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Mathematical Formulations for Contaminant Partitioning in Rivers

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Prepared for the
Westinghouse Savannah River Company
and U.S. Department of Energy
under Contract DE-AC06-76RLO 1830

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Preface

This mathematical model for contaminant transport in rivers provides a preliminary assessment of the contaminant mass and concentration using environmental partitioning. First, the model uses the advection-dispersion equation to model the river flow and contaminant transport in the water. Second, the model uses compartment modeling to partition the contaminant mass into water, sediment, bed sediment, air, fish, vegetation and free product environmental compartments. Finally, the model calculates contaminant concentration in each environmental compartment. As long as this approach is applied with an understanding of its assumptions and limitations, it can be very useful as a preliminary assessment model for contaminant transport in rivers.

The purpose of developing this approach was to provide a simple mathematical model that accounts for the time-varying partitioning of contaminant concentration at a given location along the river. This approach is intended to be used as part of the Multimedia Environmental Pollutant Assessment System (MEPAS). Currently MEPAS, and other multimedia contaminant environmental transport and exposure risk assessment methodologies, assumes that once the contaminant enters the water, it is instantaneously and completely dissolved. This assumption, that the contaminant is only present in the dissolved phase tends to over predict water contaminant levels. This approach is intended to address the partitioning of contaminants into environmental compartments in addition to the water column.

This model was tested with an illustrative example using ethylene glycol as the contaminant. The application results showed that the key model input parameters are either related to the contaminant (i.e., distribution coefficient, Henry's constant, solubility limit, and biological concentration factor for fish and vegetation) or the river (i.e., height of bed sediment, mass of fish, and mass of vegetation). This modeling effort also showed that the advection-dispersion equation being used does not account for losses due to sediment, bed sediment, or free product deposition, volatilization, or adsorption by fish or vegetation. To provide a result that addresses

these losses to the total contaminant concentration as it migrates downstream, an updated advection-dispersion equation should be developed and used with this model.

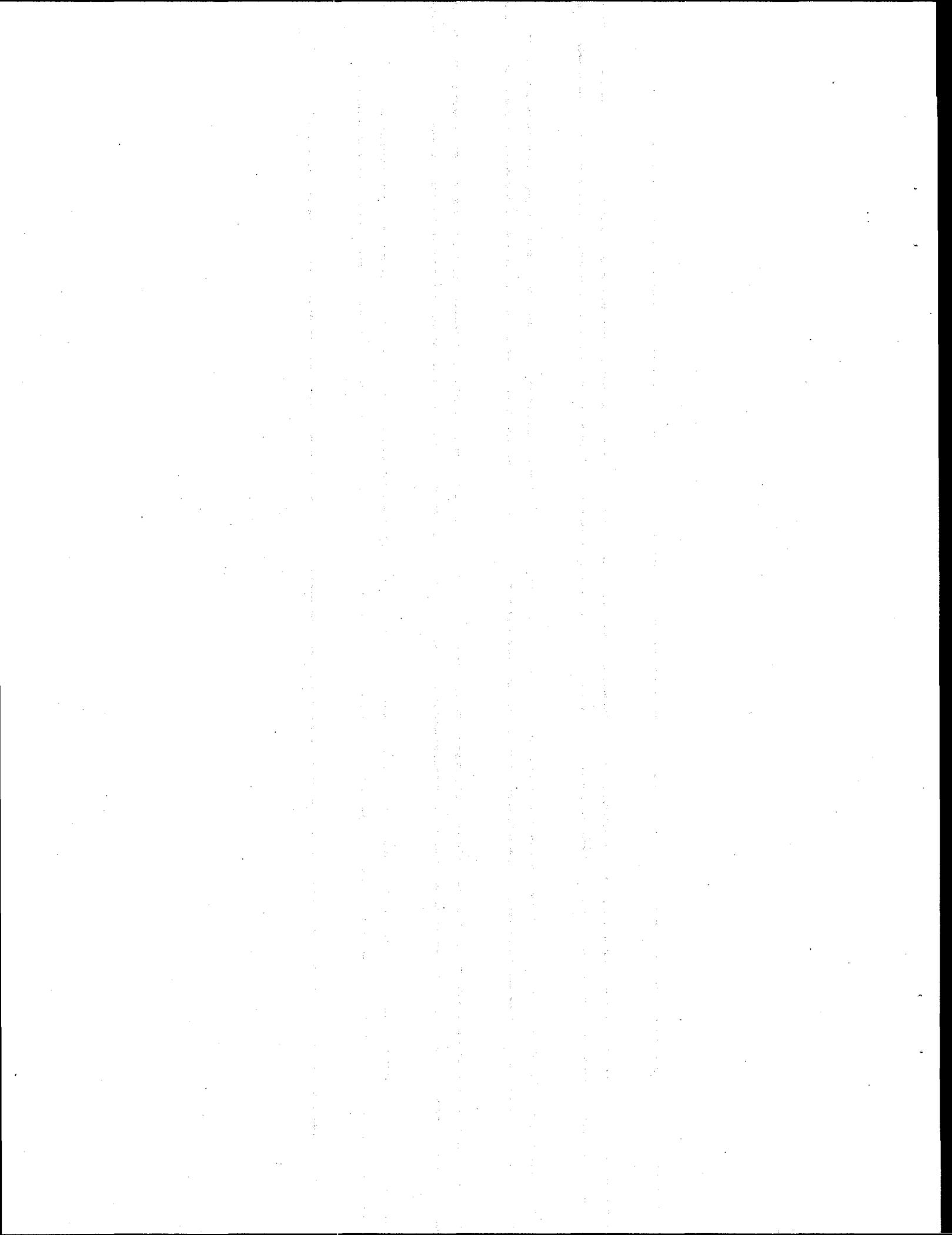
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1.0 INTRODUCTION

Mathematical modeling of contaminant transport through the environment provides a mechanism for estimating the amount of contaminant that is reaching a point of interest. River water is an important pathway for transporting contaminants to locations where humans may be directly and/or indirectly exposed to contaminants. Typical exposure pathways include the following (Cheng et al. 1995):

- ingestion of contaminated water or fish
- dermal contact of contaminated water (e.g., swimming, bathing, etc.)
- external dose of radionuclides
- inhalation of volatilized contaminants above the water
- human consumption of crops irrigated with contaminated water
- human consumption of animal products (e.g., milk and meat) following animal consumption of contaminated water or crops
- ingestion of soil contaminated by river water.

Multimedia contaminant environmental transport and exposure risk assessment methodologies, such as Multimedia Environmental Pollutant Assessment System (MEPAS), simulate the release of contaminants into the environment, their migration and fate in various sequentially connected environmental media (e.g., air, groundwater, surface water, and overland), contaminant movement through the food chain, exposure to sensitive receptors (through inhalation, ingestion, dermal contact, and external dose), and risk or hazard associated with the exposure (Buck et al. 1995). Currently, these methodologies simulate contaminant transport in rivers by way of advection and dispersion. Once the contaminant enters the water, these methodologies assume that the contaminant is instantaneously and completely dissolved. By assuming that the contaminant is only in the dissolved phase, the assessment tends to over-predict water

contaminant levels. In reality, the contaminant can partition between water, sediment, bed sediment, air, fish, vegetation, and free product, where appropriate.

The purpose of this effort is to develop a relatively simple approach that attempts to account for the time-varying partitioning of a contaminant at a given location in a river environment. This approach will eventually become a component of MEPAS and, therefore, focuses on addressing the needs of this multimedia model. The approach outlined in this paper will

- be compatible and consistent with structure and input/output requirements of the multimedia model MEPAS
- have a level of detail that is mathematically compatible (e.g., analytically, semi-analytically, and/or empirically based) with other components in MEPAS
- be based on "readily available information"
- be computationally quick
- supply the same answer, whether the analyst approaches the problem from the downstream or upstream side of the receptor location
- consider the partitioning between the water, sediment, bed sediment, air, fish, vegetation, and free product compartments
- provide time-varying environmental concentrations at receptor locations
- have a level of detail that is compatible with "order-of-magnitude" risk assessments
- account for degradation/decay.

No simplified approach will always accurately meet these constraints, but this approach attempts to provide a screening-level analysis that gives the decision-maker sufficient information to make decisions. Note that this approach is not necessarily after the numerically "right" answer, but rather providing decision-makers with a preliminary assessment that helps experts agree on answers that address the question being analyzed, such that the right decision is made. Risk (not environmental contaminant levels) and the qualitative process of decision-making are the primary

endpoints. Therefore, this approach is attempting to capture the essence of environmental partitioning without unduly burdening the analyst with data requirements and computations.

This paper addresses the need for a contaminant transport model that meets the above constraints through the following steps:

1. Transport the contaminant as a fully dissolved substance to the downstream receptor location, employing analytical and semi-analytical solutions to the advection-dispersion equation for contaminant transport.
2. Partition the contaminant between water, sediment, bed sediment, air, fish, vegetation, and free product, using a compartment model approach at the receptor location.
3. Determine the contaminant concentration in each compartment.

The mathematical approach is outlined in Section 2.0. The advection-dispersion equation, compartment model, and the concentration calculations are also outlined in Section 2.0. Section 3.0 contains the assumptions and limitations associated with this approach. Section 4.0 presents an illustrative example. Section 5.0 provides a summary and conclusions regarding this approach. Section 6.0 provides a list of references. Appendix A presents a summary list of equation variables.

2.0 APPROACH

A contaminant can sorb to washload, suspended, bedload, and bed sediment, can volatilize into the air, can be taken up by fish and vegetation, and can remain as free product in the water, if the dissolved concentration is greater than the solubility limit of the chemical. All of these different means of contaminant partitioning affect the level of exposure a receptor may receive.

To address these different contaminant transport mechanisms, this mathematical model takes the following approach:

1. Models contaminant transport to the downstream receptor location using the generic exposure scenario and the advection-dispersion equation.
2. Models contaminant mass partitioning at the receptor location into the environmental compartments: water, sediment, bed sediment, air, fish, vegetation, and free product.
3. Calculates the time-varying contaminant concentration in each environmental compartment using mass and concentration values determined in steps one and two.

The generic exposure scenario, which is illustrated in Figure 2.1, assumes a contaminant plume exists at the river's edge initially at the point where $x = 0$ and $y = 0$. The width of the contaminant plume is represented by y . As the downstream distance from the source increases, the contaminant plume makes its way across the river, until it eventually becomes uniformly mixed across the width of the river. The cross-sectional area of the river is assumed to be rectangular with the width generally exceeding the depth. The contaminant is assumed to be fully mixed over the depth of the river. Receptors are assumed to be downstream at the edge of the river (i.e., $y = 0$).

Contaminants are transported downstream via advection and dispersion, followed by the partitioning of the contaminant into various environmental compartments (i.e., water, sediment, bed sediment, air, fish, vegetation, and free product), illustrated by Figure 2.2.

Figure 2.3a presents a flow diagram highlighting the solution procedure and provides two illustrative examples of output results. Figure 2.3b illustrates the partitioning of contaminant mass into six environmental compartments. Figure 2.3c provides contaminant concentrations at a given location, as they vary with time. By using the equations described in this paper, the time-varying contaminant concentration can be computed and shown graphically.

2.1 ADVECTION-DISPERSION EQUATION

The advection-dispersion equation, as used by the MEPAS model, describes the migration of a contaminant in river water. The assumptions coinciding with this equation are as follows:

- Surface water flow is assumed to be steady and uniform over the investigated time increment.
- Longitudinal advection dominates longitudinal dispersion.
- The lateral distance to the receptor is zero.
- Contaminant releases are considered to be long-term in comparison to travel time (i.e., steady-state assumptions are appropriate).
- The river can be represented by a rectangular cross-section.
- The contaminant plume is fully mixed throughout the depth of the river (i.e., dispersion is only considered in the lateral direction).
- Contaminant degradation/decay is first-order.

