook of Chemistry and Physics* (CRC, 1981).

4.3.3.6 Anisotropy Ratio

The anisotropy ratio is a factor used to specify the relationship between the horizontal and vertical aquifer hydraulic conductivities:

$$A_r = \frac{K_x}{K_z} \tag{4.5}$$

where

A_r = anisotropy ratio = K_x/K_z.
K_x = hydraulic conductivity in the x direction (m/y)
K_z = hydraulic conductivity in the z direction (m/y)

The default value of A_r is 1, which indicates an isotropic system. In EPACMTP, the horizontal transverse hydraulic conductivity is by default set equal to the horizontal longitudinal conductivity, that is, $K_y = K_x$.

4.3.3.7 Hydraulic Gradient

Hydraulic gradient measures the head difference between two points as a function of their distance. The hydraulic gradient provides the driving force for ground-water flow.

In a typical Monte-Carlo analysis using EPACMTP, the hydraulic gradient is assigned as a regional, site-based parameter. More information about the regional, site-based methodology is provided in Section 5.5.

4.3.3.8 Seepage Velocity

The seepage velocity is related to the aquifer properties through Darcy's law. The regional seepage velocity may be input directly or it may be a derived parameter (default). In the latter case, it is computed as

$$V_x = \frac{K_x}{\phi_e} r \tag{4.6}$$

where

V_x = longitudinal ground-water seepage velocity (in the x-direction) (m/y)
K_x = longitudinal hydraulic conductivity (in the x-direction) (m/y)
ϕ_e = effective porosity (dimensionless)
r = regional hydraulic gradient (dimensionless)

Default lower and upper bounds for the seepage velocity are 0.1 and 1.1×10^4 m/y, respectively. This range of seepage velocity values is based on survey data reported by Newell et al (1990).

4.3.4 Mathematical Formulation of the Saturated-Zone Flow Submodule

The governing equation for steady-state flow in three dimensions is:

$$K_x \frac{\partial^2 H}{\partial x^2} + K_y \frac{\partial^2 H}{\partial y^2} + K_z \frac{\partial^2 H}{\partial z^2} = 0 \tag{4.7}$$

where

K_x = hydraulic conductivity in the longitudinal (x) direction (m/y)
H = hydraulic head (m)
x = principal Cartesian coordinate along the regional flow direction (m)
K_y = hydraulic conductivity in the horizontal transverse (y) direction (m/y)
y = principal Cartesian coordinate normal to the flow direction (m)
K_z = hydraulic conductivity in the vertical (z) direction (m/y)
z = principal Cartesian coordinate in the vertical direction (m)

4.3.5 Solution Methods for Flow in the Saturated Zone

As stated in Section 4.1, three simulation options are available in EPACMTP.

Option 1: Three-dimensional steady-state ground-water flow and advective-dispersive transport in an aquifer with constant saturated thickness and non-uniform recharge across the upper aquifer boundary;

Option 2: Quasi-three dimensional ground-water flow and advective-dispersive transport, through a combination of 2D areal and cross-sectional solutions; and

Option 3: One-dimensional ground-water flow and pseudo-three-dimensional advective-dispersive transport through a combination of hybrid one-dimensional numerical and two-dimensional analytical solutions.

Details of the flow component of each of the three simulation options are presented below.

4.3.5.1 <u>One-dimensional Flow Solution</u>

The steady-state flow equation in a vertical (x-z) plane may be written as:

$$K_x \frac{\partial^2 H}{\partial x^2} + K_z \frac{\partial^2 H}{\partial z^2} = 0 \qquad (4.8)$$

where

K_x = hydraulic conductivity in the longitudinal (x) direction (m/y)
H = hydraulic head (m)
x = principal Cartesian coordinate along the regional flow direction (m)
K_z = hydraulic conductivity in the vertical (z) direction (m/y)
z = principal Cartesian coordinate in the vertical direction (m)

Equation (4.8) is solved subject to the following boundary conditions:

(i) <u>Upgradient boundary</u>

$$H(0,\ z) = H_1 \qquad (4.9a)$$

(ii) <u>Downgradient boundary</u>

$$H(x_L,\ z) = H_2 \qquad (4.9b)$$

(iii) Top boundary

$$-K_z \frac{\partial H}{\partial z}(x,\ B) = I_{EFF}, \quad x_u \le x \le x_d$$
$$= I_r, \quad \textit{elsewhere} \tag{4.9c}$$

(iv) Bottom boundary

$$-K_z \frac{\partial H}{\partial z}(x,\ 0) = 0 \tag{4.9d}$$

where

$H(0,z)$	=	hydraulic head at x = 0 (m)
H_1	=	prescribed hydraulic head at the upgradient boundary (m)
$H(x_L, z)$	=	hydraulic head at x = x_L (m)
x_L	=	length of the aquifer system (m)
H_2	=	prescribed hydraulic head at the downgradient boundary (m)
K_z	=	hydraulic conductivity in the vertical (z) direction (m/y)
H	=	hydraulic head (m)
z	=	principal Cartesian coordinate in the vertical direction (m)
x	=	principal Cartesian coordinate along the regional flow direction (m)
B	=	saturated thickness of the system (m)
I_{EFF}	=	effective infiltration rate through the strip source area (m/y)
x_u	=	upgradient coordinate of the strip source area (m)
x_d	=	downgradient coordinate of the strip source area (m)
I_r	=	effective recharge rate outside the strip source area (m/y)

I_{EFF} represents the laterally-averaged vertical water flux in the source area as defined by

$$I_{EFF} = \frac{I\,y_D + I_r(y_L - y_D)}{y_L} \tag{4.10}$$

where

I_{EFF}	=	effective infiltration rate through the strip source area (m/y)
I	=	infiltration rate through the rectangular source area (m/y)
y_D	=	source width along the y-axis (m)
I_r	=	recharge rate (m/y)
y_L	=	length of the domain in the y-direction (m) (see Figure 4.1)

By vertically integrating Equation (4.8) and incorporating Equations (4.9c and 4.9d), and invoking the Dupuit-Forchheimer assumption (Bear, 1972), one obtains:

$$-K_x B \frac{\partial^2 H}{\partial x^2} = I_{EFF} \tag{4.11}$$

where

K_x	=	hydraulic conductivity in the longitudinal (x) direction (m/y)
B	=	saturated thickness of the system (m)
H	=	hydraulic head (m)
x	=	principal Cartesian coordinate along the regional flow direction (m)
I_{EFF}	=	effective infiltration rate through the strip source area (m/y)

It is possible that the Dupuit-Forchheimer assumption may be violated underneath the source where the vertical velocity component is significant. However, the assumption should remain approximately true for the rest of the flow domain. To circumvent potential limitations due to the violation of the Dupuit-Forchheimer assumption, the source dimensions on the vertical plane normal to the flow direction immediately downgradient from the WMU are determined from the condition of local mass conservation. The determination of source dimensions is discussed later in Section 4.4.5.4.

Solving Equation (4.11) subject to boundary conditions in Equations (4.9a and 4.9b), one obtains:

For $0 \le x \le x_u$

$$H(x) = \frac{-I_r}{2K_xB}x^2 + \left[\frac{I_r - I}{2K_xB}\left(\frac{x_d^2 - x_u^2}{x_L}\right) + \frac{I_r - I_{EFF}}{K_xB}(x_u - x_d) + \frac{I_r}{2K_xB}x_L + \frac{H_2 - H_1}{x_L}\right]x + H_1 \tag{4.12a}$$

For $x_u \le x \le x_d$

$$H(x) = \frac{-I_{EFF}}{2K_xB}x^2 + \left[\frac{I_r - I}{2K_xB}\left(\frac{x_d^2 - x_u^2}{x_L}\right) - \frac{I_r - I_{EFF}}{K_xB}x_d + \frac{I_r}{2K_xB}x_L + \frac{H_2 - H_1}{x_L}\right]x + \frac{I_r - I_{EFF}}{2K_xB}x_u^2 + H_1 \tag{4.12b}$$

For $x_d \le x \le x_L$

$$H(x) = \frac{-I_r}{2K_xB}x^2 + \left[\frac{I_r - I_{EFF}}{2K_xB}\left(\frac{x_d^2 - x_u^2}{x_L}\right) + \frac{I_r}{2K_xB}x_L + \frac{H_2 - H_1}{x_L}\right]x - \frac{I_r - I_{EFF}}{2K_xB}(x_d^2 - x_u^2) + H_1 \tag{4.12c}$$

where

x	=	principal Cartesian coordinate along the regional flow direction (m)
x_u	=	upgradient coordinate of the strip source area (m)
$H(x)$	=	hydraulic head at distance x (m)
I_r	=	effective recharge rate outside the strip source area (m/y)
K_x	=	hydraulic conductivity in the longitudinal (x) direction (m/y)
B	=	saturated thickness of the system (m)
I_{EFF}	=	effective infiltration rate through the strip source area (m/y)
x_d	=	downgradient coordinate of the strip source area (m)
x_L	=	length of the aquifer system (m)
H_2	=	prescribed hydraulic head at the downgradient boundary (m)
H_1	=	prescribed hydraulic head at the upgradient boundary (m)

4.3.5.2 Two-dimensional Flow Solutions

As an alternative, the flow submodule can also simulate two-dimensional (2D) steady-state ground-water flow in either the vertical (x-z) cross-section, or the areal (x-y) plane. These two options are combined with corresponding transport solutions. The 2D cross-sectional solution is appropriate for cases in which flow in the horizontal transverse (y-) direction is of minor significance. An example would be a situation in which the rate of infiltration through the patch source at the water table is relatively low compared to the regional ground-water flow rate, and the lateral extent of the source is large. Conversely, a 2D areal solution is appropriate when the contaminant mass flux into the saturated zone is relatively large and the saturated zone is relatively thin. In this case, ground-water flow in the horizontal transverse direction may be significant. In addition, the contaminant plume would be expected to quickly occupy the entire saturated aquifer thickness, allowing a 2D areal treatment.

Strictly speaking, the second condition may cause the first assumption in Section 4.3.2 to be violated because of the rise of water table due to infiltration may be significant compared with the initial aquifer saturated thickness. However, as discussed in Section 1.3, the violation of the water-table-rise assumption leads to conservative arrival times and peak concentrations of chemical constituents at receptor well locations.

Both of the 2D solutions are obtained as special cases of the general three-dimensional solution (see Section 4.3.5.3). For the vertical cross-sectional model, the horizontal transverse hydraulic conductivity, K_y, is set to zero and a computational grid is generated which is only one grid block wide and spans exactly the half-width of the source.

$$\frac{1}{2} y_L = \frac{1}{2} y_D \tag{4.13}$$

where

y_L	=	length of the model domain in the y-direction (m)
y_D	=	length of the source in the y-direction (m)

For the 2D areal solution, the vertical conductivity, K_z, is set to zero, and a one grid block thick, planar grid is generated.

The benefit of using a 2D approximation is the substantial savings in computational effort as compared to a fully 3D solution, both in terms of memory requirements and in terms of execution speed. This is especially of benefit when performing Monte-Carlo simulations. The implementation of the 2D flow and transport solutions for Monte-Carlo simulations in EPACMTP incorporates an automatic criterion for switching between cross-sectional and areal solutions based on the importance of vertical versus areal plume movement. Details of this procedure are presented later in Section 4.4.5.3.3.

4.3.5.3 Three-dimensional Flow Solution

The governing equation for steady-state flow in three dimensions is given in Equation (4.7). This equation is solved subject to the following boundary conditions:

$$H\,(0,y,z) = H_1 \tag{4.14a}$$

$$H\,(x_L,y,z) = H_2 \tag{4.14b}$$

$$-K_z \frac{\partial H}{\partial z}\,(x,y,B) = \begin{cases} I & x_u \le x \le x_d,\ -\tfrac{1}{2}y_D \le y \le \tfrac{1}{2}y_D \\ I_r & \textit{elsewhere} \end{cases} \tag{4.14c}$$

$$\frac{\partial H}{\partial y}\,(x,0,z) = 0 \tag{4.14d}$$

$$\frac{\partial H}{\partial y}\,(x,\pm\tfrac{1}{2}y_L,z) = 0 \tag{4.14e}$$

and

$$\frac{\partial H}{\partial z}\,(x,y,0) = 0 \tag{4.14f}$$

where

$H(0, y, z)$	=	hydraulic head at x = 0 (m)
H_1	=	prescribed hydraulic head at the upgradient boundary (m)
$H(x_L, y, z)$	=	hydraulic head at $x = x_L$ (m)
H_2	=	prescribed hydraulic head at the downgradient boundary (m)
K_z	=	hydraulic conductivity in the vertical (z) direction (m/y)
H	=	hydraulic head (m)
z	=	principal Cartesian coordinate in the vertical direction (m)
x	=	principal Cartesian coordinate along the regional flow direction (m)
y	=	principal Cartesian coordinate normal to the flow direction (m)
B	=	thickness of the aquifer system (m)
I	=	infiltration rate (m/y) through the rectangular source area ($x_u \le x \le x_d$, $-½\, y_D \le y \le ½\, y_D$)
x_u	=	upgradient coordinate of the strip source area (m)
x_d	=	downgradient coordinate of the strip source area (m)
y_D	=	width of the source in the y-direction (m)
I_r	=	recharge rate at the water table outside the rectangular source area (m/y)

The solution to the three-dimensional flow equation (Equation (4.7)), subject to Equations (4.14a through 4.14f), is obtained numerically using either a mesh-centered finite difference approximation with 7-point nodal connectivity, or a 27-point Galerkin finite element approximation. With the latter method, the element integrations are performed using the influence coefficient method (Huyakorn et al., 1986), which yields a very efficient solution.

The aquifer region of interest is first discretized into a grid consisting of hexahedral (brick) elements, as shown in Figure 4.2. This figure shows the local numbering of nodes associated with the element and the element dimensions represented by Δx, Δy, and Δz. The grid is the same as that used in the subsequent transport analysis and is generated internally by the saturated-zone module, based on the overall dimensions of the modeled aquifer region and location and size of the source. Nodal spacings in the latter case are automatically assigned based on the Peclet number criterion using the dispersivity values specified for the solute transport problem. The generated grid will be finest near the source, with wider nodal spacings away from the source. Details of this procedure which is automatically implemented in EPACMTP are provided in Section 4.4.5.1.

Spatial discretization by either finite differences or finite elements leads to a final matrix equation of the form:

$$[R]\,\{\tilde{H}\} = \{Q\} \tag{4.15}$$

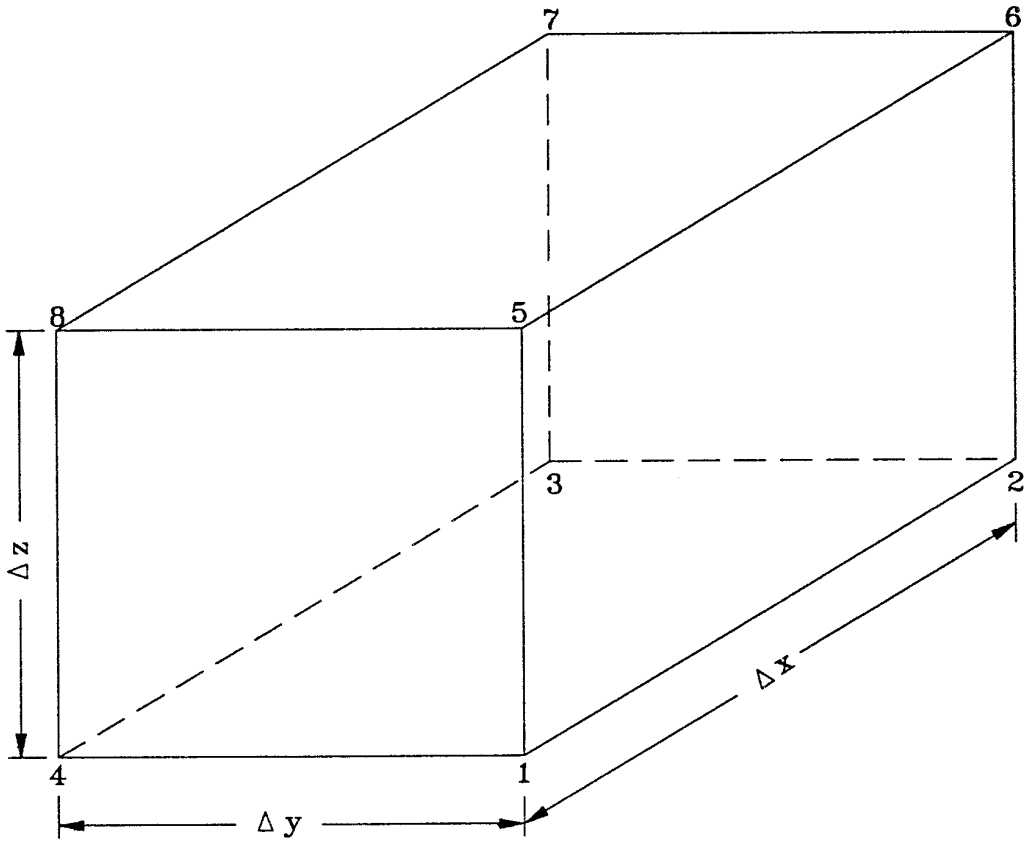

Figure 4.2 Three-dimensional Brick Element Used in Numerical Flow and Transport Model Showing Local Node Numbering Convention.

where

$[R]$ = conductance matrix (m^2/y)
$\{\tilde{H}\}$ = vector of unknown nodal head values (m)
$\{Q\}$ = vector of nodal boundary flux values (m^3/y)

The solution of Equation (4.15) is obtained using an efficient iterative matrix solver with ORTHOMIN acceleration. The solution scheme is described by Sudicky and McLaren (1991).

After the nodal head values have been obtained, the Darcy velocity values at the centroid of each element which are required for the solute transport analysis are computed from Darcy's Law as

$$V_\zeta = -K_\zeta \frac{dH}{d_\zeta} \tag{4.16}$$

where

V_ζ = Darcy velocity in the ζth direction (m/y)
K_ζ = hydraulic conductivity in the ζth direction (m/yr)
H = hydraulic head (m)
ζ = distance along a principal Cartesian coordinate direction (m)

The head derivative at the element centroid is approximated as

$$\frac{dH}{d\zeta}\Big|_{\zeta + \frac{1}{2}\Delta\zeta} \cong \frac{1}{4\Delta\zeta}\left[\sum_{i=1}^{4} H^i_{\zeta+\Delta\zeta} - \sum_{i=1}^{4} H^i_{\zeta}\right] \tag{4.17}$$

where

H = hydraulic head (m)
ζ = distance along a principal Cartesian coordinate direction (m)
i = nodal index (dimensionless)
$\Delta\zeta$ = element dimension in the direction of ζ (m)
$H^i_{\zeta+\Delta\zeta}$ = hydraulic lead at node i at distance $\zeta+\Delta\zeta$ (m)
H^i_{ζ} = hydraulic head at node i at distance ζ (m)

and where the summations are performed over the element nodes with common coordinates in the $_\zeta^{th}$ direction, that is, for each 8-noded element, four nodes will have a coordinate value of $_\zeta$ and four nodes will have a coordinate value of $_\zeta+\Delta_\zeta$.

4.3.6 Parameter Screening For Infeasible Ground-water Flow Conditions

Inherent in the Monte-Carlo process is that parameter values are drawn from multiple data sources, and then combined in each realization of the modeling process. Because the parameter values are drawn randomly from their individual probability distributions, it is possible that, in some instances, parameters are combined in ways that may be physically infeasible and may violate the validity of the EPACMTP flow model. A number of checks are implemented to eliminate or reduce these occurrences as much as possible. As a relatively simple measure, upper and lower limits are specified on individual parameter values to ensure that their randomly generated values are within physically realistic limits. Where possible, we use data sources that contain multiple parameters, and implement these in the Monte-Carlo process in a way that preserves the existing correlations among the parameters. For example, we use the HGDB database of hydrogeologic parameters (see Section 5.5.1 and Section 5.3.4 of the *EPACMTP Parameters/Data Background Document* (U.S. EPA, 2003)) in combination with knowledge of the hydrogeologic environments at each waste site location in our WMU parameter database to assign the most appropriate combinations of hydrogeological parameters to each site. Likewise, we assign climate-related parameters based on each site's proximity to an infiltration modeling database of 102 climate stations, as summarized in Section 5.5 of this

document and explained fully in Section 4.2 of the *EPACMTP Parameters/Data Background Document* (U.S. EPA, 2003).

In EPACMTP, we also specify upper and lower limits on secondary parameters whose values are calculated (derived) internally in the Monte-Carlo module as functions of the primary EPACMTP input parameters (see the *EPACMTP Parameters/Data Background Document* (U.S. EPA, 2003)) and implement a set of screening procedures to ensure that infiltration rates and the resulting predicted ground-water mounding remain physically plausible. Specifically, we screen the parameter values generated in each Monte-Carlo realization for the following conditions:

- Infiltration and recharge so high that they cause the water table to rise above the ground surface;
- Liquid level in an SI unit below the water table, causing ground water to flow into the SI; and
- Infiltration rate from an SI that exceeds the saturated hydraulic conductivity of the soil underneath.

These screening procedures are discussed in more detail below, and the mathematical algorithms for implementing the screening are presented in Appendix E. The logic diagram for the infiltration screening procedure is presented in Figure 4.3; Figure 4.4 provides a graphical illustration of the screening criteria. The numbered criteria checks in Figure 4.3 correspond to the numbered diagrams in Figure 4.4. Because high infiltration rates are most likely to occur with unlined surface impoundments, the screening procedure is the most involved for this type of WMU.

Figure 4.3(a) depicts the infiltration screening procedures for landfills, waste piles, and land application units. For these units, after the four correlated hydrogeologic parameters (depth to water table, aquifer saturated thickness, aquifer hydraulic conductivity, and regional gradient), recharge associated with the selected soil type and the nearest climate center, and source infiltration have been generated for each Monte-Carlo realization, the EPACMTP model calculates the estimated water table mounding that would result from the selected combination of parameter values. The combination of parameters is accepted if the calculated maximum water table elevation (the ground-water 'mound') remains below the ground surface elevation at the site. If the criterion is not satisfied, the selected parameters for the realization are rejected and a new data set is selected.

