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

G. Whelan
J. P. McDonald

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

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Pacific Northwest National Laboratory
Richland, Washington 99352

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 radioactive 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; transport of contaminants through the air, groundwater, surface-water, or overland pathways; and 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 platform 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 surface-water component of MEPAS.

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Summary

This report describes the mathematical formulations used for contaminant fate and transport in the riverine pathway of the Multimedia Environmental Pollutant Assessment System (MEPAS). Of the many types of surface-water bodies (e.g., nontidal rivers, estuaries, lakes, open coasts, reservoirs, impoundments, etc.) in which contaminant fate and transport could be simulated, only a nontidal river model is currently incorporated into MEPAS. Nontidal rivers refer to freshwater bodies with unidirectional flow in definable channels. Because the MEPAS methodology is compositely coupled, other surface-water models can be added when deemed necessary.

The surface-water component of MEPAS provides estimates of contaminant concentrations in a river at locations downstream from a release point. The computed contaminant concentrations are used by the exposure assessment component of MEPAS to calculate dose and the resulting health effects to the surrounding population. Potential exposure of humans to contaminants via rivers can be associated with ingestion (e.g., drinking contaminated water), inhalation of volatile pollutants (e.g., showering), dermal contact to chemicals (e.g., swimming), or external dose from radionuclides (e.g., swimming).

Because annual-average contaminant releases to a river in the MEPAS methodology are relatively long term compared to typical contaminant travel times in a river, the migration and fate of contaminants through the riverine pathway are described by the steady-state, two-dimensional advective-dispersive equation for solute transport. The results are based on an analytical solution that is well established in the scientific literature. The surface-water equation accounts for the major mechanisms of constituent persistence (i.e., degradation/decay), advection, and hydrodynamic dispersion. 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 longitudinal direction. Hydrodynamic dispersion is accounted for in the lateral direction. The processes associated with adsorption/desorption between the water column and suspended and bed sediments are not addressed. Neglecting these processes should, in most cases, represent a conservative assumption with regard to water column contaminant concentrations.

Contamination can enter the riverine environment in one of three ways. The groundwater pathway can supply transient contaminant fluxes along the stream bank adjacent to the aquifer. Overland runoff can supply nonpoint-source contaminant fluxes from the land adjacent to the stream. Finally, the surface-water component of MEPAS allows direct discharges to the stream.

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.

- Flow is steady and uniform in the longitudinal direction.

- The effects of contaminant adsorption to or desorption from sediment particles suspended in the water column or in the river bed are negligible; therefore, all contaminants travel at the same speed as the river flow.

- Contaminant releases to the riverine pathway are assumed to be long term relative to the travel time in the river. Therefore, a steady-state solution to the advective-dispersive equation is applicable for describing contaminant transport (Section 2.0).

- The river geometry can be represented by a rectangular cross-section.

- A line source along the stream bank can be approximated as a point source located at the center of the line source; therefore, only the point source equation is used in MEPAS (Section 2.1).

- Advection dominates dispersion in the longitudinal direction, and the contaminant plume is assumed to be fully mixed over the depth of the river; therefore, dispersion is only considered in the lateral direction.

- An appropriate lateral dispersion coefficient can be estimated based on the flow velocity and depth of the river (Section 2.5).

- Degradation/decay for all contaminants is first-order.

- The single concentration value specified by the user for the measured concentrations option is assumed to be temporally constant.

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The authors thank Keith Shields for his technical review of this document, Robert Buchanan for editorial review, and Vickie Atkinson for helping to prepare the manuscript. Thanks are also extended to Larry Bagaasen, John Buck, Karl Castleton, Jim Droppo, Gariann Gelston, Andre dé Hamer, Bonnie Hoopes, Chikashi Sato, Dennis Strenge, and Monique Van der Aa, 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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Figure

1.0 Introduction

This report describes the mathematical formulations used for contaminant fate and transport in the riverine 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:

- Source-Term Release (Streile et al. in press) - presents the mathematical formulations for simulating the release of contaminants from a source term to the atmospheric and waterborne transport pathways.
- Groundwater Pathway (Whelan et al. 1996) - presents the mathematical formulations for contaminant fate and transport in the groundwater pathway of MEPAS.
- Atmospheric Pathway (Droppo and Buck 1996) - presents the mathematical formulations for 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.