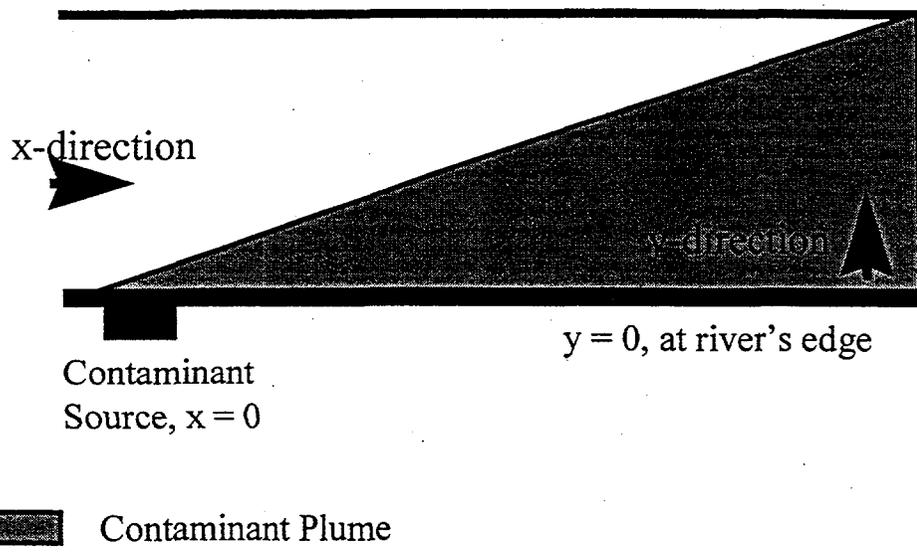


Figure 2.1. River and Contaminant Flow

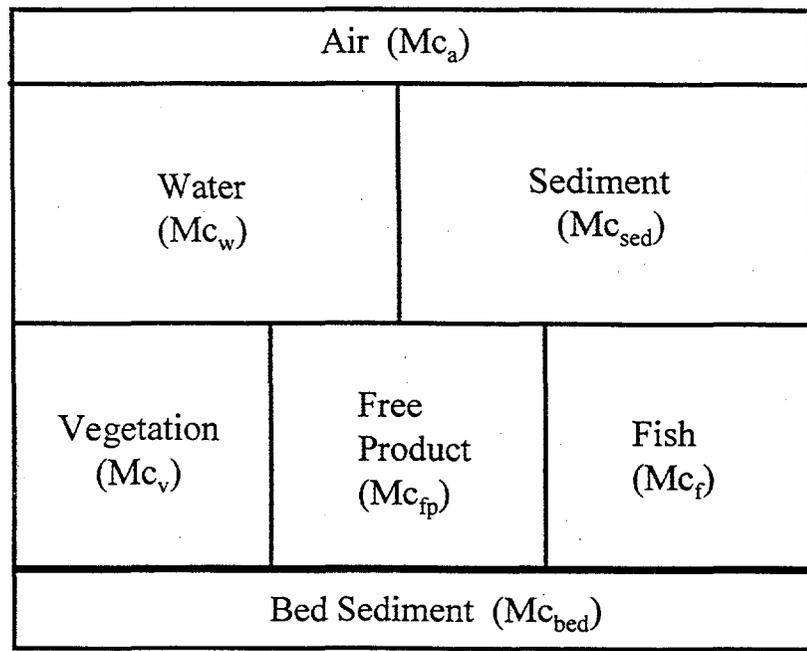


Figure 2.2. Compartment Model

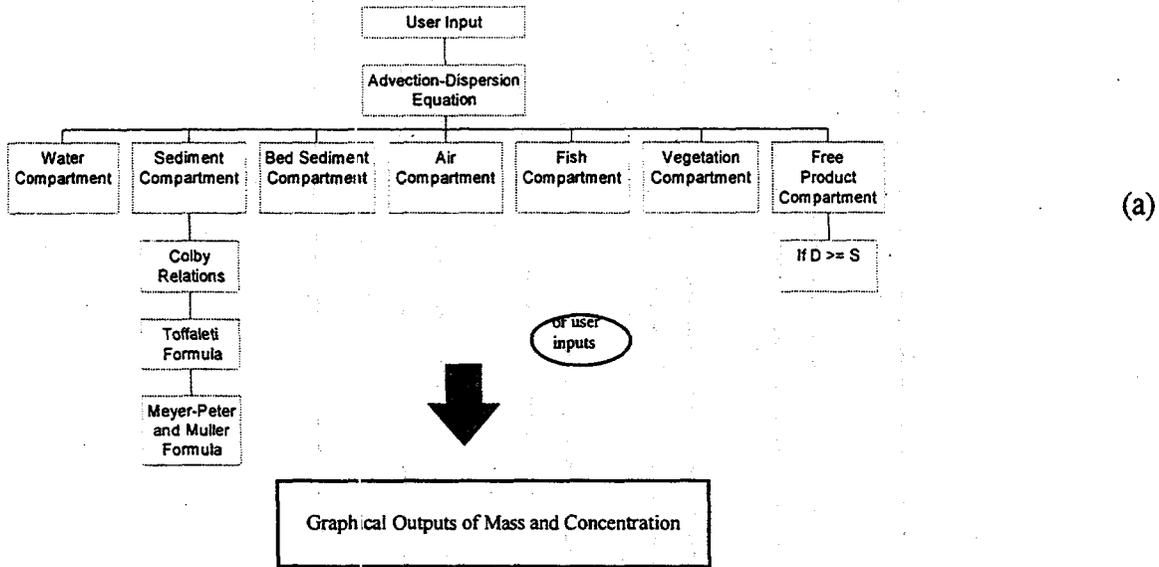


Illustration of Contaminant Mass in Environmental Compartments

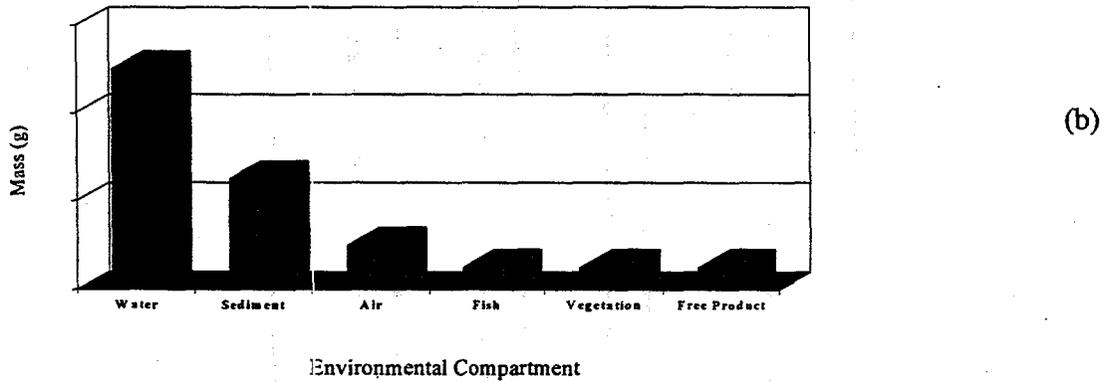


Illustration of Time-Varying Contaminant Concentration

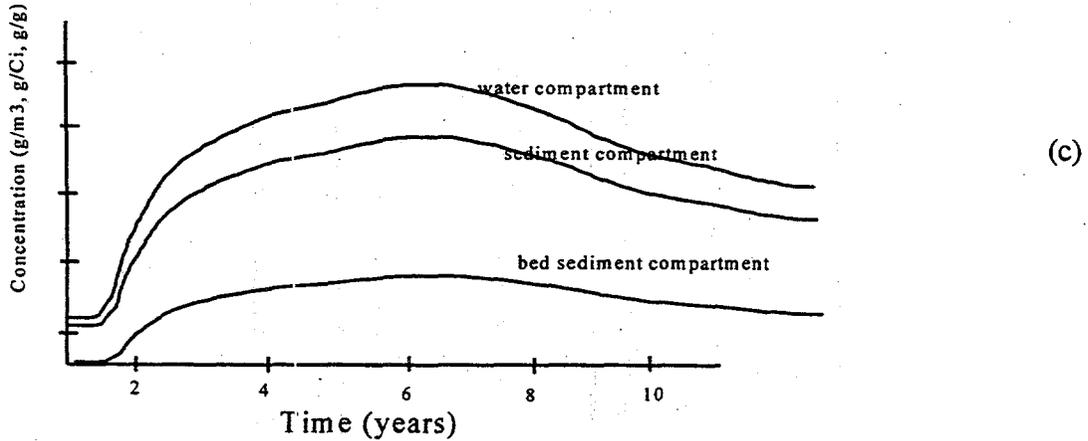


Figure 2.3. Flow Diagram

For the first river receptor, the contaminant concentration will be determined as follows (Whelan and McDonald 1996):

$$C_T = \left(\frac{Q_c}{4Bh} \right) \exp\left(-\frac{\lambda x}{u} \right) \left(1 + 2 \sum_{n=1}^{\infty} \left(\exp\left(-\frac{n^2 \pi^2 D_y x}{B^2} \right) \right) \right) \quad (2.1)$$

C_T = total contaminant concentration in stream due to advection & dispersion (g/m^3 or Ci/m^3 ; mass of contaminant/volume of water)

Q_c = contaminant flux at the source (g/s or Ci/s)

B = width of river (m)

h = depth of river (m)

λ = degradation/decay constant (s^{-1})

x = downstream distance to receptor (m)

u = average flow velocity (m/s)

D_y = dispersion coefficient in the y-direction (m^2/s)

If there are multiple downstream river receptors, the contaminant concentration will be determined as follows (Whelan and McDonald 1996):

$$C_{T(n)} = C_{n-1} \cdot \left(\frac{Q_{n-1}}{Q_n} \right) \cdot \left(\frac{l_{m(n-1)}}{l_{m(n)}} \right) \cdot \left(\frac{f_n}{f_{n-1}} \right) \quad (2.2)$$

$C_{T(n)}$ = contaminant concentration for the current receptor (g/m^3 or Ci/m^3 ; mass of contaminant/volume of water)

C_{n-1} = contaminant concentration for the previous receptor (g/m^3 or Ci/m^3 ; mass of contaminant/volume of water)

Q_n = river discharge at the current receptor location (m^3/s)

Q_{n-1} = river discharge at the previous receptor location (m^3/s)

$l_{m(n)}$ = lateral mixing length at the current receptor location (m)

$l_{m(n-1)}$ = lateral mixed length at the previous receptor location (m)

f_n = fraction of the source term upstream of the current receptor (fraction)

f_{n-1} = fraction of the source term upstream of the previous receptor (fraction)

n = number of receptors (dimensionless)

The concentration value derived from the advection-dispersion equation assumes that the only factors affecting contaminant levels are advection, dispersion, and degradation/decay. MEPAS assumes that the concentration derived from the advection-dispersion equation is the total concentration in the river and that it is completely dissolved in the water.

The total concentration is equal to the total mass of the contaminant with respect to the volume of water:

$$C_T = \left(\frac{Mc_t}{V_w} \right) \quad (2.3)$$

Mc_t = total contaminant mass (g or Ci; mass of contaminant)

V_w = volume of water (m^3)

The volume of water is equal to the river depth times the river width times the unit length of the control volume:

$$V_w = d B L \quad (2.4)$$

B = width of river (m)

d = depth of river (m)

L = unit length of control volume (m)

The total concentration can be expressed as a total contaminant mass per unit length per cross-sectional area (width times depth) of the water column:

$$C_T = \left(\frac{Mc_t}{L} \right) \left(\frac{1}{Bd} \right) \quad (2.5)$$

2.2 COMPARTMENT MODEL

A compartment model partitions the contaminant concentration into the different environmental compartments: water, sediment, bed sediment, air, fish, vegetation, and free product.

- The water compartment is used to calculate the contaminant mass and concentration dissolved in the water column.
- The sediment compartment is used to calculate the contaminant mass and concentration attached to the washload, suspended, and bedload sediments. A contaminant's likelihood of accumulating on the sediment is represented by its distribution coefficient, K_d . The sediment discharge, if not provided by the user, is determined by the Colby (1964) relations, Toffaleti (1968, 1969) formulas, or Meyer-Peter and Muller (1948) formula.
- The bed sediment compartment is used to calculate the contaminant mass and concentration attached to the bed sediment. A contaminant's likelihood of accumulating in the sediment is represented by its distribution coefficient, K_d . The K_d values for washload, suspended, and bedload sediments and bed sediments are not necessarily the same.
- The air compartment is used to calculate the contaminant mass and concentration that volatilizes to the air above the river. A contaminant's likelihood of volatilizing to the air is represented by its Henry's Constant, K_H .
- The fish compartment is used to calculate the contaminant mass and concentration associated with fish uptake through ingestion, adsorption, and respiration.
- The vegetation compartment is used to calculate the contaminant mass and concentration associated with vegetation uptake.
- The free product compartment is used to calculate the contaminant mass that is above the solubility limit and, therefore, in the free product phase (precipitants).

For a graphical representation of the compartment model, see Figure 2.2. A compartment model is based on the assumption that the total contaminant mass (M_c) equals the sum of its parts (mass balance):

$$Mc_t = Mc_w + Mc_{sed} + Mc_{bed} + Mc_a + Mc_v + Mc_f + Mc_{fp} \quad (2.6)$$

Mc_w = mass of contaminant in water compartment (g or Ci; mass of contaminant)
 Mc_{sed} = mass of contaminant in sediment compartment (g or Ci; mass of contaminant)
 Mc_{bed} = mass of contaminant in the bed sediment compartment (g or Ci; mass of contaminant)
 Mc_a = mass of contaminant in air compartment (g or Ci; mass of contaminant)
 Mc_v = mass of contaminant in aquatic vegetation compartment (g or Ci; mass of contaminant)
 Mc_f = mass of contaminant in fish compartment (g or Ci; mass of contaminant)
 Mc_{fp} = mass of contaminant in free product compartment (g or Ci; mass of contaminant)

Dividing both sides of Equation (2.6) by Mc_w gives:

$$\frac{Mc_t}{Mc_w} = \left(\frac{Mc_w}{Mc_w} + \frac{Mc_{sed}}{Mc_w} + \frac{Mc_{bed}}{Mc_w} + \frac{Mc_a}{Mc_w} + \frac{Mc_v}{Mc_w} + \frac{Mc_f}{Mc_w} + \frac{Mc_{fp}}{Mc_w} \right) \quad (2.7)$$

Therefore, the inverse of Equation (2.7) is the ratio of the mass of contaminant in the water to the total contaminant mass, represented by the following equation:

$$\frac{Mc_w}{Mc_t} = \left(\frac{1}{\frac{Mc_w}{Mc_w} + \frac{Mc_{sed}}{Mc_w} + \frac{Mc_{bed}}{Mc_w} + \frac{Mc_a}{Mc_w} + \frac{Mc_v}{Mc_w} + \frac{Mc_f}{Mc_w} + \frac{Mc_{fp}}{Mc_w}} \right) \quad (2.8)$$

Sections 2.2.1 through 2.2.7 define each of the compartment ratios (e.g., Mc_w/Mc_w , Mc_{sed}/Mc_w , etc.) and the contaminant concentration in each compartment using either user input, existing data tables, and/or values calculated from equations in this document.

2.2.1 Water Compartment

The water compartment contains the portion of the contaminant that is dissolved in the river water. The water compartment ratio (i.e., water factor) equals unity:

$$\frac{Mc_w}{Mc_w} = 1 \quad (2.9)$$

The contaminant concentration in the water compartment is the contaminant mass in the water per unit volume of water:

$$C_{C(w)} = \left(\frac{Mc_w}{V_w} \right) \quad (2.10)$$

Or,

$$C_{C(w)} = \left(\frac{Mc_t}{V_w} \right) \left(\frac{Mc_w}{Mc_t} \right) \quad (2.11)$$

$C_{C(w)}$ = contaminant concentration in the water compartment (g/m^3 or Ci/m^3 ; mass of contaminant/volume of water)

Combining Equation (2.1) or (2.2) and Equation (2.8), the contaminant concentration in the water compartment can be defined by:

$$C_{C(w)} = C_T \left(\frac{Mc_w}{Mc_t} \right) \quad (2.12)$$

If free product forms, the dissolved concentration is set equal to the solubility limit of the contaminant.

2.2.2 Sediment Compartment

Contaminants tend to accumulate onto sediment (Buck et al. 1995). Depending on the contaminant's distribution coefficient (K_d) and the concentration of sediment (C_{sed}), sediment transport may be a significant transport mechanism. The sediment compartment, as used here, contains the portion of contaminant attached to the washload, suspended, and bedload sediment. The bed sediment compartment is being considered a separate compartment and is discussed in Section 2.2.3.

