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Multimedia Environmental Pollutant Assessment System (MEPAS®): Groundwater Pathway Formulations

G. Whelan
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June 1996

Prepared for the U.S. Department of Energy
under Contract DE-AC06-76RLO 1830

Pacific Northwest National Laboratory
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(a) Idaho State University, Pocatello, Idaho.

Preface

The Multimedia Environmental Pollutant Assessment System (MEPAS) is a physics-based environmental analysis code integrating source-term, transport, and exposure models for concentration, dose, or risk endpoints. Developed by Pacific Northwest National Laboratory[a] for the U.S. Department of Energy, MEPAS is designed for site-specific assessments using readily available information. Endpoints are computed for chemical and radioactive pollutants. For human health impacts, risks are computed for radionuclide and hazardous carcinogens and hazard quotients for noncarcinogens. This system has wide applicability to environmental problems using air, groundwater, surface-water, overland, and exposure models. MEPAS enables users to simulate release of contaminants from a source; the transport of contaminants through the air, groundwater, surface water, or overland pathways; and the transfer of contaminants through food chains and exposure pathways to the exposed individual or population. Whenever available and appropriate, guidance and/or models from the U.S. Environmental Protection Agency, International Commission on Radiological Protection, and National Council on Radiation Protection and Measurements were used to facilitate compatibility and acceptance.

Although based on relatively standard transport and exposure computation approaches, MEPAS uniquely integrates these approaches into a single system providing a consistent basis for evaluating health impacts for a large number of problems and sites. Implemented on a desktop computer, a user-friendly shell allows the user to define the problem, input the required data, and execute the appropriate models. This document describes the mathematical formulations used in the groundwater component of MEPAS.

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Summary

The groundwater component of the MEPAS methodology models solute transport through the groundwater environment (i.e., partially saturated and saturated zones). Specifically, this component provides estimates of groundwater contaminant fluxes at various transporting medium interfaces (e.g., water table or aquifer/river interface) and contaminant concentrations at withdrawal wells. Contaminant fluxes at transporting medium interfaces represent boundary conditions for the next medium in which contaminant migration and fate is to be simulated (e.g., groundwater contamination entering a surface-water environment). Contaminant concentrations at withdrawal wells provide contaminant levels for the exposure assessment component of MEPAS. This document describes the mathematical formulations for the groundwater pathway.

The migration and fate of contaminants through the groundwater environment are described by the three-dimensional, advective-dispersive equation for solute transport. The results are based on semi-analytical solutions (i.e., solutions that require numerical integration) that are well established in the scientific literature. The groundwater model accounts for the major mechanisms of constituent mobility (i.e., adsorption/desorption), persistence (i.e., degradation or decay), advection, and hydrodynamic dispersion. Mobility is described by an equilibrium coefficient that assumes instantaneous adsorption/ desorption between the soil matrix and the pore water. Persistence is described by a first-order degradation/decay coefficient. Radionuclide decay products are also accounted for. Advection is described by constant, unidirectional flow in the vertical direction in the partially saturated (vadose) zone and in the longitudinal direction in the saturated zone. Hydrodynamic dispersion is described in one dimension for the partially saturated zone and three dimensions for the saturated zone.

The assumptions listed and/or discussed in this document are itemized below for easy reference. Section numbers are provided where a particular assumption is discussed in more detail.

- The groundwater environment is initially free of contamination.
- All transport media properties are homogeneous and isotropic.
- Flow in both the partially saturated and saturated zones is uniform.
- The saturated zone is of finite, constant thickness and of infinite lateral extent.
- The flow system is at steady state. Drawdown effects of withdrawal wells and other transient stresses on the aquifer are not considered by the semianalytical solutions.
- Density differences between a contaminant plume and the natural groundwater are negligible.
- The contaminant sorption process can be described by a constant (K_d) epresenting the ratio between the contaminant adsorbed to the soil matrix and the contaminant dissolved in solution (Section 2.0).

- A unit hydraulic gradient exists in the partially saturated soil beneath a waste site (Section 2.0).
- The moisture content in the partially saturated zone fluctuates between field capacity and saturation (Section 2.0).
- The soil transmission rate is the maximum possible infiltration rate for a leachate migrating through a partially saturated zone (Section 2.0).
- A unit hydraulic gradient and saturated conditions, as described by a saturated hydraulic conductivity, occurs beneath ponded sites (Section 2.0).
- If a surface-water body is part of the transport scenario, then it will be the final transporting medium, and all contaminants entering the subsurface environment will eventually enter the water body, except contaminants lost through degradation/decay.
- Contaminant diffusion through the water table does not occur once a contaminant has entered the aquifer. Thus, contaminant spreading in the vertical direction is only downward (Section 2.4).
- The leachate volume infiltrating from a waste site is insignificant compared to the total flux of contaminated water at the receptor well (Section 3.3).
- Degradation/decay is first-order for all contaminants.
- Decay products have the same equilibrium coefficient as the parent, and therefore travel at the same speed as the parent (Section 3.5).

The following assumptions are applicable to the option of using measured concentrations for evaluating health impacts (Chapter 4.0):

- The monitoring and receptor wells occur along the same groundwater flow streamline.
- The user-supplied concentration is temporally constant.
- Differences in concentrations at a monitoring well and a receptor well are due solely to vertical and lateral dispersion.

Acknowledgments

The authors thank Mark Rockhold and Keith Shields for their technical review of this document, Robert Buchanan for editorial review, and Vickie Atkinson and Text Processing staff for preparing the final manuscript. Thanks are also extended to Larry Bagaasen, John Buck, Karl Castleton, Jim Droppo, Gariann Gelston, Andre dé Hamer, Bonnie Hoopes, and Dennis Strenge, all of whom have, in some way, influenced the development of the waterborne codes with their technical guidance and suggestions. Appreciation also goes out to all the people who use MEPAS and have alerted us to potential problems in the code and offered suggestions for its improvement.

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1.0 Introduction

This report describes the mathematical formulations used for contaminant fate and transport in the groundwater pathway of the Multimedia Environmental Pollutant Assessment System (MEPAS). It is one in a series of reports that collectively describe the components of MEPAS. Other volumes address the following topics:

- Surface Hydrology (Whelan and McDonald 1996a) - describes the method used in MEPAS to compute a water mass balance in the surface soil of a waste site.

- Overland Pathway (Whelan and McDonald 1996b) - describes the method used in MEPAS to compute overland runoff and soil erosion from a waste site.

- Riverine Pathway (Whelan and McDonald 1996c) - presents the mathematical formulations for contaminant fate and transport in the surface-water component of MEPAS.

- Atmospheric Pathway (Droppo and Buck 1996) - presents the mathematical formulations for source-term volatilization and suspension, and contaminant fate and transport in the atmospheric pathway of MEPAS.

- Exposure Pathway and Human Health Impact Assessment Models (Strenge and Chamberlain 1995) - describes the methods used by MEPAS to compute dose and human health impacts to selected individuals and populations caused by exposure to pollutants.

- Source-Term Release (Streile et al. in press) - presents the mathematical formulations for a module that partitions the release of contaminants from a source term amongst the atmospheric and waterborne transport pathways. This module is planned to be incorporated into MEPAS at a later date.

The groundwater component of the MEPAS methodology models solute transport through the groundwater environment (i.e., partially saturated and saturated zones). Specifically, this component provides estimates of groundwater contaminant fluxes at various transporting medium interfaces (e.g., water table or aquifer/river interface) and contaminant concentrations at withdrawal wells. Contaminant fluxes at transporting medium interfaces represent boundary conditions for the next medium in which contaminant migration and fate is to be simulated (e.g., groundwater contamination entering a surface-water environment). Contaminant concentrations at withdrawal wells provide contaminant levels for the exposure assessment component of MEPAS. A schematic diagram illustrating the groundwater environment is presented in Figure 1.1.

The migration and fate of contaminants through the groundwater environment are described by the three-dimensional, advective-dispersive equation for solute transport. The results are based on

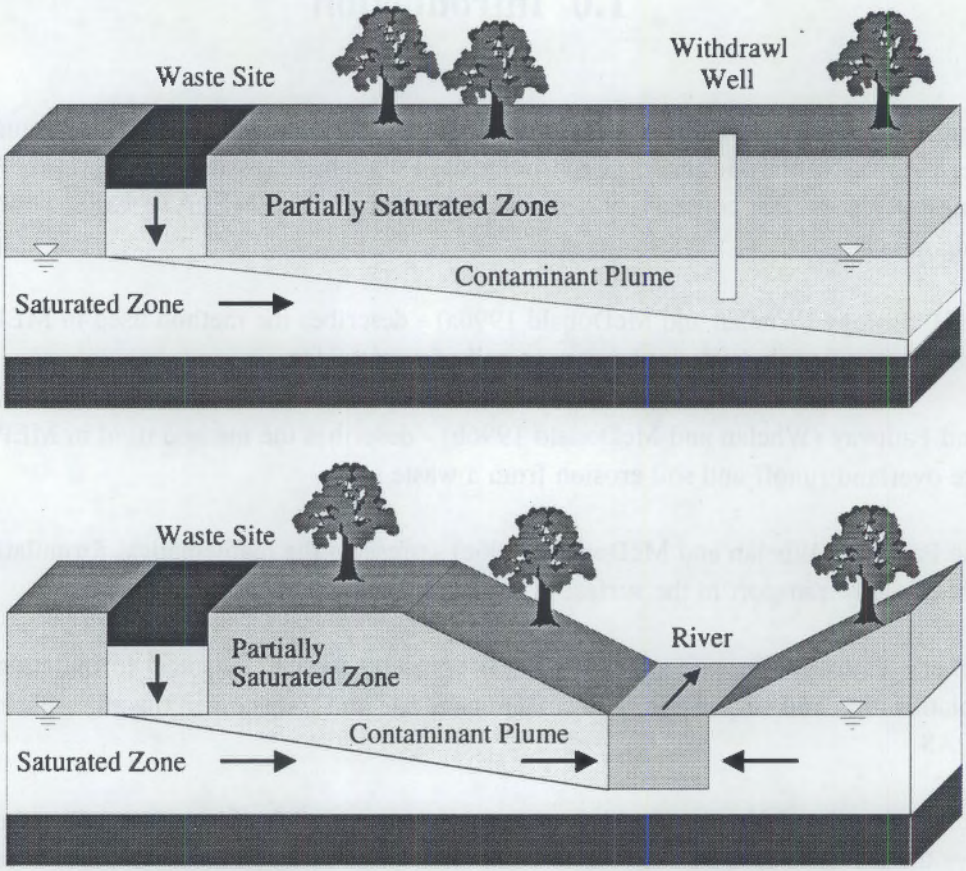

Figure 1.1. Schematic Diagram Illustrating the Groundwater Environment for the Groundwater to a Well and Groundwater to a River Transport Scenarios

semianalytical solutions (i.e., solutions that require numerical integration) that are well established in the scientific literature. To increase computational efficiency, limits of integration are also identified.

The groundwater model accounts for the major mechanisms of constituent mobility (i.e., adsorption/desorption), persistence (i.e., degradation or decay), advection, and hydrodynamic dispersion. Mobility is described by an equilibrium coefficient that assumes instantaneous adsorption/desorption between the soil matrix and the pore water. Persistence is described by a first-order degradation/decay coefficient. Radionuclide decay products are also accounted for. Advection is described by constant, unidirectional flow in the vertical direction in the partially saturated (vadose) zone and in the longitudinal direction in the saturated zone. Hydrodynamic dispersion is described in one dimension for the partially saturated zone and three dimensions for the saturated zone.

Other assumptions associated with the groundwater component of MEPAS include the following:

- The groundwater environment is initially free of contamination.

- All transport media properties are homogeneous and isotropic.

- Flow in both the partially saturated and saturated zones is uniform.

- The saturated zone is of finite, constant thickness and of infinite lateral extent.

- The flow system is at steady state. Drawdown effects of withdrawal wells and other transient stresses on the aquifer are not considered by the semianalytical solutions. Flow velocities are provided by the user.

- Density differences between a contaminant plume and the natural groundwater are negligible.

The specific topics addressed in Chapter 2.0 of this report are as follows:

- Advective-Dispersive Equation--The advective-dispersive equation describes solute migration in the groundwater environment (both partially saturated and saturated zones). The form of the equation used by the groundwater component is discussed.

- Contaminant Concentration Equations--The various semianalytical solutions (i.e., combined analytical and numerical algorithms) to the advective-dispersive equation are presented. The solutions describe solute concentrations.

- Contaminant Flux Equations--The various equations describing contaminant fluxes from one medium to another are presented. The equations describe solute movement between a series of partially saturated zones, partially saturated and saturated zones, and/or a saturated zone and a surface-water body.