The surface-water component of MEPAS provides estimates of contaminant concentrations in a river at locations downstream from a release point. The computed contaminant concentrations are used by the exposure assessment component of MEPAS to calculate dose and the resulting health effects to the exposed population. Potential exposure of humans to contaminants via rivers can be associated with ingestion (e.g., drinking contaminated water), inhalation of volatile pollutants (e.g., showering), dermal contact to chemicals (e.g., swimming), or external dose from radionuclides (e.g., swimming). A schematic diagram illustrating the riverine pathway is presented in Figure 1.1.

Because contaminant releases to a river in the MEPAS methodology are generally of long duration relative to the travel time from the point of release to a receptor, the migration and fate of contaminants through the riverine pathway are described by the steady-state, two-dimensional advective-dispersive equation for solute transport. The results are based on an analytical solution that is well established in the scientific literature. The surface-water equation accounts for the major mechanisms of constituent persistence (i.e., degradation/decay), advection, and hydrodynamic dispersion. 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 longitudinal direction. Hydrodynamic dispersion is accounted for in the lateral direction. The

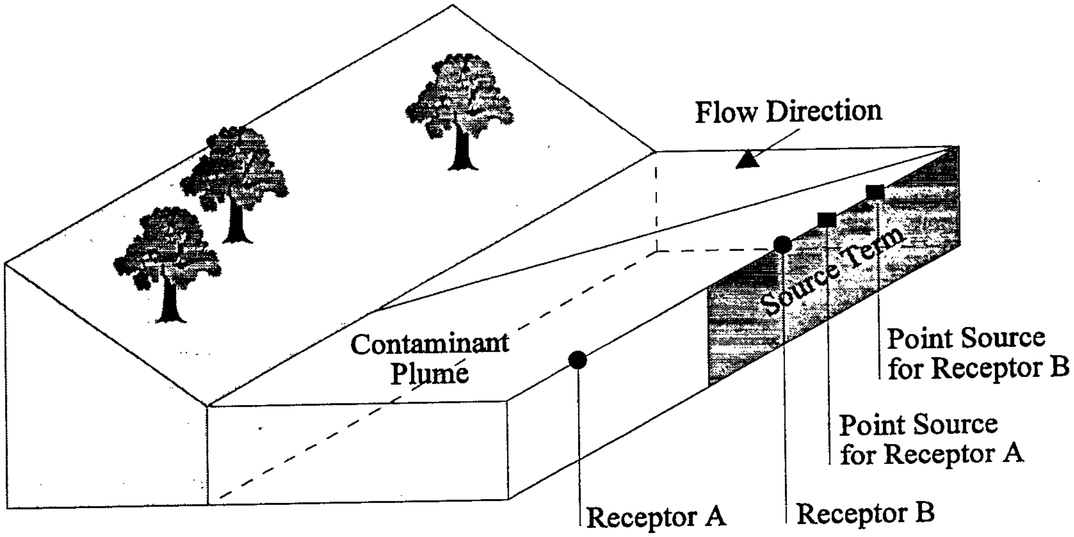

Figure 1.1. Schematic Diagram Illustrating the Riverine Pathway.

processes associated with adsorption/desorption between the water column and suspended and bed sediments are not addressed. Neglecting these processes should, in most cases, represent a conservative assumption with regard to water column contaminant concentrations.

Contamination can enter the riverine pathway in one of three ways. The groundwater pathway can supply transient contaminant fluxes along the stream bank adjacent to the aquifer. Overland runoff can supply nonpoint-source contaminant fluxes from the land adjacent to the stream. Finally, contaminants can be discharged directly to the river.