For surface impoundments, there are two additional screening steps, as depicted in Figure 4.3(b). At each Monte-Carlo realization, a surface impoundment unit is selected from the surface impoundment WMU data base. Unit-specific parameters, including ponding depth and base depth below ground surface, are retrieved from the data base. The four correlated hydrogeologic parameters are then selected from

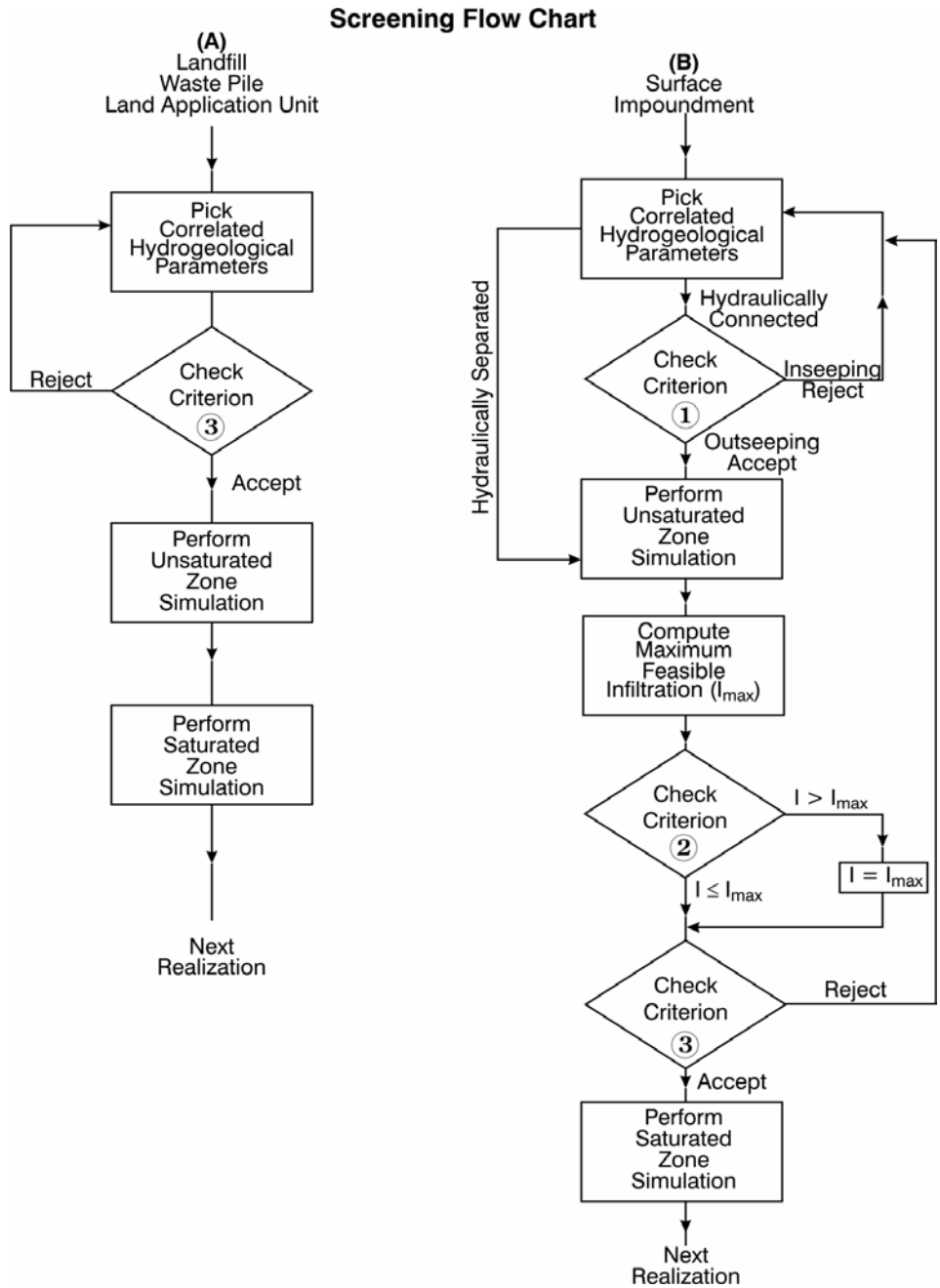

Figure 4.3 Flowchart Describing the Infiltration Screening Procedure.

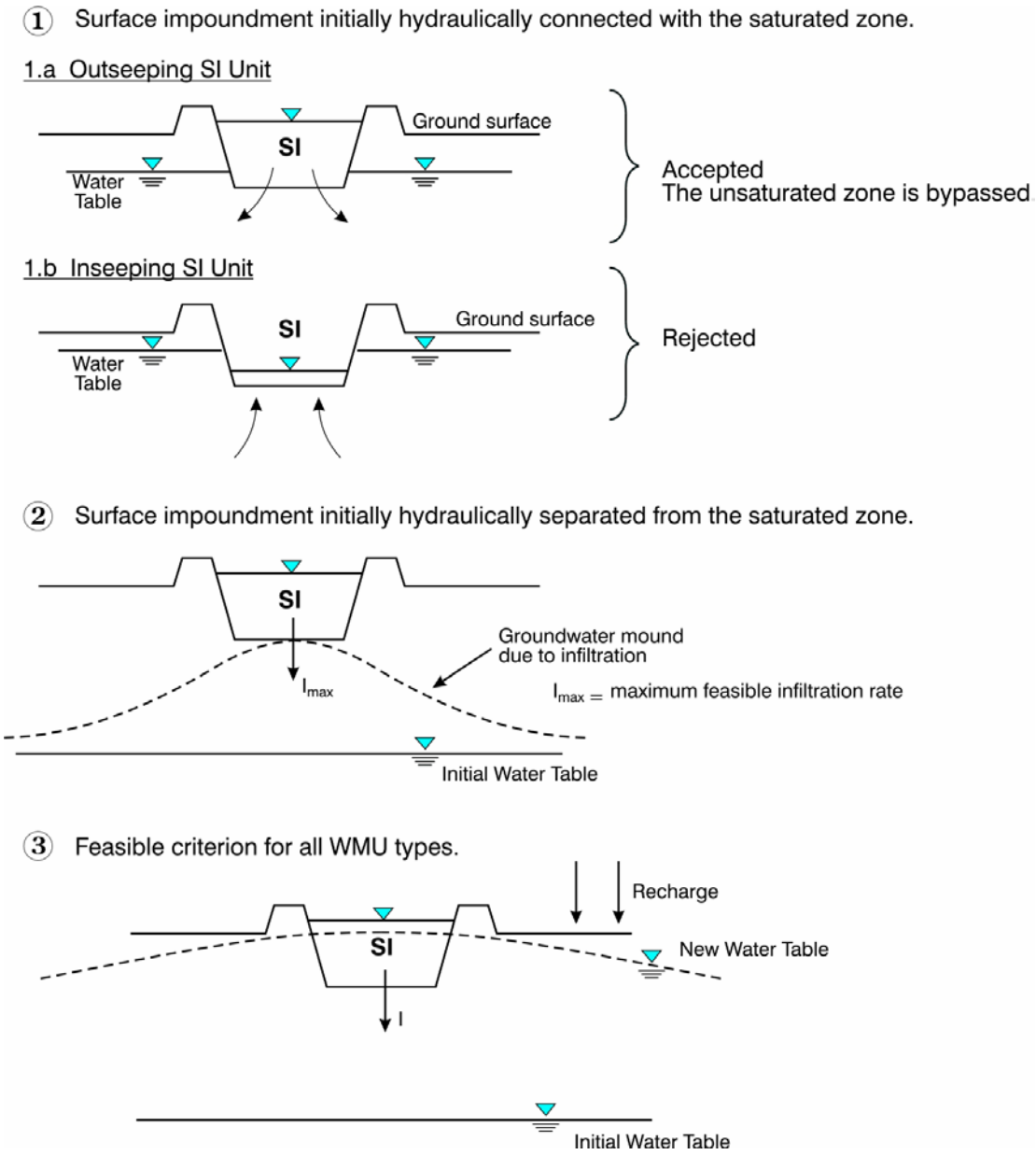

Figure 4.4 Infiltration Screening Criteria.

the hydrogeologic data base, based on the hydrogeologic environment at that WMU location. Using the information on the base depth and water table elevations, we can determine whether the surface impoundment unit is hydraulically connected to the water table. If the base of the surface impoundment is below the water table, the surface impoundment unit is said to be hydraulically connected to the water table (see Figure 4.4, Criterion 1). If the hydraulically connected surface impoundment is an inseeping type (see Figure 4.4, Criterion 1(b)), the realization is rejected, and the set of hydrogeologic parameters is regenerated. An inseeping type of surface impoundment (the elevation of the waste water surface in the impoundment is below the water table) means that ground-water transport would tend to be from the aquifer into the impoundment rather than from the impoundment into the aquifer; the model rejects this type of scenario because it is unlikely that an impoundment like this would be constructed to manage waste water. However, as long as the elevation of the waste water surface in the impoundment is **above** the water table, the first criterion is passed (Figure 4.4, Criterion 1(a)).

If the base of the unit is located above the water table, the unit is said to be hydraulically separated from the water table (see Figure 4.4, Criterion 2). However, in this case, it is necessary to ensure that the calculated infiltration rate does not exceed the maximum feasible infiltration rate. The maximum feasible infiltration rate is the maximum infiltration that allows the water table to remain hydraulically separated from the surface impoundment. In other words, it is the rate that does not allow the crest of the local ground-water mound to be higher than the base of the surface impoundment. This limitation allows us to determine a maximum infiltration rate that is based on the free-drainage condition at the base of the surface impoundment. The infiltration rate tends to decrease thereby reducing the contaminant flux if the water table is allowed to be in hydraulic contact with the base of the surface impoundment. If the maximum feasible infiltration rate (I_{max}) is exceeded, the EPACMTP model will set the infiltration rate to this maximum value.

Once the infiltration limit has been imposed, the third criterion is checked to ensure that any ground-water mounding does not result in a rise of the water table mound above the ground surface, in the same manner as done for other types of WMUs.

4.4 SATURATED-ZONE SOLUTE TRANSPORT SUBMODULE

4.4.1 Description of the Solute Transport Submodule

The saturated-zone transport submodule simulates the advective-dispersive transport of dissolved contaminants in a three-dimensional, constant thickness aquifer (Figure 4.1). The modeled region is the same as that used for flow modeling, that is, only the half of the system along the positive y-axis is actually simulated. Ambient ground-water flow is in the direction of the positive x-axis. The initial concentration of a chemical constituent in the aquifer is taken to be zero. The constituent concentration along the upgradient system boundary is held at zero throughout the simulation. The concentration gradient along the downgradient boundary is zero, and the lower aquifer boundary is assumed to be impermeable. Contaminants enter the saturated zone through a rectangular patch source of either prescribed concentration or prescribed mass flux on the upper aquifer boundary.

Recharge of contaminant-free infiltration water occurs along the upper aquifer boundary outside the patch source. Transport mechanisms considered are advection, longitudinal, vertical and transverse hydrodynamic dispersion, linear or nonlinear equilibrium sorption, zero-order production and first-order decay.

The transport submodule consists of analytical and numerical three-dimensional contaminant transport simulators. The transport submodule has the following transport options:

- Three-dimensional advective-dispersive transport in an aquifer with a steady-state flow field and a patch source of contaminants at the water table.
- Quasi-three dimensional advective-dispersive transport, through a combination of 2D areal and cross-sectional solutions.
- Pseudo-three-dimensional advective-dispersive transport through a combination of hybrid one-dimensional numerical and two-dimensional analytical solutions.

4.4.2 Assumptions Underlying the Saturated-zone Transport Submodule

The major assumptions underlying the solution of the saturated-zone transport equation are:

(1) The flow field is single phase and at steady state;

(2) The aquifer is homogeneous and initially contaminant free;

(3) Adsorption onto the solid phase is described by the Freundlich equilibrium isotherm;

(4) Chemical and/or biochemical degradation of the contaminant can be described as a first-order process;

(5) The chemical is dilute and is present only in the solution or adsorbed onto the soil matrix;

(6) Hydrodynamic dispersion can be described as a Fickian process; and

(7) The saturated zone is a chemically buffered system with constant and uniform geochemical characteristics.

4.4.3 List of Parameters for the Solute Transport Submodule

The aquifer-specific input parameters for the saturated-zone transport submodule include parameters to characterize ground-water transport in the vicinity of the waste management unit. These ground-water transport parameters, together with the ground-water flow parameters described in Section 4.3.3, are used to determine the

advective-dispersive transport of dissolved contaminants in a three-dimensional, constant thickness aquifer. The aquifer-specific parameters for the saturated-zone transport submodule are presented below and summarized in Table 4.3.

Table 4.3 Aquifer-Specific Variables for the Saturated-Zone Transport Submodule

Parameter	Symbol	Units	Section in EPACMTP Parameters/Data Background Document
Retardation Factor: a number that describes the speed of a constituent's travel through the subsurface relative to that of the bulk mass of ground water (1.0 = no sorption) (See Section 4.4.3.1)	R^s	dimensionless	5.3.7
Dispersivities: characteristic lengths that define spatial extent of dispersion of contaminants, along the flow direction, horizontally normal to the flow direction, and vertically normal to the flow direction (Section 4.4.3.2)	α_L α_T α_V	m	5.3.8
Ground-water Temperature: average regional ground-water temperature, used to derive hydrolysis rates for degrading organic constituents (Section 4.4.3.3)	T	°C	5.3.9
Ground-water pH: average regional ground-water pH, assuming that pH is not influenced by the addition of leachate from the WMU or changes in temperature, used to derive hydrolysis rates for degrading organic constituents and can be used to calculate sorption of metals (Section 4.4.3.4)	pH	std. units	5.3.10
Fractional Organic Carbon Content: the fraction of organic carbon in the aquifer material (Section 4.4.3.5)	f_{oc}^s	unitless	5.3.11
Receptor Well Parameters: • angle of well off plume centerline • radial distance to well • distance to well in x direction • distance to well in y direction • depth of well below water table (Section 4.4.3.6)	 θ_{rw} R_{rw} x_{rw} y_{rw} z_{rw}	m	6.2 through 6.6
Freundlich Sorption Coefficient: a constant used with the aqueous concentration to determine the adsorption isotherm according to the Freundlich model (Section 4.4.3.7)	k_1^s or K_d^s	cm^3/g	5.3.12
Freundlich Sorption Exponent: the exponent to which the aqueous concentration is raised in the determination of the adsorption isotherm according to the Freundlich model; when the adsorption isotherm is linear, this exponent is one (Section 4.4.3.8)	η^s	dimensionless	5.3.13

Table 4.3 Aquifer-Specific Variables for the Saturated-Zone Transport Submodule (continued)

Parameter	Symbol	Units	Section in EPACMTP Parameters/Data Background Document
Metals Sorption Coefficient: the non-linear, non-Freundlich type adsorption isotherm for metals (Section 4.4.3.9)	K_d^s	cm^3/g	3.3.3
Chemical Degradation Rate Coefficient: first order decay rate that accounts for chemical transformation only (Section 4.4.3.10)	λ_c^s	1/y	5.3.14
Biodegradation Rate Coefficient: first order decay rate that accounts for biodegradation only; the default value is zero (Section 4.4.3.10)	λ_b^s	1/y	5.3.15
Molecular diffusion coefficient: a constituent-specific parameter that accounts for the effects of molecular diffusion in free water (Section 4.4.3.11)	D_i	m^2/y	3.3.1.1
Molecular weight: the amount of mass in one mole of molecules of a constituent as determined by summing the atomic weights of the elements in that constituent, multiplied by their stoichiometric factors (Section 4.4.3.12)	MW_i	g/mole	3.3.1.3

4.4.3.1 Retardation Factor

The retardation factor is defined for a linear adsorption isotherm by

$$R_\ell^s = 1 + \frac{\rho_b K_d^s}{\phi_e} \tag{4.18}$$

where

R_ℓ^s = saturated-zone retardation factor of component species ℓ (dimensionless)
ρ_b = bulk density of the aquifer (g/cm^3)
K_d^s = distribution coefficient of the aquifer (cm^3/g)
ϕ_e = effective porosity of the aquifer (dimensionless)

When the sorption isotherm is nonlinear, R_ℓ^s is no longer constant but depends on concentration. In this case, R_ℓ^s must be given as a derived variable and the K_d-concentration relation must be specified by the user in terms of two the parameters: the Freundlich coefficient (k_1) and the Freundlich exponent (η) (see Equation (3.16)).

For the modeling of metals, the EPACMTP user has three options for specifying the relationship between dissolved and adsorbed concentrations: 1) MINTEQA2-derived

non-linear isotherms, 2) pH-dependent empirical isotherms, or 3) an empirical distribution of values. In the case of the first option, the non-linear isotherm is only used in the unsaturated zone; a linear sorption isotherm (that is, an effective K_d value) is used for the saturated zone. This effective K_d value is determined from the maximum contaminant concentration at the water table and values of the five environmental master variables (pH, iron-oxide, leachate organic matter, natural organic matter in the aquifer, and ground-water environment type (carbonate or non-carbonate)), following the procedure described in Appendix G.

The aquifer-specific input parameters for the saturated-zone transport submodule include parameters to characterize ground-water transport in the vicinity of the waste management unit. These ground-water transport parameters, together with the ground-water flow parameters described in Section 4.3.3, are used to determine the advective-dispersive transport of dissolved contaminants in a three-dimensional, constant thickness aquifer.

4.4.3.2 Dispersivity

The spreading and dilution of the contaminant plume in the saturated zone is controlled by two mechanisms: advection and dispersion. EPACMTP allows for non-uniform ground-water flow due to vertical recharge and infiltration from the waste site. The model simulates actual spreading mechanisms occurring in the field. For non-degrading chemical constituents, the dilution caused by dispersive mixing is a controlling factor in determining the constituent concentration observed at a receptor well. In Monte-Carlo analyses, transport is a relatively insensitive to dispersion. The reason for this is that low dispersivities lead to a compact, concentrated plume. If the plume is relatively small, the likelihood that the receptor well will intercept the plume is reduced, but the concentration in the well, if it does, will be relatively high. High dispersivities will lead to a more dilute plume which occupies a greater volume, thereby increasing the likelihood that a receptor well will intercept the plume. Concentrations in the plume however, are likely to be lower than in the first case. In the case of a full Monte-Carlo analysis, the resultant distribution will tend not to be sensitive to dispersivity.

The model computes the longitudinal, lateral, and vertical dispersion coefficients as the product of the seepage velocity and longitudinal (α_L), transverse (α_T) and vertical (α_V) dispersivities. A literature review indicated the absence of a generally accepted theory to describe dispersivities, although a strong dependence on scale has been noted (Gelhar et al., 1985; Gelhar et al., 1992).

In the absence of user-specified values or distributions, the default probabilistic distribution (see Section 5.4.9.1 of this document and Section 5.3.8 of the *EPACMTP Parameters/Data Background Document* (U.S. EPA, 2003)) is used. Within each of the discrete intervals of the probabilistic distribution, the longitudinal dispersivity is assumed to be uniform. The values of longitudinal dispersivity in each interval are based on a receptor well distance of 152.4 m. For distances other than 152.4 m, the following equations are used to adjust the sampled value of dispersivity:

$$\alpha_L(x_t) = \alpha_{Ref}\left(\frac{x_t}{152.4}\right)^{\frac{1}{2}} \tag{4.19}$$

$$x_t = \frac{1}{2}x_w + x_{rw} \tag{4.20}$$

where

α_L	=	longitudinal dispersivity (m)
x_t	=	average travel distance in the x direction (m)
α_{Ref}	=	reference longitudinal dispersivity, as determined from the probabilistic distribution (m)
x_w	=	length of the WMU in the x-direction (parallel to ground-water flow) (m)
x_{rw}	=	distance from the downgradient boundary of the WMU to the receptor well (m)

In other words, the travel distance x_t is equal to the distance of the receptor well (x_{rw}) from the downgradient facility boundary, plus one-half of the facility dimension. The average distance for all of the contaminants to migrate to the edge of the waste management unit is equal to one half the length of the unit or ½ x_w. Within the EPACMTP model, the minimum allowed value of α_L is 0.01 m.

By default, the transverse (α_T) and vertical (α_V) dispersivities are calculated by the EPACMTP model as a fraction of the longitudinal dispersivity. The default values for the ratio of the longitudinal to the transverse dispersivity, α_L/α_T, and the ratio of the longitudinal to the vertical dispersivity, α_L/α_V, are 8 and 160, respectively. The rationale for these values is presented below.

The dispersivity relationship described above has been derived based on a review of available data. More recently, Gelhar et al. (1992) have compiled and documented results from a large number of studies in which dispersivity values have been reported. These studies represent a wide range of spatial scales, from a few meters to over ten-thousand meters. The data as presented by Gelhar et al. (1992) show a clear correlation between scale and apparent dispersivity. The dispersivity relationship used in EPACMTP describes the observed data reasonably well. The field data suggest a somewhat steeper slope of the distance-dispersivity relation on a log-log scale than is used in the modeling analyses. A sensitivity analysis performed using EPACMTP has shown that the model results are virtually identical when the slope is varied from 0.5 to 1.5. For this reason the original relationship as shown above has been retained. The data presented by Gelhar et al. (1992) also show that the ratios between longitudinal, and horizontal and vertical transverse dispersivities used in the nationwide modeling, are consistent with published data.

4.4.3.3 Ground-water Temperature

In a typical Monte-Carlo analysis using EPACMTP, the ground-water temperature is assigned as a regional site-based parameter based on the location of the waste management unit. The map shown in Figure 4.2 of the *EPACMTP Parameters/Data Background Document* (U.S. EPA, 2003) was used to assign the ground-water temperature to each facility in the database of waste sites. For each waste site, the assigned temperature is obtained from averaging the upper and lower temperatures within the appropriate region. You can find more information about the regional, site-based methodology in Section 5.5. Additionally, the EPACMTP model uses the temperature of the ground water in the aquifer as the temperature of the ground water within the unsaturated zone.