- Steady-State Groundwater Equations--This section describes the steady-state solutions to the advective-dispersive equation for contaminant transport in the partially saturated and saturated zones.

- Mixing Length--Lateral and vertical mixing lengths are defined; these describe the lateral and vertical distances over which a migrating solute plume can be considered to be fully mixed. The time for the contaminant to travel from the waste site through groundwater media to a receptor of concern is described. The travel time is used in determining mixing lengths.

The specific topics addressed in Chapter 3.0 of this report are as follows:

- Integration Limits--Because the solutions to the advective-dispersive equation are semianalytical and must be integrated over time, integration limits that increase computational efficiency are described.

- Adaptive Simpson's Quadrature Integration Routine--This section briefly describes the integration scheme that is employed for the groundwater environment.

- Features for Far-Field/Near-Field Situations--Techniques that enhance the groundwater component's performance under near- and far-field conditions are discussed.

- Groundwater Mass Balance at the Source--This section briefly describes the features that ensure mass is conserved in the analysis.

- Contaminant Degradation/Decay--The technique for computing the degradation of chemicals and/or the decay of radionuclides is described.

Chapter 4.0 of this report discusses measured concentrations in the groundwater environment. This chapter describes the option within the methodology of using measured environmental contaminant levels in the assessment of health impacts to surrounding sensitive receptors as opposed to performing transport calculations to estimate these environmental concentrations.

Chapter 5.0 provides a listing of the equation notations found throughout the report.

2.0 Advective-Dispersive Equation

The advective-dispersive equation for solute movement through a porous medium with a constant, steady-state flow velocity forms the basis of all groundwater solution algorithms. As noted by Codell et al. (1982), the algorithms are developed for the limiting case of unidirectional advective transport with three-dimensional dispersion in a homogeneous aquifer. Let n and n_e represent total and effective porosities, respectively; then $n - n_e$ is the remaining void fraction devoted to immobile pore water. A mass balance on the differential volume $dV = dx\,dy\,dz$ gives the expression:

$$\underset{\text{(a)}}{n_e \frac{\partial C}{\partial t}} + \underset{\text{(b)}}{(n - n_e)\frac{\partial G}{\partial t}} + \underset{\text{(c)}}{\rho_s (1 - n)\frac{\partial P}{\partial t}} + \underset{\text{(d)}}{n_e u \frac{\partial C}{\partial x}} = \underset{\text{(e)}}{n_e \left[D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} + D_z \frac{\partial^2 C}{\partial z^2} \right]} +$$

$$\underset{\text{(f)}}{(n - n_e)\left[D_x' \frac{\partial^2 G}{\partial x^2} + D_y' \frac{\partial^2 G}{\partial y^2} + D_z' \frac{\partial^2 G}{\partial z^2} \right]} - \underset{\text{(g)}}{n_e \lambda C} - \underset{\text{(h)}}{(1 - n)\rho_s \lambda P} - \underset{\text{(i)}}{(n - n_e)\lambda G} \qquad (2.1)$$

where n = total porosity (dimensionless)
n_e = effective porosity (dimensionless)
C = dissolved concentration in the mobile liquid phase (g/mL or Ci/mL)[a]
ρ_s = soil particle density (g/cm^3)
t = time (s)
G = dissolved concentration in the immobile liquid phase (g/mL or Ci/mL)
P = particulate concentration on the solid phase (g/g or Ci/g)
u = the x-component groundwater velocity (also referred to as pore-water, seepage, or average linear velocity) (cm/s)
D_x, D_y, D_z = the dispersion coefficients for the mobile liquid phase in the x-, y-, and z-directions, respectively (cm^2/s)
D_x', D_y', D_z' = the diffusion coefficients for the immobile liquid phase in the x-, y-, and z-directions, respectively (cm^2/s)
λ = the decay constant [(ln 2)/(half-life)] (s^{-1}).

The following list describes the terms in Equation 2.1:

(a) accumulation (storage) in the mobile liquid phase

(b) accumulation in the immobile liquid phase

(a) When two sets of units are provided, the first refers to chemicals, and the second refers to radionuclides.

(c) accumulation in the solid phase

(d) x-direction advective transport of the mobile liquid phase

(e) dispersive transport of the mobile liquid phase in the x-, y-, and z-directions, respectively

(f) diffusive transport of the immobile liquid phase in the x-, y-, and z-directions, respectively

(g) degradation/decay in the mobile liquid phase

(h) degradation/decay in the solid phase

(i) degradation/decay in the immobile liquid phase.

Equation 2.1 can be streamlined with two simplifying assumptions. First, there is no diffusion of contaminant into the immobile liquid phase. Field studies indicate that including this phenomenon produces inappropriate analyses, as the retardation factor can never approach unity when the total porosity does not equal the effective porosity (see Equation 2.5). Second, the contaminant sorption process can be described by a constant (Kd) representing the ratio between the contaminant adsorbed to the soil matrix (P) and the contaminant dissolved in solution (C). Using these assumptions, Equation 2.1 can be rewritten as

$$\frac{\partial C}{\partial t} + \frac{u}{R_{fl}}\frac{\partial C}{\partial x} = \frac{D_x}{R_{fl}}\frac{\partial^2 C}{\partial x^2} + \frac{D_y}{R_{fl}}\frac{\partial^2 C}{\partial y^2} + \frac{D_z}{R_{fl}}\frac{\partial^2 C}{\partial z^2} - \lambda C \tag{2.2}$$

in which

$$R_{fl} = 1 + \frac{\beta_d}{n_e} Kd \tag{2.3}$$

and

$$D = \alpha u + D_{mol} \tag{2.4}$$

where R_{fl} = retardation factor (dimensionless)
β_d = bulk density (g/cm^3)
Kd = equilibrium (partition or distribution) coefficient (mL/g)
α = dispersivity in the x-, y-, or z-direction (cm)
D_{mol} = molecular diffusion [= 0.52 cm^2/d, which is the upper value of a range of experimentally determined molecular diffusion coefficients for trivalent and monovalent ions in fine sand found by Duursma (1966) as reported by Mills et al. (1985)].

The retardation factor is used as a measure of the mobility of constituents in a porous medium. It represents the ratio of the mean pore-water velocity to the mean contaminant migration velocity and can be expressed in a number of ways. Other forms describing the retardation factor have also appeared in the literature (e.g., any groundwater textbook) and have been expressed by

$$R_{f2} = \frac{n}{n_e} + \frac{\beta_d}{n_e} Kd \tag{2.5}$$

$$R_{f3} = 1 + \frac{\beta_d}{n} Kd \tag{2.6}$$

$$R_{f4} = 1 + \frac{\beta_d}{\theta} Kd \tag{2.7}$$

where θ = moisture content of the partially saturated zone (dimensionless).

Equations 2.3 and 2.7 are currently used in MEPAS, because the assumptions that form the basis of these equations are consistent with those used to simplify the advective-dispersive equation (Equation 2.2). Equation 2.5 assumes that the porous medium is composed of interconnected pore spaces through which flow occurs (n_e) and dead-end pore spaces through which no flow occurs ($n - n_e$). The contaminant in Equation 2.5 is assumed to migrate through the interconnected pore spaces, diffuse into dead-end pore spaces, and instantaneously adsorb to or desorb from the soil matrix where fluid is and is not flowing. Equation 2.5 also assumes that the solute concentration in the dead-end pore spaces is equivalent to the solute concentration in the free-flowing spaces and that the dispersion coefficients in both locations are equivalent. Equation 2.3 includes the same processes as Equation 2.5 except that the contaminant does not diffuse into dead-end pore spaces. Equation 2.6 includes the same phenomena as Equation 2.5 except that the porous medium contains no dead-end pore spaces. Equations 2.6 and 2.7 describe the retardation of the contaminant in a similar manner; the major difference between them is that the porosity in Equation 2.6 is replaced by the moisture content to give Equation 2.7. Equations 2.3, 2.5 and 2.6 are associated with the saturated zone, while Equation 2.7 is used in the partially saturated zone. By making the following substitutions

$$u' = \frac{u}{R_f} \tag{2.8}$$

and

$$D' = \frac{D}{R_f} \tag{2.9}$$

Equation 2.2 can be rewritten as

$$\frac{\partial C}{\partial t} + u^* \frac{\partial C}{\partial x} = D_x^* \frac{\partial^2 C}{\partial x^2} + D_y^* \frac{\partial^2 C}{\partial y^2} + D_z^* \frac{\partial^2 C}{\partial z^2} - \lambda C \tag{2.10}$$

As written, Equation 2.1 specifically addresses the general conditions for saturated flow and solute movement. However, Equation 2.1 can also be applied to the partially saturated zone if the total and effective porosities are assumed to be equal to the soil moisture content. In addition, one-dimensional, unidirectional flow and dispersion are assumed only in the vertical (z) direction in the partially saturated zone. Note that with these assumptions, Equation 2.7 defines the retardation factor, and Equation 2.10 is applicable if the coordinate system is rotated such that the x-axis corresponds to the z-direction and dispersion is only considered in the flow direction (i.e., D_y^* and D_z^* equal zero).

The solution algorithm to the advective-dispersive equation is based on homogeneous and isotropic soil parameters (Van Genuchten and Alves 1982; Donigian et al. 1983). The partially saturated soil beneath the waste site is assumed at a unit hydraulic gradient, and the moisture content is assumed to fluctuate between field capacity and saturation. The hydraulic conductivity is based on an empirical equation proposed by Gardner (1960), Gardner et al. (1970), Campbell (1974), and Clapp and Hornberger (1978) and is expressed as (Hillel 1980)

$$K(\theta) = K_s \left(\frac{\theta}{n} \right)^{1/m} \tag{2.11}$$

in which

$$m = \frac{1}{2b + 3} \tag{2.12}$$

where $K(\theta)$ = hydraulic conductivity (cm/s)
K_s = saturated hydraulic conductivity (cm/s)
m = empirically based parameter that is a function of soil properties (dimensionless)
b = soil type coefficient (dimensionless).

Hillel (1980) notes that although attempts have been made to develop theoretically based equations relating hydraulic conductivity to moisture content, the state of the art is such that consistently accurate *a priori* predictions of $K(\theta)$ from basic soil properties are difficult.

Whelan et al. (1986) note that if the rate of water infiltration from the waste site (i.e., leach rate) is less than the soil transmission rate, as described by the general equation for liquid flow in the partially saturated zone (i.e., the Richards equation) (Hanks and Ashcroft 1980; Hillel 1980), the water moves through the soil at the infiltration rate, accounting for adjustments in the soil moisture content.

Applying Darcy's law and the unit hydraulic gradient assumption, the hydraulic conductivity is equal to the infiltration rate. Thus, Equation 2.11 is used to compute the soil moisture content. For an infiltration rate equal to or greater than the transmission rate, the leachate is assumed to move at the transmission rate of the soil, which is equal to the saturated hydraulic conductivity (because of the unit hydraulic gradient assumption).

For ponded waters, Hillel (1971) notes that the downward infiltration into an initially partially saturated soil generally occurs under the combined influence of suction and gravity gradients. As the water penetrates deeper and the wetted part of the profile lengthens, the average suction gradient decreases, because the overall difference in pressure head (between the saturated soil surface and the unwetted soil inside the profile) divides itself along an ever-increasing distance. This trend will continue until eventually the suction gradient in the upper part of the profile becomes negligible, leaving the constant gravitational gradient as the only remaining force moving water downward in this upper or transmission zone. Because the gravitational head gradient has the value of unity, it follows that the water flux tends to approach the saturated hydraulic conductivity as the limiting value. Therefore, in a uniform soil without crust under prolonged ponding, as the water content of the wetted zone approaches saturation, the infiltration rate approaches the saturated hydraulic conductivity. Based on this reasoning, a unit hydraulic gradient and saturated conditions, as described by a saturated hydraulic conductivity, are assumed for the subsurface region below ponded sites.

2.1 Contaminant Concentration Equations

By solving Equation 2.10 with the appropriate boundary and initial conditions, a set of semi-analytical expressions is obtained that characterize the transport of contaminants through the partially saturated and saturated zones. These expressions are based on Green's functions and have been reported by several researchers (e.g., Selim and Mansell 1976; Yeh and Tsai 1976; Yeh 1981; Codell et al. 1982). Various analytical expressions describing solute concentrations at selected locations and times can be described by one basic equation:

$$Ci_\ell = \alpha_m X_i Y_j Z_k \tag{2.13}$$

where Ci_ℓ = solute concentration per unit mass/activity at location x, y, z and time t for an instantaneous source release for the ℓ-th solution (cm^{-3})[(a)(b)]

α_m = parameter that ensures mass balance and that is based on initial and boundary conditions for the m-th assumption (dimensionless)

X_i = Green's function in the x-direction for the i-th solution (cm^{-1})

Y_j = Green's function in the y-direction for the j-th solution (cm^{-1})

Z_k = Green's function in the z-direction for the k-th solution (cm^{-1}).