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 riverine environment. The form of the equation used is briefly discussed.
- Contaminant Concentration Equation - The solution to the advective-dispersive equation used in the riverine component is presented. The solution describes contaminant concentrations.

- Multiple River Receptors - The technique employed to estimate concentrations for more than one river receptor is presented.

- Mixing Length - A lateral mixing length is defined, which describes the lateral distance in which the migrating solute plume can be considered to be fully mixed, and is used in the multiple river receptor estimation technique. The time for the contaminant to travel from the waste site through the river to a receptor of concern as well as the lateral dispersion coefficient are also described. Both are used in determining mixing lengths.

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

- Contaminant Degradation/Decay - The technique for computing the degradation of chemicals and/or the decay of radionuclides is described, as well as the algorithms used to assess degradation/decay at the source of contamination only, in the environment only, or both.

- Surface Water Mass Balance at the Source - This section briefly describes the features included in the MEPAS methodology to ensure that mass is conserved in the analysis.

- Measured Concentrations in the Riverine Environment - This section describes the option within the methodology of using measured environmental contaminant levels in the assessment of health impacts to downstream sensitive receptors, as opposed to performing transport calculations to estimate these environmental concentrations.

Chapter 4.0 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 river forms the basis of the mathematical algorithm used by the riverine component. The surface-water flow is assumed to be steady and uniform; the algorithms are developed for the limiting case of unidirectional advective transport with three-dimensional (longitudinal, lateral, and vertical) dispersion. The advective-dispersive equation for solute movement in a river can be described by the following expression:

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = D_x\frac{\partial^2 C}{\partial x^2} + D_y\frac{\partial^2 C}{\partial y^2} + D_z\frac{\partial^2 C}{\partial z^2} - \lambda C \qquad (2.1)$$

where

C = dissolved instream contaminant concentration (g mL^{-1} or Ci mL^{-1})[(a)]

u = average instream flow velocity (cm s^{-1})

D_x,D_y,D_z = dispersion coefficients in the x-, y-, and z-directions, respectively (cm^2 s^{-1})

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

Equation 2.1 does not take into account the effects of contaminant adsorption to or desorption from sediment particles suspended in the water column or in the river bed. As explained in Chapter 1.0, this should result in conservative aqueous concentrations in most cases.

Contaminant releases to the riverine pathway in the MEPAS methodology are generally of long duration relative to the travel time from the point of release to the receptor. Because transient solutions for contaminant migration and fate are most applicable for batch and infrequent releases over relatively short periods of time (Codell et al. 1982), a steady-state solution to the advective-dispersive equation is used in the riverine component of MEPAS. The steady-state, vertically-integrated, mass-balance equation for transport in a river (where longitudinal advection dominates longitudinal dispersion) can be written as follows:

$$u\frac{\partial C}{\partial x} = D_y\frac{\partial^2 C}{\partial y^2} - \lambda C \qquad (2.2)$$

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

in which

$$\frac{\partial C}{\partial y} = 0 \tag{2.3}$$

at y = 0 and y = B

where

B = width of stream channel (cm).

2.1 Contaminant Concentration Equation

When Equation 2.2 is solved with the appropriate boundary conditions (i.e., Equation 2.3), the riverine pathway is described by an analytical expression that characterizes the transport of contaminants through a river. For a point-source[(a)] contaminant release from the bank of a stream having a rectangular cross-section, the solution to Equation 2.2 employing the boundary conditions defined by Equation 2.3 is very similar to those outlined by Codell et al. (1982), Strenge et al. (1986), and Whelan et al. (1986):

$$C = \left(\frac{Qc}{uBh}\right) \exp\left(-\frac{\lambda x}{u}\right) \left\{1 + 2\sum_{n=1}^{\infty} \left[\exp\left(-\frac{n^2\pi^2 D_y x}{uB^2}\right)\left(\cos\frac{n\pi y}{B}\right)\right]\right\} \tag{2.4}$$

where

Qc = contaminant flux at the source (g s^{-1} or Ci s^{-1})
h = depth of stream (cm)
x = downstream distance to receptor (cm)
y = lateral distance to receptor (cm).