4.4.3.4 Ground-water pH

A nationwide ground-water pH distribution was derived from EPA's STORET data base. The model assumes that the ground water is sufficiently buffered such that pH is not influenced by the input of contaminants from the waste management unit located above or changes in temperature. The default distribution for ground-water pH is an empirical distribution with a median value of 6.8 and lower and upper bounds of 3.2 and 9.7, respectively. The complete distribution is presented in Table 5.6 of the *EPACMTP Parameters/Data Background Document* (U.S. EPA, 2003). Additionally, the EPACMTP model uses the pH of the ground water in the aquifer as the pH of the ground water within the unsaturated zone.

4.4.3.5 Fractional Organic Carbon Content

The organic carbon content, f_{oc}^{s}, is used to determine the linear distribution coefficient, K_d^s. This approach is valid for organic contaminants containing hydrophobic groups. These chemicals will tend to sorb preferentially on non-polar natural organic compounds in the soil or aquifer. Unfortunately, few if any comprehensive subsurface characterizations of organic carbon content exist. In general, the reported values are low, typically less than 0.01. A low range for f_{oc}^{s} was assumed and the distribution shape was based on the distribution of measured dissolved organic carbon recorded as entries to EPA's STORET data base. The default distribution for fractional organic carbon content is a Johnson SB distribution with a mean and standard deviation in arithmetic space of 4.32×10^{-4} and 0.0456, respectively and upper and lower limits of 0.064 and 0.0, respectively. The complete distribution is presented in Table 5.6 of the *EPACMTP Parameters/Data Background Document* (U.S. EPA, 2003). In the case of metals, the sorption is controlled by complex geochemical interactions which are simulated using MINTEQA2 (U.S. EPA, 1996c).

4.4.3.6 Receptor Well Location and Depth

A receptor well is a drinking water well (actual or hypothetical) that is located downgradient of the waste management unit in consideration. It represents the location at which the potential exposure to the ground water is measured. In a typical Monte-Carlo simulation performed with EPACMTP, the primary model output

for each realization is the exposure concentration at a receptor well located downgradient from the waste site. When site-specific data on the receptor well location are not available, the EPA typically uses a default database of downgradient distances to the nearest receptor well obtained from the OSW landfill survey (see the *EPACMTP Parameters/Data Background Document* (U.S. EPA, 2003)). At most waste sites included in this survey, the direction of ambient ground-water flow was not known exactly; therefore, it cannot be ascertained that the nearest receptor well is located directly along the plume centerline (where the highest concentrations would be expected). Therefore, when site-specific data are not available, the modeled well can be positioned a variable x-distance from the downgradient edge of the waste management unit and at a variable y-distance from the plume centerline to reflect uncertainties and variations in the location of the receptor well in relation to the direction of ambient ground-water flow. In the Monte-Carlo model, a realization is associated with a single receptor well. Multiple receptor wells are not allowed.

The EPACMTP model requires that the receptor well location be specified in the x-, y-, and z*-directions as follows:

x_{rw} = distance from the waste unit (m)
y_{rw} = perpendicular distance from the plume centerline (m)
z^*_{rw} = well depth within the saturated zone, measured vertically downward from the water table (m)

A receptor well can be located horizontally 1) anywhere downgradient of the waste management unit (by using default settings for radial distance R_{rw} and angle θ_{rw}, for example), 2) within the areal extent of the contaminant plume, or 3) along the contaminant plume centerline (by setting the angle θ_{rw} to zero, as described below). The vertical position of the receptor well can be anywhere within the saturated zone or restricted to lie within the vertical extent of the contaminant plume; additionally, there are several options within EPACMTP that can be used to specify the well depth. Details of the various well-location options are presented below.

4.4.3.6.1 Horizontal Well Location

EPACMTP incorporates two Well-Location Options for determining the x- and y-coordinates of the receptor well: 1) Well-Location Option 1: specifying the well location as a function of radial distance and angle off the plume centerline or 2) Well-Location Option 2: specifying it directly so that the resulting distribution of locations is varied according to a particular type of distribution between the plume centerline and the areal plume boundary (a uniform distribution is the default type for this option). These two options are further explained below.

<u>Well-Location Option 1</u>

When using Well-Location Option (1) (specifying R_{rw} and θ_{rw}), the user has a choice about how the point along the downgradient edge of the waste unit (from which the radial distance to the well is measured) is determined. This point can either be constrained to always lie at the center of the downgradient edge of the WMU or it can vary along this downgradient edge according to the relationship between the

magnitude of R_{rw} and width of the WMU. That is, in Well-Location Option (1a), the radial distance to the well is always measured from the center of the downgradient edge of the WMU; in Well-Location Option (1b), the radial distance to the well is measured from a randomly varying point somewhere between the upper corner and the center of the downgradient edge of the WMU. These two options for measuring R_{rw} have been included as a means of reducing the bias introduced by large WMUs. When R_{rw} is always measured from the center of the downgradient edge of the WMU, receptor well locations are more likely to lay inside the areal extent of the contaminant plume as the size of the WMU increases, biasing exposure concentrations upward.

Well-Location Option (1a) involves determining the x- and y-coordinates of the receptor well as a function of its radial distance, R_{rw}, from the center of the downgradient edge of the waste unit, and the angle off-center, θ_{rw}. In this case the x- and y-coordinate values must be specified in the data input file as derived variables and are computed as

$$x_{rw} = R_{rw} \cos \theta_{rw} \tag{4.21}$$

$$y_{rw} = R_{rw} \sin \theta_{rw} \tag{4.22}$$

where

x_{rw}	=	distance from the waste unit (m)
R_{rw}	=	radial distance between waste management unit and well measured from the center of the downgradient edge of waste management unit (m)
θ_{rw}	=	angle measured counter-clockwise from the plume centerline (degrees)
y_{rw}	=	perpendicular distance from the plume centerline (m)

The default setting is to consider any well located downgradient of the waste unit; in this case, the angle θ_{rw} is taken to be uniformly distributed between 0 and 90° $(\frac{\pi}{2}\text{radians})$. However, if the user wishes to constrain the receptor well to the plume centerline, the angle θ_{rw} should be set to zero.

In Well-Location Option 1b; the receptor well may be located in one of two zones, as shown in Figure 4.5.

Zone 1 is defined by

$$0 \le x_{rw} \le \infty \tag{4.23a}$$

$$0 \le y_{rw} \le \frac{1}{2} y_D \tag{4.23b}$$

where

x_{rw} = distance from the waste unit (m)
y_D = width of the WMU normal to the flow direction (m)
y_{rw} = perpendicular distance from the plume centerline (m)

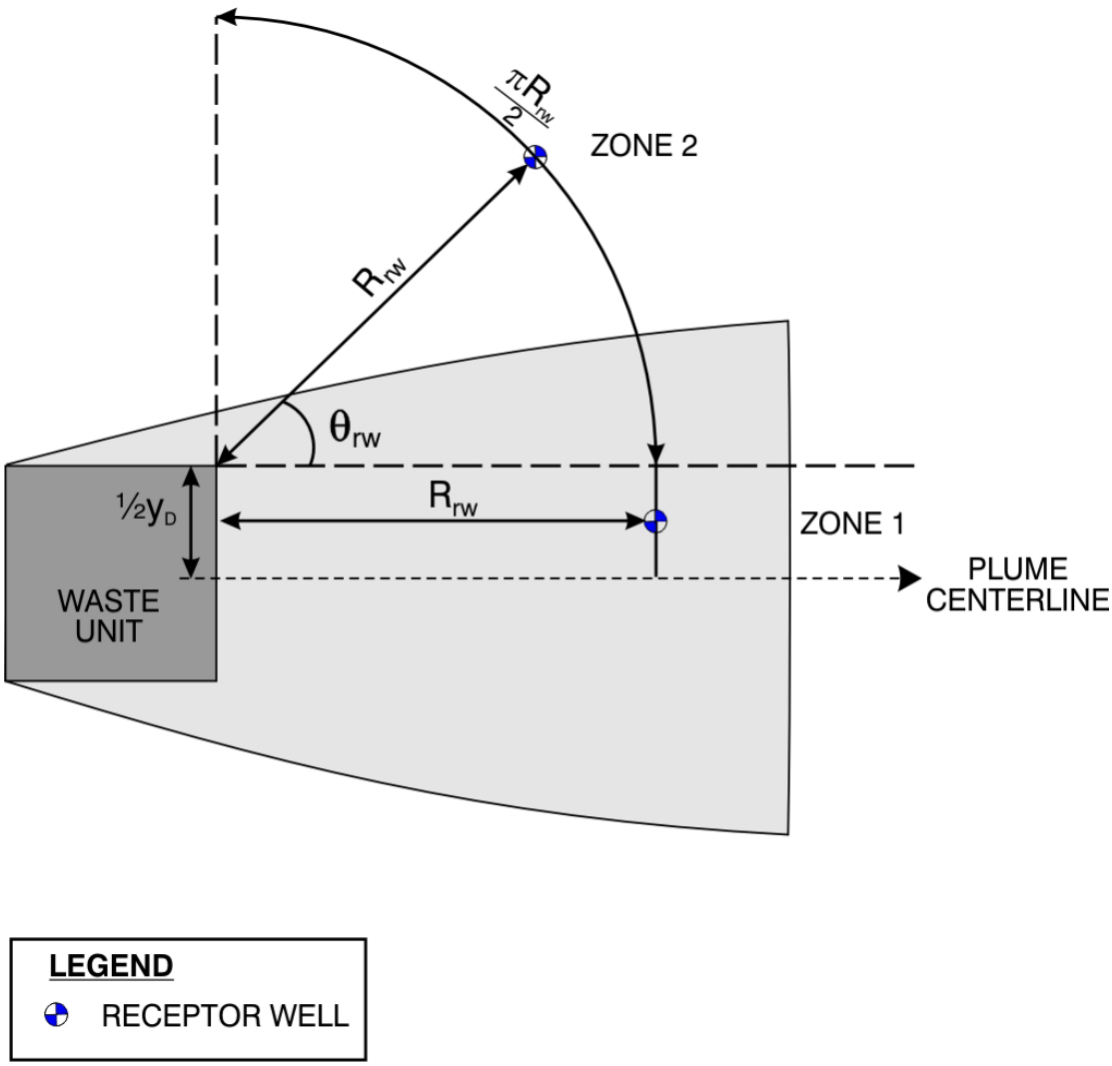

Figure 4.5 Schematic View of the Two Possible Zones for Receptor Well Location.

Zone 2 is defined by

$$0 \leq x_{rw} \leq \infty \tag{4.24a}$$

$$\tfrac{1}{2}\, y_D \leq y_{rw} \leq \infty \tag{4.24b}$$

where

x_{rw} = distance from the waste unit (m)
y_D = width of the WMU normal to the flow direction (m)
y_{rw} = perpendicular distance from the plume centerline (m)

In Zone 1, the well location coordinates (x_{rw}, y_{rw}), measured in the (x, y) coordinates defined above, are given by:

$$x_{rw} = R_{rw} \tag{4.25a}$$

$$y_{rw} = \tfrac{1}{2}\, y_D\, U(0,1) \tag{4.25b}$$

where

x_{rw}	=	distance from the waste unit (m)
R_{rw}	=	radial distance between waste management unit and well (m)
y_{rw}	=	perpendicular distance from the plume centerline (m)
y_D	=	width of the WMU normal to the flow direction (m)
$U(0, 1)$	=	uniform random number varying between 0 and 1 (dimensionless)

Similarly, in Zone 2, the well location coordinates are defined by:

$$\theta_{rw} = \frac{\pi}{2}\, U(0,1) \tag{4.26a}$$

$$x_{rw} = R_{rw} \cos(\theta_{rw}) \tag{4.26b}$$

$$y_{rw} = \tfrac{1}{2}\, y_D + R_{rw} \cdot \sin(\theta_{rw}) \tag{4.26c}$$

where

θ_{rw}	=	angle measured counter-clockwise from the plume centerline (degrees)
$U(0, 1)$	=	uniform random number varying between 0 and 1 (dimensionless)
x_{rw}	=	distance from the waste unit (m)
R_{rw}	=	radial distance between waste management unit and well (m)
y_{rw}	=	perpendicular distance from the plume centerline (m)
y_D	=	width of the WMU normal to the flow direction (m)

Based on the above description, it can be readily seen that:

- In Zone 1, the well is located at the distance of R_{rw}, along the x direction, from the down-gradient edge of the WMU; and
- In Zone 2, the well is located at the radial distance of R_{rw} from a down-gradient corner of the WMU within a quadrant defined by two lines that traverse the corner along (in the x direction) and normal to (in the y direction) the flow direction.

When using Well-Location Option (1b), the probabilities of a receptor well being located in Zones 1 and 2 are: 1 - p_{rw}, and p_{rw}, respectively, where the probability, p_r, is defined as:

$$p_{rw} = \frac{\frac{\pi R_{rw}}{2}}{\frac{1}{2} y_D + \frac{\pi R_{rw}}{2}} \tag{4.27}$$

where

p_{rw}	=	probability that the receptor well will be located in Zone 2 (dimensionless) (see Figure 4.5)
R_{rw}	=	radial distance between waste management unit and well (m)
y_D	=	width of the WMU normal to the flow direction (m)

In addition, when using Well-Location Options (1a) and (1b), the y-coordinate of the well can be optionally constrained to lie within the areal extent of the main contaminant plume as defined by

$$y_{rw} \leq \frac{1}{2} y_D + 3[2\alpha_T(x_w + x_{rw})]^{1/2} \tag{4.28}$$

where

y_{rw}	=	perpendicular distance from the plume centerline (m)
y_D	=	width of the WMU normal to the flow direction (m)
α_T	=	horizontal transverse dispersivity (m)
x_w	=	length of WMU in the x-direction (parallel to ground-water flow) (m)
x_{rw}	=	distance from the waste unit (m)

This approximation for the lateral extent of the contaminant plume is based on the assumption that plume spreading in the horizontal-transverse direction is caused by dispersive mixing, which results in a Gaussian profile as the edge of the plume cross-section. The limit of y_{rw} in Equation (4.28) above implies that at least 99.7% of the contaminant mass will be present inside the transverse plume limit.

When using Well-location Option (2) to determine the receptor well location, the well position is generated directly for each model realization so that at the conclusion of the Monte-Carlo analysis, the resulting distribution of locations is varied according to a particular type of distribution between the plume centerline and the areal plume boundary, for any given x-distance. A uniform distribution is the default type for this option. For Well-location Option (2), an x-distance is typically generated from the empirical distribution presented in Table 6.2 of the *EPACMTP Parameters/Data Background Document* (U.S. EPA, 2003), and the y-coordinate of the well is typically generated from a uniform distribution with a minimum value of zero and a maximum value given by Equation (4.26c).

4.4.3.6.2 Vertical Well Location

In addition to Well-Location Options (1) and (2) which are used to determine the x- and y-coordinates of the receptor well, three well depth options (described below) are available for specifying the vertical position of the well intake point below the water table.

Well-depth Option (1) is the default and is used to specify that the vertical position of the well be uniformly distributed between the water table (z* = 0) and the saturated aquifer thickness. This option is selected by specifying the z*-position as a uniformly distributed relative depth below water table (EPACMTP distribution type code 0; see Table 5.1 and Section 5.4.1) with lower and upper limits of 0.0 and 1.0. EPACMTP will multiply this uniformly generated value by the saturated-zone thickness to yield the actual receptor well depth below the water table for each Monte-Carlo iteration.

In Well-depth Option (2), data on the depth of receptor wells obtained from Agency surveys can be used directly in the model as an empirical distribution (EPACMTP distribution type code 6; see Table 5.1 and Section 5.4.7). The data values range from 15 ft (4.5 m) to 301 ft (90.9 m), and the complete distribution is presented in Table 6.2 of the *EPACMTP Parameters/Data Background Document* (U.S. EPA, 2003). When the generated value for the vertical position of the receptor well intake point is either above the top or below the bottom of the aquifer (physically impossible conditions), a new well position is generated to ensure that the well depth is always located within the aquifer.

In Well-depth Option (3), the receptor well depth can be specified as a constant absolute depth below the water table (that is, not a relative depth as in Well-depth Option (1) above). In this case, one of the special distribution types in EPACMTP – the vertical well position distribution (EPACMTP distribution type code 12; see Table 5.1 and Section 5.4.9.2) – should be used and the well depth below the water table should be entered in meters.

For Well-depth Options (1) and (2) listed above, the vertical position of the observation well can also be optionally constrained to lie within the approximate vertical penetration depth of the contaminant plume emanating from the waste unit, with the z*-coordinate of the receptor well (z^*_{rw}) constrained to lie within the approximate vertical extent of the contaminant plume as defined by:

$$z^*_{rw} \le 2.5 \left\{ \frac{Q_3^F + Q_4^F}{Q_1^F} B + \left[\alpha_v (x_w + x_{rw}) + \alpha_L \left(\frac{Q_3^F + Q_4^F}{Q_1^F} B \right) + \phi_e D^{s*} \right]^{1/2} \right\} = z^*_{rwmax}$$

(4.29)

where

z^*_{rw}	=	z^*-coordinate of the receptor well, positive downward from the water table (m)
Q_1^F - Q_4^F	=	components of fluxes in the ground-water flow field (m^2/y) (see Figure 4.6)
B	=	saturated-zone thickness (m)
α_V	=	vertical dispersivity (m)
x_w	=	length of WMU in the x-direction (parallel to ground-water flow) (m)
x_{rw}	=	distance from the waste unit (m)
α_L	=	longitudinal dispersivity (m)
ϕ_e	=	effective porosity of the aquifer (dimensionless)
D^{s*}	=	effective molecular diffusion coefficient in the aquifer (m^2/y)
$z^*_{rw\,max}$	=	maximum allowable z^*-coordinate of the receptor well; that is, the approximate vertical penetration depth of the contaminant plume (m)

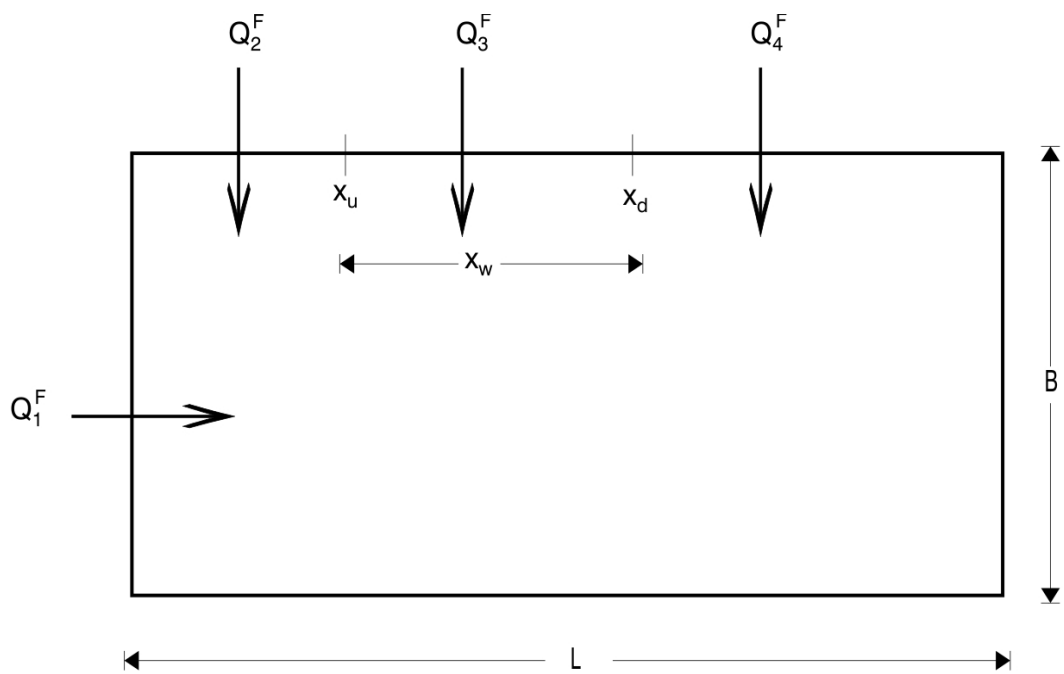

Figure 4.6 Schematic Cross-sectional View of the Aquifer Showing the Contributing Components of the Ground-water Flow Field.

4.4.3.7 Freundlich Isotherm Coefficient

For organic constituents, EPACMTP version 2.0 only allows using a linear Freundlich isotherm to describe the constituent's sorption behavior. In this case, the leading Freundlich coefficient is known as the solid-liquid phase distribution coefficient (K_d). The distribution coefficient may be specified directly or as a derived parameter. In the latter case, it is computed according to the following relationship:

$$K_d^s = k_{oc} f_{oc}^s \tag{4.30}$$

where

K_d^s = solid-liquid phase distribution coefficient (cm^3/g)
k_{oc} = distribution coefficient with respect to organic carbon (cm^3/g)
f_{oc}^s = fractional organic carbon content of the aquifer material (dimensionless)

The above relationship does not apply to simulations of metals transport. For metals that are modeled using MINTEQA2-derived isotherms or pH-dependent empirical isotherms, the K_d data is either read in from an auxiliary input file or internally calculated based on the ground-water pH. In both cases, the Freundlich isotherm coefficient is not used; see Section 4.4.3.9 below. Alternatively, metals can be modeled using an empirical distribution of distribution coefficients (e.g., based on reported K_d values in the scientific literature).

4.4.3.8 Freundlich Isotherm Exponent

For organic constituents, EPACMTP version 2.0 only allows using a linear Freundlich isotherm to describe the constituent's sorption behavior. That is, the Freundlich isotherm exponent (η) must be set equal to 1.0. If this parameter is omitted from the input data file, it is assigned a default value of 1.0, which is equivalent to specifying a linear sorption isotherm.

For metals that are modeled using MINTEQA2-derived isotherms or pH-dependent empirical isotherms, the K_d data is either read in from an auxiliary input file or internally calculated based on the ground-water pH. In both cases, the Freundlich isotherm exponent is not used; see Section 4.4.3.9 below.. Alternatively, metals can be modeled using an empirical distribution of distribution coefficients (e.g., based on reported K_d values in the scientific literature); in this case, the Freundlich isotherm exponent should be set to its default value of 1.0.

4.4.3.9 Sorption Coefficient for Metals

In general, there are three options available within EPACMTP for modeling metals transport: 1) use non-linear isotherms generated by the MINTEQA2 geochemical model, 2) use pH-dependent empirical isotherms, and 3) use an empirical distribution of values for K_d^s. For Options (1) and (2), the Freundlich isotherm coefficient and exponent are not used. However, for metals that are modeled using

an empirical distribution of values for the saturated-zone K_d^s, the Freundlich isotherm exponent should be specified as 1.0.