The sediment type may include sand, silt, clay and organic matter. Because most sediment in United States rivers is alluvial in nature, it is assumed that the sand fraction alone equals unity unless the sediment discharge rates and/or the sediment mass flux rates can be provided for the silt, clay, and organic matter fractions. The sum of the sediment type fractions equals unity:

$$\text{sand} + \text{silt} + \text{clay} + \text{OM} = 1 \quad (2.13)$$

sand = fraction of sand in sediment (fraction)

silt = fraction of silt in sediment (fraction)

clay = fraction of clay in sediment (fraction)

OM = fraction of organic matter in sediment (fraction)

The sum of the contaminant masses associated with the size fractions of sand, silt, clay, and organic matter is as follows:

$$Mc_{sed} = Mc_{sand} + Mc_{silt} + Mc_{clay} + Mc_{OM} \quad (2.14)$$

Mc_{sand} = mass of contaminant on sand portion of the sediment compartment (g or Ci; mass of contaminant)

Mc_{silt} = mass of contaminant on silt portion of the sediment compartment (g or Ci; mass of contaminant)

Mc_{clay} = mass of contaminant on clay portion of the sediment compartment (g or Ci; mass of contaminant)

Mc_{OM} = mass of contaminant on organic matter portion of the sediment compartment (g or Ci; mass of contaminant)

The sediment compartment is defined by the ratio of the mass of contaminant adsorbed on the sediment to the mass of contaminant in the water (i.e., sediment factor):

$$\frac{Mc_{sed}}{Mc_w} = \frac{Mc_{sand}}{Mc_w} + \frac{Mc_{silt}}{Mc_w} + \frac{Mc_{clay}}{Mc_w} + \frac{Mc_{OM}}{Mc_w} \quad (2.15)$$

The concentration of the sediment is equal to the sum of the concentration of the sand, silt, clay, and organic matter concentrations:

$$C_{sed} = C_{sand} + C_{silt} + C_{clay} + C_{OM} \quad (2.16)$$

In which,

$$C_{sed} = \frac{M_{sed}}{V_w} \quad (2.17)$$

$$C_{sed} = \frac{g_{ss}}{Q} \quad (2.18)$$

$$C_{sed} = \frac{(g_{ss}) (sand)}{Q} + \frac{(g_{ss}) (silt)}{Q} + \frac{(g_{ss}) (clay)}{Q} + \frac{(g_{ss}) (OM)}{Q} \quad (2.19)$$

C_{sed} = sediment concentration in the sediment compartment (g/m^3 ; mass of sediment/volume of water)

C_{sand} = concentration of sand in water compartment (g/m^3 or Ci/m^3 ; mass of sand/volume of water)

C_{silt} = concentration of silt in water compartment (g/m^3 or Ci/m^3 ; mass of silt/volume of water)

C_{clay} = concentration of clay in water compartment (g/m^3 or Ci/m^3 ; mass of clay/volume of water)

C_{OM} = concentration of organic matter in water compartment (g/m^3 or Ci/m^3 ; mass of organic matter/volume of water)

M_{sed} = sediment mass (g; mass of sediment)

g_{ss} = sediment mass flux rate (g/s)

Q = water discharge rate (m^3/s)

The individual contaminant mass associated with the sand, silt, clay and organic matter fractions, can be expressed as follows:

$$\frac{Mc_{sand}}{Mc_w} = K_{d(sand)} \cdot \rho_{sand} \cdot \frac{V_{sand}}{V_w} = K_{d(sand)} C_{sand} \quad (2.20)$$

$$\frac{Mc_{silt}}{Mc_w} = K_{d(silt)} \cdot \rho_{silt} \cdot \frac{V_{silt}}{V_w} = K_{d(silt)} C_{silt} \quad (2.21)$$

$$\frac{Mc_{clay}}{Mc_w} = K_{d(clay)} \cdot \rho_{clay} \cdot \frac{V_{clay}}{V_w} = K_{d(clay)} C_{clay} \quad (2.22)$$

$$\frac{Mc_{OM}}{Mc_w} = K_{d(OM)} \cdot \rho_{OM} \cdot \frac{V_{OM}}{V_w} = K_{d(OM)} C_{OM} \quad (2.23)$$

In which,

$$C_{sand} = \frac{(g_{ss}) (sand)}{Q} \quad (2.24)$$

$$C_{silt} = \frac{(g_{ss}) (silt)}{Q} \quad (2.25)$$

$$C_{\text{clay}} = \frac{(g_{\text{ss}}) (\text{clay})}{Q} \quad (2.26)$$

$$C_{\text{OM}} = \frac{(g_{\text{ss}}) (\text{OM})}{Q} \quad (2.27)$$

- $K_{\text{d(sand)}}$ = contaminant distribution coefficient for sand (m^3/g ; volume of water/mass of sand)
 ρ_{sand} = density of sand portion of sediment (g/m^3 ; mass of sand/volume of sand)
 V_{sand} = volume of sand in water compartment (m^3 ; volume of sand)
 $K_{\text{d(silt)}}$ = contaminant distribution coefficient for silt (m^3/g ; volume of water/mass of silt)
 ρ_{silt} = density of silt portion of sediment (g/m^3 ; mass of silt/volume of silt)
 V_{silt} = volume of silt in water compartment (m^3 ; volume of silt)
 $K_{\text{d(clay)}}$ = contaminant distribution coefficient for clay (m^3/g ; volume of water/mass of clay)
 ρ_{clay} = density of clay portion of sediment (g/m^3 ; mass of clay/volume of clay)
 V_{clay} = volume of clay in water compartment (m^3 ; volume of clay)
 $K_{\text{d(OM)}}$ = contaminant distribution coefficient for organic matter (m^3/g ; volume of water/mass of organic matter)
 ρ_{OM} = density of organic matter portion of sediment (g/m^3 ; mass of organic matter/volume of organic matter)
 V_{OM} = volume of organic matter in water compartment (m^3 ; volume of organic matter)

Lyman et al. (1982) notes that because $K_{\text{d(OM)}}$ is not routinely measured in the laboratory, the organic-carbon partition coefficient (K_{oc}), which is routinely measured more directly, generally is more available in the literature. The K_{oc} is defined as the ratio of the amount of chemical adsorbed per unit weight of organic carbon (OC) in the sediment or soil to the concentration of the chemical in solution at equilibrium. Lyman et al. (1982) also notes that the ratio of organic matter to organic carbon varies somewhat from soil to soil, but a value of $\sqrt{3}$ is often assumed when conversion is necessary. Therefore, the fraction of organic matter can be defined as $\text{OM} = \sqrt{3} \text{OC}$, and the organic matter partition coefficient can be defined as $K_{\text{d(OM)}} = \sqrt{3} K_{\text{oc}}$.

The sediment discharge rates (i.e., g_s or g_{si}) or mass flux rates (i.e., g_{ss}) will be provided by user input or calculated using the Colby (1964) relations, Toffaleti (1968, 1969) formulas, or Meyer-Peter and Muller (1948) formula discussed in Section 2.3.

The contaminant concentration in the sediment compartment is the contaminant mass in sediment divided by the dry mass of sediment:

$$C_{C(sed)} = \left(\frac{Mc_{sed}}{M_{sed}} \right) \quad (2.28)$$

Or,

$$C_{C(sed)} = \left(\frac{Mc_t}{V_w} \right) \left(\frac{Mc_w}{Mc_t} \right) \left(\frac{Mc_{sed}}{Mc_w} \right) \left(\frac{V_w}{M_{sed}} \right) \quad (2.29)$$

$C_{C(sed)}$ = adsorbed contaminant concentration in the sediment compartment (g/g or Ci/g; mass of contaminant/mass of sediment)

Equation (2.29) can be expressed by combining Equation (2.1) or (2.2) with Equations (2.8), (2.15) and (2.17):

$$C_{C(sed)} = C_T \left(\frac{Mc_w}{Mc_t} \right) \left(\frac{Mc_{sed}}{Mc_w} \right) \left(\frac{1}{C_{sed}} \right) \quad (2.30)$$

2.2.3 Bed Sediment Compartment

The bed sediment compartment involves the sand, silt, clay, and organic matter contained in the bed sediment. The sum of the mass of these components is equal to the total mass of the sediment:

$$M_{c_{bed}} = M_{c_{bed(sand)}} + M_{c_{bed(silt)}} + M_{c_{bed(clay)}} + M_{c_{bed(OM)}} \quad (2.31)$$

$M_{c_{bed(sand)}}$ = mass of contaminant in sand portion of the bed sediment compartment (g; mass of contaminant)

$M_{c_{bed(silt)}}$ = mass of contaminant in silt portion of the bed sediment compartment (g; mass of contaminant)

$M_{c_{bed(clay)}}$ = mass of contaminant in clay portion of the bed sediment compartment (g; mass of contaminant)

$M_{c_{bed(OM)}}$ = mass of contaminant in organic matter portion of the bed sediment compartment (g; mass of contaminant)

Likewise, the mass of sediment in the contaminated portion of the bed sediment equals the sum of the masses for sand, silt, and clay, recognizing that the mass of organic matter is usually insignificant:

$$M_{c_{bed}} = M_{c_{bed(sand)}} + M_{c_{bed(silt)}} + M_{c_{bed(clay)}} \quad (2.32)$$

In which,

$$M_{c_{bed(sand)}} = \beta_{d(sand)} \nabla_{bed} \quad (2.33)$$

$$M_{c_{bed(silt)}} = \beta_{d(silt)} \nabla_{bed} \quad (2.34)$$

$$M_{c_{bed(clay)}} = \beta_{d(clay)} \nabla_{bed} \quad (2.35)$$

$$\nabla_{bed} = B L H_{bed} \quad (2.36)$$

∇_{bed} = volume of bed sediment (m^3)

$\beta_{d(sand)}$ = bulk density of sand portion of bed sediment (g/m^3 ; mass of sand/volume of water)

$\beta_{d(silt)}$ = bulk density of silt portion of bed sediment (g/m^3 ; mass of silt/volume of water)

$\beta_{d(clay)}$ = bulk density of clay portion of bed sediment (g/m^3 ; mass of clay/volume of water)

H_{bed} = height of contamination in bed sediment (m)

The bed sediment compartment is defined by the ratio of the mass of contaminant sorbed to the bed to the mass of the contaminant in the water (i.e., bed sediment factor):

$$\frac{Mc_{bed}}{Mc_w} = \frac{Mc_{bed(sand)}}{Mc_w} + \frac{Mc_{bed(silt)}}{Mc_w} + \frac{Mc_{bed(clay)}}{Mc_w} \quad (2.37)$$

The individual contaminant mass associated with the sand fraction is expressed as follows:

$$\frac{Mc_{bed(sand)}}{Mc_w} = K_{d(sand)} \cdot \rho_{sand} \cdot \left(\frac{V_{sand}}{V_{water}} \right) \quad (2.38)$$

Or,

$$\frac{Mc_{bed(sand)}}{Mc_w} = K_{d(sand)} \cdot \rho_{sand} \cdot (sand) (1-n) \left(\frac{V_{bed}}{V_{water}} \right) \quad (2.39)$$

In which,

$$\frac{V_{sand}}{V_{water}} = (sand) (1-n) \left(\frac{V_{bed}}{V_{water}} \right) \quad (2.40)$$

$$n = 1 - \frac{\beta_d}{\rho} \quad (2.41)$$

$$\beta_{d(sand)} = (sand) \beta_{d.bed} \quad (2.43)$$

$$\beta_{d.bed} = \frac{M_{bed}}{V_w} \quad (2.44)$$

∇_{sand} = volume of sand in bed sediment (m^3)

$(1 - n)$ = total porosity fraction (fraction)

∇_{bed} = volume of bed sediment (m^3)

$\beta_{\text{d}(\text{bed})}$ = bulk density of bed sediment (g/m^3 ; mass of sediment/volume of water)

M_{bed} = mass of bed sediment in the contaminated portion of the bed (g; mass of sediment)

Substituting Equations (2.4), (2.36) and (2.43) into (2.39) and simplifying, gives:

$$\frac{Mc_{\text{bed}(\text{sand})}}{Mc_w} = K_{\text{d}(\text{sand})} \cdot \beta_{\text{d}(\text{bed})} \cdot (\text{sand}) \cdot \frac{H_{\text{bed}}}{d} \quad (2.45)$$

Similar expressions can be developed for silt and clay:

$$\frac{Mc_{\text{bed}(\text{silt})}}{Mc_w} = K_{\text{d}(\text{silt})} \cdot \beta_{\text{d}(\text{bed})} \cdot (\text{silt}) \cdot \frac{H_{\text{bed}}}{d} \quad (2.46)$$

$$\frac{Mc_{\text{bed}(\text{clay})}}{Mc_w} = K_{\text{d}(\text{clay})} \cdot \beta_{\text{d}(\text{bed})} \cdot (\text{clay}) \cdot \frac{H_{\text{bed}}}{d} \quad (2.47)$$

The contaminant concentration in the bed sediment compartment is the contaminant mass in the bed sediment per unit mass of bed sediment:

$$C_{\text{C}(\text{bed})} = \left(\frac{Mc_{\text{bed}}}{M_{\text{bed}}} \right) \quad (2.48)$$

Or,

$$C_{\text{C}(\text{bed})} = \left(\frac{Mc_t}{\nabla_w} \right) \left(\frac{Mc_w}{Mc_t} \right) \left(\frac{Mc_{\text{bed}}}{Mc_w} \right) \left(\frac{\nabla_w}{M_{\text{bed}}} \right) \quad (2.49)$$

$C_{C(\text{bed})}$ = contaminant concentration in the bed sediment compartment (g/g or Ci/g; mass of contaminant/mass of bed sediment)

Equation (2.49) can be expressed by combining Equation (2.1) or (2.2) with Equations (2.8), (2.37) and (2.44) to give:

$$C_{C(\text{bed})} = C_T \left(\frac{M_{c_w}}{M_{c_t}} \right) \left(\frac{M_{c_{\text{bed}}}}{M_{c_w}} \right) \left(\frac{1}{\beta_{d(\text{bed})}} \right) \quad (2.50)$$

2.2.4 Air Compartment

The air portion of the contaminant transport represents the quantity of contaminant volatilized to the air from the river. Volatilized contaminants will result in a lower concentration in the water and impose an additional risk to receptors breathing the air near the river. The air compartment is defined by the ratio of the mass of contaminant in the air to that in the water (i.e., air factor):

$$\frac{M_{c_a}}{M_{c_w}} = K_H' \left(\frac{V_a}{V_w} \right) \quad (2.51)$$

Or,

$$\frac{M_{c_a}}{M_{c_w}} = K_H' \frac{H_{\text{air}}}{d} \quad (2.52)$$

In which,

$$K_H' = \frac{K_H}{RT} \quad (2.53)$$

$$V_a = H_{\text{air}} B L \quad (2.54)$$

K_H' = Henry's constant (dimensionless)

V_a = volume of air (m^3)

K_H = Henry's constant ($atm\ m^3/mole$)

R = universal gas constant [8.2057×10^{-5} ($atm\ m^3$)/($mole\ K$)]

T = temperature (Kelvin)

H_{air} = height of the air compartment (m)

The contaminant concentration in air is the contaminant mass in air per unit volume of air:

$$C_{C(air)} = \frac{Mc_a}{V_a} \quad (2.55)$$

Or,

$$C_{C(air)} = \left(\frac{Mc_t}{V_w} \right) \left(\frac{Mc_a}{Mc_w} \right) \left(\frac{Mc_w}{Mc_t} \right) \left(\frac{V_w}{V_a} \right) \quad (2.56)$$