The concentration at y = 0 is used in computing contaminant levels for the exposure component of the MEPAS methodology. By assuming that y equals 0, Equation 2.4 reduces to

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(a) The term "point source" refers to the source-term configuration, which reflects simplifying assumptions, and does not refer to the exact technical definition associated with the concentration equation. Note, for example, that a vertically averaged point source represents a point source in the x and y directions, and a line source in the z-direction.

$$C = \left(\frac{Qc}{uBh}\right) \exp\left(-\frac{\lambda x}{u}\right) \left\{1 + 2\sum_{n=1}^{\infty} \left[\exp\left(-\frac{n^2\pi^2 D_y x}{uB^2}\right)\right]\right\} \tag{2.5}$$

A line source along the edge of the stream can be represented as a series of point sources along the length of the line source. As the downstream receptor location is moved farther away, the line source resembles a point source located at the center of the line source (Receptor A in Figure 1.1). As the receptor location is moved closer to the center of the line source, only that portion of the source term upstream of the receptor has an opportunity to influence contaminant levels at the receptor; in effect, the strength of the source term is reduced. Under these circumstances, the line source can be approximated as a point source that is located at one-half the distance between the receptor location and the upstream end of the line source (Receptor B in Figure 1.1), and the reduced strength of the source is accounted for by multiplying Equation 2.5 by the fraction of the source term upstream of the receptor:

$$f = \frac{l_{ur}}{l_s} \tag{2.6}$$

where

f = fraction of the source term upstream of the receptor (dimensionless)
l_{ur} = length of the source term upstream of the receptor (cm)
l_s = total length of the source term (cm).

Therefore, only the point source solution is used in the surface-water component of MEPAS.

Discharge in a river channel varies along the length of the river, generally increasing in the downstream direction due to inflowing tributary streams and groundwater. The riverine component accounts for an increase in discharge between the source location and the receptor location by using a dilution ratio:

$$Q_{ratio} = \frac{Q_r}{Q_s} \tag{2.7}$$

where

Q_{ratio} = dilution ratio (dimensionless)
Q_r = river discharge at the receptor location ($cm^3\ s^{-1}$)

Q_s = river discharge at the source location (cm^3 s^{-1}).

Incorporating Equations 2.6 and 2.7 into Equation 2.5 gives the final form of the steady-state equation used to simulate concentrations in the riverine component of MEPAS:

$$C = Q_{ratio} \cdot f \cdot \left(\frac{Qc}{uBh} \right) \exp\left(-\frac{\lambda x}{u} \right) \left\{ 1 + 2 \sum_{n=1}^{\infty} \left[\exp\left(-\frac{n^2 \pi^2 D_y x}{uB^2} \right) \right] \right\} \tag{2.8}$$

2.2 Multiple River Receptors

When more than one river receptor is specified in a MEPAS run, an estimation technique is employed to calculate concentrations at the second and subsequent receptors, rather than using Equation 2.8. The method estimates contaminant concentrations for the current receptor based on concentrations for the previous receptor as follows:

$$C_n = C_{n-1} \cdot \frac{Q_{r(n-1)}}{Q_{r(n)}} \cdot \frac{l_{m(n-1)}}{l_{m(n)}} \cdot \frac{f_n}{f_{n-1}} \tag{2.9}$$

where

C_n = contaminant concentration for the current receptor (g mL^{-1} or Ci mL^{-1})
C_{n-1} = contaminant concentration for the previous receptor (g mL^{-1} or Ci mL^{-1})
$Q_{r(n)}$ = river discharge at the current receptor location (mL s^{-1})
$Q_{r(n-1)}$ = river discharge at the previous receptor location (mL s^{-1})
$l_{m(n)}$ = lateral mixing length at the current receptor location (cm)
$l_{m(n-1)}$ = lateral mixing length at the previous receptor location (cm)
f_n = fraction of the source term upstream of the current receptor (dimensionless)
f_{n-1} = fraction of the source term upstream of the previous receptor (dimensionless).