(a) Based on a unit mass in grams, or a unit activity in curies.

(b) When included in an equation, "Ci" refers to instantaneous solute concentration; otherwise, "Ci" refers to the unit "curies."

α_m is given by the following equations:

$$\alpha_1 = \frac{1}{R_{f1} n_e} \tag{2.14}$$

$$\alpha_2 = \frac{1}{R_{f2} n_e} \tag{2.15}$$

$$\alpha_3 = \frac{1}{R_{f3} n} \tag{2.16}$$

$$\alpha_4 = \frac{1}{R_{f4} \theta} \tag{2.17}$$

Currently, α_1 and α_4 are used in the groundwater pathway.

2.1.1 Green's Functions

The various solutions associated with X_i, Y_j, and Z_k in Equation 2.13 can be derived using Green's relationships (Carslaw and Jaeger 1959; Yeh and Tsai 1976; Yeh 1981) or by the method of separation of variables (Ritger and Rose 1968; Codell et al. 1982). X_i, Y_j, and Z_k reflect the geometry associated with the source (i.e., boundary conditions) releasing the contaminants. For example, a point source and a line source will each have a different solution. The expressions describing X_i, Y_j, and Z_k by source-term type that are incorporated into MEPAS are as follows:

$$X_1 = \left[\frac{1}{4\pi D_x^* t}\right]^{1/2} \exp(-\lambda t) \exp\left[-\frac{(x - u^* t)^2}{4 D_x^* t}\right] \tag{2.18}$$

with $C = 0$ at $t = 0$ or $x = \pm\infty$

where X_1 = the point-source solution in the x-direction with flow in the x-direction (cm^{-1})
x = distance of travel in the x-direction (cm).

$$X_2 = \frac{1}{2l}\exp(-\lambda t)\left\{\operatorname{erf}\left[\frac{x+\frac{l}{2}-u^{*}t}{(4D_x^{*}t)^{1/2}}\right]-\operatorname{erf}\left[\frac{x-\frac{l}{2}-u^{*}t}{(4D_x^{*}t)^{1/2}}\right]\right\} \tag{2.19}$$

with $C = 0$ at $t = 0$ or $x = \pm\infty$

where X_2 = line-source solution in the x-direction with flow in the x-direction (cm^{-1})
l = length of contaminated line source in the x-direction (cm).

$$Y_1 = \left[\frac{1}{4\pi D_y^{*}t}\right]^{1/2}\exp\left[-\frac{y^2}{4D_y^{*}t}\right] \tag{2.20}$$

with $C = 0$ at $t = 0$ or $y = \pm\infty$

where Y_1 = point-source solution in the y-direction with flow in the x-direction for an aquifer of infinite width (cm^{-1})
y = distance of travel in the y-direction (cm).

$$Y_2 = \frac{1}{2b}\left\{\operatorname{erf}\left[\frac{y+\frac{b}{2}}{(4D_y^{*}t)^{1/2}}\right]-\operatorname{erf}\left[\frac{y-\frac{b}{2}}{(4D_y^{*}t)^{1/2}}\right]\right\} \tag{2.21}$$

with $C = 0$ at $t = 0$ or $y = \pm\infty$

where Y_2 = line-source solution in the y-direction with flow in the x-direction for an aquifer of infinite width (cm^{-1})
b = length of contaminated line or area source in the y-direction (cm).

$$Z_1 = \left[\frac{1}{4\pi D_z^{*}t}\right]^{1/2}\exp(-\lambda t)\exp\left[-\frac{(z-w^{*}t)^2}{4D_z^{*}t}\right] \tag{2.22}$$

with $C = 0$ at $t = 0$ or $z = \pm\infty$

where Z_1 = point-source solution in the z-direction with flow in the z-direction (cm^{-1}) (Note: This expression represents the one-dimensional solution of the advective-dispersive transport equation (i.e., Equation 2.10 in the z-direction.)
z = distance of travel in the z-direction (cm)
w^{*} = flow velocity in the z-direction, adjusted for retardation (i.e., ratio of the leach rate and retardation factor) (cm/s).

The point source solution, which is bounded in the vertical direction by the water-table on top and an aquitard on the bottom, is adapted from Yeh (1981), and is given as

$$Z_2 = \frac{1}{h}\left\{1 + 2\sum_{N=1}^{\infty}\left[\exp\left(-\frac{N^2\pi^2 D_z^* t}{h^2}\right)\cos\left(\frac{N\pi z}{h}\right)\right]\right\} \tag{2.23}$$

with $\partial C/\partial z = 0$ at $y = 0$ and $y = h$

where Z_2 = solution in the z-direction for flow in the x-direction (cm^{-1})
z = depth below water table of calculated concentration at the receptor (cm)
h = thickness of aquifer (cm).

In MEPAS, when the exact formulation for the solution in the z-direction (Equation 2.23) does not converge within an adequate time frame, the following equation is used as an approximation (Yeh 1981):

$$Z_2 = \frac{1}{\sqrt{4D_z^* t}}\left\{2\sum_{N=1}^{\infty}\left[\exp\left(-\frac{(z-2Nh)^2}{4D_z^* t}\right)\right] + \sum_{N=1}^{\infty}\left[\exp\left(-\frac{[z-2(N-1)h]^2}{4D_z^* t}\right)\right] + \sum_{N=1}^{\infty}\left[\exp\left(-\frac{[z-2(N+1)h]^2}{4D_z^* t}\right)\right]\right\} \tag{2.24}$$

Under fully mixed conditions in the z-direction, Equation 2.23 reduces to the vertically averaged solution over the total aquifer thickness:

$$Z_2 = \frac{1}{h} \tag{2.25}$$

2.1.2 Solute Concentrations

Solute concentrations are computed by combining Green's functions (i.e., X_i, Y_j, and Z_k) in a multiplicative manner. The types of configurations at the source considered in MEPAS are point source, line

source (in both the x- and y-directions), and area source (in the x-y plane). The various instantaneous solute concentration options addressed by MEPAS for the saturated zone are presented in a form similar to that expressed by Equation 2.13, and are as follows:

Point Source

$$Ci_1 = \alpha_1 X_1 Y_1 Z_2 \tag{2.26}$$

where Ci_1 = solute concentration per unit mass/activity at location x, y, z for an instantaneous release from a point source at the water table (cm^{-3}).

Line Source

$$Ci_3 = \alpha_1 X_2 Y_1 Z_2 \tag{2.28}$$

$$Ci_2 = \alpha_1 X_1 Y_2 Z_2 \tag{2.27}$$

where Ci_2 = solute concentration per unit mass/activity at location x, y, z for an instantaneous release from a line source in the y-direction at the water table (cm^{-3})

Ci_3 = solute concentration per unit mass/activity at location x, y, z for an instantaneous release from a line source in the x-direction at the water table (cm^{-3}).

Area Source

$$Ci_4 = \alpha_1 X_2 Y_2 Z_2 \tag{2.29}$$

where Ci_4 = solute concentration per unit mass/activity at location x, y, z for an instantaneous release from line sources in the x- and y-directions (i.e., horizontal area source) at the water table (cm^{-3}).

Note that when two line-source solutions corresponding to orthogonal directions (e.g., X_2 and Y_2 in Equation 2.29) are combined, a solution results for an area source.

The following equation can be used for calculating concentrations in the partially saturated zone. Although this computation is not performed in MEPAS, this equation is used as the basis for deriving the contaminant flux equation for the partially saturated zone (Equation 2.38):

$$Ci_5 = \frac{\alpha_4 Z_1}{bl} \tag{2.30}$$

where Ci_5 = solute concentration per unit mass/activity at location z, with flow only in the z-direction for an instantaneous release from a point source (cm^{-3}).

Note that Equations 2.13 through 2.30 have been formulated in terms of an instantaneous contaminant release (i.e., a pulse release over zero time). Codell et al. (1982) note that these equations can be generalized for arbitrary time-varying releases by using the convolution integral

$$C(\tau) = \int_0^{\tau} f(t)\, Ci_\ell(\tau - t)\, dt \tag{2.31}$$

where $C(\tau)$ = solute concentration at time τ (g/mL or Ci/mL)
τ = the time over which contaminant concentration is computed (s)
$f(t)$ = source term expressed as a temporally varying contaminant flux (g/s or Ci/s).

2.2 Contaminant Flux Equations

Contaminant fluxes are computed to indicate the transfer of contaminants between successive media (between partially saturated layers, partially saturated and saturated zones, etc.). The fluxes are computed when they leave one medium (e.g., the saturated zone) and act as boundary conditions for the next medium to be modeled (e.g., the surface-water environment). The MEPAS methodology can calculate the flux of a contaminant between partially saturated layers, between a partially saturated layer and the saturated zone, and at the interface where the saturated zone discharges into a surface-water body. It is assumed that if a surface-water body is part of the transport scenario, then it will be the final transporting medium, and all contaminants entering the subsurface environment will eventually enter the water body, except contaminants lost through degradation/decay.

The MEPAS methodology assumes a unidirectional flow field and bases its flux computations on contaminated material crossing a plane perpendicular to the flow axis. Using the saturated zone as an example, the instantaneous flux across a plane oriented perpendicular to the x-direction (i.e., the direction of flow) can be described by the following equation:

$$\frac{dFi_\ell}{dA} = n_e\left(u\,Ci_\ell - D_x\frac{\partial Ci_\ell}{\partial x}\right) \tag{2.32}$$

where Fi_ℓ = contaminant flux per unit mass/activity resulting from an instantaneous release (s^{-1})
A = cross-sectional area perpendicular to the flow direction ($dA = dy\,dz$) (cm^2).

The total flux across the plane is, therefore, described by laterally and vertically integrating Equation 2.32:

$$Fi_\ell = n_e\int_0^{h}\int_{-\infty}^{+\infty}\left(u\,Ci_\ell - D_x\frac{\partial Ci_\ell}{\partial x}\right)dy\,dz \tag{2.33}$$

The temporally distributed contaminant flux (Fi_1) in the longitudinal direction due to an instantaneous release from a point source at $x = 0$ and $t = 0$, as described by Equation 2.26, is given by

$$Fi_1 = \left[\frac{x + u^* t}{(16\pi D_x^* t^3)^{1/2}}\right] \exp\left\{-\left[\frac{(x - u^* t)^2}{4 D_x^* t} + \lambda t\right]\right\} \tag{2.34}$$

The temporally distributed contaminant flux (Fi_2) in the longitudinal direction due to an instantaneous release from an area source at $x = 0$ and $t = 0$, as described by Equation 2.29, is given by

$$Fi_2 = \left[\frac{\exp(-\lambda t)}{l}\right]\left[\frac{1}{4\pi D_x^* t}\right]^{1/2}\left\{u^*(\pi D_x^* t)^{1/2}\left[\text{erf}(A_1) - \text{erf}(A_2)\right]\right. \\ \left. - D_x^*\left[\exp(-A_1^2) - \exp(-A_2^2)\right]\right\} \tag{2.35}$$

in which

$$A_1 = \frac{x + \frac{l}{2} - u^* t}{(4 D_x^* t)^{1/2}} \tag{2.36}$$

$$A_2 = \frac{x - \frac{l}{2} - u^* t}{(4 D_x^* t)^{1/2}} \tag{2.37}$$

The contaminant flux in the vertical direction with flow in the vertical direction (Fi_3) due to an instantaneous release from a point source at $z = 0$ and $t = 0$, as described by Equation 2.30, is given by

$$Fi_3 = \left[\frac{z + w^* t}{(16\pi D_z^* t^3)^{1/2}}\right] \exp\left\{-\left[\frac{(z - w^* t)^2}{4 D_z^* t} + \lambda t\right]\right\} \tag{2.38}$$

where z = distance of travel in the z-direction (cm).

Equations 2.34, 2.35, and 2.38 have been formulated in terms of an instantaneous contaminant release. These equations can be generalized for arbitrary time-varying releases by the use of the convolution integral:

$$F(\tau) = \int_0^\tau f(t) Fi_x(\tau - t)\, dt \tag{2.39}$$

where $F(\tau)$ = contaminant flux at time τ (g/s or Ci/s).

Note that when Equations 2.34, 2.35, and 2.38 were derived, the α_m terms factored out of the solutions.

2.3 Steady-State Groundwater Equations

This section presents the solutions to the three-dimensional advective-dispersive equation under steady-state conditions (Section 2.1 presents the transient solutions). The steady-state solutions were used to verify the transient equations.