For Options (1) and (2), the K_d^s is either provided in tabular form as a function of the concentration value or calculated as a function of pH, respectively. For Option (3), the saturated-zone K_d^s should be specified using an empirical distribution (EPACMTP distribution type code 6; see Table 5.1 and Section 5.4.7)) and this distribution should be appended to the end of the input file.

Further details of metals sorption coefficients can be found in Section 3.3.3 of the *EPACMTP Parameters/Data Background Document* (U.S. EPA, 2003).

4.4.3.10 Chemical & Biological Transformation Coefficients

The overall decay coefficient (the sum of the chemical and biological transformation coefficients) can be expressed as a distribution of values or as a constant value. The saturated-zone derivation of the overall decay is calculated in the same manner as that for the unsaturated zone (see Section 3.3.3.7). Although the temperature and pH values are assumed not to vary between the saturated and unsaturated zones, the porosity and bulk density values may differ, leading to a difference in the decay coefficients for the two zones.

4.4.3.11 Molecular Diffusion Coefficient

EPACMTP accounts for molecular diffusion in the saturated zone as part of hydrodynamic dispersion. Further details of molecular diffusion in the saturated-zone hydrodynamic dispersion can be found in Section 4.4.4.1.

4.4.3.12 Molecular Weight

EPACMTP accounts for concentrations of degradation products via stoichiometry. A degradation-product concentration is determined by converting its concentration from moles/L to mg/L using its molecular weight.

4.4.4 Mathematical Formulation of the Saturated-zone Solute Transport Submodule

The governing equation for 3D transport is:

$$\frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial c_\ell}{\partial x_j}\right) - V_i\frac{\partial c_\ell}{\partial x_i} = \phi_e Q_\ell \lambda_\ell^s c_\ell + \phi_e R_\ell^s \frac{\partial c_\ell}{\partial t} - \phi_e \sum_{m=1}^{M} \xi_{\ell m} Q_m \lambda_m^s c_m, \quad \begin{matrix} \ell = 1, n_c \\ i,j = 1,2,3 \end{matrix} \qquad (4.31)$$

where

x_i, x_j = Cartesian coordinates with
- x_1 = x coordinate (m)
- x_2 = y coordinate (m)
- x_3 = z coordinate (m)

i,j = directional indices (dimensionless) (i,j = 1,2,3)
ℓ = component species being evaluated (dimensionless)
n_c = number of component species in the decay chain (dimensionless)
D_{ij} = dispersion coefficient tensor (m^2/y)
c_ℓ = aqueous concentration of the ℓth component species in the decay chain (mg/L)
V_i = Darcy velocity in the ith direction (m/y)
Φ_e = effective porosity of the aquifer (dimensionless)
Q_ℓ = coefficient to incorporate decay of sorbed phase species ℓ (dimensionless)
λ^s_ℓ = first-order decay coefficient for species ℓ (1/y)
R^s_ℓ = saturated-zone retardation factor for species ℓ (dimensionless)
t = time (y)
m = immediate parent of the component species being evaluated (dimensionless)
M = number of parent species (dimensionless)
$\xi_{\ell m}$ = stoichiometric fraction of parent m that degrades into degradation product ℓ (dimensionless)
Q_m = coefficient to incorporate sorbed phase decay of parent m (dimensionless)
λ^s_m= first-order decay coefficient for parent m (1/y)
c_m = concentration of parent m (mg/L)

Parameters, and initial and boundary conditions for Equation (4.31) are described below.

4.4.4.1 Dispersion Coefficients

For computation of the longitudinal, horizontal transverse, and vertical dispersion coefficients (D_{11}, D_{22}; and D_{33} which can be written as D_{xx}, D_{yy}, and D_{zz}), the conventional dispersion tensor for isotropic porous media is modified to allow the use of different horizontal transverse and vertical dispersivities (Burnett and Frind, 1987). The dispersion coefficients are given by:

$$D_{xx} = \alpha_L \frac{V_x^2}{|V|} + \alpha_T \frac{V_y^2}{|V|} + \alpha_V \frac{V_z^2}{|V|} + \phi_e D_\ell^{s*} \tag{4.32a}$$

$$D_{yy} = \alpha_L \frac{V_y^2}{|V|} + \alpha_T \frac{V_x^2}{|V|} + \alpha_V \frac{V_z^2}{|V|} + \phi_e D_\ell^{s*} \tag{4.32b}$$

$$D_{zz} = \alpha_L \frac{V_z^2}{|V|} + \alpha_v \frac{V_y^2}{|V|} + \alpha_V \frac{V_z^2}{|V|} + \phi_e D_\ell^{s*} \tag{4.32c}$$

$$D_{xy} = D_{yx} = (\alpha_L - \alpha_T)\ V_x V_y\ /\ |V| \tag{4.32d}$$

$$D_{xz} = D_{zx} = (\alpha_L - \alpha_v)\ V_x V_z\ /\ |V| \tag{4.32e}$$

$$D_{yz} = D_{zy} = (\alpha_L - \alpha_v)\ V_y V_z\ |iv| \tag{4.32f}$$

$$D_\ell^{s*} = \phi_e^{1/3}\ D_i \tag{4.32g}$$

where

D_{xx}	=	longitudinal dispersion coefficient (m^2/y)
α_L	=	longitudinal dispersivity (m)
V_x	=	longitudinal Darcy velocity (m/y)
$\|V\|$	=	absolute value of the Darcy velocity (m/y)
α_T	=	horizontal transverse dispersivity (m)
V_y	=	horizontal transverse Darcy velocity (m/y)
α_V	=	vertical dispersivity (m)
V_z	=	vertical Darcy velocity (m/y)
ϕ_e	=	effective porosity (dimensionless)
D_ℓ^{s*}	=	effective molecular diffusion for species ℓ (m^2/y)
D_{yy}	=	horizontal transverse dispersion coefficient (m^2/y)
D_{zz}	=	vertical dispersion coefficient (m^2/y)
D_{xy}, D_{yx}	=	off-diagonal dispersion coefficients for the x-y plane (m^2/y)
D_{xz}, D_{zx}	=	off-diagonal dispersion coefficients for the x-z plane (m^2/y)
D_{yz}, D_{zy}	=	off-diagonal dispersion coefficients for the y-z plane (m^2/y)

The effects of molecular diffusion are incorporated into hydrodynamic dispersion using the last terms of Equations (4.32a), (4.32b), and (4.32c). Equation (4.32g) is adapted from Equation (3.15) with water saturation equal to unity.

4.4.4.2 Retardation Factor

The saturated-zone retardation factor for each of the member species (R_ℓ^s) is given by

$$R_\ell^s = 1 + \frac{\rho_b}{\phi_e}\frac{ds_\ell}{dc_\ell} \tag{4.33}$$

where

R_ℓ^s	=	saturated-zone retardation factor for species ℓ (dimensionless)
ρ_b	=	bulk density of the aquifer (g/cm^3)

s_ℓ	=	adsorbed concentration of the ℓth component species (mg/kg)
ϕ_e	=	effective porosity of the aquifer (dimensionless)
c_ℓ	=	aqueous concentration of the ℓth component species (mg/L)

Assuming the adsorption isotherm follows the equilibrium Freundlich equation:

$$s_\ell = k_1 c_\ell^{\eta^s} \tag{4.34}$$

where

s_ℓ	=	adsorbed concentration of the ℓth component species (mg/kg)
k_1^s	=	Freundlich coefficient (dimensionless)
c_ℓ	=	aqueous concentration of the ℓth component species (mg/L)
η^s	=	Freundlich exponent (dimensionless)

Then the retardation factor can be written as:

$$R_\ell^s = 1 + \frac{\rho_b}{\phi_e} k_1^s \eta^s c_\ell^{\eta^s - 1} \tag{4.35}$$

where

R_ℓ^s	=	saturated-zone retardation factor for species ℓ (dimensionless)
ρ_b	=	bulk density of the aquifer (g/cm^3)
ϕ_e	=	effective porosity (dimensionless)
k_1^s	=	Freundlich coefficient (dimensionless)
η^s	=	Freundlich exponent (dimensionless)
c_ℓ	=	aqueous concentration of the ℓth component species (mg/L)

4.4.4.3 Coefficient Q_ℓ

The coefficient Q_ℓ is given by

$$Q_\ell = 1 + \frac{\rho_b}{\phi_e} k_1^s c_\ell^{\eta^s - 1} \tag{4.36}$$

where

Q_ℓ	=	coefficient to incorporate decay of sorbed phase species ℓ (dimensionless)
ρ_b	=	bulk density of the porous media (aquifer material) (g/cm^3)
ϕ_e	=	effective porosity (dimensionless)
k_1^s	=	Freundlich coefficient (dimensionless)
c_ℓ	=	aqueous concentration of the ℓth component species (mg/L)
η^s	=	Freundlich exponent (dimensionless)

In general, the retardation factor is a nonlinear function of concentration. The Freundlich isotherm becomes linear when the exponent $\eta^s = 1.0$. The Freundlich coefficient k_1^s in this case is the same as the familiar solid-liquid phase partition coefficient, K_d^s. When sorption is linear, the coefficients R_ℓ^s and Q_ℓ also become identical.

4.4.4.4 Degradation Products Terms

The summation term on the right-hand side of Equation (4.31) represents the production of species ℓ due to decay (U.S. EPA 1996a) of its immediate parents, c_m, with m varying from 1 to M. The coefficient $\xi_{\ell m}$ is called the stoichiometric fraction which expresses how many units of species ℓ are produced in the decay of each unit of parent m. The value of the stoichiometric fraction is thus determined by the reaction stoichiometry, as well as the units used to express concentration. For instance, consider the following hydrolysis reaction in which 2 moles of degradation product B_{cp} and 1 mole of degradation product C_{cp} are formed from the hydrolysis of 3 moles of parent A_{cp}:

$$3A_{cp} + 2H_2O \rightarrow 2B_{cp}\,(OH)^- + 2H^+ + C_{cp} \tag{4.37}$$

where

A_{cp}	=	parent compound A_{cp}
H_2O	=	water molecule
B_{cp}	=	degradation product B_{cp}
C_{cp}	=	degradation product C_{cp}
$(OH)^-$	=	hydroxide ion
H^+	=	hydrogen ion

In this example, ξ_{BA} is equal to $\frac{2}{3}\frac{MW_B}{MW_A}$ and ξ_{CA} is equal to $\frac{1}{3}\frac{MW_C}{MW_A}$

where

MW_ℓ	=	molecular weight of species ℓ
ξ_{BA}	=	speciation factor between parent A_{cp} and degradation product B_{cp}
ξ_{CA}	=	speciation factor between parent A_{cp} and degradation product C_{cp}

4.4.4.5 Initial Condition

The saturated zone is taken to be initially contaminant free

$$c_\ell(x,\ y,\ z,\ t=0) = 0 \tag{4.38}$$

where

c_ℓ	=	ground-water (aqueous) concentration of the ℓth component species (mg/L)

x	=	x coordinate (m)
y	=	y coordinate (m)
z	=	z coordinate (m)
t	=	time – a value of zero indicates the beginning of the leaching duration (y)

4.4.4.6 Boundary Conditions

Boundary conditions are as follows (see Figure 4.1 for references axes):

(i) Upgradient boundary

$$c_\ell = 0 \qquad \begin{matrix} x = 0 \\ -\tfrac{1}{2}y_L \le y \le \tfrac{1}{2}y_L \\ 0 \le z \le B \end{matrix} \tag{4.39a}$$

(ii) Top boundary

$$c_\ell\,(x,y,B,t) = c_\ell^{\,o}\,(t), \qquad \begin{matrix} x_u \le x \le x_d, \\ -\tfrac{1}{2}y_D \le y \le \tfrac{1}{2}\,y_D \end{matrix} \tag{4.39b}$$

or

$$\left[-D_{zz}\frac{\partial c_\ell}{\partial z} + V_z c_\ell\right]_{z=B} = c_\ell^{\,o}(t)\,I, \qquad \begin{matrix} x_u \le x \le x_d, \\ -\tfrac{1}{2}y_D \le y \le \tfrac{1}{2}\,y_D \end{matrix} \tag{4.39c}$$

The second boundary condition in Equation (4.39c), is more general as it reflects the preservation of mass flux at the water table. Equation (4.39c) is implemented in EPACMTP.

$$\left[-D_{zz}\frac{\partial c_\ell}{\partial z} + V_z c_\ell\right]_{z=B} = 0, \qquad \begin{matrix} x<x_u\ ,\ x>x_d \\ \text{and} \\ y<-\tfrac{1}{2}y_D,\ y>\tfrac{1}{2}y_D \end{matrix} \tag{4.39d}$$

and

(iii) Downgradient boundary

$$\frac{\partial c_\ell}{\partial x} = 0, \quad x = x_L,\ -\tfrac{1}{2}y_L \le y \le \tfrac{1}{2}y_L,\ 0 \le z \le B \tag{4.39e}$$

(iv) Left boundary

$$\frac{\partial c_\ell}{\partial y} = 0, \quad 0 \le x \le x_L\ ,\ y = -\tfrac{1}{2}y_L,\ \ 0 \le z \le B \tag{4.39f}$$

(v) Right boundary

$$\frac{\partial c_\ell}{\partial y} = 0 \ , \quad 0 \le x \le x_L \ , \ y = +\tfrac{1}{2} y_L \ , \ 0 \le z \le B \qquad (4.39g)$$

(vi) Bottom boundary

$$\frac{\partial c_\ell}{\partial z} = 0, \quad 0 < x \le x_L, \ -\tfrac{1}{2} y_L \le y \le \tfrac{1}{2} y_L, \ z = 0 \qquad (4.39h)$$

where

c_ℓ	=	aqueous concentration of the ℓth component species (mg/L)
x	=	x coordinate (m)
y_L	=	length of the aquifer system in the y-direction (m)
B	=	thickness of the aquifer system (m)
t	=	time (y)
c^o_ℓ	=	source concentration (mg/L)
x_u	=	upgradient coordinates of the patch source (m)
x_d	=	downgradient coordinates of the patch source (m)
y_D	=	width of the source in the y-direction (m)
D_{zz}	=	vertical dispersion coefficient (m^2/y)
z	=	z coordinate (m)
V_z	=	vertical ground-water velocity (m/y)
I	=	infiltration rate of water through the source (m/y)
x_L	=	length of the aquifer system in the x-direction (m)
y	=	y coordinate (m)

Equation (4.39a) describes a zero-concentration condition at the upgradient boundary of the model domain. This condition ensures that no contaminant enters the model through this boundary. However, in cases representing high infiltration from the waste source, the ground-water flow direction in the vicinity of the source may be opposite to the regional ground-water flow direction, with outflow rather than inflow across the upgradient boundary. Setting the concentration to be zero in this case means that the boundary acts as a sink, resulting in excessive loss of contaminant mass from the system. Therefore, when the local flow direction at the upgradient boundary is outward from the domain, condition Equation (4.39a) is replaced by a zero concentration gradient condition to minimize the loss of contaminant mass. Boundary conditions Equation (4.39b) and Equation (4.39c) correspond to a prescribed source concentration and prescribed source contaminant mass flux, respectively.

4.4.4.7 Source Concentration

The source concentration, c^o_ℓ, in Equations (4.39b and 4.39c) is generally time-dependent to reflect possible decay or other concentration variations at the source. The source concentration component of the saturated-zone module provides source

concentration directly to the water table. For a multi-species decay chain, the source concentration at time *t* is determined by the Bateman equation:

$$\frac{dc_\ell^{\,o}}{dt} = -\lambda_\ell^s\, c_\ell^{\,o} + \sum_{m=1}^{M} \xi_{\ell m}\lambda_m^s\, c_m^o \tag{4.40a}$$

subject to

$$c_\ell^{\,o}(t=o) = \hat{c}_\ell^{\,o} \tag{4.40b}$$

where

$c_\ell^{\,o}$	=	source concentration of the ℓth component species in the decay chain (mg/L)
t	=	time (y)
λ_ℓ^s	=	first-order decay coefficient for species ℓ (1/y)
m	=	immediate parent of the ℓth component species (dimensionless)
M	=	number of parent species (dimensionless)
$\xi_{\ell m}$	=	stoichiometric fraction, expressing how many units of species ℓ are produced in the decay of each unit of parent *m* (dimensionless)
λ_m^s	=	first-order decay coefficient for parent m (1/y)
c^0_m	=	source concentration of parent species m (mg/L)
$\hat{c}_\ell^{\,o}$	=	initial source concentration of the ℓth component species in the decay chain (mg/L)

For a decay chain having n_c members (with ℓ varying from 1 to n_c), the solution of Equation (4.40a) subject to Equation (4.40b) is obtained most conveniently by applying the Laplace transform (see below) to Equation (4.40a). The Laplace-transformed solution takes the simple form:

$$\bar{c}_\ell^{\,o}(p) = \frac{1}{p+\lambda_\ell^s}\left[\hat{c}_\ell^{\,o} + \sum_{m=1}^{M} \xi_{\ell m}\,\lambda_m^s\,\bar{c}_m^o(p)\right] \tag{4.41}$$

where

$\bar{c}_\ell^{\,0}$	=	Laplace-transformed source concentration of species ℓ (y-mg/L)
p	=	Laplace transform parameter (1/y)
λ_ℓ^s	=	first-order decay coefficient for species ℓ (1/y)
$\hat{c}_\ell^{\,o}$	=	initial source concentration of the ℓth species in the decay chain (mg/L)

m	=	immediate parent of the ℓth component species (dimensionless)
M	=	number of parent species (dimensionless)
$\xi_{\ell m}$	=	stoichiometric fraction, expressing how many units of species ℓ are produced in the decay of each unit of parent m (dimensionless)
λ_m^s	=	first-order decay coefficient for parent m (1/y)
$\bar{c}_m^0$	=	Laplace-transformed concentration of parent species m (y-mg/L)

The desired concentration $c_\ell^o(t)$ is subsequently obtained by numerically inverting Equation (4.41) using the de Hoog algorithm (de Hoog et al., 1982).

4.4.4.8 Treatment of Nonlinear Isotherms

Although EPACMTP can be run using nonlinear adsorption in both the unsaturated and saturated zones in the deterministic case (in other words, for a single set of hydrogeological parameters), the computer processing time required for a Monte-Carlo analysis that includes nonlinear adsorption in both zones is prohibitive. For that reason, a technique was developed that calculates a single value of K_d^s from a nonlinear isotherm. This "linearized" single K_d^s value can then be used as a linear partition coefficient in the model, which decreases computer processing time dramatically (from tens of hours to a few seconds per realization). Obviously, when the original nonlinear isotherm from which the linear K_d^s is calculated is almost linear to begin with, the impact of reducing it to a linear K_d^s is small. Conversely, the error associated with using a linear approximation is increased for highly nonlinear isotherms. The linearization in EPACMTP is such that errors are minimized or conservative results are obtained.

In EPACMTP, two methods are provided for approximating a linear isotherm from a nonlinear isotherm. In the first method, a concentration-interval weighted approach is used to compute a single K_d^s from the nonlinear K_d^s versus dissolved (aqueous) concentration curve. In effect, the technique simply calculates an average K_d^s over the range of dissolved metal concentrations represented by the isotherm. Concentration-interval weighting is used to account for the fact that the dissolved concentration values are not evenly spaced on the isotherm. This method is an option for the EPACMTP model in the unsaturated zone. In the second method (that EPACMTP uses in the saturated zone), the K_d^s corresponding to the peak water table metal concentration is used for linear partitioning. The procedure involves the following steps: First, a saturated-zone isotherm is specified by Monte-Carlo selection of values for the five geochemical master variables. Then, the peak dissolved metal concentration at the water table is determined, and the K_d^s corresponding to this dissolved concentration is obtained from the isotherm by searching for the minimum K_d^s on the isotherm between the minimum concentration and the peek dissolved metal concentration at the water table. This search is conducted to ensure that conservative results are always obtained, even though the isotherm is monotonically increasing with dissolved metal concentration.

4.4.5 Solution Methods for the Solute Transport Submodule

As stated in Section 4.1, three simulation options are available in EPACMTP for modeling ground-water fate and transport in the saturated zone. The saturated-zone transport submodule of EPACMTP contains numerical and analytical solution options for: (i) three-dimensional transport; (ii) numerical solutions for quasi three-dimensional and two-dimensional areal solute transport; and (iii) a hybrid numerical-analytical solution for pseudo-three-dimensional transport.

The three options above are ranked in descending order for accuracy and in ascending order for computational efforts required. In general, the third option (the pseudo three-dimensional solution) is preferred due to its acceptable accuracy (see verification results in Appendix D) and relatively low computational efforts required. It is several times faster than the first two solution options.

4.4.5.1 <u>Aquifer Discretization and Solution Method Selection</u>

For most model applications, no matter what solution method is used for saturated-zone transport, it will be convenient to use the option to automatically discretize the model domain; this option generates the computational grid without requiring detailed user input on node numbers and element sizes. The procedure involves two main steps. The first involves determination of the overall dimensions, that is, length, width, and height of the aquifer region to be modeled. The second step involves generating a computational grid representing the model domain.

4.4.5.1.1 Determination of Model Domain Dimensions

The model domain is determined based upon the length and width of the contaminant source, location(s) of receptor well(s), and the aquifer saturated thickness. The length of the model domain is determined to be sufficiently long that the source itself and any receptor wells are included. In addition, the boundaries are placed far enough upgradient of the source, and downgradient of the farthest receptor well, to minimize boundary effects in the flow field and simulated contaminant plume. Particular care is given to the distance between the upgradient model boundary and the source. It is desirable to place this boundary far enough away from the source to be outside the influence of a ground-water mound resulting from the locally higher infiltration through the source area. This involves determining the location of the stagnation point along the x-axis upgradient of the source, that is, the point at which the hydraulic head gradient vanishes. An analytical flow solution (see Appendix C) for areal recharge in a finite domain is used to evaluate the head gradient. The Newton-Raphson method is used to locate the x-coordinate at which the gradient becomes zero. The upgradient boundary in the model domain is then placed at a distance equal to three times the upgradient distance of the stagnation point, away from the source.