2.3 Lateral Mixing Length

The mixing length is the distance over which contamination is considered fully mixed in the lateral direction and is used in Equation 2.9. The 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

$$\frac{\partial C}{\partial t} = D_y \frac{\partial^2 C}{\partial y^2} \tag{2.10}$$

The unit area solution to Equation 2.10 in a river of infinite lateral extent is described by

$$C = \left(\frac{M}{\sigma_l (2\pi)^{1/2}} \right) \exp\left(-\frac{y^2}{2\sigma_l^2} \right) \tag{2.11}$$

in which

$$\sigma_l = (2 D_y t_t)^{1/2} \tag{2.12}$$

where

M = contaminant mass or activity per unit area (g cm^{-2} or Ci cm^{-2})
σ_l = standard deviation in the lateral direction (cm)
t_t = representative contaminant travel time (s).

With the assumption that contaminant dispersion does not occur through the river banks once the contaminant has entered the river, contaminant spreading is only in the lateral direction. Therefore, the lateral mixing length for the fully mixed condition is assumed as the dispersive distance associated with one-half the standard deviation:

$$l_m = \frac{1}{2}\sigma_l = \left(\frac{D_y t_t}{2} \right)^{1/2} \tag{2.13}$$

where

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

To illustrate that Equation 2.13 has a physical basis, a similar mixing-length expression can be developed by defining a time scale associated with complete lateral mixing as similar to the one found in Codell et al. (1982):

$$t_m = \xi \frac{(l_m')^2}{D_y} \tag{2.14}$$

where

t_m = time to achieve the fully mixed condition (i.e., representative contaminant travel time) (s)

ξ = proportionality coefficient (dimensionless)

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

By rearranging Equation 2.14, the effective length, which represents the fully mixed condition, can be solved for

$$l_m' = (\phi t_m D_y)^{1/2} \tag{2.15}$$

in which

$$\phi = \frac{1}{\xi} \tag{2.16}$$

where

ϕ = proportionality constant (dimensionless).

Codell et al. (1982) note that when $\phi \leq 3.3$, the fully mixed condition can be assumed. When ϕ is between 3.3 and 12, the release is considered to be neither fully mixed over the width of the river nor unaffected by the river boundary. Because Equation 2.13 represents a more conservative expression than Equation 2.15 when ϕ equals 3.3, Equation 2.13 is used to describe the lateral mixing length in the riverine environment.

The MEPAS methodology computes l_m to identify the mixing width. If l_m is larger than the width of the river, l_m is set equal to the width of the river. This procedure ensures a continuous transition between the fully mixed condition and non-fully mixed condition.

2.4 Representative Contaminant Travel Time

To use Equation 2.13, a representative travel time has to be identified. The MEPAS waterborne components recognize three travel times: 1) the advective travel time, 2) the travel time due to advection and dispersion, 3) the time to the peak flux or concentration (which includes advection, dispersion, and decay). Longitudinal dispersion is not considered by the riverine component, because advection is assumed to dominate dispersion in the flow direction. In addition, including the effects of decay produces an apparent travel time that is not indicative of the average time required for a particle to travel from the source to the receptor. Thus, the advective travel time is used in Equation 2.13:

$$t_t = \frac{x}{u} \tag{2.17}$$

The use of advective travel time in Equation 2.13 is consistent with the riverine mixing zone equation given in Mills et al. (1985).