The steady-state, one-dimensional, advective-dispersive equation with degradation/decay is used to describe steady-state contaminant transport through the partially saturated zone and is presented as follows:

$$u^* \frac{\partial C}{\partial z} = D_z^* \frac{\partial^2 C}{\partial z^2} - \lambda C \tag{2.40}$$

The solution to Equation 2.40 has been reported by Van Genuchten and Alves (1982) and is presented as follows:

$$C(z) = \left[\frac{2u^* C_o}{u^* + [(u^*)^2 + 4\lambda D_z^*]^{1/2}}\right] \exp\left\{\left[\frac{z}{2D_z^*}\right]\left[u^* - \left((u^*)^2 + 4\lambda D_z^*\right)^{1/2}\right]\right\} \tag{2.41}$$

where $C(z)$ = steady-state contaminant concentration at location z (g/mL or Ci/mL)
C_O = initial contaminant concentration at the source (g/mL or Ci/mL).

The steady-state, vertically averaged, two-dimensional, advective-dispersive equation with degradation/decay is used to describe steady-state contaminant transport through the saturated zone and is presented as follows:

$$u^* \frac{\partial C}{\partial x} = D_x^* \frac{\partial^2 C}{\partial x^2} + D_y^* \frac{\partial^2 C}{\partial y^2} - \lambda C \tag{2.42}$$

The solution to Equation 2.42 has been reported by Sayer (1973) and Reckhow and Chapra (1983) and is presented as follows:

$$C(x,y) = \left[\frac{Qc}{2\pi h_m (D_x^* D_y^*)^{1/2}}\right] \exp\left(\frac{u^* x}{2D_x^*}\right) \text{Ko}\left[\left(x^2 + \frac{D_x^* y^2}{D_y^*}\right)^{1/2}\left[\frac{\lambda}{D_x^*} + \left(\frac{u^*}{2D_x^*}\right)^2\right]^{1/2}\right] \quad (2.43)$$

where $C(x,y)$ = steady-state contaminant concentration at location x and y (g/mL or Ci/mL)
Qc = contaminant flux (boundary condition) (g/s or Ci/s)
h_m = vertical distance in an aquifer over which the contaminant is assumed to be uniformly distributed (cm) (see Equation 2.51)
Ko = modified Bessel function of the second kind, zeroth order (dimensionless).

2.4 Mixing Length Equations

When a contaminant travels from a waste site to a receptor of concern (e.g., well or river), the contaminant is temporally and spatially redistributed--longitudinally, vertically, and laterally--by the transporting medium. At any given distance downgradient from a waste site releasing contaminants to an aquifer of constant thickness, contaminants near the water table can be considered to be fully mixed over some distance in both the lateral and vertical directions. As Codell et al. (1982) note, vertical dispersion close to the point of release is considered to be very small, and is not influenced by the vertical dimensions of the aquifer. As the contaminant moves downgradient from the point of release, the mixed region increases in vertical extent while the aquifer geometry becomes more of an influence in the spatial distribution of contaminant. Eventually, at some distance downgradient from the source, the contaminant becomes fully mixed vertically over the aquifer thickness.

This section briefly identifies the basis for defining the spatial extent of the mixing regions used in the saturated zone component of MEPAS. Vertical and lateral mixing lengths are used when estimating the saturated zone water flux for near-field dilution (see Section 3.3) and for measured concentration scenarios (see Section 4.0). A lateral mixing length is also used to estimate the spatial extent of groundwater contamination at the edge of a surface-water body, and a vertical mixing length is needed by the steady-state equation for the saturated zone (Equation 2.43).

2.4.1 Vertical Mixing Length

The vertical mixing length is the vertical distance over which contamination at some downgradient distance from the source is considered uniformly mixed. The vertical mixing length is estimated by

employing the advective-dispersive equation and its associated Gaussian distribution solution. The one-dimensional, advective-dispersive equation in the vertical direction is written as

$$\frac{\partial C}{\partial t} = D_z^* \frac{\partial^2 C}{\partial z^2} \tag{2.44}$$

The unit area solution to Equation 2.44 in an aquifer of infinite vertical extent is described by

$$C = \frac{M}{\sigma_v (2\pi)^{1/2}} \exp\left(- \frac{z^2}{2\sigma_v^2} \right) \tag{2.45}$$

in which

$$\sigma_v = (2 D_z^* t_t)^{1/2} \tag{2.46}$$

where M = contaminant mass/activity per unit area (g/cm^2 or Ci/cm^2)
σ_v = standard deviation in the vertical direction (cm)
t_t = representative contaminant travel time (defined in Section 2.5) (s).

With the assumption that no contaminant diffusion occurs through the water table once the contaminant has entered the saturated aquifer, contaminant spreading in the vertical direction is only downward. Because of this, the vertical mixing depth for the fully mixed condition is assumed as the dispersive distance associated with one-half the standard deviation:

$$h_m = \frac{1}{2}\sigma_v = \left(\frac{D_z^* t_t}{2} \right)^{1/2} \tag{2.47}$$

where h_m = vertical distance over which the contaminant is assumed to be uniformly distributed (equivalent to one-half the standard deviation) (cm).

To illustrate that Equation 2.47 has a physical basis, a similar mixing depth expression can be developed by defining a time scale associated with complete vertical mixing as similar to the one found in Codell et al. (1982):

$$t_m = \xi \frac{(h_m')^2}{D_z^*} \tag{2.48}$$

where t_m = time to achieve the fully mixed condition (i.e., representative contaminant travel time) (s)
ξ = proportionality coefficient (dimensionless)
h_m' = alternative vertical distance over which the contaminant is assumed to be uniformly distributed (cm).

By rearranging Equation 2.48, the effective depth, which represents the fully mixed condition, can be solved for

$$h_m' = (\phi t_m D_z^*)^{1/2} \tag{2.49}$$

in which

$$\phi = \frac{1}{\zeta} \tag{2.50}$$

where ϕ = proportionality constant (dimensionless).

Codell et al. (1982) note that when $\phi \leq 3.3$, the fully mixed condition can be assumed, because the release may be considered to be unaffected by the confining layer beneath the plume. When ϕ is between 3.3 and 12, the release is considered to be neither fully mixed over the depth of the aquifer nor unaffected by the aquifer boundary. Because Equation 2.47 represents a more conservative expression than Equation 2.49 when ϕ equals 3.3, and because its derivation is consistent with other mixing-length estimations used in the MEPAS methodology, Equation 2.47 is used to describe the vertical mixing length in the groundwater environment.

The MEPAS methodology computes h_m to identify the mixing depth. If h_m is less than the aquifer depth, h_m is used as the mixing depth. If h_m is greater than the aquifer depth, the aquifer depth is used as the mixing length.

Equation 2.47 is valid as long as the waste site remains above the water table. When the waste site penetrates the aquifer (i.e., a portion of the waste site is situated below the water table), the vertical mixing zone is increased by that portion of the waste site below the water table. For a partially penetrating waste site, the mixing depth can be expressed as

$$h_m = \left(\frac{D_z^* t_t}{2} \right)^{1/2} + h_w \tag{2.51}$$

where h_w = depth of the waste site below the water table (cm).

2.4.2 Lateral Mixing Length

The groundwater pathway interacts with the surface-water pathway by supplying the necessary boundary conditions (i.e., temporally varying contaminant fluxes). Unfortunately, the lateral distance over which the groundwater pathway supplies contaminated water may be considered infinite. To alleviate this problem, the MEPAS methodology computes an effective length for the line source used as

the source term for the surface-water transport computations. The lateral mixing length for a conservative substance identifies the extent over which contamination at the groundwater/surface-water interface is considered fully mixed in the lateral direction. The contaminant level is assumed to be uniformly distributed over this lateral region and is used in computing the boundary conditions for modeling the surface-water environment.

As in the case of the vertical mixing length, the lateral mixing length is estimated by employing the advective-dispersive equation and its associated Gaussian distribution solution. The one-dimensional, advective-dispersive equation in the lateral direction is written as

$$\frac{\partial C}{\partial t} = D_y^* \frac{\partial^2 C}{\partial y^2} \tag{2.52}$$

The unit area solution to Equation 2.52 in an aquifer of infinite lateral extent is described by

$$C = \left[\frac{M}{\sigma_l (2\pi)^{1/2}}\right] \exp\left(-\frac{y^2}{2\sigma_l^2}\right) \tag{2.53}$$

in which

$$\sigma_l = (2D_y^* t_l)^{1/2} \tag{2.54}$$

where σ_l = standard deviation in the lateral direction (cm).

The lateral mixing distance for the fully mixed condition, approximately adjusted for a source term of width b, is assumed equal to the dispersion distance associated with one standard deviation:

$$l_m = \sigma_l + b = (2D_y^* t_l)^{1/2} + b \tag{2.55}$$

where l_m = lateral distance over which the contaminant is assumed to be uniformly mixed (cm).

To illustrate that Equation 2.55 has a physical basis, a similar mixing width expression can be developed by equating the longitudinal travel time to the receptor of concern with the time for complete lateral mixing. An estimate of the time scale associated with complete lateral mixing is given by

$$t_m = \xi \frac{(l_m')^2}{D_y^*} \tag{2.56}$$

where l_m' = alternative lateral distance over which the contaminant is assumed to be uniformly distributed (cm).

By rearranging Equation 2.56, an effective width that represents the fully mixed condition can be calculated:

$$l_m' = (\phi t_m D_y^*)^{1/2} \tag{2.57}$$

The mixing length, when approximately adjusted for a source term of width b, can be estimated as

$$l_m' = (\phi t_m D_y^*)^{1/2} + b \tag{2.58}$$

As noted in the previous section, when $\phi \leq 3.3$ in a flow field with a fixed width, the fully mixed condition can be assumed. Because Equation 2.55 represents a more conservative expression than Equation 2.58 when $\phi = 3.3$ and because its derivation is consistent with the other mixing-length estimations used in the MEPAS methodology, Equation 2.55 is used to describe the lateral mixing length in the groundwater environment.

2.5 Travel Time and Time to Peak Equations

To define a vertical or lateral mixing length (see Equations 2.51 and 2.55), a representative travel time has to be identified. As the plume migrates downgradient from the source, some contaminant particles migrate faster than others (i.e., attenuation effect); therefore, a representative travel time must be determined. One technique of estimating the travel time of a contaminant in a groundwater system is to divide the distance the contaminant travels by the flow velocity, adjusted for retardation:

$$t_t = \frac{x}{u^*} \tag{2.59}$$

where t_t = representative contaminant travel time (s)
x = longitudinal distance traveled (cm).

This is the travel time used in the mixing-length equations (discussed in the previous section).

Equation 2.59 usually provides a good estimate of the time to peak of the solute concentration due to an instantaneous release. However, it assumes that dispersion in the flow direction and degradation/decay are negligible. A more precise estimate of the time to peak of a contaminant that does account for dispersion and degradation/decay can be developed. The time to the peak concentration can be estimated by 1) assuming a point source and its accompanying analytical Green's function solution in the direction of flow for an instantaneous release (e.g., Equation 2.18 or 2.22), 2) taking its derivative with respect to time, 3) setting the derivative to zero, and 4) solving for the time to peak. The point-source solution is used, as opposed to the line-source solution, because tests indicate that it

provides an accurate estimation of the time to peak and because its formulation is less complicated than that of a line source. Using Equation 2.18 as an example, we have

$$X_1 = \left(\frac{1}{4 \pi D_x^* t_p} \right)^{1/2} \exp(-\lambda t_p) \exp\left[- \frac{(x - u^* t_p)^2}{4 D_x^* t_p} \right] \tag{2.60}$$

where t_p = time to the peak contaminant concentration (s).

Setting the derivative of Equation (2.60) to zero and solving for the time to maximum concentration gives

$$t_p = \frac{\left[(u^* x)^2 + 4 \lambda D_x^* x^2 + (D_x^*)^2 \right]^{1/2} - D_x^*}{4 \lambda D_x^* + (u^*)^2} \tag{2.61}$$

If degradation/decay is negligible, an estimate of the travel time, which includes advection and dispersion, can be developed:

$$t_t = \frac{\left[(u^* x)^2 + (D_x^*)^2 \right]^{1/2} - D_x^*}{(u^*)^2} \tag{2.62}$$

If dispersion and degradation/decay are negligible, Equations 2.61 and 2.62 reduce to Equation 2.59, as expected.

3.0 Computational Methods

This chapter describes the techniques used to analyze Equations 2.31 and 2.39. In addition, methods employed for near-field/far-field situations, mass conservation, and decay chains are presented.