$C_{C(air)}$ = contaminant concentration in the air compartment (g/m^3 or Ci/m^3 ; mass of contaminant/volume of air)

Equation (2.56) can be expressed by combining Equations (2.1) or (2.2) with Equations (2.4), (2.8), and (2.52) to give:

$$C_{C(air)} = C_T K_H' \left(\frac{H_{air}}{d} \right) \left(\frac{Mc_w}{Mc_t} \right) \left(\frac{d B L}{H_{air} B L} \right) \quad (2.57)$$

Or,

$$C_{C(air)} = C_T K_H' \left(\frac{Mc_w}{Mc_t} \right) \quad (2.58)$$

2.2.5 Fish Compartment

The fish portion of the contaminant transport represents the quantity of contaminant adsorbed or ingested by the fish in the contaminant plume. The fish compartment is defined by the ratio of the mass of contaminant in the fish to the mass of contaminant in water (i.e., fish factor):

$$\frac{Mc_f}{Mc_w} = \rho_f \frac{V_f}{V_w} BCF_f' \quad (2.59)$$

Or,

$$\frac{Mc_f}{Mc_w} = BCF_f' \cdot \beta_{d(\text{fish})} \quad (2.60)$$

In which,

$$\rho_f = \frac{M_f}{V_f} \quad (2.61)$$

$$\beta_{d(\text{fish})} = \frac{M_f}{V_w} \quad (2.62)$$

ρ_f = density of fish (g/m^3 ; mass of fish/volume of fish)

V_f = volume of fish (m^3)

BCF_f' = biological concentration factor for fish (m^3/g ; volume of water/mass of fish)

M_f = mass of fish in water (g)

$\beta_{d(\text{fish})}$ = bulk density of fish (g/m^3 ; mass of fish/volume of water)

The contaminant concentration in the fish compartment is the contaminant mass of fish per unit mass of fish:

$$C_{C(\text{fish})} = \frac{M_{c_f}}{M_f} \quad (2.63)$$

Or,

$$C_{C(\text{fish})} = \left(\frac{M_{c_t}}{V_w} \right) \left(\frac{M_{c_w}}{M_{c_t}} \right) \left(\frac{M_{c_f}}{M_{c_w}} \right) \left(\frac{V_w}{M_f} \right) \quad (2.64)$$

$C_{C(\text{fish})}$ = contaminant concentration in the fish compartment (g of contaminant/g of fish or Ci/g; mass of contaminant/mass of fish)

Equation (2.64) can be expressed by combining Equations (2.1) or (2.2) with Equations (2.8), (2.59), and (2.62) to give:

$$C_{C(\text{fish})} = C_T \left(\frac{M_{c_w}}{M_{c_t}} \right) \left(\frac{M_{c_f}}{M_{c_w}} \right) \left(\frac{1}{\beta_{d(\text{fish})}} \right) \quad (2.65)$$

2.2.6 Vegetation Compartment

The vegetation portion of the contaminant transport represents the quantity of contaminant adsorbed by the vegetation within the contaminant plume. The vegetation compartment is defined by the ratio of the mass of contaminant in the vegetation to the mass of contaminant in water (i.e., vegetation factor):

$$\frac{M_{c_v}}{M_{c_w}} = \rho_v \frac{V_v}{V_w} BCF'_v \quad (2.66)$$

Or,

$$\frac{M_{c_v}}{M_{c_w}} = BCF'_v \cdot \beta_{d(\text{veg})} \quad (2.67)$$

In which,

$$\rho_v = \frac{M_v}{V_v} \quad (2.68)$$

$$\beta_{d(\text{veg})} = \frac{M_v}{V_w} \quad (2.69)$$

ρ_v = density of vegetation (g/m^3 ; mass of vegetation/volume of fish)

V_v = volume of vegetation (m^3)

BCF_v' = biological concentration factor for vegetation (m^3/g ; volume of water/mass of fish)

M_v = total mass of vegetation in water (g; mass of vegetation)

$\beta_{d(\text{veg})}$ = bulk density of vegetation (g/m^3 ; mass of vegetation/volume of water)

The contaminant concentration in the vegetation compartment is the contaminant mass of vegetation per unit mass of vegetation:

$$C_{C(\text{veg})} = \frac{M c_v}{M_v} \quad (2.70)$$

Or,

$$C_{C(\text{veg})} = \left(\frac{M c_t}{V_w} \right) \left(\frac{M c_w}{M c_t} \right) \left(\frac{M c_v}{M c_w} \right) \left(\frac{V_w}{M_v} \right) \quad (2.71)$$

$C_{C(\text{veg})}$ = contaminant concentration in the vegetation compartment (g/g or Ci/g ; mass of contaminant/mass of vegetation)

Equation (2.71) can be expressed by combining Equations (2.1) or (2.2) with Equations (2.8), (2.66), and (2.69) to give:

$$C_{C(\text{veg})} = C_T \left(\frac{Mc_w}{Mc_t} \right) \left(\frac{Mc_v}{Mc_w} \right) \left(\frac{1}{\beta_{d(\text{veg})}} \right) \quad (2.72)$$

2.2.7 Free Product Compartment

The free product portion of the contaminant transport represents the quantity of contaminant that exceeds the chemical's solubility limit (S) for water. This portion of the contaminant is the solid or liquid form of the chemical that is traveling as a precipitant (e.g., oil traveling on the surface of the water, solid chemical settling to the bottom of the river, etc.). Two conditions need to be considered for the free product compartment. Condition 1 is when the dissolved concentration is less than the solubility limit ($C_{C(w)} < S$). At that time the mass of the free product is zero ($Mc_{fp} = 0$). Condition 2 occurs when the dissolved concentration is greater than or equal to the solubility limit ($C_{C(w)} \geq S$). Under those circumstances, the dissolved concentration is set equal to the solubility limit ($C_{C(w)} = S$), and mass of the free product equals:

$$Mc_{fp} = Mc_t - S \nabla_w \left(\frac{Mc_w}{Mc_w} + \frac{Mc_{sed}}{Mc_w} + \frac{Mc_{bed}}{Mc_w} + \frac{Mc_a}{Mc_w} + \frac{Mc_f}{Mc_w} + \frac{Mc_v}{Mc_w} \right) \quad (2.73)$$

S = solubility limit (g/m³ or Ci/m³; mass of contaminant/volume of water)

The mass of contamination as a free product per mass of contaminant in the water compartment is calculated by dividing Equation (2.73) by $S \nabla_w$:

$$\frac{Mc_{fp}}{Mc_w} = \left(\frac{Mc_t}{\nabla_w} \right) \left(\frac{1}{S} \right) - \left(\frac{Mc_w}{Mc_w} + \frac{Mc_{sed}}{Mc_w} + \frac{Mc_{bed}}{Mc_w} + \frac{Mc_a}{Mc_w} + \frac{Mc_f}{Mc_w} + \frac{Mc_v}{Mc_w} \right) \quad (2.74)$$

2.3 SEDIMENT EQUATIONS^a

Many empirical and semi-empirical approaches have been developed to model contaminant transport via sediment movement. In this approach, the Colby (1964) relations, Toffaleti (1968, 1969) formulas, and Meyer-Peter and Muller (1948) formula, as seen in Sedimentation Engineering (Vanoni 1975), will be used to determine the sediment fraction of the contaminant concentration. Although these approaches have been initially chosen to represent the sediment transport rate within this framework, other approaches can be easily included, if appropriate or necessary. Colby's relations, Toffaleti's formulas, and the Meyer-Peter and Muller formula are intended for sand- or gravel-bed sediment types. The ability of these methods to determine the sediment discharge rate is demonstrated in Figures 2.4 and 2.5. The Colorado and Niobrara Rivers have bed sediment with medium-sized sand and stream depths of 1-12 feet. The Colby and Toffaleti methods agree well with the observed sediment discharge in these rivers. The Meyer-Peter and Muller estimates are low (Vanoni 1975).^b

For this approach, the Meyer-Peter and Muller formula will be used only for sediment beds with relatively coarse sediments. Colby and Toffaleti will be used for all other sediment beds, even though it is recognized that they were intended for use only on sand sediment beds. The sediment mass flux rate (g_{ss}) needed to calculate the sediment compartment (Section 2.2.2) is equal to the sediment discharge rate (g_s or g_i), determined from Colby, Toffaleti, and Meyer-Peter and Muller, times the contaminant plume's width at the receptor location. The approach described in this paper is the first step to account for the sediment transport effect on contaminant transport for multimedia models like MEPAS. Other sediment formulas are necessary to estimate sediment transport of silt, clay, and organic matter.

(a) Many of the sediment transport formulations, figures, tables, and correction factors are in English units, which will be presented when consistent with the original published procedure.

(b) Figures 2.4 through 2.10 were reproduced from Sedimentation Engineering (V. A. Vanoni 1975) with permission from the publisher, American Society of Civil Engineers, 1996.

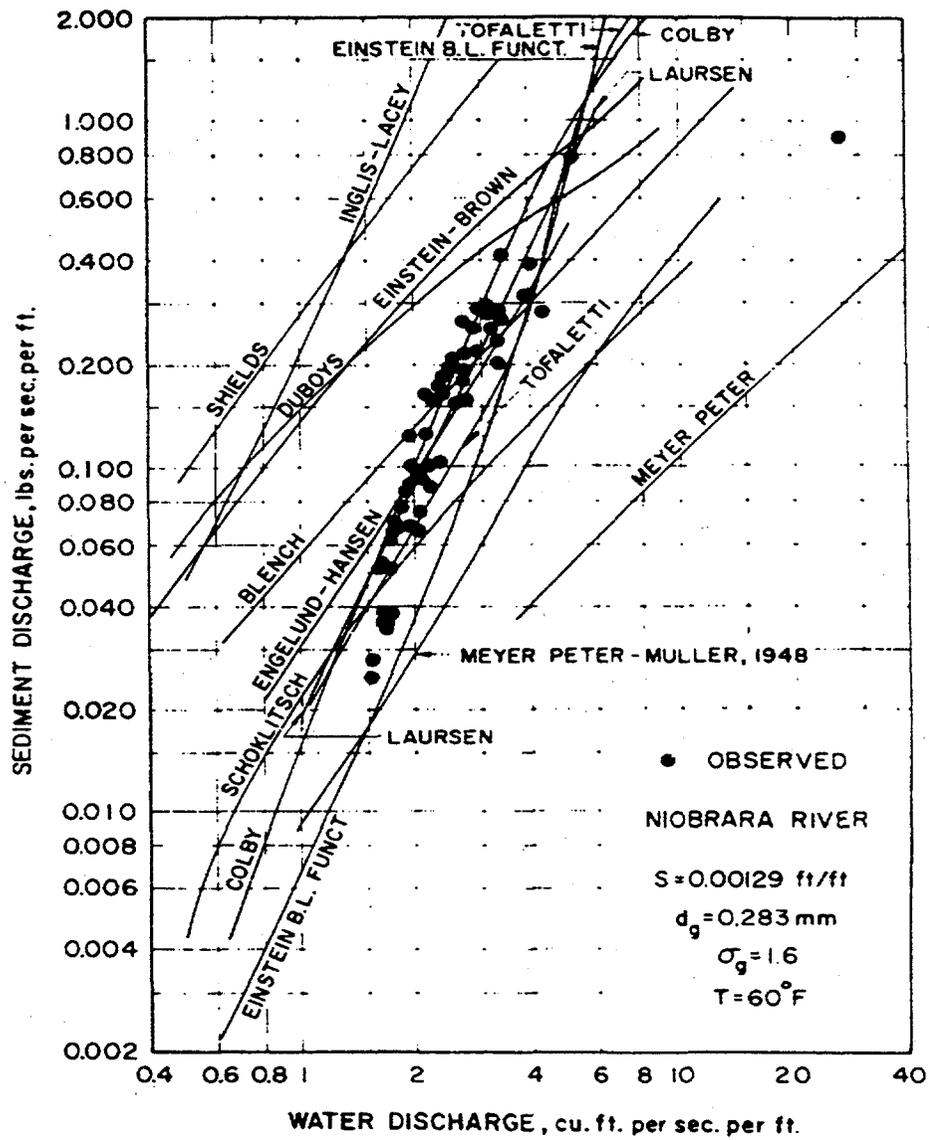


Figure 2.4. Sediment Discharge for the Niobrara River near Cody, Nebraska (from Vanoni 1975 with permission from the publisher, the American Society of Civil Engineers)

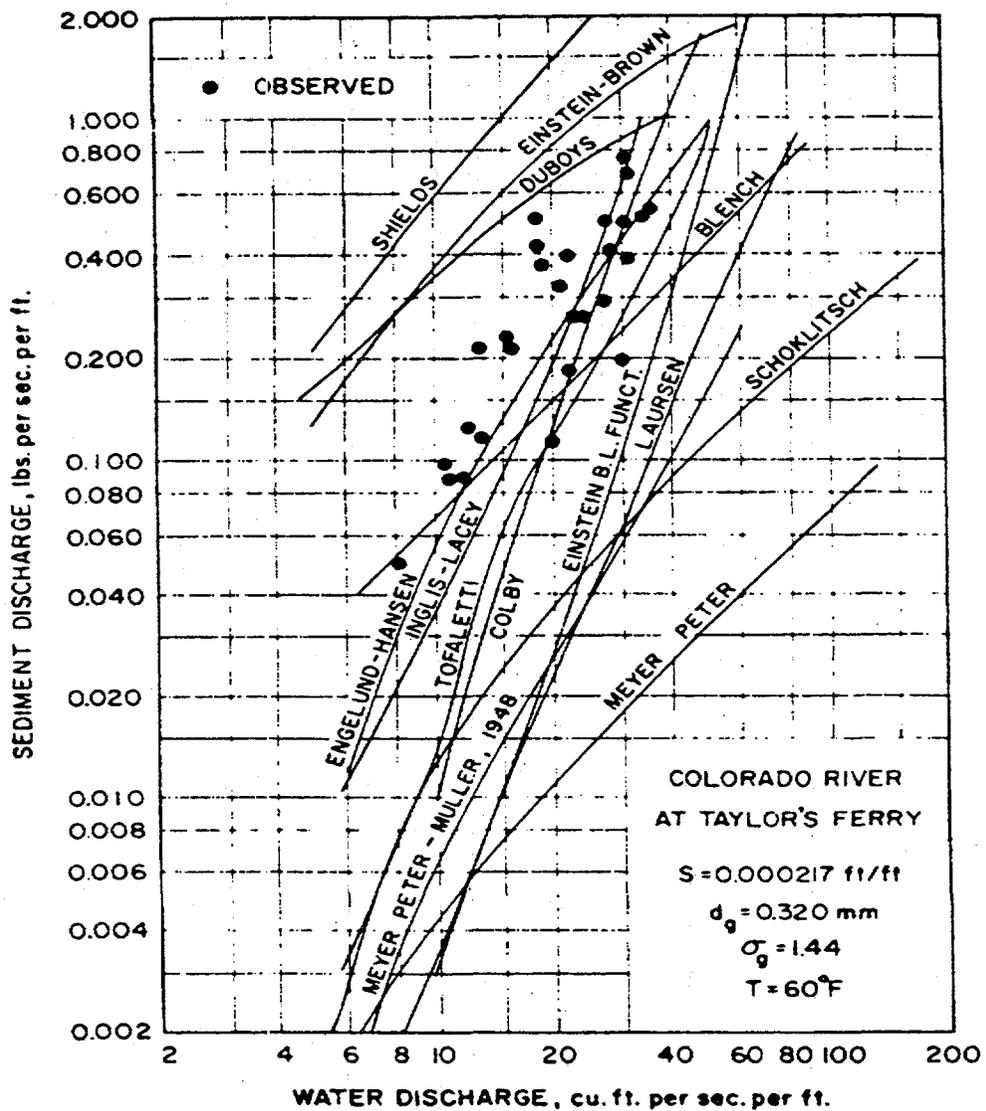


Figure 2.5. Sediment Discharge for the Colorado River at Taylor's Ferry (from Vanoni 1975 with permission from the publisher, the American Society of Civil Engineers)