The factor of three is an empirically chosen safety factor to ensure that the boundary location is well away from the region of influence of the source. To ensure that the upgradient boundary is not located either too far from the source which might lead to an excessively large computational grid, or too close to the source, the distance, x_s,

(see Figure 4.7) between the upgradient domain boundary and the upgradient edge of the source is always constrained to fall within the following upper and lower bounds:

$$x_s^{max} \geq x_s \geq 0.5\, x_s^{max} \tag{4.42a}$$

$$x_s^{max} = \min(20\alpha_L, 2x_w) \tag{4.42b}$$

where

x_s^{max}	=	maximum allowable distance between the upgradient domain boundary and the upgradient edge of the source (m)
x_s	=	distance between the upgradient domain boundary and the upgradient edge of the source (m)
α_L	=	longitudinal dispersivity (m)
x_w	=	length of the source in the x-direction (m) (see Figure 4.7)

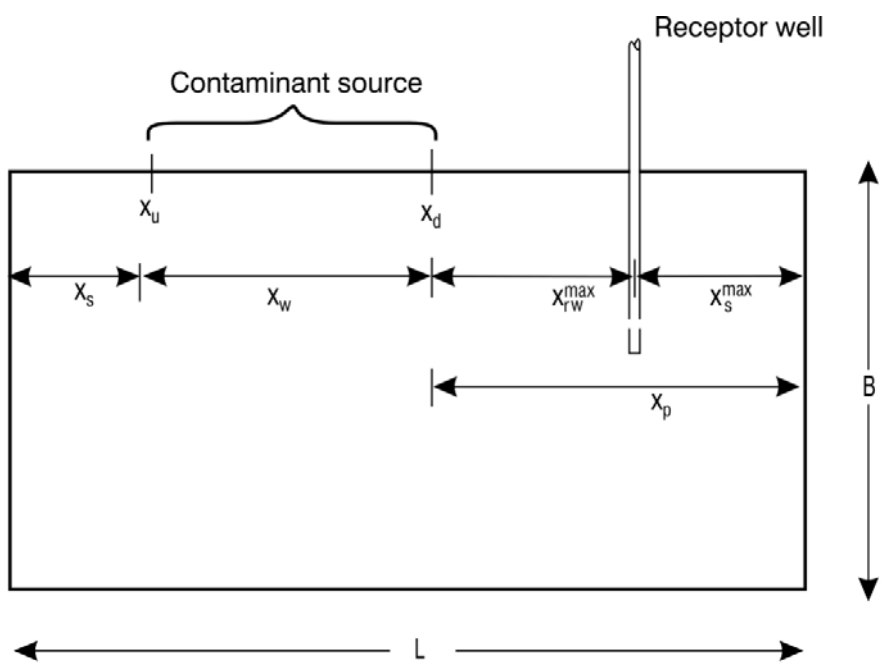

Figure 4.7 Schematic Cross-sectional View of the Aquifer, Illustrating the Procedure for Determining the X-Dimension of the Model Domain.

The parameter x_s^{max} is determined as a function of the longitudinal dispersivity (α_L) to reflect the dependence of nodal spacings in the computational grid on the Peclet number ($\Delta s/\alpha_L$, where Δs is the grid dimension (m), and α_L the longitudinal dispersivity (m)). Small dispersivity values will lead to a closer spacing of nodal

points. In this case, Equation (4.42b) will have the effect of reducing the length of the domain upgradient of the source to ensure that the number of elements required to discretize this portion of the domain does not become too large. The opposite is true when the dispersivity is large, in which case a greater distance to the upgradient boundary is allowed since the code will use a coarser grid.

The length of the model domain downgradient of the source, x_p, is determined from the position of the receptor well located farthest away from the source, as

$$x_p = x_{rw}^{max} + x_s^{max} \tag{4.43}$$

where

x_p	=	length of the model domain downgradient of the source (m)
x_{rw}^{max}	=	farthest horizontal distance between the receptor well and the downgradient edge of the source area (m)
x_s^{max}	=	maximum allowable distance between the upgradient domain boundary and the upgradient edge of the source (m)

The overall length of the model domain in the x-direction is thus equal to

$$L = x_s + x_w + x_p \tag{4.44}$$

where

L	=	overall length of the model domain in the x-direction (m)
x_s	=	distance between the upgradient domain boundary and the upgradient edge of the source (m)
x_w	=	length of the source in the x-direction (m) (see Figure 4.7)
x_p	=	length of the model domain downgradient of the source (m)

The dimension of the domain in the y-direction is determined as

$$y_L = \max(y_{rw}^{max}, y_{plume}) \tag{4.45a}$$

where

y_L	=	length of the model domain in the y-direction (m)
y_{rw}^{max}	=	farthest horizontal distance between the receptor well and the plume centerline (m)
y^{plume}	=	transverse extent of the plume (m)

And the transverse extent of the plume is approximated by

$$y_{plume} = \tfrac{1}{2}\, y_D + 3\sqrt{2\,\alpha_T(x_{rw}^{max} + x_w)} \tag{4.45b}$$

where

y^{plume}	=	transverse extent of the plume (m)
y_D	=	source width (m)
α_T	=	horizontal transverse dispersivity (m)
x_{rw}^{max}	=	farthest horizontal distance between the receptor well and the downgradient edge of the source area (m)
x_w	=	length of the source in the x-direction (m) (see Figure 4.7)

The last term on the right-hand side of Equation (4.45b) represents the transverse plume spreading due to dispersive mixing.

The dimension of the model domain in the y-direction, y_L, is determined based on the assumption that the infiltration rate is small relative to the lateral ambient ground-water flux. However, in the event that the infiltration rate is large, the model results will be conservative. In this case, the width of the model domain will be underestimated and the predicted ground-water velocity will be overestimated, thereby causing the modeled contaminants to arrive at receptors sooner and with greater peak concentrations (due to less dilution and less degradation).

The vertical dimension of the model domain is equal to the saturated aquifer thickness, B, except in cases involving very thick saturated zones and shallow contaminant plumes. In these cases, only the upper portion of the saturated zone is actually included in the model domain, based on the approximate vertical extent of the contaminant plume. The vertical extent of the model domain below the water table is determined using Equation (4.71) (see Section 4.4.5.3.3), with the adjustment factor, δ_{ad}, set equal to 7.5. A relatively large value for δ_{ad} is used to minimize boundary influence on the modeling results. The final vertical dimension of the model domain is taken to be the lesser of the value obtained using Equation (4.71) (see Section 4.4.5.3.3) and the physical thickness of the saturated zone.

4.4.5.1.2 Discretization of Model Domain

Following determination of the model dimensions, the domain is discretized. Since simple hexagonal (brick) elements are used, the discretization step involves determining the spacings of the grid lines, which is done sequentially for the x-, y-, and z-directions. The nodal spacings are smallest near the source and increase with distance away from the source. The magnitude of nodal spacing, Δs, is controlled by the dispersivity with

$$2.5\alpha_L \le \Delta s \le 7.5\alpha_L \tag{4.46}$$

where

α_L	=	longitudinal dispersivity (m)
Δs	=	magnitude of nodal spacing (m)

This results in grid Peclet numbers varying between 2.5 and 7.5.

The transport equation can be solved numerically using spatial discretization schemes based on either 7-point or 27-point nodal connectivity. The 7-point scheme is equivalent to a typical finite difference method, while the 27-point scheme is usually encountered in finite element schemes. The 7-point finite difference scheme leads to a reduced matrix bandwidth and thus less memory requirements, as well as reduced computational effort during the matrix assembly stage. The option to use either a 7-point finite difference or a 27-point finite element spatial discretization is selected by the user. The use of the 7-point scheme results in an approximately four-fold savings in CPU time and matrix storage requirements as compared to the 27-point scheme. Since the loss in accuracy in the solution is relatively small, in many cases, this is an attractive option to use.

4.4.5.1.3 Solution Method Selection

The applicability and appropriateness of using each of the transport solution options (fully 3D, quasi-3D a combination of (cross-sectional and areal solutions), pseudo-3D (hybrid analytical and numerical solution), and analytical solution options) depends on the problem considered.

Using the quasi three-dimensional option instead of the fully three-dimensional option, will result in a greater savings of CPU time and memory requirements. For Monte-Carlo uses of the code, as in the composite EPACMTP model, the appropriate 2D areal or cross-sectional solution can be selected automatically using the criterion discussed in Section 4.4.5.3.3. The pseudo-3D solution is the most computationally efficient of the four solutions available.

Use of the analytical solution is restricted to situations when the criteria for using the analytical solution are satisfied, that is, single species transport with regional ground-water flow only in the horizontal direction. In this case, the influences of infiltration and recharge are negligibly small. Moreover, use of the analytical solution is attractive only when the number of observation points (n_{obs}) and observation times (n_t) is relatively small, that is, $n_{obs} \times n_t \leq 20$. When these conditions are satisfied, the analytical solution is much faster than the numerical one.

A practical criterion for determining whether the assumption of one-dimensional regional ground-water flow is satisfied is given by the ratio of infiltration and recharge flux to the regional, longitudinal ground-water flux. Shown in Figure 4.7 is a schematic vertical cross-section of an aquifer system, identifying the various contributing components of the ground-water flow field. Q_1^F represents the "background" ground-water flux. Q_2^F and Q_4^F are recharge fluxes and Q_3^F is the infiltration flux through the source. Each of these components is obtained by multiplying the Darcy flow rate by the length of the appropriate boundary segment, that is, Q_3^F is the infiltration rate times the length of the source. Next, Q_r^F is defined as the ratio

$$Q_r^F = \frac{Q_2^F \frac{x_u}{L} + Q_3^F \frac{x_d - x_u}{L} + Q_4^F \frac{L - x_d}{L}}{Q_1^F} \tag{4.47}$$

where

Q_r^F	=	ratio of the background ground-water flux to that near the source (dimensionless)
Q_2^F	=	recharge flux upgradient of the source (m^2/y)
x_u	=	upgradient coordinates of the source (m)
L	=	overall length of the model domain in the x-direction (m)
x_d	=	downgradient coordinates of the source (m)
Q_3^F	=	infiltration flux through the source (m^2/y)
Q_4^F	=	recharge flux downgradient of the source (m^2/y)
Q_1^F	=	background ground-water flux (m^2/y)

Shown in Figure 4.8 is the difference between the results of the analytical and numerical solutions in a randomly located downgradient well as a function of Q_r^F. In this figure, the difference is calculated as the relative concentration difference, $(c_{analytical}-c_{numerical})/C_0$, where C_0 is the source concentration. This figure was obtained by performing a hundred simulations with both the analytical and numerical solutions. In these simulations, the well location, source and aquifer parameters were varied randomly according to probability distributions for Subtitle D surface impoundments. The figure clearly illustrates that as the value of Q_r^F decreases (as the ground-water flow field becomes one-dimensional), the analytical and numerical solutions converge. For most practical purposes, a value of $Q_r^F = 0.02$ is a good upper limit for using the analytical solution. The upper limit for Q_r^F, Q_{max}^F, is a user-specified variable. For every problem, the code evaluates Q_r^F using Equation (4.47). If this value is less than the specified Q_{max}^F, the analytical transport solution is used, otherwise, the numerical solution is used.

4.4.5.2 Three-dimensional Transport Solutions

4.4.5.2.1 Laplace Transform Galerkin Solution

For time-dependent simulations with linear adsorption ($\eta^s = 1.0$, see Equation (4.35)), the governing Equation (4.31) with initial and boundary conditions Equation (4.36) through Equation (4.40) is solved using the Laplace Transform Galerkin (LTG) technique. The method is described in detail by Sudicky (1989), and only the most important steps are given here. The Laplace transform, $\bar{f}(p)$, of a function $f(t)$ is defined as

$$\mathcal{L}[f(t)] = \bar{f}(p) = \int_0^\infty f(t) \exp(-pt)\, dt \tag{4.48}$$

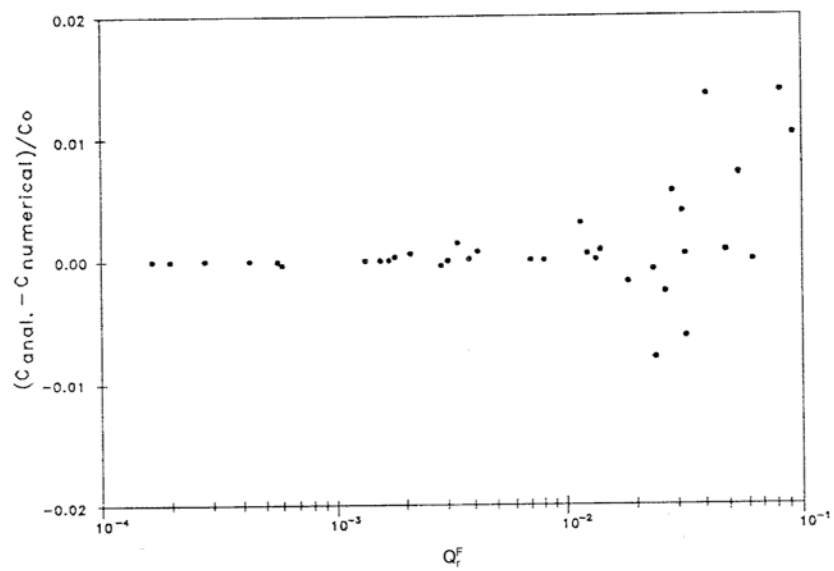

Figure 4.8 Difference ($C_{analytical}$ -$C_{numerical}$)/c_0 Between Analytical and Numerical Transport Solutions as a Function of Q_r^F (ratio of regional flux to near-source flux). C_0 Is the Source Concentration.

where

$\mathcal{L}(\cdot)$	=	Laplace transform operator (dimensionless)
$f(p)$	=	Laplace transformed function (original dimension · y)
p	=	Laplace transform variable (1/y)
t	=	time (y)

Application of the Laplace transformation to the governing transport equation leads to

$$\frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial \bar{c}_\ell}{\partial x_j}\right) - V_i\frac{\partial \bar{c}_\ell}{\partial x_i} = \phi_e Q_\ell \lambda^s_\ell \bar{c}_\ell + \phi_e R^s_\ell p \bar{c}_\ell - \phi_e \sum_{m=1}^{M} \xi_m \lambda^s_m Q_m \bar{c}_m \quad (4.49)$$

where

i,j	=	directional indices for x, y, and z (dimensionless)
x_i	=	spatial coordinate in the ith direction (m)
x_j	=	spatial coordinate in the jth direction (m)
		x_1 = x coordinate (m)
		x_2 = y coordinate (m)
		x_3 = z coordinate (m)
D_{ij}	=	dispersion coefficient tensor (m^2/y)
$\bar{c}_\ell$	=	$\bar{c}_\ell(x, y, z, p)$, Laplace-transformed concentration of species ℓ (y-mg/L)
V_i	=	Darcy velocity in the ith direction (m/y)

Φ_e = effective porosity of the aquifer (dimensionless)
Q_ℓ = coefficient to incorporate sorbed phase decay of species ℓ (dimensionless)
λ^s_ℓ = first-order decay coefficient for species ℓ (1/y)
R^s_ℓ = saturated-zone retardation factor for species ℓ (dimensionless)
p = Laplace transform variable (1/y)
m = immediate parent of the ℓth component species (dimensionless)
M = number of parent species (dimensionless)
ξ_m = stoichiometric fraction, expressing how many units of species ℓ are produced in the decay of each unit of parent m (dimensionless)
λ^s_m = first-order decay coefficient for parent m (1/y)
Q_m = coefficient to incorporate sorbed phase decay of parent m (dimensionless)
$\bar{c}_m$ = Laplace-transformed concentration of parent species m (y-mg/L)

Equation (4.49) together with the transformed boundary conditions is solved employing either 7-point finite difference or 27-point finite element spatial discretization schemes. In both cases, a rectangular, three-dimensional grid is employed. This grid is the same as that used for the steady-state ground-water flow solution. It yields a final matrix equation of the form

$$([P] + p[S])\,\{\bar{c}\} - \{\bar{b}\} = 0 \tag{4.50}$$

where

$[P]$ = advective-dispersive transport matrix, including the decay term λ
$[S]$ = Laplace-transformed mass matrix
p = Laplace transform variable (1/y)
$\{\bar{c}\}$ = Laplace-transformed concentration vector
$\{\bar{b}\}$ = a vector containing the known transformed natural boundary conditions, as well as contributions from decaying parents

The species index, ℓ, has been dropped to simplify the notation.

The solution of Equation (4.50) is obtained using the iterative ORTHOMIN matrix solver also employed for the ground-water flow solution. This solution yields the transformed concentration $\bar{c}(x,y,z,p)$. The last step in the solution process is inversion of the transformed concentration. The inverse Laplace transformation is carried out numerically using the de Hoog algorithm (de Hoog et al., 1982). The concentration at node j of the finite element grid, $c_j(t)$, is found from $\bar{c}_j$ using the Fourier series approximation

$$c_j(t) = \frac{1}{T}\exp(p^o t)\left[\frac{1}{2}\,\bar{c}_j(p^o) + \sum_{k=0}\left(Re\{\bar{c}_j(p_k)\}\cos(k\pi t/T) - Im\{\bar{c}_j(p_k)\}\sin(k\pi t/T)\right)\right] + E \tag{4.51}$$

where

$c_j(t)$	=	concentration at node *j* of the finite element grid at time *t* (mg/L)
T	=	one-half of the fundamental period of the Fourier series approximating the inverse function on the interval [0, *2T*] (y)
p^o	=	real constant for the inversion of Laplace transform (1/y)
t	=	time (y)
$\bar{c}_j$	=	Laplace-transformed concentration (y-mg/L)
N	=	number of terms in the series (dimensionless)
k	=	index of the series (dimensionless)
Re	=	real part of the complex $\bar{c}_j$ values (y-mg/L)
p_k	=	k^{th} term of the parameter in the Laplace inversion series (1/y)
Im	=	imaginary part of the complex $\bar{c}_j$ values (y-mg/L)
E	=	error term arising because the Fourier coefficients are approximations obtained from $\bar{c}_j$ rather than $c_j(t)$ and because the series is truncated after 2*N* terms (mg/L)

The parameter p^o is evaluated as:

$$p^o = \frac{-\ln E}{1.6\ t_{max}} \tag{4.52}$$

where

p^o	=	real constant for the inversion of Laplace transform (1/y)
E	=	error term arising because the Fourier coefficients are approximations obtained from $\bar{c}_j$ rather than $c_j(t)$ and because the series is truncated after 2*N* terms (mg/L)
t_{max}	=	maximum simulation time (y)

The *k* discrete values of the Laplace variable p_k are related to the parameter p^o according to the relationship

$$p_k = p^o + \frac{k\pi i}{T} \tag{4.53}$$

where

p_k	=	k^{th} term of the parameter in the Laplace inversion series (1/y)
p^o	=	real constant for the inversion of Laplace transform (1/y)
k	=	index of the series (dimensionless)
i	=	an imaginary number equal to $\sqrt{-1}$
T	=	one-half of the fundamental period of the Fourier series approximating the inverse function on the interval [0, *2T*] (y)

The truncation error in Equation (4.51) is reduced, and, therefore, convergence is accelerated by applying a quotient difference acceleration scheme algorithm (MacDonald, 1964).