3.1 Integration Limits

Equations 2.31 and 2.39 are evaluated in MEPAS by a modified Simpson's quadrature for numerical integration (Lyness 1969, 1970). However, as noted by Codell et al. (1982), several special precautions are taken to preserve computational accuracy and efficiency. The terms within the integral sign of the equations can be nearly equal to zero over part of the computational range, if f(t) is equal to zero or if $Ci_i(\tau - t)$ or $Fi_i(\tau - t)$ is equal or nearly equal to zero. If we ensure that $Ci_i(\tau - t)$ or $Fi_i(\tau - t)$ is small enough to provide little to the integration, then integration limits can be developed that improve the computational efficiency of the numerical integration scheme.

Solutions to the advective-dispersive equation (i.e., Equation 2.10) for an instantaneous release have been provided in Equations 2.18 through 2.30 and 2.32 through 2.38. These equations are generalized for arbitrary time-varying releases using the convolution integral (Equations 2.31 and 2.39). Whelan et al. (1987) evaluated Equations 2.31 and 2.39 by a standard Simpson's rule for numerical integration. In an attempt to preserve computational accuracy and to help ensure efficient run times, upper and lower integration limits were defined such that a reasonable and efficient time frame could be developed for defining the source term and routing contaminants through successive media. The method identified by Whelan et al. (1987) made use of the error function argument of the area-source solution (i.e., Equation 5.42 of Whelan et al. 1987). This works well under most situations, but the range that defines the lower and upper limits of integration (i.e., Equations 5.48 through 5.50 in Whelan et al. 1987) was found to be too large at times, resulting in computational inefficiencies. The integration limits identified by Whelan et al. (1987), although correct, were found to be too conservative for groundwater analyses where the flow is relatively slow (e.g., integration of excess zero values). In addition, if the source-term boundary condition (i.e., f(t) in Equation 2.31) has a duration less than the assessment interval "Δt,"[(a)] the integration limits could miss an important portion of the integration, depending on the velocity of groundwater flow.

To ensure that the analysis is covering only the significant portion of the integration, the upper and lower limits are based on the temporal location of the inflection points on the rising and falling limbs of

(a) Note that "Δt" is defined by the difference in the upper and lower integration limits divided by the number of evaluation intervals. For example, if concentrations are analyzed for every 10 years, then Δt equals 10 years. If the peak concentration occurs within the first 10-year interval, then the peak is missed.

the solute concentration for an instantaneous release (e.g., Equation 2.18). These integration limits are then checked against a solution of the product of solute concentration for an instantaneous release and source-term flux as well as the final solution, to ensure that only the significant portion of the integration is included in the analysis.

The integration limits can be approximated by 1) assuming a point source and its accompanying analytical Green's function solution in the direction of flow (e.g., Equation 2.18 or 2.22), 2) taking the second derivative with respect to time, 3) setting the derivative to zero, and 4) iteratively solving for the upper and lower integration limits. The point-source solution is used as opposed to the line- or area-source solution, because tests indicate that it provides an adequate estimation of integration limits under all conditions and because its formulation is less complicated than that of the line or area source.

Setting the second derivative of Equation 2.18 to zero provides the appropriate solution for identifying the inflection points as follows:

$$\frac{d^2(X_1)}{dt^2} = 0 = \left[\frac{-2(u^*)^2}{4D_x^* t}\right] - \left[\frac{16u^* D_x^*(x-u^* t)}{(4D_x^* t)^2}\right] - \left[\frac{32(D_x^*)^2(x-u^* t)^2}{(4D_x^* t)^3}\right] + \left\{\left[\frac{-2u^*(x-u^* t)}{4D_x^* t}\right] - \left[\frac{4D_x^*(x-u^* t)^2}{(4D_x^* t)^2}\right] + \lambda\right\}^2 + \left\{\left[\frac{-2u^*(x-u^* t)}{4D_x^* t}\right] - \left[\frac{4D_x^*(x-u^* t)^2}{(4D_x^* t)^2}\right] + \lambda\right\}\left(\frac{1}{t}\right) + \frac{3}{4t^2} \quad (3.1)$$

Equation 3.1 is solved by iteration to define the lower and upper inflection points, which are used to define the limits of integration.

The integration limits are calculated as a factor of the difference between the time to peak and the inflection point of the instantaneous solution of the advective-dispersive equation for a point source (Equation 2.26). This difference is designated as δ, where the inflection point is defined by Equation 3.1:

$$\delta = t_p - t_{lip} = t_{uip} - t_p \quad (3.2)$$

where t_p = time to peak, where the first derivative of the instantaneous solution to the advective-dispersive equation for a point source is zero (s) (see Equation 2.61)
t_{lip} = lower inflection point (s)
t_{uip} = upper inflection point (s).

The lower (t_1) and upper (t_2) integration limits (prior to the convolution integral transformation) are calculated as

$$t_1 = \begin{cases} t_{lip} - K\delta & \text{for } t_{lip} - K\delta > 0 \\ 0 & \text{for } t_{lip} - K\delta \leq 0 \end{cases} \tag{3.3}$$

$$t_2 = t_{uip} + K\delta \tag{3.4}$$

where t_1 = lower integration limit (s)
t_2 = upper integration limit (s)
K = constant (dimensionless).

The constant K is chosen to ensure that the peak concentration is many orders of magnitude higher than the concentrations associated with the upper or lower integration limit.

3.2 Adaptive Simpson's Quadrature Integration Routine

To help increase the computational efficiency and flexibility of simulating contaminant transport in a series of environmental media, an Adaptive Simpson's Quadrature integration scheme is used. The convolution integrations identified by Equations 2.31 and 2.39 were originally solved by a standard Simpson's rule for numerical integration. Typical problems encountered using a standard Simpson's rule for numerical integration included the following:[a]

- When the difference in the error functions used in the area-source analysis (see Equations 2.19 and 2.21) approaches zero, a round-off error can be propagated in the integration.

- The integration is based on a chosen fixed time step (i.e., Δt). As the time step approaches zero, the integration should approach the true solution. Unfortunately, as the time step approaches zero, the computational efficiency decreases.

To correct these concerns, a modified Simpson's quadrature called the Adaptive Simpson's Quadrature routine is used that varies the magnitude of the integration time step to more accurately reflect variations in the function. In addition, the solution algorithms allow for a dynamic check on accuracy.

The Adaptive Simpson's Quadrature routine is an adaptive numerical integration procedure designed to approximate definite integrals to a specified precision. As used here, an adaptive algorithm is one that automatically changes the solution strategy as the problem being solved becomes easier or more difficult. In simplified form, this procedure is as follows: the integration process is a calculation

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(a) Note that Simpson's rule for numerical integration forms the basis for many specialized integration techniques, including the Adaptive Simpson's Quadrature briefly outlined in this section.

of the area under a function f(t), where t lies within specified time limits. Numerically, this is done by breaking the range of time into a number of time steps, and approximating the area within each. The approximation of the integral is then the sum of the area associated with the individual time steps. More time steps are needed where f(t) changes rapidly than when f(t) changes gently. An adaptive routine automatically determines when f(t) is rapidly changing based on concentration gradients, and reduces the size of each time step.

The Adaptive Simpson's Quadrature routine is based on Simpson's rule and uses an accuracy control feature that dynamically adjusts the tolerance (required accuracy) of the integrand. The tolerance of the integrand is computed by estimating the peak concentration for the integrand and setting the tolerance to be a function of the peak concentration (this tolerance has been tested and is based on the required accuracy of the groundwater model). This accuracy control feature provides reduced computational times while maintaining the desired accuracy of the results. Specific algorithms used are described in Lyness (1969, 1970).

3.3 Features for Far-Field/Near-Field Situations

A given modeling scenario can be considered near-field or far-field depending on several criteria. When a receptor well is located far from a source, the physical dimensions of the source have a negligible effect on receptor concentrations. Under these conditions, a scenario is said to be spatially far-field, and the equations for an area source release reduce to those of a point source release. In other words, from the point of view of the receptor well, the source term looks like a point source. Figure 3.1 shows receptor concentrations for a spatially far-field scenario arbitrarily chosen for illustrative purposes. This chart shows that whether the source term has an areal extent of 0.093 m^2 or 93,000 m^2, concentrations at the receptor well are essentially the same. A scenario in which the physical dimensions of the source have a significant effect on receptor concentrations would be a spatially near-field scenario.

A modeling scenario can also be considered temporally far-field. This occurs when the duration of release from the source is small relative to the time required for the contaminant to travel from the source to the receptor. Thus, the numerically integrated solutions (i.e., Equations 2.31 and 2.39) reduce to the analytical solutions for an instantaneous release. From the point of view of the receptor well, the duration of time over which contaminant is released from the source has little effect on receptor concentrations, so the source-term flux looks like an instantaneous release. A scenario in which the duration of release has a noticeable effect on receptor concentrations would be a temporally near-field scenario.

Under temporally far-field conditions, the groundwater component of MEPAS uses the analytical solutions for an instantaneous release, instead of performing numerical integration. The advantage of this approach is that run times are significantly reduced. For each groundwater medium (i.e., partially

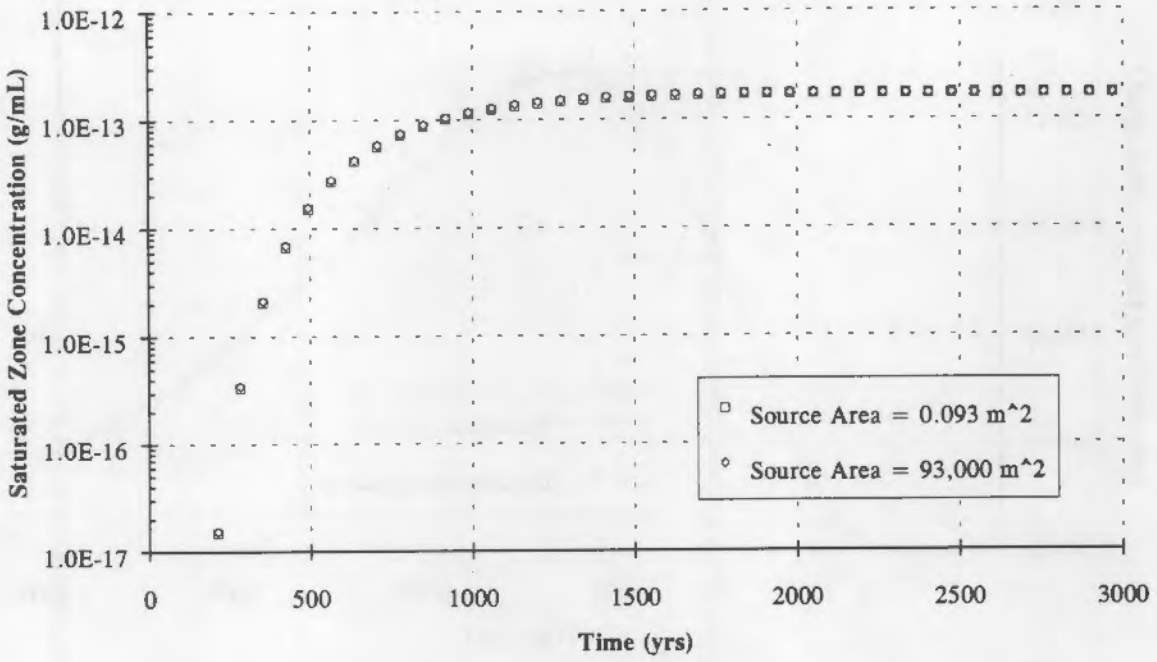

Figure 3.1. Saturated Zone Concentrations for a Spatially Far-Field Scenario

saturated and saturated zones), the ratio of representative travel time to the duration of time over which a contaminant is released to that medium (i.e., the boundary condition) is used to determine if contaminant migration through the medium is temporally far-field:

$$T_{ratio(i)} = \frac{t_{r(i)}}{t_{r(i)}} \tag{3.5}$$

where $T_{ratio(i)}$ = ratio of representative contaminant travel time to the duration of time over which contaminant is released to the i-th medium (dimensionless)

$t_{t(i)}$ = representative travel time for a contaminant in the i-th medium (s) (see Equation 2.59)

$t_{r(i)}$ = duration of time over which a contaminant is released to the i-th medium (s).

Testing has shown that a $T_{ratio(i)}$ of 30 constitutes an appropriate rule-of-thumb threshold value. Thus, if $T_{ratio(i)}$ is greater than or equal to 30, contaminant migration through that medium is considered to be temporally far-field, and the analytical equations for an instantaneous release are used. Otherwise, numerical integration is performed. Figure 3.2 shows both the numerical and instantaneous solutions for a temporally far-field case arbitrarily chosen for illustrative purposes.