2.3.1 Colby Relations

The Colby (1964a and 1964b) relations relate the discharge of sands in terms of mean velocity for six median sediment sizes, four flow depths at water temperatures of 15.6°C (60°F). Colby's relations will be used for stream depths 3 meters (10 feet) or less. Based on velocity, depth, and mean particle size, the uncorrected sediment discharge rate can be read from Figure 2.6:

$$g_{si} = f(V, d, d_{50}) \quad (2.75)$$

g_{si} = sediment discharge as a function of V, d, and d_{50} (tons/day/ft)

V = mean velocity (ft/s)

d = stream depth (ft)

d_{50} = mean particle size (mm)

Under conditions when the temperature is not equal to 15.6°C (60°F), there is more than a negligible amount of fine sediment, or the mean particle size is >0.3 mm or <0.2 mm, the sand discharge rate [i.e., Equation (2.75)] requires adjustment. Correction factors for these conditions (Figure 2.7) should be used in the following equation to adjust the sand sediment discharge rate:

$$g_s = (1 + (k_1 k_2 - 1) 0.01 k_3) g_{si} \quad (2.76)$$

g_s = sediment discharge (tons/day/ft)

k_1 = water temperature correction factor (° F)

k_2 = presence of fine sediment correction factor

k_3 = sediment size correction factor

Colby's relations, as reported in Vanoni (1975), were compared to observed river data from several U.S. rivers (see Figure 2.8). These rivers ranged in depth from one to over 50 feet and median bed sediment size from 0.2 to 0.4 mm. Although the median bed size did not vary significantly, this figure demonstrates that the theoretical basis of Colby's relations can be applied to rivers with somewhat different characteristics and still retain a reasonable amount of confidence in the results.

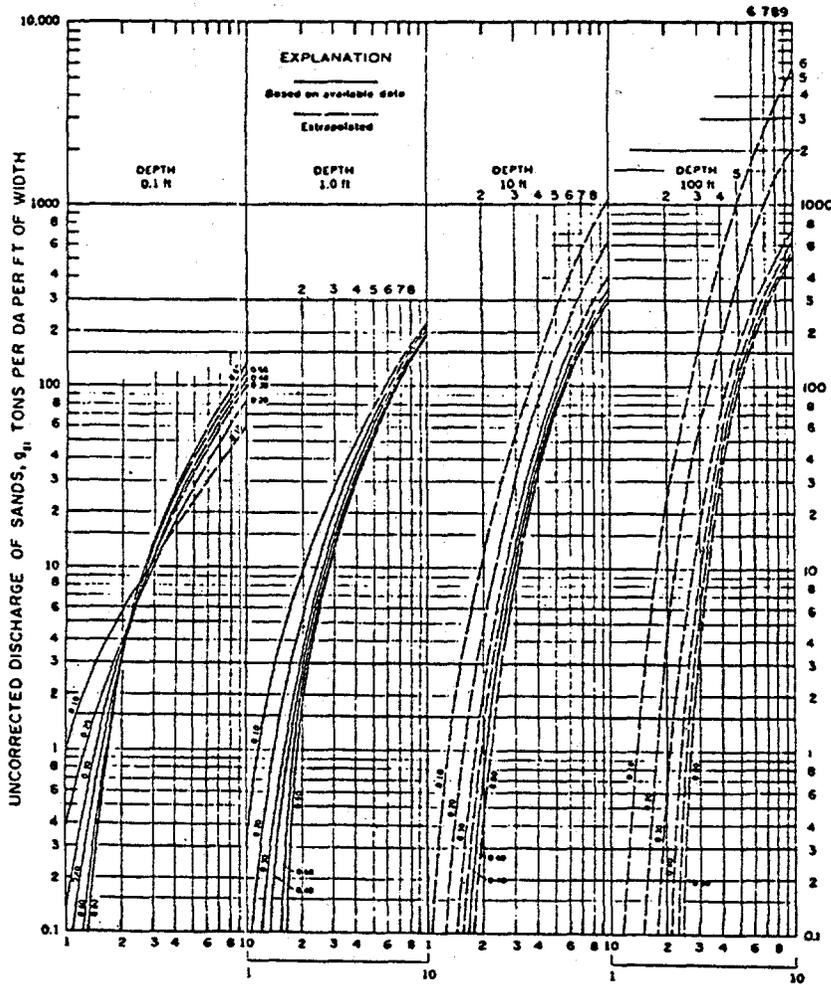


Figure 2.6. Colby's (1964b) Relationship for Discharge of Sands in Terms of Mean Velocity for Six Median Sizes of Bed Sands, Four Depths of Flow, and Water Temperature of 60°F (from Vanoni 1975 with permission from the publisher, the American Society of Civil Engineers)

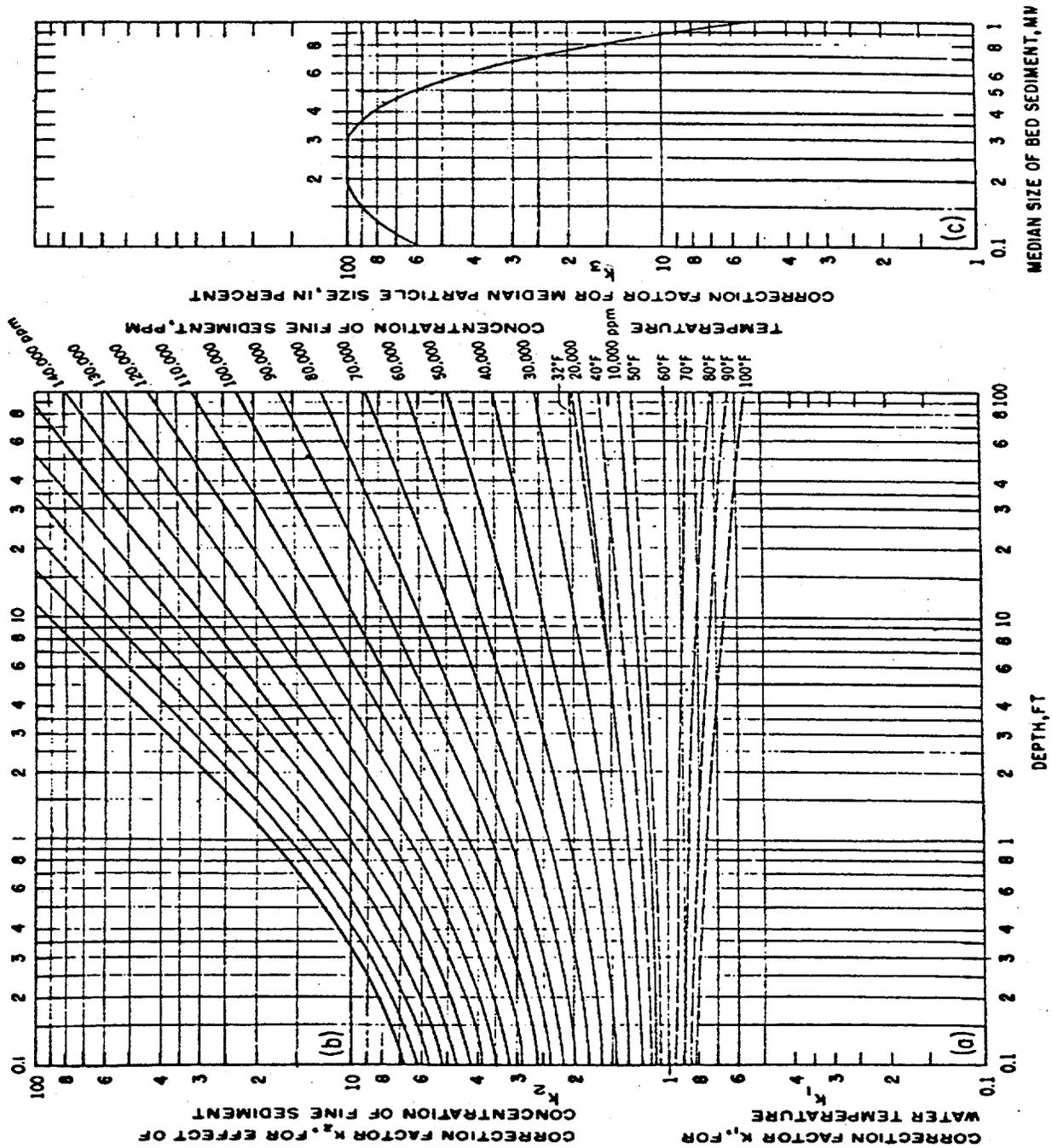


Figure 2.7. Colby's (1964b) Correction Factors for Effect of Water Temperature, Concentration of Fine Sediment, and Sediment Size to be Applied to Uncorrected Discharge of Sand Given by Figure 2.6 (from Vanoni 1975 with permission from the publisher, the American Society of Civil Engineers)

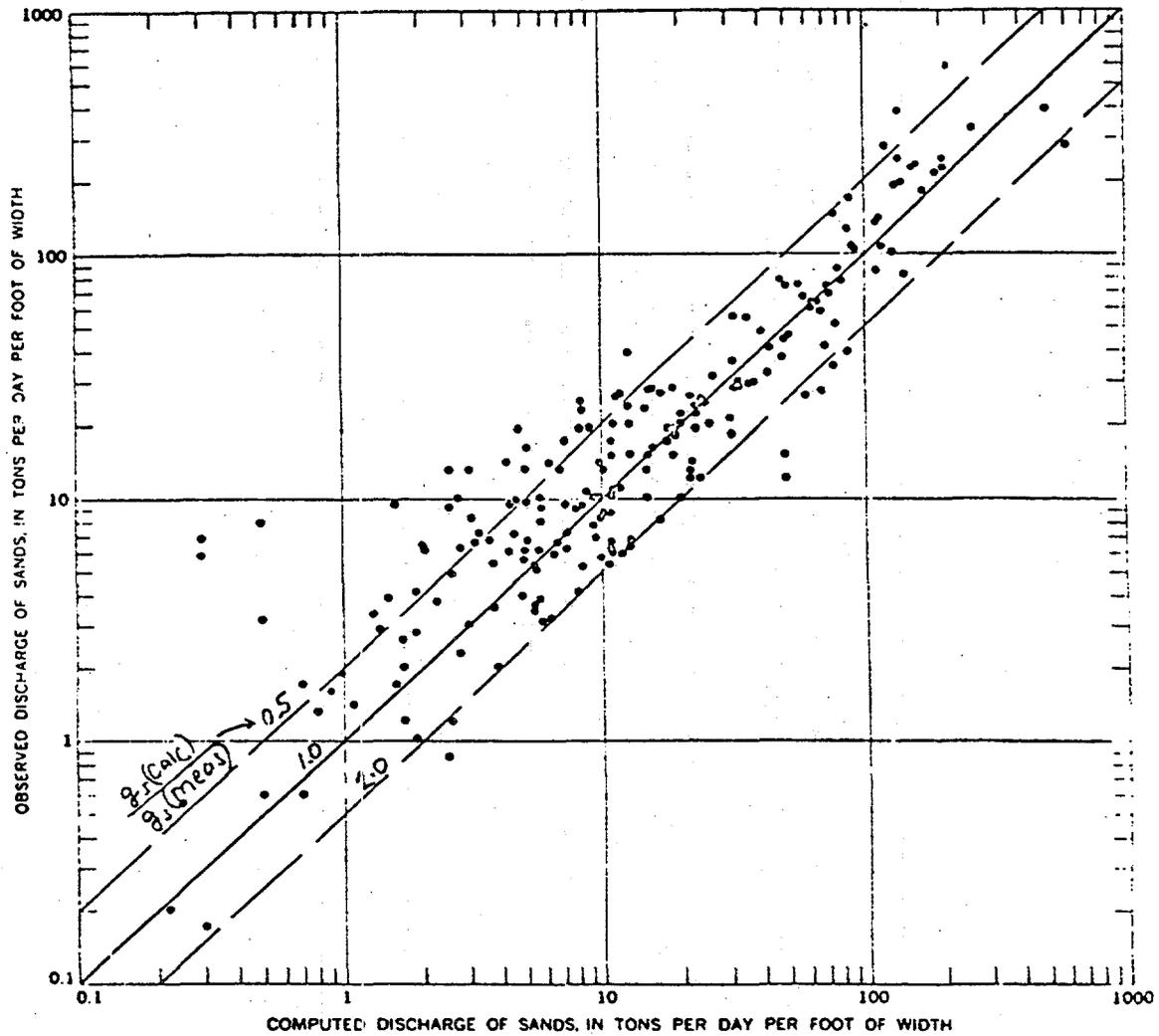


Figure 2.8. Comparison of Bed Sediment Discharge Calculated by Colby Relation and Observed on Several U.S. Rivers (from Vanoni 1975 with permission from the publisher, the American Society of Civil Engineers)

2.3.2 Toffaleti Formulas

In this approach, the Toffaleti (1968, 1969) formulas will be used for streams with depths greater than 3 meters (10 feet). The depth of the stream is divided into four zones as shown in Figure 2.9. The total sediment load discharge is determined by the sum of these four zones:

$$g_{si} = (g_{sbi} + g_{ssLi} + g_{ssMi} + g_{ssUi}) \quad (2.77)$$

g_{si} = total sediment discharge (tons/day/ft)

g_{sbi} = bed load sediment discharge (tons/day/ft)

g_{ssLi} = suspended sediment load discharge in lower zone (tons/day/ft)

g_{ssMi} = suspended sediment load discharge in middle zone (tons/day/ft)

g_{ssUi} = suspended sediment load discharge in upper zone (tons/day/ft)