Application of the Laplace transform method requires that the boundary conditions be transformed along with the transport equation itself (Equation (4.31)). In the case of a constant source concentration, $c^o_\ell(t) = C^o_\ell$, the transformed boundary condition is simply

$$\bar{c}^o_\ell(p) = \frac{1}{p} C^o_\ell \tag{4.54}$$

where

$\bar{c}^o_\ell(p)$	=	Laplace transform of the source function (y-mg/L)
p	=	Laplace transform variable (1/y)
C^o_ℓ	=	constant source concentration (mg/L)

When the source concentration is described by the Bateman equation (Equation (4.40a)), the transformed boundary condition is given by Equation (4.41). EPACMTP furthermore allows the source concentration $c^o_\ell(t)$ to vary as an arbitrary function of time. To make this case amenable to solution by the Laplace transform method, the source function $c^o_\ell(t)$ is approximated as a sequence of Heaviside step functions. Dropping the species subscript ℓ to simplify the notation, this can be expressed as

$$c^o(t) \simeq \sum_{i=1}^{N_s} C^o_{iave} [H_v(t - t_i^{on}) - H_v(t - t_i^{off})] \tag{4.55}$$

where

$c^0(t)$	=	source concentration at time t (mg/L)
i	=	step index (dimensionless)
N_s	=	number of steps into which $c^o(t)$ is discretized (dimensionless)
C^0_{iave}	=	average concentration value during the time interval $[t_i^{on}, t_i^{off}]$ (mg/L)
H_v	=	Heaviside step function (dimensionless) (see Equation 4.56)
t	=	time (y)
t_i^{on}	=	beginning of the time interval of step i (y)
t_i^{off}	=	end of the time interval of step i (y)
exp(·)	=	exponential operator (dimensionless)

The Heaviside step function is defined as

$$H_v(t - t_i^{on}) = \begin{cases} 0, & t < t_i^{on} \\ 1, & t \geq t_i^{on} \end{cases}, \tag{4.56}$$

where

H_v	=	Heaviside step function (dimensionless)
t	=	time (y)
t_i^{on}	=	beginning of the time interval of step *i* (y)

The Laplace transform of the source function, $\bar{c}^o(p)$, then becomes

$$\bar{c}^o(p) = \frac{1}{p} \sum_{i=1}^{N_s} C_{iave}^o \left[\exp(-pt_i^{on}) - \exp(-pt_i^{off})\right] \tag{4.57}$$

where

$\bar{c}_\ell^o(p)$	=	Laplace transform of the source function (y-mg/L)
p	=	Laplace transform variable (1/y)
i	=	step index
N_s	=	number of steps into which $c^o(t)$ is discretized (dimensionless)
C_{iave}^o	=	average concentration during time interval $[t_i^{on}, t_i]$ (mg/L)
t_i^{on}	=	beginning of the time interval of interest (y)
t_i^{off}	=	end of the time interval of interest (y)

The LTG solution scheme offers additional advantages when it is desired to compute ground-water concentration values that represent temporal averages rather than instantaneous values. For instance, for risk assessment purposes, exposure is often defined as the average concentration over a specified exposure period, that is,

$$C_A = \frac{1}{t_2 - t_1} \int_0^{t_2} c(x,y,z,t)\,dt. \tag{4.58}$$

where

C_A	=	average ground-water concentration over a specified exposure period (mg/L)
t_1	=	beginning of the time interval of interest (y)
t_2	=	end of the time interval of interest (y)
$c(x,y,z,t)$	=	concentration at x,y,z at time t (mg/L)
t	=	time (y)

Noting the Laplace transform property

$$\mathcal{L}\left[\int_0^t f(t)\,dt\right] = \frac{1}{p}\bar{f}(p), \tag{4.59}$$

where

$\mathcal{L}(\cdot)$	=	Laplace transformation operator (dimensionless)
t	=	time (y)
p	=	Laplace transform variable (1/y)
$\bar{f}(p)$	=	Laplace–transformed function (original unit · y)

the desired time-averaged concentration can be conveniently obtained as

$$C_A = \frac{1}{t_2 - t_1}\left[\int_0^{t_2} c(x,y,z,t)\,dt - \int_0^{t_1} c(x,y,z,t)\,dt\right] \tag{4.60}$$

$$= \frac{1}{t_2 - t_1}\left\{\mathcal{L}^{-1}\left[\frac{1}{p}\bar{c}(x,y,z,p)\right]_{t_2} - \mathcal{L}^{-1}\left[\frac{1}{p}\bar{c}(x,y,z,p)\right]_{t_1}\right\} \tag{4.61}$$

where

C_A	=	average ground-water concentration over a specified exposure period (mg/L)
t_2	=	end of the time interval of interest (y)
t_1	=	beginning of the time interval of interest (y)
$c(x,y,z,t)$	=	concentration at x,y,z at time t (mg/L)
x	=	x coordinate (m)
y	=	y coordinate (m)
z	=	z coordinate (m)
t	=	time (y)
$\mathcal{L}(\cdot)$	=	Laplace transformation operator (dimensionless)
p	=	Laplace transform variable (1/y)
$\bar{c}(x,y,z,t)$	=	Laplace-transformed concentration at x, y, z at time t (y-mg/L)

4.4.5.2.2 Solution for Steady-state and Nonlinear Transport

A major advantage of the LTG method for linear transport problems compared with conventional time marching numerical approaches is that in order to obtain the solution for any arbitrary time value, the governing equation (Equation (4.49)) needs to be solved only 2*N*+1 times where *N* is typically 5 or 7. When the solution is required for multiple time values, only the inversion of the Laplace transformed solution needs to be repeated. This advantage disappears when only the steady-state solution is desired. In this situation the solution, using conventional time discretization, can be obtained in a single step by setting the time derivative to zero, whereas the LTG method still requires 2*N*+1 steps. Moreover, the LTG method cannot be used for problems with nonlinear adsorption isotherms. For this purpose, EPACMTP contains a separate standard Galerkin finite element numerical solution (Huyakorn and Pinder, 1983) for the steady-state or nonlinear transient transport equation. Compared to the Laplace Transform method, standard numerical transport solution schemes are more susceptible to oscillatory behavior in the

computed concentration profiles when the grid Peclet number $\Delta s/\alpha_L$, where Δs is the grid dimension, increases. Upgradient weighting (Huyakorn and Nilkuha, 1979) is therefore used to reduce numerical oscillations in the predicted concentrations. In the case of nonlinear sorption, a central difference time stepping solution is used with Picard iteration (Huyakorn and Pinder, 1983) to resolve the non-linearity.

4.4.5.2.3 Analytical Solution

In situations where the vertical and transverse components of ground-water flow are negligibly small, and sorption is linear, the ground-water transport problem may be solved analytically. The analytical solution is reserved for single component simulations. The species subscript will therefore be omitted in the remainder of this section. When ground-water flow is in the longitudinal direction only, and considering only the half of the system along the positive y-axis, the governing three-dimensional transport equation can be written as

$$D_{xx}\frac{\partial^2 c}{\partial x^2} + D_{yy}\frac{\partial^2 c}{\partial y^2} + D_{zz}\frac{\partial^2 c}{\partial z^2} - V_x\frac{\partial c}{\partial x} +$$

$$M_s\ [\{H_v(x-x_u) - H_v(x-x_d)\}\ \{H_v(y+y_0) - H_v(y-y_0)\}\ \delta(z-B)\ ] = \phi_e R^s\left(\frac{\partial c}{\partial t} + \lambda^s c\right) \tag{4.62}$$

where

D_{xx}	=	longitudinal dispersion coefficient (m^2/y)
c	=	contaminant concentration in the aqueous phase (mg/L)
x	=	x coordinate (m)
D_{yy}	=	horizontal transverse dispersion coefficient (m^2/y)
y	=	y coordinate (m)
D_{zz}	=	vertical transverse dispersion coefficient (m2/y)
z	=	z coordinate (m)
V_x	=	Darcy velocity in the x-direction (m/y)
M_s	=	contaminant mass flux ($mg/m^2 \cdot y$) which is applied over the rectangular area given by $x_u \le x \le x_d$ and $0 \le y \le y_0$
$H_v(\bullet)$	=	Heaviside step function (dimensionless)
x_u	=	upgradient coordinates of the source (m)
x_d	=	downgradient coordinates of the source (m)
y_0	=	one-half the source width (Y_D) (m)
$\delta(\bullet)$	=	Dirac Delta function (dimensionless)
B	=	aquifer thickness (m)
ϕ_e	=	effective porosity (dimensionless)
R^s	=	retardation factor for the saturated zone (dimensionless)
t	=	time (y)
λ^s	=	first-order decay constant (1/y)

Equation (4.62) is solved analytically for a zero concentration initial condition

$$c\ (x,y,z,0) = 0 \tag{4.63a}$$

where

c(x, y, z, 0) = concentration at x, y, z at time 0 (mg/L)

and boundary conditions

$$\frac{\partial c}{\partial x} = 0 \qquad y = \pm\infty \tag{4.63b}$$

$$\frac{\partial c}{\partial y} = 0 \qquad y = 0,\ y = \infty \tag{4.63c}$$

$$\frac{\partial c}{\partial z} = 0 \qquad z = 0,\ z = B \tag{4.63d}$$

where

c	=	contaminant concentration in the aqueous phase (mg/L)
x	=	x coordinate (m)
y	=	y coordinate (m)
z	=	z coordinate (m)
B	=	aquifer thickness (m)

Since flow in the saturated zone is taken to be in the longitudinal direction only, the components of the dispersion tensor now become

$$D_{xx} = \alpha_L V_x + \phi_e D_\ell^{s*} \tag{4.64a}$$

$$D_{yy} = \alpha_T V_x + \phi_e D_\ell^{s*} \tag{4.64b}$$

$$D_{zz} = \alpha_v V_x + \phi_e D_\ell^{s*} \tag{4.64c}$$

where

D_{xx}	=	longitudinal dispersion coefficient (m^2/y)
α_L	=	longitudinal dispersivity (m)
V_x	=	longitudinal ground-water velocity (m/y)
ϕ_e	=	effective porosity (dimensionless)

D_ℓ^{s*}	=	effective molecular diffusion coefficient for species ℓ (m^2/y)
D_{yy}	=	horizontal transverse dispersion coefficient (m^2/y)
α_T	=	horizontal transverse dispersivity (m)
D_{zz}	=	vertical transverse dispersion coefficient (m^2/y)
α_V	=	vertical transverse dispersivity (m)

The solution of Equations (4.62 through 4.64) is given by

$$c(x,y,z,t) = \frac{M_s}{4R^s} \sum_{q=0}^{\infty} G_q \int_0^t \exp\left(\frac{-\psi_q^2 D_{zz}}{R^s} - \lambda^s\right) \tau_t \bullet$$

(4.65a)

$$\left\{-\,erfc\left[(x_d - x)\left(\frac{R^s}{4D_{xx}\tau_t}\right)^{1/2} + V_x\left(\frac{\tau_t}{4D_{xx}R^s}\right)^{1/2}\right] + erfc\left[(x_u - x)\left(\frac{\tau_t}{4D_{xx}\tau_t}\right)^{1/2} + V_x\left(\frac{\tau_t}{4D_{xx}R^s}\right)^{1/2}\right]\right\}$$

$$\cdot \left\{erfc\left[(y - y_0)\left(\frac{R^s}{4D_{yy}\tau_t}\right)^{1/2}\right] - erfc\left[(y + y_0)\left(\frac{R^s}{4D_{yy}\tau_t}\right)^{1/2}\right]\right\} d\tau_t$$

with

$$\psi_q = \pi q/B \qquad q = 0,\ 1,\ \ldots \tag{4.65b}$$

$$G_q = \begin{cases} 1/B & q = 0 \\ \dfrac{2\cos(\psi_q z)}{B} & q = 1,\ 2,\ \ldots \end{cases} \tag{4.65c}$$

where

$c(x,y,z,t)$	=	concentration at x, y, z at time t (mg/L)
M_s	=	contaminant mass flux ($mg/m^2 \cdot y$) which is applied over the rectangular area given by $x_u \le x \le x_d$ and $0 \le y \le y_0$
R^s	=	retardation factor for the saturated zone (dimensionless)
q	=	index of the series (dimensionless)
G_q	=	m^{th} coefficient described by Equation (4.65c) (1/m)
ψ_q	=	constant described by Equation (4.65b) (1/m)
D_{zz}	=	vertical transverse dispersion coefficient (m^2/y)
R^s	=	retardation factor (dimensionless)
λ^s	=	first-order decay coefficient (1/y)
τ_t	=	time integration variable (y)

x_d	=	downgradient coordinates of the source (m)
x	=	x coordinate (m)
D_{xx}	=	longitudinal dispersion coefficient (m^2/y)
V_x	=	longitudinal ground-water velocity (m/y)
x_u	=	upgradient coordinates of the source (m)
y	=	y coordinate (m)
y_0	=	half-source width (m)
	=	one-half the source width (Y_D) (m)
D_{yy}	=	horizontal transverse dispersion coefficient (m^2/y)
B	=	saturated thickness of the aquifer (m)
q	=	index of terms in the summation (dimensionless)
z	=	z coordinate (m)

The solution presented in Equation (4.65a) is a transient solution. The analytical steady-state solution is obtained by using a large *t* value in Equation (4.65a).

4.4.5.3 Two-dimensional Transport Solutions

Consistent with the 2D cross-sectional and 2D areal ground-water flow options of the model (see Section 4.3.5.2), the transport module includes options to ignore horizontal transverse advection and vertical advection, respectively.

4.4.5.3.1 Two-dimensional Cross-sectional Transport Solution

For the case in which 2D cross-sectional flow is considered, EPACMTP contains a corresponding transport solution which does not consider advection in the horizontal transverse (y-direction). The solution, however, does take into account dispersion in the y-direction, thus yielding a quasi three-dimensional contaminant transport approximation. The governing transport Equation (4.31) is rigorously solved in the two-dimensional, cross-sectional (x-z) plane, using either the Laplace transform or standard Galerkin numerical schemes. The same one grid block-wide grid employed for the two-dimensional, cross-sectional ground-water flow equation is used. Since the transverse ground-water flow rate, V_y, obtained from the flow solution is zero and the grid spans exactly the half source width, a two-dimensional transport solution is obtained. To account for dispersion in the y-direction, the analytical method of Domenico and Robbins (1985) is used. The computation of horizontal transverse dispersion from a point in the x-z plane (x_c, 0, z_c) involves the use of the travel time t' which is defined as the time required for a particle of water to travel a distance d_c from a point at the water table underneath the patch source to the downgradient location x_c. The distance d_c is defined as

$$d_c = \max(0,\ x_c - x_u) \tag{4.66a}$$

$$t' = \frac{d_c}{\bar{V}_x} \tag{4.66b}$$

where

d_c = distance from a point at the water table underneath the patch source to the downgradient location x_c (m)
x_c = downgradient location at which dispersion is calculated (m)
x_u = upgradient location underneath the patch source (m)
t' = travel time from x_u to x_c (y)
$\overline{V_x}$ = average longitudinal ground-water velocity (m/y)

The governing equation for one-dimensional dispersive transport in the horizontal transverse direction is

$$D_{yy} \frac{\partial^2 c_\ell}{\partial y^2} = R_\ell^s \frac{\partial c_\ell}{\partial t'} \tag{4.67}$$

where

D_{yy} = horizontal transverse dispersion coefficient (m^2/y)
c_ℓ = aqueous concentration of the species ℓ (mg/L)
y = y coordinate (m)
R_ℓ^s = retardation factor for the saturated zone of the species ℓ (dimensionless)
t' = travel time from x_u to x_c (y)

with the initial condition

$$c_\ell(y, t = 0) = 0 \tag{4.68a}$$

where

$c_\ell(y, t = 0)$ = initial aqueous concentration of the species ℓ at y at the beginning of the leaching duration (t = 0) (mg/L)

and boundary conditions

$$c_\ell(y, t) \,|_{x,z} = c_\ell(x, z, t) \quad 0 \le y \le y_o \tag{4.68b}$$

$$\frac{\partial c_\ell}{\partial y} = 0 \qquad y \to \infty \tag{4.68c}$$

where

$c_\ell(y, t = 0)$ = aqueous concentration of the species ℓ at y at the beginning of the leaching duration (t = 0) (mg/L)
x = x coordinate (m)
z = z coordinate (m)

$c_\ell(x, z, t)$	=	aqueous concentration of the species ℓ at x, z at time *t* (mg/L)
y	=	y coordinate (m)
y_o	=	one-half the source width (y_o) (m)
c_ℓ	=	aqueous concentration of the species ℓ (mg/L)

The one-dimensional transverse and two-dimensional cross-sectional transport solutions are coupled through the boundary condition presented in Equation (4.68b). The transverse dispersion coefficient D_{yy} is given by

$$D_{yy} = \alpha_T \bar{V}_x + \phi_e D_\ell^{s*} \tag{4.69}$$

where

D_{yy}	=	horizontal transverse dispersion coefficient (m^2/y)
α_T	=	horizontal transverse dispersivity (m)
$\bar{V}_x$	=	average longitudinal ground-water velocity (m/y)
Φ_e	=	effective porosity (dimensionless)
D_ℓ^{s*}	=	effective molecular diffusion coefficient of species ℓ (m^2/y)

The final three-dimensional solution is obtained by multiplication of the two-dimensional and one-dimensional solutions

$$c_\ell(x,y,z,t) = c_\ell(x,z,t)\frac{1}{2}\left[erfc\left\{\frac{y-y_o}{2\left(\frac{D_{yy}t'}{R_\ell^s}\right)^{1/2}}\right\} - erfc\left\{\frac{y+y_o}{2\left(\frac{D_{yy}t'}{R_\ell^s}\right)^{1/2}}\right\}\right] \tag{4.70}$$

where

$c_\ell(x, y, z, t)$	=	aqueous concentration of the species ℓ at x, y, z at time *t* (mg/L)
$c_\ell(x, z, t)$	=	aqueous concentration of the species ℓ at x, z at time *t* on a vertical plane with y = o (mg/L)
x	=	x coordinate (m)
y	=	y coordinate (m)
z	=	z coordinate (m)
y_o	=	one-half the source width (y_D) (m)
D_{yy}	=	horizontal transverse dispersion coefficient (m^2/y)
t'	=	travel time from x_u to x_c (y)
R_ℓ^s	=	retardation factor for the saturated zone of the species ℓ (dimensionless)

The contaminant decay constant λ_ℓ does not appear explicitly in Equation (4.70). The effects of degradation are implicitly accounted for through the linking term, $c_\ell(x, z, t)$, with the two-dimensional solution.

4.4.5.3.2 Two-dimensional Areal Transport Solution

For the case in which ground-water flow in the vertical direction is ignored, the module contains a two-dimensional areal transport solution. This solution yields a vertically averaged concentration distribution, representing the case in which the contaminant plume occupies the entire saturated aquifer thickness with complete vertical mixing. This solution employs the 2D areal grid used in the two-dimensional areal flow solution. This grid is one grid block deep with a thickness equal to the saturated aquifer thickness. The source mass flux is apportioned equally to the upper and lower plane of the grid, with each receiving one-half of the total mass flux. This ensures a correct mass balance and yields a vertically averaged solution.

4.4.5.3.3 Criterion for selecting Two-dimensional Solutions

As mentioned before, it is expected that the 2D cross-sectional flow and transport solutions will be most accurate in situations involving a large waste facility overlying a deep saturated zone, while the 2D areal approximation is expected to be most accurate in cases with a thin saturated zone. For Monte-Carlo applications of the model, the 2D approximations will result in substantial savings of computational effort as compared to the fully 3D solution. In order to implement these options for Monte-Carlo applications, a suitable criterion for selecting either a 2D vertical or a 2D areal solution is required.

The criterion for automatic switching between the cross-sectional and areal solutions is based on the penetration depth of the contaminant plume in the quasi-3D saturated zone. If the plume has reached the base of the saturated zone when it reaches the nearest observation well, the areal solution is used. In other cases, the cross-sectional approximation is used. The approximation for the plume depth, B', takes into account both advective and dispersive movement of the contaminant, and takes the form
where

B' = estimated plume depth (m)
δ_{ad} = empirical adjustment factor (dimensionless)

$$B' = \delta_{ad} \left\{ \frac{Q_3^F + Q_4^F}{Q_1^F} B + \left[\alpha_v (x_w + x_{rw}) + \alpha_L \left(\frac{Q_3^F + Q_4^F}{Q_1^F} B \right) \right]^{1/2} \right\} \quad (4.71)$$

Q_1^F = background ground-water flux (m^2/y)
Q_3^F = infiltration flux through the source (m^2/y)
Q_4^F = recharge flux downgradient of the source (m^2/y)
α_v = transverse vertical dispersivity (m)
x_w = length of the source along the flow direction (m)

x_{rw} = horizontal distance between the source and receptor well (m)
α_L = longitudinal dispersivity (m)
B = saturated thickness of the aquifer (m)

Each of the Q^F terms is obtained by multiplying the areal flux by the length of the corresponding boundary segment; for example, Q_1^F equals the ambient ground-water flow rate times the saturated aquifer thickness. The first term in the right-hand side of Equation (4.71) includes the ratio of vertical to horizontal ground-water flow components. It approximates the extent of vertical plume movement due to advection. The second term in Equation (4.71) describes the downward plume movement due to dispersive action. The adjustment factor, δ_{ad}, is introduced to account for the approximate nature of Equation (4.71). Its value is determined such that differences between the fully 3D and quasi-3D transport solutions are minimized. A value of δ_{ad} = 0.65 was determined by evaluating 1,000 randomly generated aquifer realizations, and comparing the differences in predicted plume concentration values at a randomly located receptor well between the fully 3D and quasi-3D solutions, as a function of δ_{ad}. The simulation was conducted using the Monte-Carlo procedure implemented in the composite EPACMTP code and representative landfill parameter distributions.

The approximation for the vertical plume extent is useful also to determine whether an observation well lies within the plume at all, or lies underneath the plume and samples only pristine ground water. The latter case would obviate the need to perform the transport simulation at all. In this case, a conservative approach to determining whether a receptor well lies outside of the plume is adopted. This is achieved by setting the adjustment factor in Equation (4.71) to δ_{ad} = 2.5. This value was determined also by simulating 1,000 randomly generated aquifer realizations. By using a value of δ_{ad} = 2.5, virtually all cases with a non-zero receptor well concentration were accounted for. Out of 1,000 random realizations, the highest normalized observation well concentration value that was missed was 5 x 10^{-6} mg/L. This value is smaller than the numerical accuracy of the transport solution.

4.4.5.4 Pseudo-3D Transport Solution

Assuming that equilibrium exists between the solid and aqueous phases and that the dimension in the y direction is infinite, the transport in the saturated zone may be described as :

$$\frac{\partial}{\partial t} c_\ell [\phi_e + (1-\phi_e)\rho_s \frac{\partial s_\ell}{\partial c_\ell}] + \frac{\partial}{\partial x_i}[V_i c_\ell - D_{ij}\frac{\partial c_\ell}{\partial x_i}] + \lambda_\ell^s [c_\ell \phi_e + (1-\phi_e)\rho_s s_\ell] - \sum_{m=1}^{M} \lambda_m^s [c_m \phi_e + (1-\phi_e)\rho_s s_m] \xi_{\ell m} = 0 \qquad (4.72)$$

i, j = 1, 2, 3.

where

t	=	time (y)
c_ℓ	=	concentration of species ℓ in the aqueous phase (mg/L)
ϕ_e	=	effective porosity (dimensionless)
ρ_s	=	density of the solid phase (g/cm^3)
s_ℓ	=	concentration of species ℓ in the solid (adsorbed) phase (mg/kg)
x_i	=	Cartesian coordinates in the ith direction (the 1st, 2nd, and 3rd directions correspond to the x, y, and z directions, respectively) (m)
V_i	=	ground-water velocity in the ith direction (aqueous phase) (m/y)
D_{ij}	=	dispersion coefficient tensor (aqueous phase) (m^2/y)
x_j	=	Cartesian coordinates in the jth direction (the 1st, 2nd, and 3rd directions correspond to the x, y, and z directions, respectively) (m)
λ_ℓ^s	=	degradation constant for the ℓth species (1/y)
m	=	immediate parent of the component species being evaluated (dimensionless)
M	=	total number of parent chemicals (dimensionless)
λ_m^s	=	degradation constant for parent m (1/y)
c_m	=	concentration of parent species m in the aqueous phase (mg/L)
s_m	=	concentration of parent species m in the solid (adsorbed) phase (mg/kg)
$\xi_{\ell m}$	=	constant related to decay reaction stoichiometry of the mth parent chemical and the ℓth chemical which is a degradation product of the mth parent chemical (dimensionless)

<u>Boundary and Initial Conditions</u>

The saturated zone is taken to be initially contaminant free, that is,

$$c_\ell\ (x,\ y,\ z,\ 0) = 0 \tag{4.73}$$

where

c_ℓ (x, y, z, 0) = initial concentration of species ℓ at x, y, z (mg/L)

Boundary conditions are as follows:

(i) <u>Upgradient boundary</u>

$$c_\ell = 0 \qquad \begin{array}{c} x = 0 \\ -\infty \le y \le +\infty \\ 0 \le z \le B \end{array} \tag{4.74a}$$

(ii) <u>Top boundary</u>

$$c_\ell\ (x,y,B,t) = c_\ell^{\,o}\ (t), \qquad x_u \le x \le x_d, \quad -\frac{y_D}{2} \le y \le \frac{y_D}{2} \tag{4.74b}$$

or

$$[-D_{zz}\frac{\partial c_\ell}{\partial z} + V_z c_\ell]_{z=B} = c_\ell^{\,o}\ (t)\ I, \qquad x_u \le x \le x_d, \quad -\frac{y_D}{2} \le y \le \frac{y_D}{2} \tag{4.74c}$$

and

$$[-D_{zz}\frac{\partial c_\ell}{\partial z} + V_z c_\ell]_{z=B} = 0, \qquad x < x_u\ ,\ x > x_d,\ or\ y < -\frac{y_D}{2}\ ,\ y > \frac{y_D}{2} \tag{4.74d}$$

(iii) <u>Downgradient boundary</u>

$$\frac{\partial c_\ell}{\partial x} = 0, \quad x = x_L,\ -\infty \le y \le +\infty,\ 0 \le z \le B \tag{4.74e}$$

(iv) <u>Left and right boundaries</u>

$$c_\ell \to 0, \quad 0 \le x \le x_L\ ,\ y \to \pm\infty, \quad 0 \le z \le B \tag{4.74f}$$

or, alternatively,

$$\frac{\partial c_\ell}{\partial y} \to 0\ ,\ 0 \le x \le x_L\ ,\ y \to \pm\infty, \quad 0 \le z \le B \tag{4.74g}$$

(v) Bottom boundary

$$\frac{\partial c_\ell}{\partial z} = 0, \quad 0 < x \le x_L, \; -\infty \le y \le +\infty, \; z = 0 \tag{4.74h}$$

where

c_ℓ = aqueous concentration of species ℓ (mg/L)
x = x coordinate (m)
y = y coordinate (m)
z = z coordinate (m)
B = aquifer thickness (m)
c_ℓ^o = source concentration for species ℓ (mg/L)
x_u = upgradient coordinate of the source (m)
x_d = downgradient coordinate of the source (m)
y_D = source dimension in the y direction (m)
D_{zz} = vertical transverse dispersion coefficient (m^2/y)
V_z = vertical ground-water velocity (m/y)
I = infiltration rate through the source (see Figure 4.1) (m/y)
x_L = downgradient coordinate of the transport domain (m)

The boundary condition in Equation (4.74d) indicates the finiteness of the source in the y direction, and the boundary conditions in Equations (4.74b and 4.74c) correspond to a prescribed source concentration and prescribed source contaminant mass flux, respectively.