Contaminated water from a site leaches from the source through the vadose zone to the water table. The contaminated leachate then mixes with the saturated zone water while migrating to the receptor. This results in a mixing zone or plume in the saturated zone that expands as the contaminant migrates

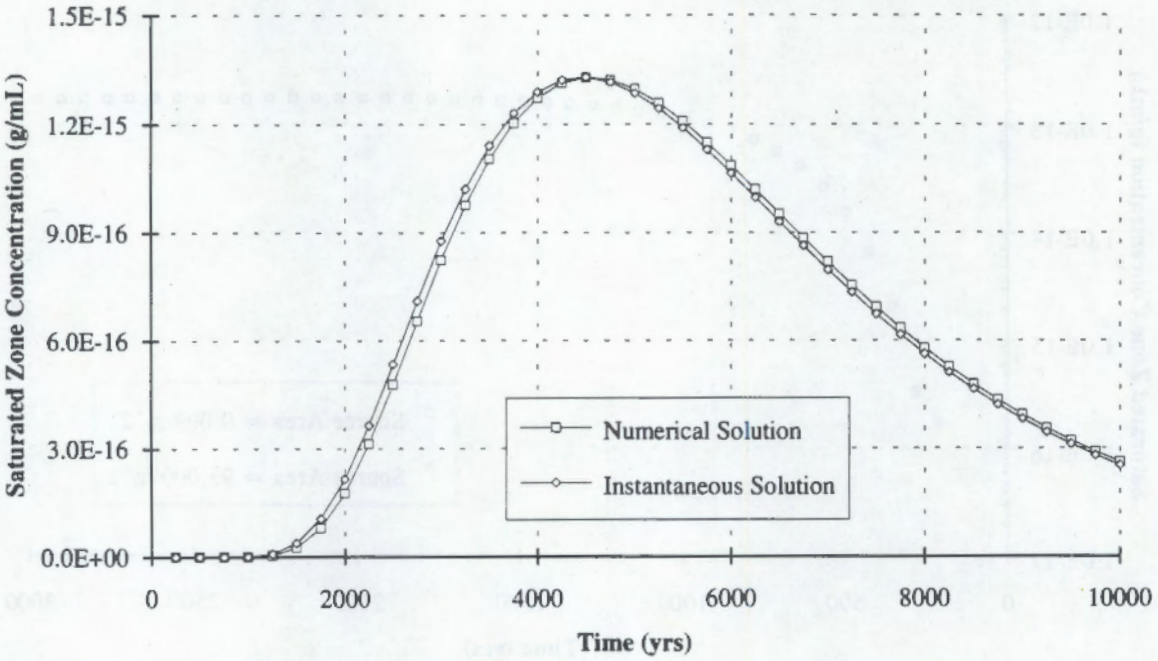

Figure 3.2. Saturated Zone Concentrations for a Temporally Far-Field Scenario ($T_{ratio} = 31$)

from the waste site. MEPAS, as with other flux boundary condition analytical models, assumes that the amount of water entering from the vadose zone is relatively insignificant as compared to the flux of contaminated water at the receptor. Because the cross-sectional area of the plume is a function of distance from the waste site and approaches zero near the waste site for point, line, and area sources at the water table, the volume of water percolating from the vadose zone may be significant relative to the flux of contaminated water at receptor locations near the source. Under these conditions, the assumptions of the model may be violated resulting in over predicted concentrations for receptors near the waste site. As long as the receptor distance from the waste site is sufficiently large, hydrodynamic dispersion will lower the concentrations to more reasonable levels. Because large percolation rates are associated with ponded sites, they create a special concern.

In an attempt to account for the flux of water from the partially saturated zone, MEPAS uses a near-field dilution ratio:

$$W_{ratio} = \frac{Q_{sz}}{Q_{sz} + Q_{psz}} \tag{3.6}$$

where W_{ratio} = ratio of saturated zone water flux to total water flux at the receptor well (dimensionless)

Q_{sz} = saturated zone water flux (cm^3/s)

Q_{psz} = partially saturated zone water flux beneath the source (cm^3/s).

Concentrations at a receptor well computed according to the equations presented in Section 2.1, are multiplied by W_{ratio}, for releases from an area source to the partially saturated zone:

$$C_f = C \cdot W_{ratio} \tag{3.7}$$

where C = computed concentration [Ci_t or $C(\tau)$] (g/mL or Ci/mL)
C_f = final reported solute concentration (g/mL or Ci/mL).

Under near-field conditions, $W_{ratio} < 1$, which accounts for water entering from the partially saturated zone. Under far-field conditions, the saturated zone water flux is much larger than the partially saturated zone water flux, and W_{ratio} approaches unity.

Using a hypothetical example, Figure 3.3 presents receptor concentrations with and without the near-field correction. This example illustrates that the near-field effects of dilution can extend

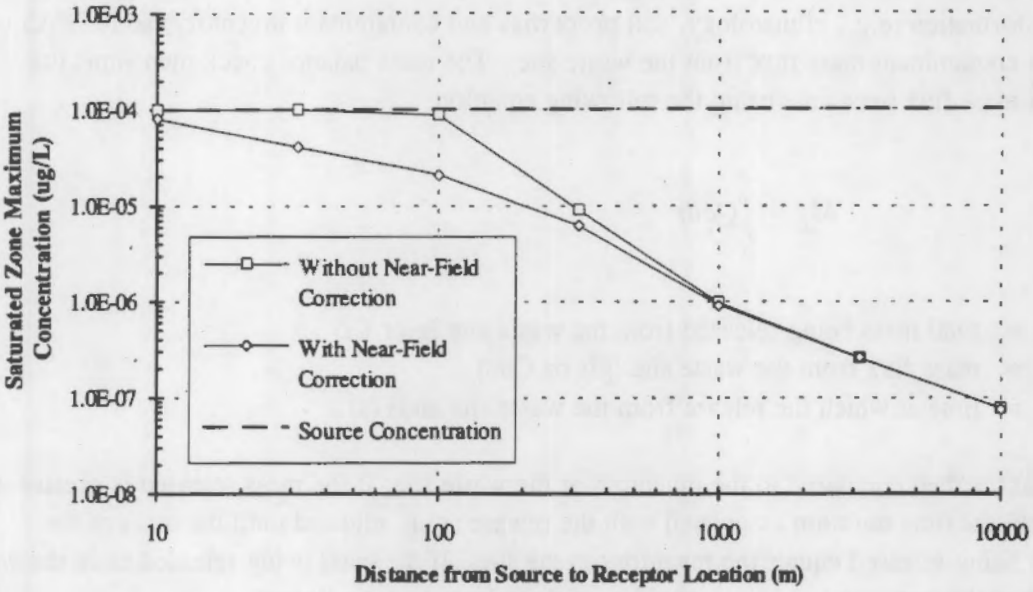

Figure 3.3. Effect of Near-Field Dilution Ratio on Saturated Zone Concentrations for a Near-Field Scenario

significant distances. The figure also demonstrates that for all source term and release type configurations, the code will set receptor concentrations that exceed the source concentration equal to the source concentration. The use of the near-field correction is summarized by the following equation:

$$C_f = \begin{cases} C \cdot W_{ratio}, & C \cdot W_{ratio} < C_o \\ C_o, & C \cdot W_{ratio} \geq C_o \end{cases} \quad (3.8)$$

where C_o = initial contaminant concentration at the source (g/mL or Ci/mL).

3.4 Groundwater Mass Balance at the Source

The analytical equations, in particular Equations 2.33 and 2.39, by definition, conserve mass as the contaminant migrates through the groundwater environment. As a check on the information supplied by the investigator, MEPAS includes a contaminant mass balance check at the source. The investigator either indicates the contaminant mass entering the environment from the waste site, or provides the necessary information (e.g., climatology, soil properties and contaminant inventory) so MEPAS can compute the contaminant mass flux from the waste site. The mass balance check then sums the contaminant mass flux over time using the following equation:

$$M_T = \int_0^{\tau} Qc\, dt \quad (3.9)$$

where M_T = total mass being released from the waste site (g or Ci)
Qc = mass flux from the waste site (g/s or Ci/s)
τ = time at which the release from the waste site ends (s).

The total mass is then compared to the inventory at the waste site; if the mass released is greater than the inventory, the time duration associated with the release (τ) is adjusted until the mass of the contaminant being released equals the inventory at the site. If the mass being released from the waste site is less than the inventory, the time duration of the release is not adjusted.

3.5 Contaminant Degradation/Decay

Although many chemicals have degradation rates that are different for dissolved and adsorbed phases, known degradation rates in many cases are lacking for each. Therefore, MEPAS assumes first-order degradation/decay for all contaminants. For radionuclides that produce decay products, the groundwater model transports the decay products like the parent radionuclide. Once the parent reaches the receptor of concern, the temporal distributions of the important decay products are computed using the Bateman equation (Bateman 1910):

$$C_i = \left(\frac{\lambda_i C_p}{\lambda_1}\right)\left(\prod_{j=1}^{i-1}\lambda_j\right)\left\{\sum_{j=1}^{i}\left[\frac{e^{-\lambda_j t}}{\prod_{\substack{r=1 \\ r\neq j}}^{i}(\lambda_r - \lambda_j)}\right]\right\} \qquad (3.10)$$

where C_p = undecayed parent concentration (Ci/mL)
λ_1 = radiological decay coefficient of the parent (s^{-1})
C_i = decayed concentration of the i-th member of the decay chain (i=1 for the parent, i=2 for the first decay product, etc.) (Ci/mL)
λ_i = radiological decay coefficient of the i-th member of the decay chain (s^{-1}).

Performing the decay computation after transporting the parent radionuclide to the receptor allows for more manageable computations.

Using the Bateman equation to compute decay product concentrations has important consequences. Decay products have chemical properties different from the parent and, in all probability, are absorbed on the soil medium to a greater or lesser extent than the parent. This has two implications (Codell et al. 1982):

- The decay product travels in the ground faster or slower than the parent.
- The decay product is partitioned between the soil and interstitial water differently from the parent. The concentration of the decay radionuclide in the groundwater must, therefore, be corrected for its equilibrium coefficient.

The assumption of equal transport speeds may produce difficulties in a risk analysis when a decay product has a significantly shorter travel time than the parent, a higher dose-conversion factor than the parent, and is persistent enough to reach a receptor. As an indication of how often this may occur, the parent radionuclide constituents having at least one decay product in the MEPAS chemical database were assessed for these conditions. Estimated distribution coefficients for a sandy soil under neutral pH conditions were used as a relative indicator of mobility. Where distribution coefficients were not provided in the database, they were obtained from Serne and Wood (1990). These distribution coefficients are not universally applicable and should not be assumed to apply to any particular site.

Of the 38 decay chains assessed, only six have a decay product with an estimated distribution coefficient at least 20% smaller than the parent, a dose-conversion factor larger than the parent, and a half-life of at least one year. The six parent constituents along with the decay product of concern in their decay chains are listed in Table 3.1. As shown in the table, five of the parents have half-lives less than one year. Thus, it is unlikely that these five would be the subject of a waste site assessment, because of their lack of persistence. One would most likely consider their first decay product as the parent radionuclide. This leaves thorium-230 as the only potential problem, and the dose conversion factor of its decay product of concern is only a factor of two greater. Thus, no decay chains were

Table 3.1. Parent Radionuclides in the MEPAS Chemical Database Having a Decay Product of Greater Toxicity and a Higher Potential Mobility in a Sandy Soil of Neutral pH Conditions. (Note: The constituent in parentheses is one isotope from the parent's decay chain, and thus, is not necessarily the first decay product)

Parent (Decay Product)	Kd (mL/g)	Half-Life (years)	Ingestion Dose-Conversion Factor (rem/pCi)
Ac-228	228.0	7.0E-04	2.2E-07
(Th-228)	100.0	1.9E+00	4.0E-07
Am-242	82.0	1.8E-03	1.4E-09
(Pu-242)	10.0	3.8E+05	3.4E-06
Cm-242	82.0	4.5E-01	1.2E-07
(Pu-238)	10.0	8.8E+01	3.2E-06
Pu-237	10.0	1.2E-01	4.4E-10
(Np-237)	3.0	2.1E+06	4.4E-06
Th-230	**100.0**	**7.7E+04**	**5.5E-07**
(Ra-226)	**24.3**	**1.6E+03**	**1.3E-06**
Th-231	100.0	2.9E-03	1.4E-09
(Pa-231)	0.0	3.3E+04	1.3E-06

identified that would likely pose a significant concern to the results of a risk analysis because such results are considered to be an order of magnitude estimate. While site-specific conditions can certainly alter this conclusion, this short study does indicate that the conditions under which the equal transport speed assumption would pose a significant problem in a risk analysis should not occur very often.