The velocity profile is represented by:

$$U = (1 + n_v) V \left(\frac{y}{r} \right)^{n_v} \quad (2.78)$$

In which,

$$n_v = 0.1198 + 0.00048T \quad (2.79)$$

U = flow velocity at distance y above bed (ft/s)

V = mean velocity (ft/s)

y = distance above sediment bed (ft)

r = depth of stream (ft)

T = temperature ($^{\circ}$ F)

The concentration profile is defined as follows:

$$C_i = C_{Li} \left(\frac{y}{r} \right)^{-0.756z_i} \quad (2.80)$$

C_i = concentration
 C_{Li} = concentration in lower zone
 C_{Mi} = concentration in middle zone
 C_{Ui} = concentration in upper zone
 w_i = fall velocity
 S = slope of real stream

When $z_i < n_v$, set $z_i = 1.5n_v$. As Vanoni (1975) notes, the expressions for the suspended load discharges in the lower, middle, and upper zones are obtained by substantiating Equation (2.78) and the appropriate expression for C_i [i.e., Equation (2.80), (2.81), or (2.82)] and integrating between the appropriate limits for depth. The suspended sediment load in each region is calculated as follows:

$$g_{ssLi} = \frac{0.600 p_i}{\left(\frac{T_r A k_4}{V^2} \right)^{\frac{5}{3}} \left(\frac{d_{si}}{0.0058} \right)^{\frac{5}{3}}} \quad (2.85)$$

$$g_{ssLi} = M_i \left(\frac{\left(\frac{r}{11.24} \right)^{1+n_v-0.758z_i} - (2d_{si})^{1+n_v-0.756z_i}}{1+n_v-0.756z_i} \right) \quad (2.86)$$

$$g_{ssMi} = M_i \left(\frac{\left(\frac{r}{11.24} \right)^{0.244z_i} \left(\left(\frac{r}{2.5} \right)^{1+n_v-z_i} - \left(\frac{r}{11.24} \right)^{1+n_v-z_i} \right)}{1+n_v-z_i} \right) \quad (2.87)$$

$$g_{ssUi} = M_i \left(\frac{\left(\frac{r}{11.24} \right)^{0.244z_i} \left(\frac{r}{2.5} \right)^{0.5z_i} \left(r^{1+n_v-1.5z_i} - \left(\frac{r}{2.5} \right)^{1+n_v-1.5z_i} \right)}{1+n_v-1.5z_i} \right) \quad (2.88)$$

$$g_{sbi} = M_i (2d_{si})^{1 + n_v - 0.758z_i} \quad (2.89)$$

A = function of $10^5 U^{1/3} / 10 U_*$ as given in Figure 2.10

p_i = weight fraction

k_4 = correction factor from Figure 2.10

U_*' = shear velocity (ft/s)

d_{si} = sand size (ft)

In which,

$$T_r = 1.10 (0.051 + 0.00009T) \quad (2.90)$$

$$M_i = 43.2 p_i C_{Li} (1 + n_v) V_r^{0.758z_i - n_v} \quad (2.91)$$

When $Ak_4 < 16.0$, set $Ak_4 = 16$. To ensure that g_{sbi} is not unrealistically high, the concentration at $2d_{si}$ must be calculated:

$$C_i(y=2d_{si}) = C_{Li} \left(\frac{2d_{si}}{r} \right)^{-0.756z_i} \quad (2.92)$$

$C_i(y=2d_{si})$ = concentration at $y = 2d_{si}$ (lbs/ft³)

If $C_i(y=2d_{si}) > 100$ lb/ft³, C_{Li} must be reduced so that $C_i(y=2d_{si}) = 100$ lb/ft³, and then all of the sediment discharge calculations must be recalculated. Solutions to Equations (2.86) through (2.89) are based on knowing M_i and, hence, C_{Li} . M_i is determined by equating Equations (2.85) and (2.86), and C_{Li} is determined from Equation (2.91).

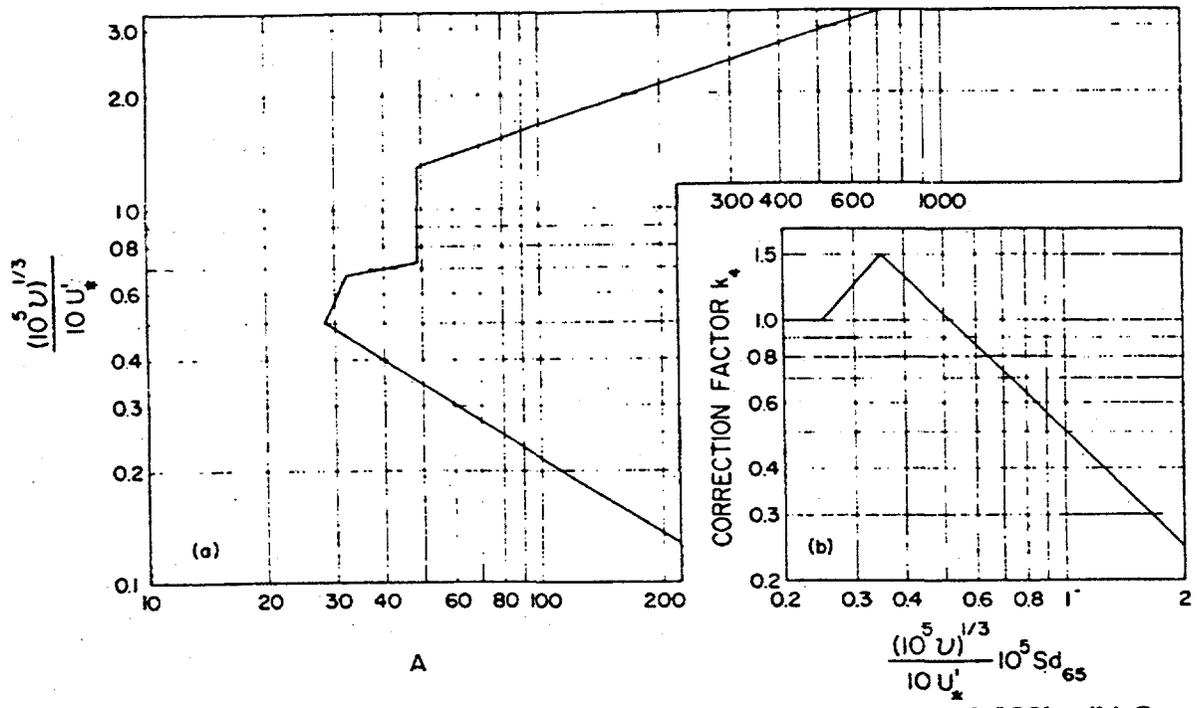


Figure 2.10. Factors in Toffaleti Relations (from Vanoni 1975 with permission from the publisher, the American Society of Civil Engineers)

Although the Toffaleti Formulas were intended for sand beds, this approach assumes they can be applied with reasonable results to all bed types. Comparisons of the sediment discharge calculated by Toffaleti to those observed in United States rivers were similar to those of Colby, as shown in Figure 2.8.

2.3.3 Meyer-Peter and Muller Formula

Most of the data upon which the Meyer-Peter and Muller Formula (1948) is based were obtained in flows with little or no suspended sediment. Therefore, this formula is not valid for flows with appreciable suspended sediment loads. The Meyer-Peter and Muller Formula will be used for

ivers and streams with median grain sizes ranging from coarse sand (0.4 mm) to coarse gravel (30 mm) (Vanoni 1975).

$$\left(\frac{k_r}{k_r'}\right)^{\frac{3}{2}} \gamma r_b S = 0.047(\gamma_s - \gamma)d_m + 0.25\left(\frac{\gamma}{g}\right)^{\frac{1}{3}}\left(\frac{\gamma_s - \gamma}{\gamma_s}\right)^{\frac{2}{3}} g_s^{\frac{2}{3}} \quad (2.93)$$

In which,

$$\frac{k_r}{k_r'} = \sqrt{\frac{f_b'}{8}} \frac{V}{\sqrt{g r_b S}} \quad (2.94)$$

$$d_m = \sum_i p_i d_{si} \quad (2.95)$$

g_s = sediment discharge (lbs/s/ft)

S = slope of stream (ft/ft)

r_b = depth of bed (ft)

γ = specific weight of water

γ_s = specific weight of sediment

g = acceleration due to gravity

f_b' = Darcy-Weisbach bed friction factor

p_i = fraction by weight of fraction of bed with mean size d_{si}

d_{si} = mean size fraction of sediment (ft)

3.0 ASSUMPTIONS AND LIMITATIONS

Many assumptions have been made to represent the contaminant mass and concentration in each of the environmental compartments. The assumptions include the following:

- Tables for the K_d , K_H , BCF_f' , BCF_v' , and S values are appropriate for partitioning chemicals in the environment.
- River is instantly and fully mixed over its depth.
- Contaminant releases to the river are assumed to be long-term relative to the contaminant travel time in the river.
- Washload is not specifically singled out or addressed in the sediment compartment.
- Type of sediment bed forms is not considered.
- Degradation/decay for all contaminants is first-order.
- Dispersion in the water column is only considered in the lateral direction.
- Flow is steady-state and uniform in the longitudinal direction over a given time interval.
- Colby (1964) relations, Toffaleti (1968, 1969) formulas, and Meyer-Peter and Muller (1948) formula are assumed appropriate for the estimation of sediment transport.

For this approach to be useable, the following contaminant characteristics are required:

- Distribution coefficient (K_d)
- Henry's Constant (K_H)
- Biological Concentration Factor (BCF_f') for fish
- Biological Concentration Factor (BCF_v') for vegetation
- Solubility Limit (S)

K_d values need to be available for all relevant contaminants and to be sensitive to the type of sediment the river contains (e.g., sand, silt, clay, or organic matter). K_H values need to be available for all relevant contaminants. BCF' factors for fish and vegetation need to be available for all relevant contaminants. The Solubility Limit needs to be available for all relevant contaminants. Currently, the MEPAS chemical database contains a protocol for each of these parameters. However, the K_d , K_H , BCF'_f, BCF'_v (use above-ground vegetation values if nothing else is available), and S values should be used as estimation tools only because these values change with temperature, pressure, sediment type, and much more. The total approach can be no more accurate than values selected for these parameters.

According to Guy (1964), there are many different factors affecting sediment transport:

- seasonal changes
- net surface runoff
- groundwater runoff
- long-term mean air temperature
- peak rate of water discharge
- storm intensity
- aerial mean precipitation
- aerial mean precipitation intensity.

These factors may affect the washload, suspended sediment and/or bed load sediment transport mechanisms. Changes in the bed action and different types of sediment bed forms could play a factor in the sediment movement and, therefore, the risk associated with the sediment compartment. The sediment compartment equations do not include these attributes for simplification purposes.

This approach considers several mechanisms that may account for additional losses to the total contaminant concentration downstream:

- degradation/decay
- deposition of sediment with adsorbed contaminant
- uptake of contaminants by fish
- uptake of contaminants by vegetation
- deposition of free product
- volatilization.

4.0 APPLICATION

To demonstrate the application of the methodology, an example has been selected from Cheng et al. (1995). This example assumes that liquid ethylene glycol is discharged into the river from a point source beside the river. The discharge of ethylene glycol is assumed to be small in relation to the discharge of the river. The contaminant migrates downstream, mixing laterally as it travels. The ethylene glycol contaminant release occurs over a 10-year time frame with a maximum inflow rate of $3.17 \times 10^{-5} \text{ mg s}^{-1}$. The river width is assumed to be 30.5 meters. The river depth is assumed to be 3.05 meters. The river is assumed to be straight with steady-state, constant flow. The river discharge is $56.7 \text{ m}^3 \text{ s}^{-1}$.

Two receptor scenarios are considered for this example, near-field and far-field. Both receptors are assumed to be on the same side of the river as the contaminant source. The near-field receptor location is 100 meters downstream from the contaminant source. The near-field scenario assumes that the contaminant has not fully mixed across the width of the river. For these calculations, it is assumed that the contaminant plume is 1/4 of the way laterally across the river. The far-field receptor location is 10,000 meters downstream from the contaminant source. The far-field scenario assumes that the contaminant is now fully mixed in the lateral direction across the entire width of the river. In general, this approach would either require the user to provide the lateral mixing width or it could be estimated using the dispersive distance associated with one-half the standard deviation, as is done in MEPAS (Whelan and McDonald 1996). Figure 4.1 shows the example that is used to illustrate the approach.

4.1 NUMERICAL DESCRIPTION OF STREAM

To perform the environmental compartment calculations, many river and contaminant characteristics must be identified. This section identifies the data used and assumptions made to

determine the contaminant mass and concentration for the illustrative example provided in Cheng et al. (1995).