2.5 Lateral Dispersion Coefficient

The transverse dispersion coefficient is required by Equations 2.8 and 2.13. Accurately defining this parameter for all riverine systems under all conditions is difficult. The coefficient is, therefore, defined such that representative properties of the water body are considered in the estimation.

Fischer et al. (1979) note that dispersion in rivers is generally related to the characteristics of the river using the following relationship:

$$D_y = \beta h u^* \tag{2.18}$$

where

β = proportionality constant (dimensionless)
u^* = shear velocity (cm s^{-1}).

Fischer[(a)] and Fischer et al. (1979) note that researchers (e.g., Orlob 1959; Sayre and Chamberlain 1964; Sayre and Chang 1968; Engelund 1969; Prych 1970; Elder 1959; Okoye 1970; Glover 1964; Fischer 1967; Yotsukura et al. 1970) have defined a range of values for β. In laboratory flumes, β ranges from 0.5 to 2.4. For practical purposes, Fischer (1967) suggests that $\beta = 0.6$.

The shear velocity is estimated by Fischer (1974) by assuming that it is directly proportional to the average flow velocity of the stream (u):

$$u^* = 0.10u \tag{2.19}$$

(a) Fischer, H. B. Date Unknown. "Longitudinal Dispersion and Turbulent Mixing in Open Channel Flow." Working Paper. University of California at Berkeley. California.

Equation 2.19 was suggested for streams with Manning's roughness coefficients on the order of 0.04. By combining Equations 2.18 and 2.19 with $\beta = 0.6$, the dispersion coefficient in the lateral direction used by the riverine component is given by:

$$D_y = 0.06hu \tag{2.20}$$

3.0 Computational Techniques

This chapter describes the techniques employed for radionuclide decay chains, mass conservation, and the measured concentration option.

3.1 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 riverine model transports the decay products like the parent radionuclide. Once the parent reaches the receptor of concern, the model corrects for radiological decay in a separate calculation and the temporal distributions of the important decay products are computed using the Bateman equation (Bateman 1910):

$$C_i = \left(\frac{\lambda_i C_p}{\lambda_1}\right)\left(\prod_{j=1}^{i-1} \lambda_j\right)\left\{\sum_{j=1}^{i}\left[\frac{e^{-\lambda_j t}}{\prod_{\substack{r=1 \\ r\neq j}}^{i} (\lambda_r - \lambda_j)}\right]\right\} \tag{3.1}$$

where

C_p = undecayed parent concentration (Ci mL^{-1})
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^{-1})
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.

By using the Bateman equation to compute concentrations of decay products, the assumption is tacitly made that decay products travel at the same speed as the parent. This assumption poses no complications for the riverine pathway because no sediment adsorption is assumed to occur. Thus, all constituents travel at the same speed as the river flow velocity.

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 a river 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). After assessing a number of waste sites, it became apparent that this time frame was not necessarily the appropriate time to use for degradation/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 is then 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 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.

In addition to degradation/decay, mass loss by volatilization can also occur in the riverine environment. This loss is not computed by the surface-water component, but is taken into account by the exposure component of MEPAS. The mass loss is first order using the transit time in the surface water between the source and the receptor location along with a surface-water volatilization half-time, as described in Strenge and Chamberlain (1995).

3.2 Surface Water Mass Balance at the Source

Because the solution to the surface-water transport algorithm is exact and in a closed form, the analytical algorithm, by definition, conserves mass as the contaminant migrates through the surface-water environment. Note that Equation 2.8 conserves mass once the contaminant has been released into the environment and does not account for the amount of contaminant remaining in the waste site. 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:

(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.

$$M_T = \int_0^{\tau} Qc\,dt \tag{3.2}$$

where

M_T = total mass or activity being released from the waste site (g or Ci)
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.

3.3 Measured Concentrations in the Groundwater Environment

Contaminant levels are often measured in surface-water bodies 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 analysis 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 single concentration value is assumed to be temporally constant, although first-order degradation/decay can be included in the analysis.