When a contaminant has been disposed of, it spends a portion of its time at the source prior to release into the environment, and a portion of its time migrating in the environment (e.g., through the groundwater system). The time frame associated with the solutions to the advective-dispersive equations with flux boundary conditions inherently includes the total time (i.e., time the contaminant is at the source and in the environment). As with most numerically integrated analytical transport equations, degradation/decay occurs over this total simulation time frame. After assessing a number of waste sites, it became apparent that this time frame was not necessarily the appropriate time to use for decay computations. The use of total simulation time is only appropriate if the contaminant degrades/decays at the same rate at the source as in the environment. For example, if a mass of radionuclide is placed in a landfill at the start of a simulation, it will decay at the same rate at the source and in the environment, and the use of total simulation time is appropriate. Under other circumstances, use of the total simulation time (which is standard practice) is inappropriate. Some examples are as follows:

Scenario 1: A production facility continually produces a waste at a given contaminant level; the waste is continually disposed of at a waste site (i.e., source). The contaminant then leaches or is directly released into the environment to migrate.

Under this scenario, the source is continually replenished with new waste at the original contaminant level. In effect, there is no apparent reduction in the contaminant level at the source (i.e., no apparent degradation/decay). Degradation/decay only occurs while the contaminant is in the environment. Therefore, the time used in computing the degradation/decay should be equal to the time in the environment only.

Scenario 2: A waste is disposed of at a waste facility, and its only significant degradation occurs at the source (e.g., photodegradation); no significant degradation occurs in the environment at this particular site.

Under this scenario, the waste degrades at the source but not in the environment. The time used in computing degradation should only be the time the contaminant remains at the source.

Scenario 3: A waste is disposed of at a waste facility, and the only significant degradation occurs in the environment (e.g., microbial degradation); no significant degradation occurs while the waste is in the waste site proper at this particular site.

Under this scenario, the waste degrades in the environment but not at the source. The time used in computing degradation should be the time in the environment only.

Based on these discussions, three conditions for calculating degradation/decay can exist. These are 1) degradation/decay at the source and in the environment, 2) degradation/decay at the source but not in the environment, and 3) degradation/decay in the environment but not at the source. The MEPAS methodology can handle all of these situations, because it allows the user to specify the correct conditions under which the contaminants will degrade/decay.[a] For the first condition, the total simulation time is used for computing degradation/decay, for the second, only the time at the source is used, and for the third, only the time in the environment is used.

When simulating degradation/decay through multiple environmental media, using the flux from the previous medium as a boundary condition for the succeeding medium (i.e., sequential modeling of media), only the travel times through the succeeding media should be included in the subsequent

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(a) Only one degradation rate can be specified; the degradation/decay rate assumed at the source is equal to that in the environment, if degradation/decay occurs in both. Different degradation rates are not possible using the semianalytical solutions in the MEPAS methodology; mass balance would be violated if different rates were identified. The user has to decide *a priori* where degradation/decay will dominate (i.e., at the source, in the environment, or in both), based on the characteristics at the site.

degradation/decay computations. If the total simulation time is included in the calculation, then degradation/decay in the previous media will be accounted for more than once. MEPAS has been formulated to assure that over accounting for decay does not occur.

4.0 Measured Concentrations in the Groundwater Environment

Contaminant levels are often measured in nearby drinking-water or observation wells prior to a complete remedial investigation at a waste site. Instances also occur where monitored contaminant levels are available, but the nature, extent, and sometimes source of contamination are unknown. A risk assessment methodology should be flexible enough to handle those situations where only monitored information is available from which to perform an analysis.

The MEPAS methodology allows and encourages investigators to assess human health impacts using monitored data whenever possible. As opposed to relying only on transport modeling with its inherent uncertainties to predict contaminant concentrations, actual observed concentrations can be used in the assessment. The concept is that monitoring data are usually more accurate than information resulting from a model simulation. If an investigator selects the measured concentrations option, no transport modeling is performed, and the investigator is required to supply a representative concentration for each constituent being analyzed. This concentration is assumed to be temporally constant, and after the concentration is adjusted as appropriate (see Section 4.3), it is passed to the exposure component of MEPAS to be used in the health assessment.

The MEPAS methodology allows the user to implement measured data scenarios in groundwater, surface-water, surface soil, and atmospheric environments. Of these, the groundwater environment represents a particular challenge. Unlike the other environments, samples cannot easily be collected, as sampling wells must be established for this purpose. As such, the sampling or monitoring well may not represent the same well from which drinking-water supplies are gathered.

In the past, the MEPAS methodology recommended that if monitoring information were available "near" the receptor well of concern, the user should use the monitoring well information as the concentration in the receptor well. Recognizing the deficiencies associated with this approach, MEPAS has been modified to estimate the receptor well concentration, if monitoring well information is available. These estimates do not account for degradation/decay and assume that the monitoring and receptor wells are along the same streamline. The estimate also depends on the distance from the source to both the monitoring and receptor wells. If the source is unknown, then it is still recommended that the monitoring well concentration be used as the receptor well concentration.[a]

The difference in concentrations between the receptor and monitoring wells is assumed to be due to spreading (i.e., dispersion) along the same streamline. For pure plug flow, the concentrations at the monitoring and receptor wells would be the same, as there is no dispersion. When dispersion occurs, the concentration in the upgradient well is higher than the concentration in the downgradient well.

(a) The updated methodology presented here requires the investigator to supply the distances from the source to the monitoring and receptor wells. To use the monitoring well concentration as the receptor well concentration, the investigator would set these two distances equal to the same value. This causes the mixing length ratios in the equations presented in Section 4.3 to reduce to unity.

4.1 Contaminant Spreading in the Vertical Direction

The degree of spreading in the vertical direction can be described by Equation 2.47 in Section 2.4:

$$h_m = \left[\frac{D_z^* t_t}{2}\right]^{1/2} \tag{4.1}$$

in which

$$D_z^* = \frac{D_z}{R_f} \tag{4.2}$$

$$t_t = \frac{x}{u^*} = \frac{xR_f}{u}; \quad u = \frac{xR_f}{t_t} \tag{4.3}$$

$$D_z = u\alpha_z \tag{4.4}$$

$$\alpha_z = \beta x \tag{4.5}$$

where α_z = dispersivity in the z-direction (cm)
β = constant used to determine α_z ($\beta = 1.16 \cdot 10^{-4}$, Mills et al. 1985).

Combining Equations 4.1 through 4.5 and simplifying produces the following expression for vertical mixing length:

$$h_m = \left(\frac{\beta}{2}\right)^{1/2} x \approx 7.62 \cdot 10^{-3} x \tag{4.6}$$

$$h_{mm} = 7.62 \cdot 10^{-3} x_m \tag{4.7}$$

$$h_{mr} = 7.62 \cdot 10^{-3} x_r \tag{4.8}$$

where h_{mm} = vertical mixing length at the monitoring well (cm)
x_m = distance from source to monitoring well (cm)
h_{mr} = vertical mixing length at the receptor well (cm)
x_r = distance from source to receptor well (cm).

4.2 Contaminant Spreading in the Lateral Direction

The degree of spreading in the lateral direction can be described by Equation 2.54 in Section 2.4:

$$l_m = \sigma_l = (2D_y^* t_t)^{1/2} \tag{4.9}$$

in which

$$D_y^* = \frac{D_y}{R_f} \tag{4.10}$$

$$t_t = \frac{x}{u^*} = \frac{xR_f}{u} \; ; \quad u = \frac{xR_f}{t_t} \tag{4.11}$$

$$D_y = u\alpha_y \tag{4.12}$$

$$\alpha_y = \gamma x \tag{4.13}$$

where α_y = dispersivity in the y-direction (cm)
γ = constant used to determine α_y (γ = 0.02, Mills et al. 1985).

Combining Equations 4.9 through 4.13 and simplifying produces the following expression for lateral mixing length:

$$l_m = (2\gamma)^{1/2} x = 0.2x \tag{4.14}$$

$$l_{mm} = 0.2x_m \tag{4.15}$$

$$l_{mr} = 0.2x_r \tag{4.16}$$

where l_{mm} = lateral mixing length at the monitoring well (cm)
l_{mr} = lateral mixing length at the receptor well (cm).

4.3 Equations for Determining Receptor Well Concentrations

Because the difference in concentrations between the receptor and monitoring wells is assumed to be due to dispersion, the ratio of the degree of spreading at these wells can provide the concentration at

the receptor well, if the concentration at the monitoring well is known. The fundamental equation for calculating the concentration at the receptor well, based on a known concentration at a monitoring well, is

$$C_R = C_M \frac{h_{mm}}{h_{mr}} \frac{l_{mm}}{l_{mr}} \tag{4.17}$$

where C_R = concentration at the receptor well (g/mL or Ci/mL)
C_M = concentration at the monitoring well (g/mL or Ci/mL).

Using Equation 4.17, four different conditions can be analyzed; these are as follows and coincide with Figures 4.1 through 4.4, respectively:

- **Condition 1)** - $h \geq h_{mm}$ and $h \geq h_{mr}$ -- Under this condition, the aquifer depth (h) exceeds the mixing depths at both the monitoring and receptor wells, and Equation 4.17 reduces to

$$C_R = C_M \left(\frac{x_m}{x_r} \right)^2 \tag{4.18}$$

Thus, the receptor well concentration is higher than the monitoring well concentration if the receptor well is closer to the source than the monitoring well, and lower if the receptor well is farther from the source. Figure 4.1 illustrates both of these conditions.

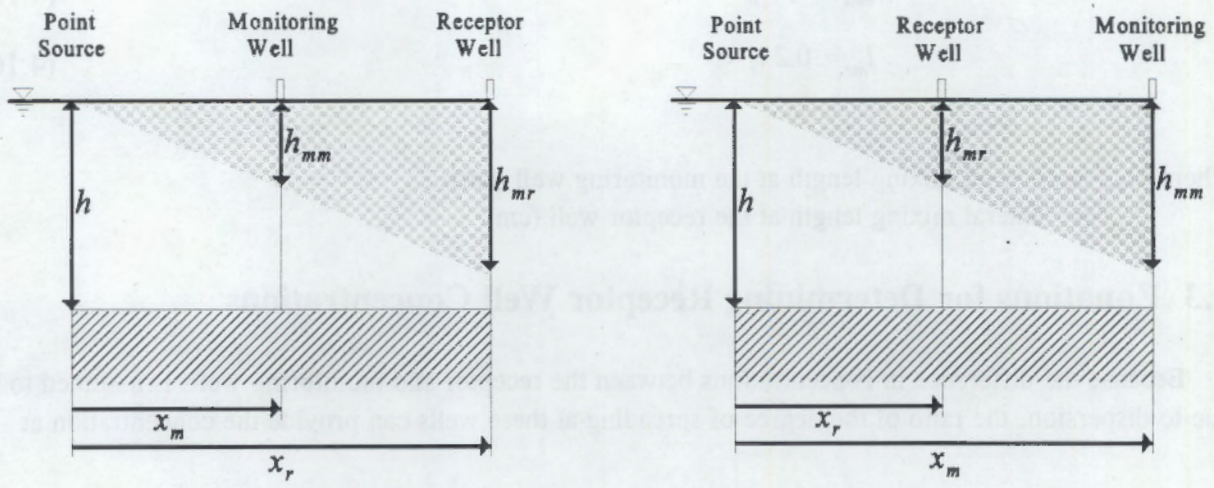

Figure 4.1. Contaminant Plume Not Fully Mixed Over the Aquifer Depth at Either the Monitoring or Receptor Well

- **Condition 2)** - $h \leq h_{mm}$ and $h \leq h_{mr}$ -- Under this condition, the contaminant is fully mixed over the aquifer depth at both wells. Dispersion of contaminant in the z-direction no longer occurs, and Equation 4.17 reduces to

$$C_R = C_M \frac{x_m}{x_r} \tag{4.19}$$

Again, receptor concentrations are higher than the monitoring well concentration if the receptor well is closer to the source than the monitoring well, and lower if the receptor well is farther from the source. Figure 4.2 illustrates this condition.

- **Condition 3)** - $h > h_{mm}$ and $h \leq h_{mr}$ -- Under this condition, the contaminant at the receptor well is fully mixed over the aquifer depth, but is not fully mixed at the monitoring well. In this case, Equation 4.17

$$C_R = C_M \frac{h_{mm} x_m}{h x_r} \tag{4.20}$$

This condition can only occur if the receptor well is farther from the source than the monitoring well (Figure 4.3).