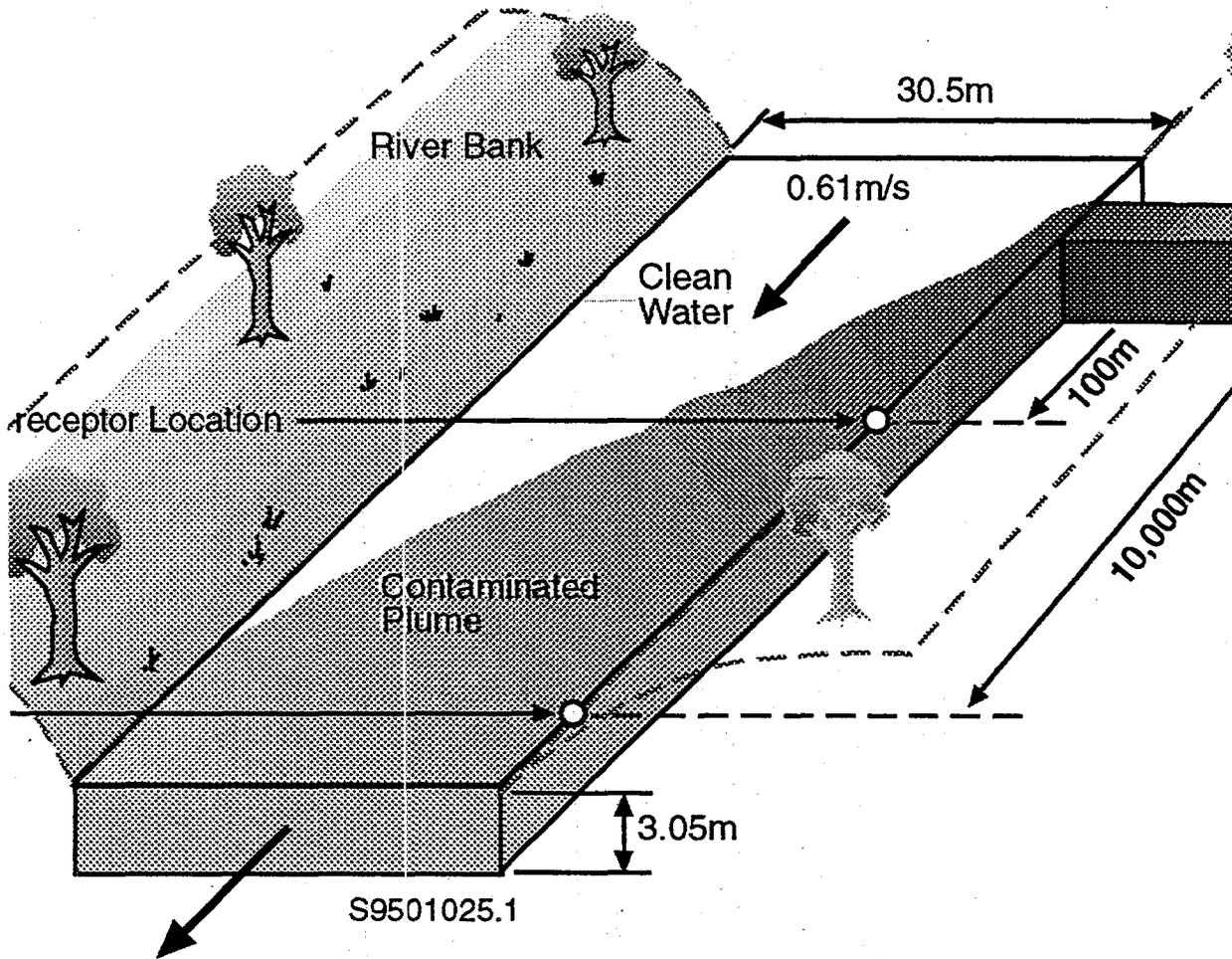


Figure 4.1. Example Illustration of River Environment used in Compartment Model Application (from Cheng et al. 1995)

First, the mixing width of the contaminant plume (W) for the near-field receptor (100 meters) was calculated, assuming that the contaminant was laterally mixed across one-quarter of the river. In general, this approach would require that the user enter the mixing width or a model like MEPAS would provide it:

$$W \text{ (near-field)} = \frac{1}{4} (30.5\text{m}) = 7.625\text{m} \quad (4.1)$$

The mixing width for the far-field receptor (10,000 meters) is assumed to be the full width of the river, 30.5 m. Using the near- and far-field widths, the volume of water was calculated for the near- and far-term receptors:

$$V_w \text{ (near-field)} = 7.625\text{m} \cdot 3.05\text{m} \cdot 100\text{m} = 2325.6\text{m}^3 \quad (4.2)$$

$$V_w \text{ (near-field)} = 30.5\text{m} \cdot 3.05\text{m} \cdot 100\text{m} = 930250\text{m}^3 \quad (4.3)$$

It was assumed that the sediment type was 100% medium sand. To assign the bed sediment bulk density, Table 4.1 was used and the representative soil type selected was sand. In general, this approach would require the user to provide the percent sand, silt, clay, and organic matter, bulk density, and porosity of the sediment. If the percent of sand, silt, clay and organic matter, porosity, or bulk density are unknown, representative values could be assigned based on the "Representative Soil Characteristics" provided in Table 4.1.

The height of the sediment bed was assumed to be 5 cm. The water temperature of the river is assumed to be 60°F. The height of the air column is assumed to be 3.05 meters. This approach requires the user to provide these values.

To determine the near- and far-field bulk density of the fish, it was assumed the river contained one fish every 10 meters and that an average fish weighed 0.5 kilograms:

Table 4.1. Representative Soil Characteristics (from Buck et al, 1995)

Soil-Texture Classification	Soil Composition (based on USDA Textural Diagram)			Porosity, %	Bulk Density, g/cm ³	USLE K-Factor Organic Matter Content		
	% Sand	% Silt	% Clay			<0.5%	2%	4%
Sand	92	5	3	38.0	1.64	0.05	0.03	0.02
Loamy Sand	83	11	6	43.7	1.49	0.12	0.10	0.08
Sandy Loam	65	25	10	44.2	1.48	0.27	0.24	0.19
Loam	42	38	20	46.6	1.42	0.38	0.34	0.29
Silty Loam	20	65	15	46.3	1.42	0.48	0.42	0.33
Silt	7	88	5	44.2	1.48	0.60	0.52	0.42
Sandy Clay Loam	60	14	26	39.8	1.60	0.27	0.25	0.21
Clay Loam	32	35	33	47.7	1.39	0.28	0.25	0.21
Silty Clay Loam	10	57	33	49.0	1.35	0.37	0.32	0.26
Sandy Clay	52	7	41	43.0	1.51	0.14	0.13	0.12
Silty Clay	7	46	47	48.6	1.36	0.25	0.23	0.19
Clay	20	20	60	47.5	1.39	0.25	0.23	0.19

$$\beta_{d(\text{fish})} (\text{near-field}) = \left(\frac{0.5\text{kg}}{3.05\text{m} \cdot 7.625\text{m} \cdot 10\text{m}} \right) \left(\frac{\text{m}^3}{1000\text{L}} \right) = 2.15 \times 10^{-6} \text{ kg/L} \quad (4.4)$$

$$\beta_{d(\text{fish})} (\text{far-field}) = \left(\frac{0.5\text{kg}}{3.05\text{m} \cdot 30.5\text{m} \cdot 10\text{m}} \right) \left(\frac{\text{m}^3}{1000\text{L}} \right) = 5.37 \times 10^{-7} \text{ kg/L} \quad (4.5)$$

To determine the near- and far-field bulk density of the vegetation, it was assumed the river contained 10 kilograms of vegetation every 100 meters:

$$\beta_{d(\text{veg})} (\text{near-field}) = \left(\frac{10\text{kg}}{3.05\text{m} \cdot 7.625\text{m} \cdot 100\text{m}} \right) \left(\frac{\text{m}^3}{1000\text{L}} \right) = 4.3 \times 10^{-6} \text{ kg/L} \quad (4.6)$$

$$\beta_{d(\text{veg})} (\text{far-field}) = \left(\frac{10\text{kg}}{3.05\text{m} \cdot 30.5\text{m} \cdot 100\text{m}} \right) \left(\frac{\text{m}^3}{1000\text{L}} \right) = 1.07 \times 10^{-6} \text{ kg/L} \quad (4.7)$$

Values for the Henry's Constant, Gas Law Constant, Biological Concentration Factor for fish and vegetation, Carbon Matter Partition Coefficient, and Solubility Limit were found in the MMEDE database (Warren and Strenge 1994), and the MEPAS chemical database (Strenge et al. 1989). Table 4.2 is a summary of the data input values used in this illustrative example. Table 4.3 contains some of the conversion factors used to assist with the calculations.

4.2 COMPARTMENT CALCULATIONS

Using the data inputs defined in Section 4.1, each environmental compartment's mass and concentration were calculated. It was discovered, after the initial set of calculations were made, that the distribution coefficient of ethylene glycol was too small to allow the Cheng et al. (1995) example to illustrate the potential effects that partitioning contaminants into the various environmental compartments could have on the contaminant mass and concentration values.

Table 4.2. Summary of Data Inputs

Variable		Value
River Depth	D	3.05 m
Contaminant Plume Width (Near-Field)	W	7.625 m
Contaminant Plume Width (Far-Field)	W	30.5 m
River Length (Near-Field)	L	100 m
River Length (Far-Field)	L	10,000 m
River Volume (Near-Field)	V_w	2325.6 m ³
River Volume (Far-Field)	V_w	930250 m ³
River Flow Velocity	U	0.61 m/s
Water Discharge Rate	Q	56.7 m ³ /s
Height of Air Column	H _{air}	3.05 m
Height of Sediment Bed	H _{bed}	0.05 m
Bulk Density of Fish (Near-Field)	$\beta_{d(\text{fish})}$	2.15 x 10 ⁻⁶ kg/L
Bulk Density of Fish (Far-Field)	$\beta_{d(\text{fish})}$	5.37 x 10 ⁻⁷ kg/L
Bulk Density of Vegetation (Near-Field)	$\beta_{d(\text{veg})}$	4.3 x 10 ⁻⁶ kg/L
Bulk Density of Vegetation (Far-Field)	$\beta_{d(\text{veg})}$	1.07 x 10 ⁻⁶ kg/L
Temperature	T	60°F, 15.6°C, 288.75 K
Henry's Constant	K _H	9.97 x 10 ⁻⁹ atm · m ³ /mole
Gas Law Constant	R	0.08314 L · bar/K · mole
Bulk Density of Bed Sediment	$\beta_{d(\text{bed})}$	1.64 g/m ³
Biological Concentration Factor for Fish BCF _f '		2 x 10 ⁻² L/kg
Biological Conc. Factor for Vegetation BCF _v '		1.3 x 10 ² mL/kg
Carbon Matter Partition Coefficient	K _{oc}	2.7 x 10 ⁻² L/g
Solubility Limit	S	5.82 x 10 ⁵ mg/L

Table 4.3. Conversion Factors

1 L	10^{-3}m^3
C	$5/9(\text{F}-32)$
K	$273.15 + \text{C}$
1 atm	1.01325 bar
1 kg	1000 g
1 m	100 cm
1 ft	0.3048 m
1 ton	907185 g

To demonstrate the potential affects a higher distribution coefficient could have on concentration levels, two additional distribution coefficient values were tested (Example 2: $K_d = 100 \text{ mL/g}$, and Example 3: $K_d = 6000 \text{ mL/g}$). The Cheng et al. (1995) example results are described as Example 1 or the illustrative example. The calculations will be shown for Example 1, but only a summary of the results for Examples 2 and 3 are provided in this report.

Eight time-varying total concentration values were used from Cheng et al. (1995) to determine the concentration distribution in the environmental compartments. Table 4.4 provides the values that were used. Figure 4.2 shows the distribution of the contaminant concentration over time.

4.2.1 Water Compartment

The water compartment mass ratio equals unity.

Table 4.4. Time-Varying Concentration of Ethylene Glycol

Year	Near-Field Concentration (mg/L)	Far-Field Concentration (mg/L)
0	0	0
2	1.48×10^{-9}	1.4×10^{-10}
4	2.2×10^{-9}	2.8×10^{-10}
6	2.2×10^{-9}	2.8×10^{-10}
8	2.2×10^{-9}	2.8×10^{-10}
10	2.2×10^{-9}	2.8×10^{-10}
12	8.2×10^{-10}	1.4×10^{-10}
14	1×10^{-10}	0
16	0	0

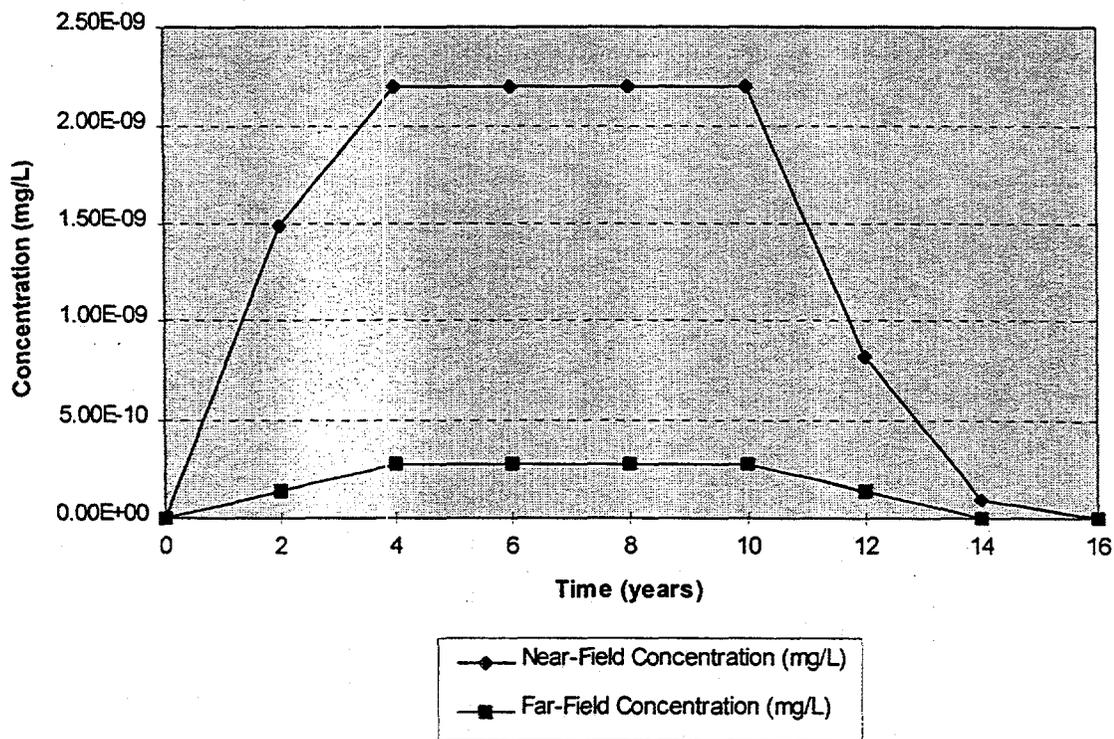


Figure 4.2. Time-Varying Concentration of Ethylene Glycol Calculated by MEPAS for Illustrative Example in Cheng et al. (1995).