In order to obtain a computationally efficient solution for Equation (4.72), the following assumptions are adopted:

- Ground-water velocity in the x direction is uniform.
- Ground-water flow in the lateral and vertical directions is negligible compared with the flow along the x direction.
- Contaminant mass entering the saturated zone at the water table within the source area is instantaneously transported to a vertical plane that is coplanar with the downgradient boundary of the strip source. All the fluid particles entering the water table at the same time are assumed to arrive simultaneously at the vertical plane.
- The source may be represented by an equivalent source on the plane described in the previous assumption. The dimension of the source on this plane is such that the mass conservation principle is not violated.

Utilizing the first and second assumptions, Equation (4.72) becomes

$$\phi_e R_\ell^s \frac{\partial c_\ell}{\partial t} + \overline{V}_x \frac{\partial c_\ell}{\partial x} - D_{xx}\frac{\partial^2 c_\ell}{\partial x^2} - D_{yy}\frac{\partial^2 c_\ell}{\partial y^2} - D_{zz}\frac{\partial^2 c_\ell}{\partial z^2}$$

$$+ \lambda_\ell^s c_\ell \phi_e Q_\ell - \sum_{m=1}^{M} \lambda_m^s c_m \phi_e Q_m \xi_{\ell m} = 0 \qquad (4.75)$$

where

$$R_\ell^s = 1 + \frac{(1-\phi_e)\ \rho_s}{\phi_e}\frac{\partial s_\ell}{\partial c_\ell} \qquad (4.76)$$

$$Q_\ell = 1 + \frac{(1-\phi_e)\ \rho_s}{\phi_e}\frac{s_\ell}{c_\ell} \qquad (4.77)$$

and

$$\overline{q}_x = \frac{\int_{x_d}^{x} -K_x \frac{\partial H}{\partial x} dx}{x - x_d}, \quad x > x_d \qquad (4.78)$$

where

ϕ_e	=	effective porosity (dimensionless)
R_ℓ^s	=	retardation factor of species ℓ (dimensionless)
c_ℓ	=	aqueous concentration of species ℓ (mg/L)
t	=	time (y)
$\overline{V}_x$	=	average Darcy velocity in the x direction between the downgradient edge of the source and the point of interest along the x direction (m/y)
x	=	x coordinate (m)
D_{xx}	=	longitudinal dispersion coefficient (m^2/y)
D_{yy}	=	horizontal transverse dispersion coefficient (m^2/y)
y	=	y coordinate (m)
D_{zz}	=	vertical dispersion coefficient (m^2/y)
z	=	z coordinate (m)
λ_ℓ^s	=	degradation constant for the ℓth species (1/y)
Q_ℓ	=	coefficient to incorporate sorbed phase decay of species ℓ (dimensionless)

m	=	immediate parent of the component species being evaluated (dimensionless)
M	=	total number of parent chemicals (dimensionless)
λ_m^s	=	degradation constant for parent m (1/y)
c_m	=	concentration of parent species m in the aqueous phase (mg/L)
Q_m	=	coefficient to incorporate sorbed phase decay of species m (dimensionless)
$\xi_{\ell m}$	=	constant related to decay reaction stoichiometry of the mth parent chemical and the ℓth chemical which is a degradation product of the mth parent chemical (dimensionless)
ρ_s	=	density of the solid phase (g/cm^3)
s_ℓ	=	concentration of species ℓ in the solid (adsorbed) phase (mg/kg)
$\bar{q}_x$	=	average Darcy velocity in the x direction between the downgradient edge of the source and the point of interest along the x direction (m/y)
K_x	=	hydraulic conductivity in the x direction (m/y)
H	=	hydraulic head (m)
x_d	=	downgradient coordinate of the source (m)

According to the third and fourth assumptions, the vertical plane that is coplanar with the downgradient edge of the source area is defined by:

$$x = x_d; \quad -\infty \le y \le +\infty; \quad 0 \le z \le B \tag{4.79}$$

where

x	=	x coordinate (m)
x_d	=	downgradient coordinate of the source (m)
y	=	y coordinate (m)
z	=	z coordinate (m)
B	=	aquifer thickness (m)

The dimension of the source on this plane is defined by the following conditions:

$$c_\ell(x_d, y, z, t) = c_\ell^o(t) \tag{4.80}$$

$$-\frac{1}{2}y_S \le y \le \frac{1}{2}y_S \tag{4.81}$$

$$B - z_S - D_R \le z \le B - D_R \tag{4.82}$$

where

$c_\ell\ (x_d, y, z, t)$	=	aqueous concentration of species ℓ at x_d, y, z at time t (mg/L)
c_ℓ^o	=	source concentration for species ℓ (mg/L)
t	=	time (y)
y_S	=	width of the source on the source plane in the y direction (m)
y	=	y coordinate (m)
B	=	aquifer thickness (m)
z_S	=	width of the source on the source plane in the z direction (m)
D_R	=	average penetration depth due to recharge between the downgradient edge of the source and the observation point (m)
z	=	z coordinate (m)

Outside the source area on the source plane, the source concentration is absent.

The average penetration depth due to recharge may be determined from:

$$D_R = \int_{x_d}^{x_d + \frac{x - x_d}{2}} \frac{I_r}{\bar{q}_x} dx \tag{4.83}$$

where

D_R	=	average penetration depth due to recharge between the downgradient edge of the source and the observation point (m)
x_d	=	downgradient coordinate of the source (m)
x	=	x coordinate (m)
I_r	=	recharge rate outside the source area (m/y)
$\bar{q}_x$	=	average Darcy velocity in the x direction between the downgradient edge of the source and the point of interest along the x direction (m/y)

The average penetration depth is used to replace the boundary condition between the downgradient edge of the source and the point of interest (typically the location of an observation well; presented as Equation (4.74c)). It represents the influx of recharge and the average vertical displacement of the bulk of the plume between the source plane and the point of interest.

As a first approximation, the width of the source on the vertical source plane, y_S, is determined as the width resulting from a particle advected from the most upgradient location ($x_u \le x \le \max(x_{crest}, x_d)$ (see Equation (4.84)) along the side of the source (where $y = ½\ y_D$) to the vertical plane at $x = x_d$. The particle is advected within the horizontal plane using a two-dimensional flow field described by a two-dimensional

analytical solution presented in Appendix C. The source half width is assumed to be equal to the distance from $y = 0$ to the point where the advected particle transverses the vertical plane at $x = x_d$. The source half width is not allowed to be smaller than $\frac{1}{2}y_D$. The vertical source dimension is approximated by the following expression (U.S. EPA, 1990):

$$z_S = \sqrt{2\alpha_V f(x_d - x_u)} + B\left[1 - \exp\left(\frac{-f(x_d - x_u)I}{B\overline{q_x}}\right)\right] \tag{4.84}$$

where

z_S	=	width of the source on the source plane in the z direction (m)
α_v	=	vertical transverse dispersivity (m)
f	=	fraction of the source that migrates downgradient in the event that a water table crest occurs within the source area (dimensionless)
x_d	=	downgradient coordinate of the source (m)
x_u	=	upgradient coordinate of the source (m)
B	=	aquifer thickness (m)
I	=	areal infiltration rate (m/y)
$\bar{q}_x$	=	average Darcy velocity in the x direction between the downgradient edge of the source and the point of interest along the x direction (m/y)

The first term on the right hand side of Equation (4.84) accounts for potential mixing due to transverse dispersion in the vertical direction, while the second term accounts for vertical displacement due to infiltration in the source area.

In Equation (4.84), the fraction, f, indicates the fraction of the source that migrates downgradient in the event that a water table crest occurs within the source area. The water table crest within the source area occurs when the hydraulic gradient in that area vanishes. The location of the water table crest is determined by differentiating Equation (4.84) with respect to x and equating the resulting derivative to zero, so that:

$$x_{crest} = \frac{K_x B}{I}\left[\frac{I_r - I}{2K_x B}\left(\frac{x_d^2 - x_u^2}{x_L}\right) - \frac{I_r - I}{K_x B}x_d + \frac{I_r}{2K_x B}x_L + \frac{H_2 - H_1}{x_L}\right] \tag{4.85}$$

where

x_{crest}	=	x-coordinate of the crest of the water table (m)
K_x	=	longitudinal hydraulic conductivity along the flow direction (m/y)
B	=	aquifer thickness (m)
I	=	infiltration rate (m/y)

I_r	=	recharge rate (m/y)
x_d	=	downgradient coordinate of the source (m)
x_u	=	upgradient coordinate of the source (m)
x_L	=	x-coordinate at the downgradient end of the domain (m)
H_2	=	hydraulic head at the downgradient end of the domain (m)
H_1	=	hydraulic head at the upgradient end of the domain (m)

The fraction of the source, *f*, is then determined from the following expression:

$$f = \frac{x_d - x_{crest}}{x_d - x_u} \tag{4.86}$$

where

f	=	fraction of the source that migrates downgradient in the event that a water table crest occurs within the source area (dimensionless)
x_d	=	downgradient coordinate of the source (m)
x_{crest}	=	x-coordinate of the crest of the water table (m)
x_u	=	upgradient coordinate of the source (m)

One can readily see that if *f* is negative, the crest occurs at $x > x_d$ from the source area and all the contaminant mass migrates towards the origin of the x-axis. Similarly, if *f* is greater than unity, the crest occurs at $x < x_u$, and all the contaminant mass migrates downgradient. In the event that *f* is negative, the solution is trivial, and the contaminant concentration at each observation well location is set to zero. In the determination of the source dimension, the fraction *f* is limited to the following range:

$$0 \le f \le 1 \tag{4.87}$$

where

f	=	fraction of the source that migrates downgradient in the event that a water table crest occurs within the source area (dimensionless)

In the event that *f* is greater than unity, the source will not be partitioned, and *f* is set to unity in Equation (4.87) as well as in the procedure shown below. The release location of the advected particle is also determined by the location of the water table crest. If $x_u \le x_{crest} \le x_d$, the release location is (x_{crest}, $\frac{1}{2}y_D$). If $x_{crest} < x_u$, the release location is (x_u, $\frac{1}{2}y_D$).

To account for source partitioning, the boundary condition described by Equation (4.80) must be adjusted to reflect the change in source location and dimension. Letting $c_k^s(t)$ represent the adjusted boundary condition, the following statement results from the principle of mass conservation:

$$c_k^o(t)\, I f x_w y_D = c_k^S(t)\, \overline{V_x}\, z_S y_S \tag{4.88}$$

where

$c_k^o(t)$	=	aqueous concentration of species $_k$ within the source (mg/L)
I	=	infiltration rate (m/y)
f	=	fraction of the source that migrates downgradient in the event that a water table crest occurs within the source area (dimensionless)
x_w	=	length of the source along the flow direction ($x_w = x_d - x_u$) (m)
y_D	=	source dimension in the y direction (m)
$c_k^s(t)$	=	equivalent aqueous concentration of species $_k$ on the vertical plane at the downgradient edge of the source (mg/L)
$\overline{V}_x$	=	average Darcy velocity in the x direction between the downgradient edge of the source and the point of interest along the x direction (m/y)
z_s	=	equivalent source dimension in the vertical direction on the vertical plane at the downgradient edge of the waste management unit (m)
y_s	=	equivalent source dimension in the direction normal to the regional flow direction on the vertical plane at the downgradient edge of the waste (m)

Rearranging Equation (4.88), we get a concentration ratio, F_c, which can be applied to the contaminant concentration within the waste management unit:

$$\frac{c_k^S(t)}{c_k^o(t)} = \frac{I f x_w y_D}{\overline{V_x}\, z_S y_S} = F_c \tag{4.89}$$

where

$c_k^s(t)$	=	equivalent aqueous concentration of species $_k$ on the vertical plane at the downgradient edge of the source (mg/L)
$c_k^o(t)$	=	aqueous concentration of species $_k$ within the source (mg/L)
I	=	infiltration rate (m/y)
f	=	fraction of the source that migrates downgradient in the event that a water table crest occurs within the source area (dimensionless)
x_w	=	length of the source along the flow direction ($x_w = x_d - x_u$) (m)
y_D	=	source dimension in the y direction (m)
$\overline{V}_x$	=	average Darcy velocity in the x direction between the downgradient edge of the source and the point of interest along the x direction (m/y)
z_s	=	equivalent source dimension in the vertical direction on the vertical plane at the downgradient edge of the waste management unit (m)
y_s	=	equivalent source dimension in the direction normal to the regional flow direction on the vertical plane at the downgradient edge of the waste (m)
F_c	=	concentration ratio (dimensionless)

If the source dimension in the vertical direction, determined using Equation (4.85), is such that $z_S + D_R > B$, then the vertical source dimension is set to

$$z_S^{new} = B - D_R \tag{4.90}$$

where

z_S^{new}	=	vertical source dimension on the vertical source plane, adjusted to account for the presence of recharge depth D_R (m)
B	=	aquifer thickness (m)
D_R	=	average penetration depth due to recharge between the downgradient edge of the source and the observation point (m)

and the horizontal source dimension is set to

$$y_S^{new} = \frac{y_S z_S}{z_S^{new}} \tag{4.91}$$

where

y_S^{new}	=	horizontal source dimension on the vertical source plane, adjusted to account for z_S^{new} (m)
y_s	=	equivalent source dimension in the direction normal to the regional flow direction on the vertical plane at the downgradient edge of the waste (m)
z_s	=	equivalent source dimension in the vertical direction on the vertical plane at the downgradient edge of the waste management unit (m)
z_S^{new}	=	z_s adjusted to account for the presence of recharge depth D_R (m)

Solution Method

A solution to Equation (4.75) and boundary and initial conditions in Equations (4.73 through 4.74) is sought in the form of a product solution (Carslaw and Jaeger, 1959). Assuming that the solution to Equation (4.72) may be obtained in the following product form:

$$c_\ell(x, y, z, t) = X_\ell(x, t)\, Y_\ell(x, y)\, Z_\ell(x, z) \tag{4.92}$$

where

$c_\ell\ (x,y,z,t)$	=	aqueous concentration of species ℓ at x, y, z at time t (mg/L)
t	=	time (y)
X_ℓ	=	x-direction component of the solution for species ℓ

x	=	x coordinate (m)
Y_ℓ	=	y-direction component of the solution for species ℓ
y	=	y coordinate (m)
Z_ℓ	=	z-direction component of the solution for species ℓ
z	=	z coordinate (m)

so that Equation (4.75) can be recast as

$$\phi_e R_\ell^s \frac{\partial}{\partial t} X_\ell Y_\ell Z_\ell + \overline{V}_x \frac{\partial}{\partial x}[X_\ell Y_\ell Z_\ell] - D_{xx}\frac{\partial^2}{\partial x^2}[X_\ell Y_\ell Z_\ell]$$

$$- D_{yy}\frac{\partial^2}{\partial y^2}[X_\ell Y_\ell Z_\ell] - D_{zz}\frac{\partial^2}{\partial z^2}[X_\ell Y_\ell Z_\ell]$$

$$+ \lambda_\ell^s X_\ell Y_\ell Z_\ell \phi_e Q_\ell - \sum_{m=1}^{M} \lambda_m^s X_m Y_m Z_m \phi_e Q_m \xi_{\ell m} = 0 \qquad (4.93)$$

where

ϕ_e	=	effective porosity (dimensionless)
R_ℓ^s	=	retardation factor (dimensionless)
t	=	time (y)
X_ℓ	=	x-direction component of the solution for species ℓ
Y_ℓ	=	y-direction component of the solution for species ℓ
Z_ℓ	=	z-direction component of the solution for species ℓ
$\overline{V}_x$	=	average Darcy velocity in the x direction between the downgradient edge of the source and the point of interest along the x direction (m/y)
x	=	x coordinate (m)
D_{xx}	=	longitudinal dispersion coefficient (m^2/y)
D_{yy}	=	horizontal transverse dispersion coefficient (m^2/y)
y	=	y coordinate (m)
D_{zz}	=	vertical transverse dispersion coefficient (m^2/y)
z	=	z coordinate (m)
λ_ℓ^s	=	degradation constant for the ℓth species (1/y)
Q_ℓ	=	coefficient to incorporate sorbed phase decay of species ℓ (dimensionless)
m	=	immediate parent of the component species being evaluated (dimensionless)
M	=	total number of parent chemicals (dimensionless)
λ_m^s	=	degradation constant for parent m (1/y)
X_m	=	x-direction component of the solution for species m
Y_m	=	y-direction component of the solution for species m
Z_m	=	z-direction component of the solution for species m
Q_m	=	coefficient to incorporate sorbed phase decay of species m (dimensionless)

$\xi_{\ell m}$ = constant related to decay reaction stoichiometry of the mth parent chemical and the ℓth chemical which is a degradation product of the mth parent chemical (dimensionless)

Equation (4.93) is subject to the following boundary conditions:

<u>On the source plane coplanar with the downgradient edge of the WMU</u>

$$X_\ell Y_\ell Z_\ell = c_k^0(t) F_c \; ; \; x = x_d \; , \; -\frac{y_S}{2} \le y \le +\frac{y_S}{2}, \; B - z_S - D_R \le z \le B - D_R \qquad (4.94a)$$
$$= 0, \quad \textit{elsewhere}.$$

<u>Along the top and bottom boundaries</u>

$$D_{zz}\frac{\partial}{\partial z} X_\ell Y_\ell Z_\ell = 0, \qquad z = 0, \; z = B \qquad (4.94b)$$

The boundary conditions of Equation (4.93) are used to replace the boundary conditions of Equations (4.74d and 4.74h).

<u>Along the left and right boundaries</u>

$$X_\ell Y_\ell Z_\ell \to 0, \qquad y \to \pm\infty \qquad (4.94c)$$

and, as a corollary:

$$D_{yy}\frac{\partial}{\partial y} X_\ell Y_\ell Z_\ell \to 0, \qquad y \to \pm\infty \qquad (4.94d)$$

<u>Downgradient boundary</u>

$$X_\ell Y_\ell Z_\ell \to 0, \qquad x \to +\infty \qquad (4.94e)$$

(In order to simplify the equation, the downgradient dimension of the domain is extended to infinity.)