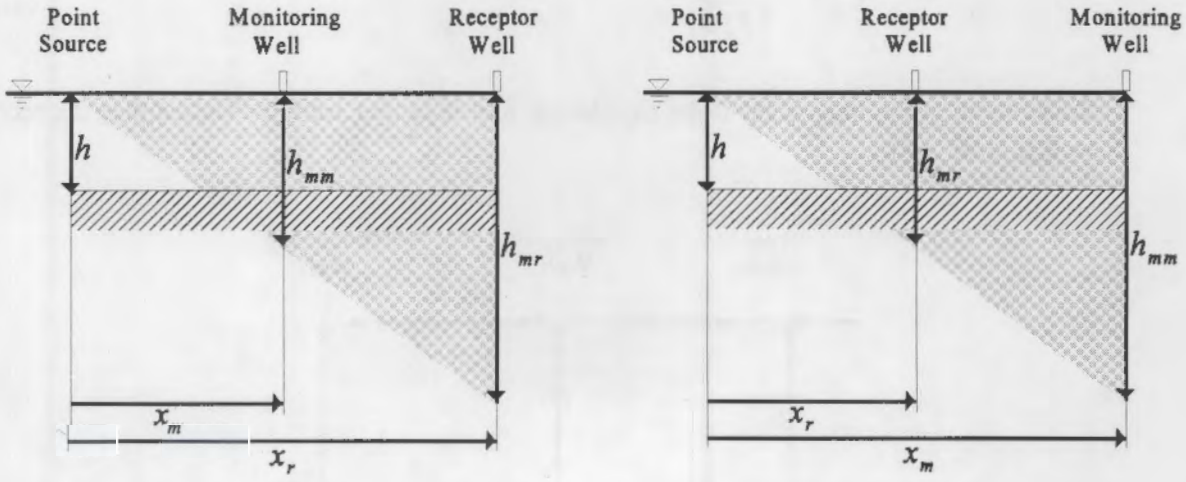

Figure 4.2. Contaminant Plume Fully Mixed Over the Aquifer Depth at Both the Monitoring and Receptor Wells

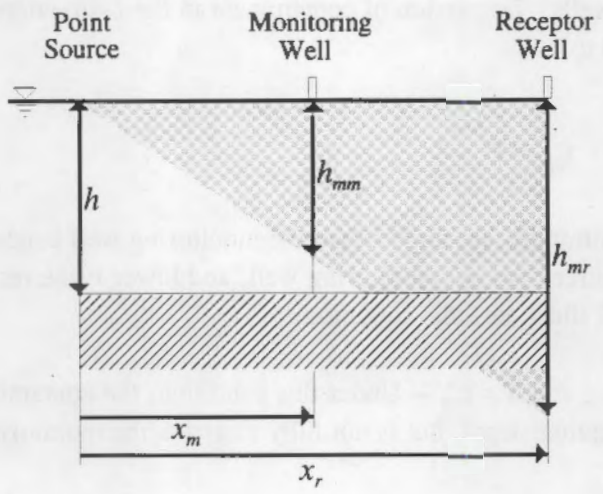

Figure 4.3. Contaminant Plume Fully Mixed Over the Aquifer Depth Only at the Receptor Well

- **Condition 4)** - $h \le h_{mm}$ and $h > h_{mr}$ -- Under this condition, the contaminant at the monitoring well is fully mixed over the aquifer depth, but is not fully mixed at the receptor well. In this case, Equation 4.17 becomes

$$C_R = C_M \frac{h x_m}{h_{mr} x_r} \tag{4.21}$$

This condition can only occur if the monitoring well is farther from the source than the receptor well (Figure 4.4).

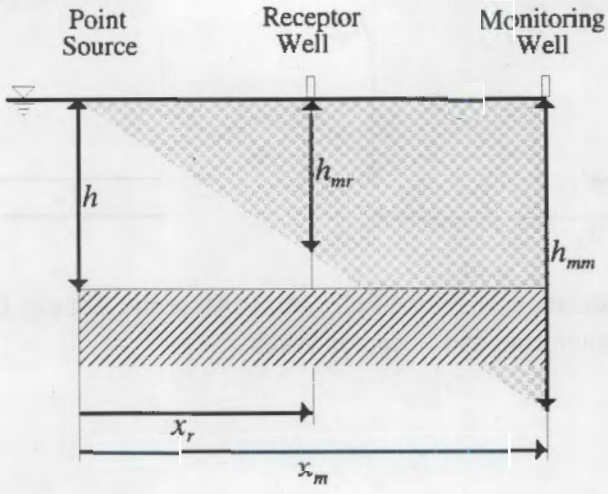

Figure 4.4. Contaminant Plume Fully Mixed Over the Aquifer Depth Only at the Monitoring Well

5.0 Equation Notation

English

A	=	cross-sectional area perpendicular to the flow direction ($dA = dy\ dz$) (cm^2)
b	=	soil type coefficient when used in Equation 2.12 (dimensionless). Length of contaminated line or area source in the y-direction when used elsewhere (cm)
C	=	dissolved concentration in the mobile liquid phase (g/mL or Ci/mL)
C_f	=	final reported solute concentration (g/mL or Ci/mL)
C_i	=	concentration of the i-th member of the decay chain (Ci/mL)
Ci_ℓ	=	solute concentration per unit mass/activity at location x, y, z and time t for an instantaneous source release for the ℓ-th solution (cm^{-3})
Ci_1	=	solute concentration per unit mass/activity at location x, y, z for an instantaneous release from a point source at the water table (cm^{-3})
Ci_2	=	solute concentration per unit mass/activity at location x, y, z for an instantaneous release from a line source in the y-direction at the water table (cm^{-3})
Ci_3	=	solute concentration per unit mass/activity at location x, y, z for an instantaneous release from a line source in the x-direction at the water table (cm^{-3})
Ci_4	=	solute concentration per unit mass/activity at location x, y, z for an instantaneous release from line sources in the x- and y-directions at the water table (i.e., horizontal area source) (cm^{-3})
Ci_5	=	solute concentration per unit mass/activity at location z with flow only in the z-direction for an instantaneous release from a point source (cm^{-3})
C_M	=	concentration at the monitoring well (g/mL or Ci/mL)
C_p	=	undecayed parent concentration (Ci/mL)
C_O	=	initial contaminant concentration at the source (g/mL or Ci/mL)
C_R	=	concentration at the receptor well (g/mL or Ci/mL)
$C(\tau)$	=	solute concentration at time τ (g/mL or Ci/mL)
$C(x,y)$	=	steady state contaminant concentration at location x and y in the saturated zone (g/mL or Ci/mL)
$C(z)$	=	steady state contaminant concentration at location z in the partially saturated zone (g/mL or Ci/mL)
D_{mol}	=	molecular diffusion (cm^2/d)
D_x, D_y, D_z	=	the dispersion coefficients for the mobile liquid phase in the x-, y-, and z-directions, respectively (cm^2/s)
D_x', D_y', D_z'	=	the diffusion coefficients for the immobile liquid phase in the x-, y-, and z-directions, respectively (cm/s)
D_x^*, D_y^*, D_z^*	=	dispersion in the x-, y-, and z-directions, respectively, divided by retardation factor, R_f (cm^2/s)
$f(t)$	=	source term expressed as a temporally varying contaminant flux (g/s or Ci/s)

Fi_t	=	contaminant flux per unit mass resulting from an instantaneous release (s^{-1})
Fi_1	=	the temporally distributed contaminant flux in the longitudinal direction due to an instantaneous release from a point source (g/s or Ci/s)
Fi_2	=	the temporally distributed contaminant flux in the longitudinal direction due to an instantaneous release from an area source (g/s or Ci/s)
Fi_3	=	the temporally distributed contaminant flux in the vertical direction due to an instantaneous release from a point source (g/s or Ci/s)
G	=	dissolved concentration in the immobile liquid phase (g/mL or Ci/mL)
h	=	thickness of aquifer (cm)
h_m	=	vertical distance in an aquifer over which the contaminant is assumed to be uniformly distributed (cm)
h'_m	=	alternative vertical distance in an aquifer over which the contaminant is assumed to be uniformly distributed (cm)
h_{mm}	=	vertical mixing length at the monitoring well (cm)
h_{mr}	=	vertical mixing length at the receptor well (cm)
h_w	=	depth of the waste site below the water table (cm)
K	=	constant when used in the integration limit equations (Equations 3.3 and 3.4) (dimensionless). Hydraulic conductivity when used elsewhere (cm/s)
Kd	=	equilibrium (partition or distribution) coefficient (mL/g)
Ko	=	modified Bessel function of the second kind, zero order (dimensionless)
K_s	=	saturated hydraulic conductivity (i.e., permeability) (cm/s)
l	=	length of contaminated line source in the x-direction (cm)
l_m	=	lateral distance in an aquifer over which the contaminant is assumed to be uniformly mixed (cm)
l'_m	=	alternative lateral distance in an aquifer over which the contaminant is assumed to be uniformly distributed (cm)
l_{mm}	=	lateral mixing length at the monitoring well (cm)
l_{mr}	=	lateral mixing length at the receptor well (cm)
M	=	contaminant mass per unit area (g/cm^2 or Ci/cm^2)
M_T	=	total mass being released from the waste site (g or Ci)
m	=	empirically based parameter that is a function of soil properties (dimensionless)
n	=	total porosity (dimensionless)
n_e	=	effective porosity (dimensionless)
P	=	particulate concentration on the solid phase (g/g or Ci/g)
Qc	=	mass flux from the waste site (g/s or Ci/s)
Q_{psz}	=	partially saturated zone water flux beneath the source (cm^3/d)
Q_{sz}	=	saturated zone flux of contaminated water past a receptor well (cm^3/d)
R_{fm}	=	retardation factor for the m-th assumption (dimensionless)
t	=	time (s)
t_1	=	lower integration limit (s)
t_2	=	upper integration limit (s)
t_{lip}	=	lower inflection point (s)
t_m	=	time to achieve the fully mixed condition (i.e., representative contaminant travel time) (s)

t_p = time to peak, where the first derivative of the instantaneous solution to the advective-dispersive equation for a point source is zero (s)

$t_{r(i)}$ = duration of time over which a contaminant is released to the i-th medium (s)

$T_{ratio(i)}$ = ratio of time to peak to duration of time over which contaminant is released to the i-th medium (dimensionless)

t_t = representative contaminant travel time (s)

$t_{t(i)}$ = representative travel time for a contaminant in the i-th medium (s)

t_{uip} = upper inflection point (s)

u = the x-component groundwater velocity (also referred to as pore-water, seepage, or average linear velocity) (cm/s)

u^* = the x-component groundwater velocity divided by retardation factor, R_f (cm/s)

W_{ratio} = ratio of saturated zone water flux to total water flux at the receptor well (dimensionless)

w^* = flow velocity in the z-direction, adjusted for retardation (i.e., ratio of the seepage rate and retardation factor) (cm/s)

X_i = Green's function in the x-direction for the i-th solution (cm^{-1})

X_1 = the point-source solution in the x-direction with flow in the x-direction (cm^{-1})

X_2 = line-source solution in the x-direction with flow in the x-direction (cm^{-1})

x = distance of travel in the x-direction (cm)

x_m = distance from source to monitoring well (cm)

x_r = distance from source to receptor well (cm)

Y_j = Green's function in the y-direction for the j-th solution (cm^{-1})

Y_1 = point-source solution in the y-direction with flow in the x-direction for an aquifer of infinite width (cm^{-1})

Y_2 = line-source solution in the y-direction with flow in the x-direction for an aquifer of infinite width (cm^{-1})

y = distance of travel in the y-direction (cm)

Z_k = Green's function in the z-direction for the k-th solution (cm^{-1})

Z_1 = point-source solution in the z-direction with flow in the z-direction (cm^{-1})

Z_2 = spatially varying solution in the z-direction (cm^{-1})

z = distance of travel in the z-direction with flow in the x-direction when used in Equations 2.22, 2.38 and 2.41 (cm). Depth below the water table of calculated concentration at the receptor when used elsewhere (cm)

Greek

α_m = parameter that ensures mass balance and that is based on initial and boundary conditions for the m-th assumption (dimensionless)

$\alpha_x, \alpha_y, \alpha_z$ = dispersivity in the x-, y-, and z-directions, respectively (cm)

β = constant used to determine α_z for measured concentrations in the groundwater environment (dimensionless)

β_d = bulk density (g/cm^3)

γ = constant used to determine α_y for measured concentrations in the groundwater environment (dimensionless)

λ = decay constant [(ln 2)/(half-life)] (s^{-1})

λ_1 = radiological decay coefficient of the parent (s^{-1})

λ_i = radiological decay coefficient of the i-th member of the decay chain (s^{-1})

θ = moisture content of the partially saturated zone (dimensionless)

ξ = proportionality constant in the alternative mixing length equations (dimensionless)

ρ_s = soil particle density (g/cm^3)

σ_l, σ_v = standard deviation of the Gaussian distribution of the one-dimensional advective-dispersive equation in the lateral and vertical directions, respectively (cm)

τ = the time over which contaminant concentration is computed (s)

ϕ = proportionality constant in the alternative mixing length equations (reciprocal of ξ) (dimensionless)

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