If a measured contaminant level is used, as opposed to modeling contaminant transport from the source to the receptor, the investigator should understand the meaning of the measured value and the implications associated with using a measured concentration. For example, if a waste site is being assessed for radionuclides, measured contaminant levels for heavy metals at an intake structure should not necessarily be attributed to that particular waste site and indiscriminantly used for that site's assessment. Also, an observed concentration implies that the concentration is constant with respect to time; this assumption may be conservative or nonconservative, depending on whether the contaminant plume has passed or is still approaching the receptor location.

If monitoring information is available at a receptor location and the nature, extent, and source of contamination are known, then the monitored information can be used to back calculate (i.e., calibrate) the transport modeling to ensure that the entire migrating plume is appropriately included in the assessment. Following the transport exercise, the monitored value is correlated to the simulated value, both spatially and temporally. Input parameters are modified, as appropriate, to ensure that the simulated and observed values match. Back calculation is an extremely powerful tool that can be used to ensure that any assumptions associated with the modeling scenario are appropriate. Failure to match observed values using input parameters that physically make sense may indicate that an important fate and transport process is not being captured by the current modeling scenario (e.g., sediment adsorption).

4.0 Equation Notation

English

B = width of stream channel (cm)
C = dissolved instream contaminant concentration (g mL^{-1} or Ci mL^{-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^{-1})
C_n = contaminant concentration for the current receptor (g mL^{-1} or Ci mL^{-1})
C_{n-1} = contaminant concentration for the previous receptor (g mL^{-1} or Ci mL^{-1})
C_p = undecayed parent concentration (Ci mL^{-1})
D_x, D_y, D_z = dispersion coefficients in the x-, y-, and z-directions, respectively (cm^2 s^{-1})
f = fraction of the source term upstream of the receptor (dimensionless)
f_n = fraction of the source term upstream of the current receptor (dimensionless)
f_{n-1} = fraction of the source term upstream of the previous receptor (dimensionless)
h = depth of stream (cm)
l_m = lateral distance over which the contaminant is assumed to be uniformly distributed (equivalent to one-half the standard deviation) (cm)
l_m' = alternative lateral distance over which the contaminant is assumed to be uniformly distributed (cm)
$l_{m(n)}$ = lateral mixing length at the current receptor location (cm)
$l_{m(n-1)}$ = lateral mixing length at the previous receptor location (cm)
l_s = total length of the source term (cm)
l_{ur} = length of the source term upstream of the receptor (cm)
M = contaminant mass or activity per unit area (g cm^{-2} or Ci cm^{-2})
M_T = total mass or activity being released from the waste site (g or Ci)
Qc = contaminant flux at the source (g s^{-1} or Ci s^{-1})
Q_r = river discharge at the receptor location (cm^3/s)
Q_{ratio} = dilution ratio (dimensionless)
$Q_{r(n)}$ = river discharge at the current receptor location (mL s^{-1})
$Q_{r(n-1)}$ = river discharge at the previous receptor location (mL s^{-1})
Q_s = river discharge at the source location (cm^3/s)
t_t = representative contaminant travel time (s)
t_m = time to achieve the fully mixed condition (i.e., representative contaminant travel time) (s)
u = average instream flow velocity (cm s^{-1})
u^* = shear velocity (cm s^{-1})
x = downstream distance to receptor (cm)

y = lateral distance to receptor (cm)

Greek

β = proportionality constant used to calculate the lateral dispersion coefficient (dimensionless)
λ = degradation/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})
ξ = proportionality constant in the alternative mixing length equation (dimensionless)
σ_l = standard deviation of the Gaussian distribution of the one-dimensional advective-dispersive equation in the lateral direction (cm)
τ = time at which the release from the waste site ends (s)
ϕ = proportionality constant in the alternative mixing length equation (reciprocal of ξ) (dimensionless)

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