<u>Initial condition</u>

From the condition stated by Equation (4.73),

$$X_\ell(t = 0) Y_\ell Z_\ell = 0, \quad \text{throughout the saturated zone} \qquad (4.94f)$$

In order to further simplify the equations, the x, y, and z coordinates are transformed as follows:

$$
\begin{aligned}
x' &= x - x_d \\
y' &= y \\
z' &= B - z - \frac{z_S}{2} - D_R
\end{aligned}
\tag{4.94g}
$$

where

X_ℓ	=	x-direction component of the solution for species ℓ
Y_ℓ	=	y-direction component of the solution for species ℓ
Z_ℓ	=	z-direction component of the solution for species ℓ
$c_\ell^o(t)$	=	aqueous concentration of species ℓ within the source (mg/L)
F_c	=	concentration ratio (dimensionless)
x	=	x coordinate (m)
x_d	=	downgradient coordinate of the source (m)
y_s	=	equivalent source dimension in the direction normal to the regional flow direction on the vertical plane at the downgradient edge of the waste (m)
y	=	y coordinate (m)
B	=	aquifer thickness (m)
z_s	=	equivalent source dimension in the vertical direction on the vertical plane at the downgradient edge of the waste management unit (m)
Y_s	=	equivalent source dimension in the vertical direction on the vertical plane at the downgradient edge of the waste management unit (m)
D_R	=	average penetration depth due to recharge between the downgradient edge of the source and the observation point (m)
z	=	z coordinate (m)
D_{zz}	=	vertical transverse dispersion coefficient (m^2/y)
D_{yy}	=	horizontal transverse dispersion coefficient (m^2/y)
t	=	time (y)
x'	=	transformed x-coordinate (m)
y'	=	transformed y-coordinate (m)
z'	=	transformed z-coordinate (m)

Since the boundary and initial conditions may be expressed as products of the three basic functions, X_ℓ, Y_ℓ, and Z_ℓ, the simplified transport equation may be separated into the following three single-unknown equations, which can be individually solved for X_ℓ, Y_ℓ, and Z_ℓ.

$$
\phi_e R_\ell^s \frac{\partial}{\partial t} X_\ell + \overline{V}_x \frac{\partial X_\ell}{\partial x'} - D_{xx} \frac{\partial^2 X_\ell}{\partial x'^2}
$$

$$+ \lambda_\ell^s \phi_e X_\ell Q_\ell - \sum_{m=1}^{M} \lambda_m^s \phi_e X_m Q_m \xi_{\ell m} = 0 \tag{4.95}$$

$$\overline{V}_x \frac{\partial Y_\ell}{\partial x'} - D_{yy} \frac{\partial^2 Y_\ell}{\partial y'^2} = 0 \tag{4.96}$$

$$\overline{V}_x \frac{\partial Z_\ell}{\partial x'} - D_{zz} \frac{\partial^2 Z_\ell}{\partial z'^2} = 0 \tag{4.97}$$

where

ϕ_e	=	effective porosity (dimensionless)
R_ℓ^s	=	retardation factor of species ℓ (dimensionless)
t	=	time (y)
X_ℓ	=	x-direction component of the solution for species ℓ
$\overline{V}_x$	=	average Darcy velocity in the x direction between the downgradient edge of the source and the point of interest along the x direction (m/y)
x'	=	transformed x-coordinate (m)
D_{xx}	=	longitudinal dispersion coefficient (m^2/y)
λ_ℓ^s	=	degradation constant for the ℓth species (1/y)
Q_ℓ	=	coefficient to incorporate sorbed phase decay of species ℓ (dimensionless)
m	=	immediate parent of the component species being evaluated (dimensionless)
M	=	total number of parent chemicals (dimensionless)
λ_m^s	=	degradation constant for parent m (1/y)
X_m	=	x-direction component of the solution for species m
Q_m	=	coefficient to incorporate sorbed phase decay of species m (dimensionless)
$\xi_{\ell m}$	=	constant related to decay reaction stoichiometry of the mth parent chemical and the ℓth chemical which is a degradation product of the mth parent chemical (dimensionless)
Y_ℓ	=	y-direction component of the solution for species ℓ
D_{yy}	=	horizontal transverse dispersion coefficient (m^2/y)
y'	=	transformed y-coordinate (m)
Z_ℓ	=	z-direction component of the solution for species ℓ
D_{zz}	=	vertical dispersion coefficient (m^2/y)
z'	=	transformed z-coordinate (m)

Upon simplification, Equations (4.96 to 4.97) require the following assumptions:

$$\left| Y_\ell Z_\ell D_{xx} \frac{\partial^2 X_\ell}{\partial x'^2} \right| \gg \left| 2D_{xx} \frac{\partial Y_\ell Z_\ell}{\partial x'} \frac{\partial X_\ell}{\partial x'} \right| \tag{4.98a}$$

$$\left| \overline{V}_x \frac{\partial Y_\ell Z_\ell}{\partial x'} \right| \gg \left| D_{xx} \frac{\partial^2 Y_\ell Z_\ell}{\partial x'^2} \right| \tag{4.98b}$$

and

$$X_\ell Y_\ell \approx X_m Y_m \tag{4.98c}$$

where

Y_ℓ	=	y-direction component of the solution for species ℓ
Z_ℓ	=	z-direction component of the solution for species ℓ
D_{xx}	=	longitudinal dispersion coefficient (m^2/y)
X_ℓ	=	x-direction component of the solution for species ℓ
x'	=	transformed x-coordinate (m)
$\overline{V}_x$	=	average Darcy velocity in the x direction between the downgradient edge of the source and the point of interest along the x direction (m/y)
X_m	=	x-direction component of the solution for species *m*
Y_m	=	y-direction component of the solution for species *m*

The proviso in Equation (4.98b) is used by Harleman and Rumer (1963) in their steady-state solution for transversal dispersion. It is approximately true in the event that the plume is extended to infinity so that the transversal dispersive flux relatively close to the source is much greater than the longitudinal dispersive flux. Equation (4.98a) is approximately true when the variation of $Y_\ell Z_\ell$ in the x-direction is negligibly small. The steady-state solutions of Equations (4.96 and 4.97) are based on an assumption that *x* is extended to infinity (see the explanation below of the solution for X_ℓ and Y_ℓ). Equation (4.98c) is predicated upon the condition that molecular diffusion coefficients are approximately the same for all chemicals.

<u>Solution for X_ℓ</u>

Equation (4.95) corresponds to the three-dimensional multi-species aqueous phase transport equation for the saturated zone in the EPACMTP code (U.S. EPA, 1996c), with uniform ground-water velocity in the x-direction and unit cross-sectional area in the y-z plane. With appropriate boundary conditions and parameters, the existing solution procedure in EPACMTP may be used to obtain X_ℓ.

Solution for Y_ℓ

Equation (4.96) is restated below:

$$\overline{V}_x \frac{\partial Y_\ell}{\partial x'} - D_{yy} \frac{\partial^2 Y_\ell}{\partial y'^2} = 0 \tag{4.99}$$

where

$\overline{V}_x$	=	average Darcy velocity in the x direction between the downgradient edge of the source and the point of interest along the x direction (m/y)
Y_ℓ	=	y-direction component of the solution for species ℓ
x'	=	transformed x-coordinate (m)
D_{yy}	=	horizontal transverse dispersion coefficient (m^2/y)
y'	=	transformed y-coordinate (m)

which is subject to the following boundary conditions:

$$\frac{\partial}{\partial y'} Y_\ell \rightarrow 0, \qquad y' \rightarrow \pm\infty \tag{4.100a}$$

$$Y_\ell \quad \textit{bounded}, \quad x \rightarrow \infty \tag{4.100b}$$

$$\begin{aligned} Y_\ell(x'=0) &= 1, \text{ with } -0.5y_S \le y' \le 0.5y_S, \\ &= 0, \; y' \le -0.5y_S, \textit{ and } y' \ge 0.5y_S, \end{aligned} \tag{4.100c}$$

where

y'	=	transformed y-coordinate (m)
Y_ℓ	=	y-direction component of the solution for species ℓ
x	=	x-coordinate (m)
x'	=	transformed x-coordinate (m)
y_s	=	equivalent source dimension in the direction normal to the regional flow direction on the vertical plane at the downgradient edge of the waste (m)

A solution to Equations (4.99 and 4.100) is given by (Carslaw and Jaeger, 1959)

$$Y_\ell = \frac{1}{2}\left(\mathit{erf}\, \frac{0.5y_S - y'}{2\sqrt{D_{yy}\frac{x}{\overline{V}_x}}} + \mathit{erf}\, \frac{0.5y_S + y'}{2\sqrt{D_{yy}\frac{x}{\overline{V}_x}}} \right) \tag{4.101}$$

where

Y_ℓ	=	y-direction component of the solution for species ℓ
y_s	=	equivalent source dimension in the direction normal to the regional flow direction on the vertical plane at the downgradient edge of the waste (m)
y'	=	transformed y-coordinate (m)
D_{yy}	=	horizontal transverse dispersion coefficient (m^2/y)
x	=	x-coordinate (m)
$\overline{V}_x$	=	average Darcy velocity in the x direction between the downgradient edge of the source and the point of interest along the x direction (m/y)
erf(·)	=	error function

<u>Solution for Z_k</u>

Equation (4.97) is restated below:

$$\overline{V}_x \frac{\partial Z_\ell'}{\partial x'} - D_{zz} \frac{\partial^2 Z_\ell'}{\partial z'^2} = 0 \tag{4.102}$$

which is subject to the following boundary conditions:

$$\frac{\partial}{\partial z'} Z_\ell' \rightarrow 0, \qquad z' \rightarrow \pm\infty \tag{4.103a}$$

$$Z_\ell' \quad \textit{bounded}, \quad z' \rightarrow \infty \tag{4.103b}$$

$$\begin{aligned} Z_\ell'(x' = 0) &= 1, \text{ with } -0.5z_S \le z' \le 0.5z_S, \\ &= 0, \text{ with } z' \le -0.5z_S,\ z' \ge 0.5z_S, \end{aligned} \tag{4.103c}$$

where

$\overline{V}_x$	=	average Darcy velocity in the x direction between the downgradient edge of the source and the point of interest along the x direction (m/y)
Z_ℓ'	=	a component of the solution for species ℓ
x'	=	transformed x-coordinate (m)
D_{zz}	=	vertical dispersion coefficient (m^2/y)
z'	=	transformed z-coordinate (m)
z_s	=	equivalent source dimension in the vertical direction on the vertical plane at the downgradient edge of the waste management unit (m)

The boundary conditions in Equations (4.103a and 4.103b) are used as intermediate boundary conditions from which the intermediate solution, Z_ℓ' may be derived. The

boundary conditions in Equation (4.93) at the top and bottom of the saturated zone are imposed through the use of the method of images (Bear, 1972).

A solution to Equations (4.102 and 4.103) is given by (Carslaw and Jaeger, 1959).

$$Z_\ell' = \frac{1}{2}\left(erf\,\frac{0.5z_S - z'}{2\sqrt{D_{zz}\frac{x}{\overline{V}_x}}} + erf\,\frac{0.5z_S + z'}{2\sqrt{D_{zz}\frac{x}{\overline{V}_x}}} \right) \tag{4.104}$$

where

Z_ℓ'	=	a component of the solution for species ℓ
z_s	=	equivalent source dimension in the vertical direction on the vertical plane at the downgradient edge of the waste management unit (m)
z'	=	transformed z-coordinate (m)
D_{zz}	=	vertical dispersion coefficient (m^2/y)
x	=	x-coordinate (m)
$\overline{V}_x$	=	average Darcy velocity in the x direction between the downgradient edge of the source and the point of interest along the x direction (m/y)
erf(·)	=	error function

The boundary conditions at the top and bottom of the saturated zone are imposed by using one image on either side. In general, it is found that multiple images are not necessary and only one image per side is adequate. The final solution for Z_ℓ at the well depth, z_{rw}^*, may be obtained by:

$$Z_\ell(x', z_{rw}^{*\prime}) = Z_\ell'(x', z_{rw}^{*\prime}) + Z_\ell'(x', z_1') + Z_\ell'(x', z_2') \tag{4.105}$$

where

$$\begin{aligned} z_{rw}^{*\prime} &= z_{rw}^* - \frac{z_S}{2} - D_R \\ z_1' &= 2B - \frac{z_S}{2} - D_R - z_{rw}^* \\ z_2' &= z_{rw}^* + \frac{z_S}{2} + D_R \end{aligned} \tag{4.106}$$

where

Z_ℓ	=	z-direction component of the solution for species ℓ
x'	=	transformed x-coordinate (m)

$z_{rw}^{*\prime}$ = transformed well depth (m)
Z'_{ℓ} = a component or an image of Z_{ℓ}
z'_1 = transformed well depth in image 1 (m)
z'_2 = transformed well depth in image 2 (m)
z_{rw}^{*} = well depth (m)
z_s = equivalent source dimension in the vertical direction on the vertical plane at the downgradient edge of the waste management unit (m)
D_R = average penetration depth due to recharge between the downgradient edge of the source and the observation point (m)
B = aquifer thickness (m)

Determination of D_{ij}

From Equations (4.32a to 4.32c), dispersion coefficients for the saturated zone may be written as follows:

$$\begin{aligned} D_{xx} &= \alpha_L \overline{V}_x + \phi_e D_k^{s*} \\ D_{yy} &= \alpha_T \overline{V}_x + \phi_e D_k^{s*} \\ D_{zz} &= \alpha_V \overline{V}_x + \phi_e D_k^{s*} \end{aligned} \tag{4.107}$$

where

D_{xx} = longitudinal dispersion coefficient (m^2/y)
α_L = longitudinal dispersivity (m)
$\overline{V}_x$ = average Darcy velocity in the x direction between the downgradient edge of the source and the point of interest along the x direction (m/y)
ϕ_e = effective porosity (dimensionless)
D_k^{s*} = effective molecular diffusion coefficient for species k (m^2/y)
D_{yy} = horizontal transverse dispersion coefficient (m^2/y)
α_T = lateral dispersivity in the horizontal direction (m)
D_{zz} = vertical dispersion coefficient (m^2/y)
α_V = lateral dispersivity in the vertical direction (m)

4.4.6 Determining the Exposure Concentration at the Receptor Well

The finite source methodology involves evaluation of the temporally averaged receptor well concentration, $\underline{C}_{RW}$. Two options have been implemented. The first is based on determining the average receptor well concentration over a specified time interval, for instance a 30 years average residence time (U.S. EPA, 1991). In order to ensure that a protective result is obtained, the exposure period is always selected to be centered about the time at which the receptor well concentration reaches its maximum value (see Figure 4.9). The second option is to forego the time-averaging and set $\underline{C}_{RW}$ equal to the peak receptor well concentration value, $\underline{C}_{RW}^{max}$. The second option will yield higher values for the receptor well concentration, $\underline{C}_{RW}$, and therefore will be more conservative with regard to health risks. As mentioned before, as the pulse duration, t_p, increases, the receptor well breakthrough curve will exhibit a

plateau with maximum concentration equal to the steady-state concentration, and eventually the time-averaged concentration will be the same as the peak concentration value (Figure 4.10).

4.4.6.1 Time-Averaged Concentration

When time-averaged receptor well concentrations are required, a two-step procedure is used. The first step is again to determine the time value at which the receptor well concentration reaches its peak, as described below in Section 4.4.6.2. Denoting this time value as t_{max} and denoting the exposure time interval of interest as t_d, the time-averaged receptor well concentration $\bar{C}_{RW}$ is computed as (Figure 4.9):

$$\bar{C}_{RW} = \frac{1}{t_d} \int_{t_{peak} - \frac{1}{2}t_d}^{t_{peak} + \frac{1}{2}t_d} C_{RW}(t)\,dt \tag{4.108}$$

$$\bar{C}_{RW} = \frac{1}{t_d} \left\{ \int_0^{t_{peak} + \frac{1}{2}t_d} C_{RW}(t)dt - \int_0^{t_{peak} - \frac{1}{2}t_d} C_{RW}(t)dt \right\} \tag{4.109}$$

where

$\bar{C}_{RW}$	=	time-averaged receptor well concentration (mg/L)
t_d	=	exposure time interval of interest (y)
t_{peak}	=	time value at which the receptor well concentration reaches its peak (y)
C_{RW}	=	instantaneous receptor well concentration (mg/L)
t	=	time (y)

Equation (4.109) is used because the Laplace Transform Galerkin (LTG) formulation in EPACMTP makes it very straightforward to directly evaluate the time-integrated concentration at any location (U.S. EPA, 1996b).

Strictly speaking, use of Equation (4.109) may not always ensure that $\bar{C}_{RW}$ is indeed the highest possible average exposure concentration. Use of Equation (4.109) will yield the maximum average exposure concentration provided the receptor well breakthrough curve is symmetrical. If the breakthrough curve is not symmetrical, the time period of the maximum average receptor well concentration may be shifted relative to the time of the peak concentration. Using Equation (4.109) has a considerable computational advantage because, after t_{peak} has been found, it requires only two quick Laplace inversions to determine $\bar{C}_{RW}$. Using a search procedure to find the maximum average receptor well concentration, versus using Equation (4.109) has been evaluated for a range of different constituents and modeling scenarios. The two approaches were found to yield almost the same

averaged exposure concentrations, but using Equation (4.109) in a Monte-Carlo simulation required only about half the CPU time of a direct search procedure.

For the pseudo three-dimensional transport equation, t_{peak} for a given receptor well is found directly from the well's breakthrough curve. Equation (4.108) is then applied to determine $\underline{C}_{RW}$.

In EPACMTP, up to 10 values of exposure duration of interest (t_d) may be specified, and multiple exposure duration values may be used with any of the transport solutions (fully 3D transport, pseudo-3D transport, and 2D transport).

4.4.6.2 Peak Concentration

The procedure for locating the receptor well concentration peak and the time-averaged concentration value is as follows. The time value at which the receptor well concentration reaches its maximum is estimated based on the distance to the receptor well and the average solute travel velocity. An empirical search procedure is then employed to locate the exact position of the peak. The search procedure is a one-dimensional search algorithm to determine the maximum concentration that occurs within a predetermined time period. The algorithm, which is similar to the Fibonacci search algorithm, attempts to decrease the time period with the maximum concentration through successive searches. The search is terminated when two successive time periods and maximum concentrations are approximately the same (or differ within a predetermined tolerance). If the analysis is based on the peak concentration value itself, this value is stored for later post-processing. For a degrading compound with degradation products that may be toxic, the peak concentrations for each member of the species may occur at different times. The searching procedure is therefore repeated for all member species.

For the pseudo three-dimensional transport solution, a complete breakthrough curve (concentration versus time) is determined for each receptor well in each model realization. The peak concentration at a given receptor well is found by performing a direct search for the maximum value of concentration in the breakthrough curve.

4.4.6.3 Time-to-Arrival of the Peak Concentration

For the pseudo three-dimensional transport equation, the time-to-arrival of the peak concentration at a given receptor well is determined by searching the well's breakthrough curve. For other solutions, the empirical search algorithm described in Section 4.4.6.2 is used.

4.4.7 Determining the Contaminant Mass Flux from Ground-water into a Surface Water Body

A ground water to surface water pathway can be included in an EPACMTP modeling analysis, however, these calculations are not incorporated into the EPACMTP model and must be done separately as a post-processing step. Determining the contaminant mass flux from the ground water into a surface water body is done by calculating the total contaminant mass flux at a given downgradient location selected to represent the intersection of the contaminant plume with a surface water body. It is assumed that the surface water body fully penetrates the aquifer and the plume fully intersects the water body. The total contaminant mass flux (in mg/y) is then calculated by multiplying the ground-water flux with the net contaminant mass across the entire plume cross section. The details of this calculation are presented in Appendix F.

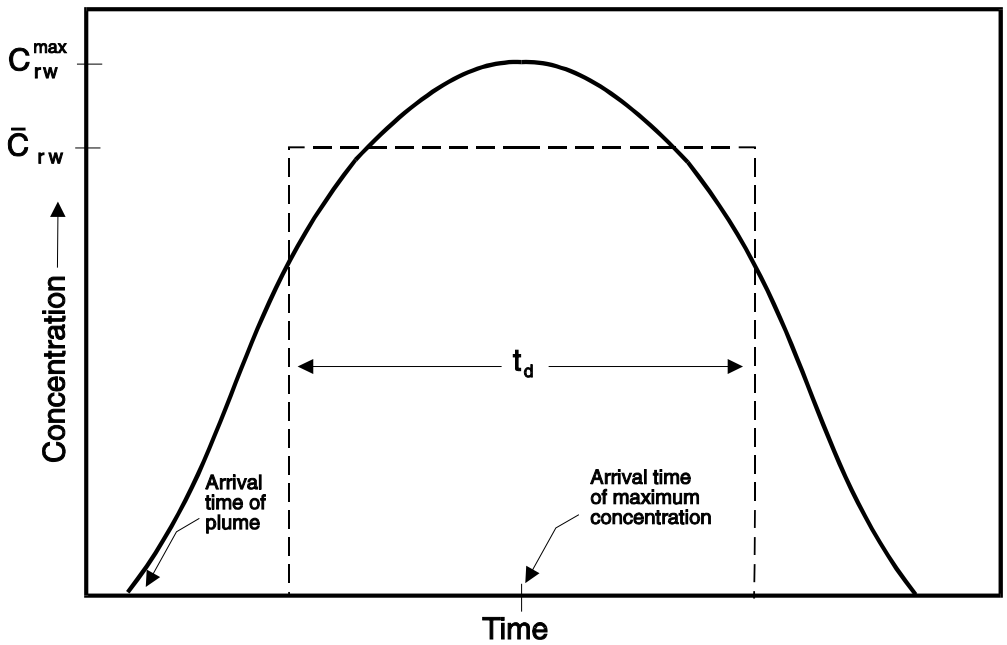

Figure 4.9 Schematic View of the Time-varying Receptor Well Concentration (Break Through Curve) and Illustration of the Procedure for Determining $\bar{C}_{rw}$.

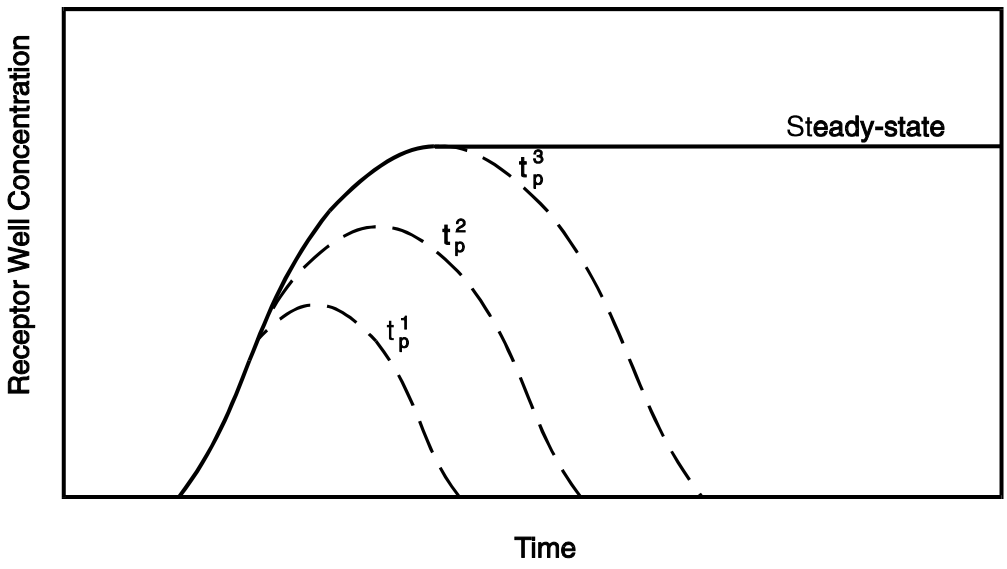

Figure 4.10 Schematic Illustration of the Effect of Increasing Pulse Duration, T_p, on the Receptor Well Break Through Curve.

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