4.2.2 Sediment Compartment

As described in Section 4.1, the sediment type is 100% medium sand and the river water temperature is 60°F. From Table 4.5, it is assumed that the mean particle size of the sediment is 0.3 mm. It is also assumed that there is minimal fine sediment present. Since the river depth is 10 feet or less, Colby's relations were used. From Figure 2.6, the sediment discharge rate (g_{si}) is 2 tons/day/ft-width. Next, the sediment discharge rate is used to calculate the sediment flux rate (g_{ss}); and the sediment flux rate and water discharge rate are used to calculate the concentration of the sediment in the water column (Equation 2.18):

Table 4.5. Sediment Grade Scale

Class Name	Size Range (mm)
Very coarse sand	2.000-1.000
Coarse sand	1.000-0.500
Medium sand	0.500-0.250
Fine sand	0.250-0.125
Very fine sand	0.125-0.062
Coarse silt	0.062-0.031
Medium silt	0.031-0.016
Fine silt	0.016-0.008
Very fine silt	0.008-0.004
Coarse clay	0.004-0.0020
Medium clay	0.0020-0.0010
Fine clay	0.0010-0.0005
Very fine clay	0.0005-0.00024

$$g_{ss}(\text{near-field}) = g_s \cdot W(\text{near-field}) \quad (4.8)$$

$$g_{ss}(\text{near-field}) = 2.0 \frac{\text{tons}}{\text{day} \cdot \text{ft}} \cdot 7.625\text{m} \cdot \frac{907185\text{g}}{\text{ton}} \cdot \frac{\text{day}}{86400\text{s}} \cdot \frac{\text{ft}}{0.3048\text{m}} = 525.3\text{g/s} \quad (4.9)$$

$$g_{ss}(\text{far-field}) = g_s \cdot W(\text{far-field}) \quad (4.10)$$

$$g_{ss}(\text{far-field}) = 2.0 \frac{\text{tons}}{\text{day} \cdot \text{ft}} \cdot 50.5\text{m} \cdot \frac{907185\text{g}}{\text{ton}} \cdot \frac{\text{day}}{86400\text{s}} \cdot \frac{\text{ft}}{0.3048\text{m}} = 2101.3\text{g/s} \quad (4.11)$$

Next, the distribution coefficient for ethylene glycol was estimated using the Carbon Matter Partition Coefficient (K_{oc}) provided by Warren and Strenge (1995) and the estimation method described in Strenge et al. (1989). In general, the approach outlined in this paper would request the user to provide the distribution coefficient.

$$K_d = 10^{-4} \cdot K_{oc} \cdot 0.005 = 1.35 \times 10^{-8} \text{ mL/g} \quad (4.12)$$

The next step was to calculate the sediment factor for the near- and far- field receptors using Equation (2.15):

$$\frac{Mc_{sed}}{Mc_w}(\text{near-field}) = K_{d(sed)} \cdot C_{sed} = 1.35 \times 10^{-8} \text{ mL/g} \cdot 9.27 \text{ mg/L} = 1.25 \times 10^{-13} \quad (4.13)$$

$$\frac{Mc_{sed}}{Mc_w}(\text{far-field}) = K_{d(sed)} \cdot C_{sed} = 1.35 \times 10^{-8} \text{ mL/g} \cdot 37.1 \text{ mg/L} = 5 \times 10^{-13} \quad (4.14)$$

4.2.3 Bed Sediment Compartment

For the bed sediment factor, the same distribution coefficient (K_d) that was calculated for the sediment factor was used. Since the user will be asked to provide a distribution coefficient for the bed sediment, it might not always be the same as the sediment factor K_d . The following calculation represents both the near- and far-field calculations for the contaminant mass in the bed sediment compartment, using Equation (2.37):

$$\frac{Mc_{bed(scd)}}{Mc_w} = (1.35 \times 10^{-8} \text{ mL/g})(1.64 \text{ g/m}^3) \left(\frac{0.05\text{m}}{3.05\text{m}} \right) = 3.63 \times 10^{-16} \quad (4.15)$$

4.2.4 Air Compartment

The following calculation represents both the near- and far-field calculations for the contaminant mass in the air compartment, using Equation (2.52):

$$\frac{Mc_a}{Mc_w} = K_H \frac{H_{air}}{d} = (4.21 \times 10^{-7}) \left(\frac{3.05\text{m}}{3.05\text{m}} \right) = 4.21 \times 10^{-7} \quad (4.16)$$

4.2.5 Fish Compartment

The following calculation represents the near-field calculations for the contaminant mass in the fish compartment, using Equation (2.60):

$$\frac{Mc_f}{Mc_w} (\text{near-field}) = (2.15 \times 10^{-6} \text{ kg/L})(2 \times 10^{-2} \text{ L/kg}) = 4.3 \times 10^{-8} \quad (4.17)$$

The following calculation represents the far-field calculations for the contaminant mass in the fish compartment:

$$\frac{Mc_f}{Mc_w} \text{ (far-field)} = (5.37 \times 10^{-7} \text{ kg/L})(2 \times 10^{-2} \text{ L/kg}) = 1.07 \times 10^{-8} \quad (4.18)$$

4.2.6 Vegetation Compartment

The following calculation represents the near-field calculations for the contaminant mass in the vegetation compartment, using Equation (2.67):

$$\frac{Mc_v}{Mc_w} \text{ (near-field)} = (4.3 \times 10^{-6} \text{ kg/L})(1.3 \times 10^2 \text{ mL/kg}) = 5.59 \times 10^{-7} \quad (4.19)$$

The following calculation represents the far-field calculations for the contaminant mass in the vegetation compartment:

$$\frac{Mc_v}{Mc_w} \text{ (far-field)} = (1.07 \times 10^{-6} \text{ kg/L})(1.3 \times 10^2 \text{ mL/kg}) = 1.4 \times 10^{-7} \quad (4.20)$$

4.2.7 Free Product Compartment

The total contaminant mass for the air factor is zero because the total concentration was not greater than the solubility limit of ethylene glycol.

4.2.8 Mass Balance and Concentration Calculations

Table 4.6 summarizes the near- and far-field contaminant mass calculations for the illustrative example.

Table 4.6. Summary of Contaminant Mass Calculations

Compartment/Variable		Near Field	Far Field
Sediment	Mc_{sed}/Mc_w	1.25×10^{-13}	5.00×10^{-13}
Bed	Mc_{bed}/Mc_w	3.63×10^{-16}	3.63×10^{-16}
Air	Mc_a/Mc_w	4.21×10^{-7}	4.21×10^{-7}
Fish	Mc_f/Mc_w	4.30×10^{-8}	1.07×10^{-8}
Vegetation	Mc_v/Mc_w	5.59×10^{-7}	1.40×10^{-7}
Water	Mc_w/Mc_w	1	1
Free Product	Mc_{fp}/Mc_w	0	0

The following calculation represents the near-field scenario ratio of contaminant mass in the water compartment to the total mass, Equation (2.8):

$$\frac{Mc_w(\text{near-field})}{Mc_t} = \left(\frac{1}{1 + (1.25E-13) + (3.63E-16) + (4.21E-7) + (4.3E-8) + (5.59E-7)} \right) \quad (4.21)$$

$$\frac{Mc_w(\text{near-field})}{Mc_t} = 0.999998977 \quad (4.22)$$

The following calculation represents the far-field scenario ratio of contaminant mass in the water compartment to the total mass:

$$\frac{Mc_w(\text{far-field})}{Mc_t} = \left(\frac{1}{1+(5E-13)+(3.63E-16)+(4.21E-7)+(1.07E-8)+(1.4E-7)} \right) \quad (4.23)$$

$$\frac{Mc_w(\text{far-field})}{Mc_t} = 0.999999428 \quad (4.24)$$

The time-varying concentration near- and far-field values for each of the environmental compartments are summarized in Table 4.7.

4.3 RESULTS AND DISCUSSION

As mentioned in Section 4.1, the ethylene glycol distribution coefficient was so small that the water factor was the primary holder of contaminant mass and concentration; the sediment factors, along with all the other environmental compartments, appeared to be insignificant. Figure 4.3 shows how the water compartment contaminant concentration dominates in the illustrative example. This illustrative example was chosen because it was used to compare the results of multimedia models, like MEPAS and MMSOILS. Although the results did not show significant partitioning of the contaminant into environmental compartments, this approach still provides the equations needed to perform a preliminary analysis of contaminant transport mechanisms that can be incorporated into multimedia models.

To determine the sensitivity of the distribution coefficient, two additional examples with higher K_d values were performed. A comparison of the percent of mass per environmental compartment is shown in Table 4.8.

Table 4.7. Time-Varying Concentrations

Compartment	Near-Field Concentration	Far-Field Concentration	Years
Water (g/m ³)	1.48 x 10 ⁻⁹	1.40 x 10 ⁻¹⁰	2
	2.20 x 10 ⁻⁹	2.80 x 10 ⁻¹⁰	4-10
	8.20 x 10 ⁻¹⁰	1.40 x 10 ⁻¹⁰	12
	1.00 x 10 ⁻¹⁰	0	14
Sediment (g/g)	1.05 x 10 ⁻²⁰	3.97 x 10 ⁻²¹	2
	1.56 x 10 ⁻²⁰	7.94 x 10 ⁻²¹	4-10
	5.82 x 10 ⁻²¹	3.97 x 10 ⁻²¹	12
	7.09 x 10 ⁻²²	0	14
Bed Sediment (g/g)	3.28 x 10 ⁻²⁵	3.10 x 10 ⁻²⁶	2
	4.87 x 10 ⁻²⁵	6.20 x 10 ⁻²⁶	4-10
	1.81 x 10 ⁻²⁵	3.10 x 10 ⁻²⁶	12
	2.21 x 10 ⁻²⁶	0	14
Air (g/m ³)	6.23 x 10 ⁻¹⁶	5.89 x 10 ⁻¹⁷	2
	9.26 x 10 ⁻¹⁶	1.18 x 10 ⁻¹⁶	4-10
	3.45 x 10 ⁻¹⁶	5.89 x 10 ⁻¹⁷	12
	4.21 x 10 ⁻¹⁷	0	14
Fish (g/g)	2.96 x 10 ⁻¹⁷	2.80 x 10 ⁻¹⁸	2
	4.40 x 10 ⁻¹⁷	5.60 x 10 ⁻¹⁸	4-10
	1.64 x 10 ⁻¹⁷	2.80 x 10 ⁻¹⁸	12
	2.00 x 10 ⁻¹⁸	0	14
Vegetation (g/g)	1.92 x 10 ⁻¹⁶	1.82 x 10 ⁻¹⁷	2
	2.86 x 10 ⁻¹⁶	3.64 x 10 ⁻¹⁷	4-10
	1.07 x 10 ⁻¹⁶	1.82 x 10 ⁻¹⁷	12
	1.30 x 10 ⁻¹⁷	0	14

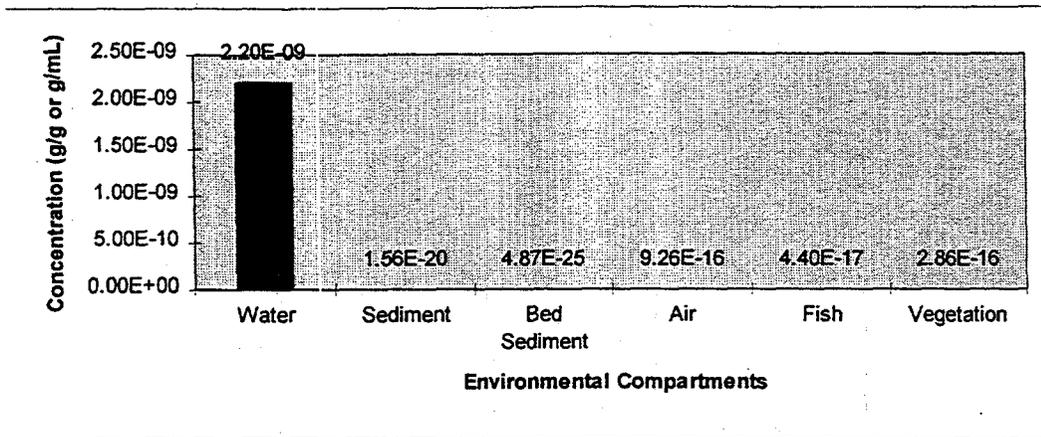


Figure 4.3. Contaminant Concentration for the Near-Field Receptor, at 4 years, in each Environmental Compartment, when $K_d = 1.35 \times 10^{-8}$ mL/g

Table 4.8. Percentage of Mass per Environmental Compartment

Compartment	$K_d = 1.35 \times 10^{-8}$ mL/g		$K_d = 100$ mL/g		$K_d = 6000$ mL/g	
	Near-Field	Far-Field	Near-Field	Far-Field	Near-Field	Far-Field
Water	100.00%	100.00%	99.91%	99.63%	94.73%	81.81%
Sediment	0.0%	0.0%	0.09%	0.37%	5.27%	18.19%
Bed Sediment	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Air	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Fish	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Vegetation	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Free Product	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%

Graphical representation of the contaminant concentration distribution in the environmental compartments for K_d values of 100 mL/g (Example 2) and 6000 mL/g (Example 3) are shown in Figures 4.4 and 4.5, respectively.

In the case of Example 3, the contaminant concentration on the sediment is greater than that in the water column by a factor of 10. The approach outlined in this report is most useful when the distribution coefficient for the contaminant is large, or any other determining factor (e.g., Henry's Constant, Biological Concentration Factors, etc.) is significant.

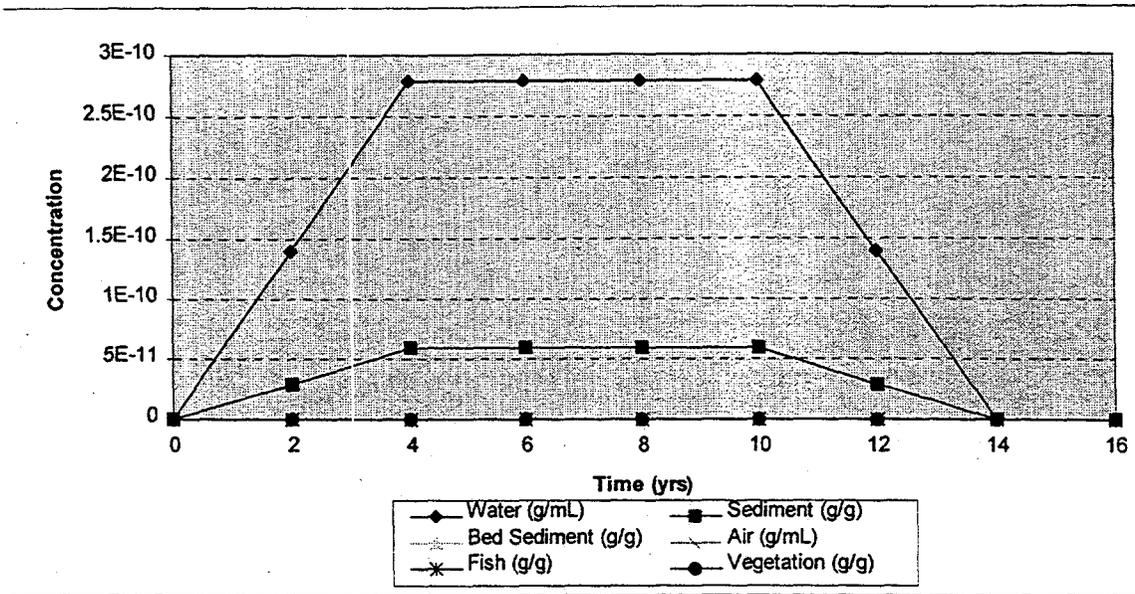


Figure 4.4. Time-Varying Contaminant Concentration for the Far-Field Receptor, in each Environmental Compartment, when $K_d = 100 \text{ mL/g}$

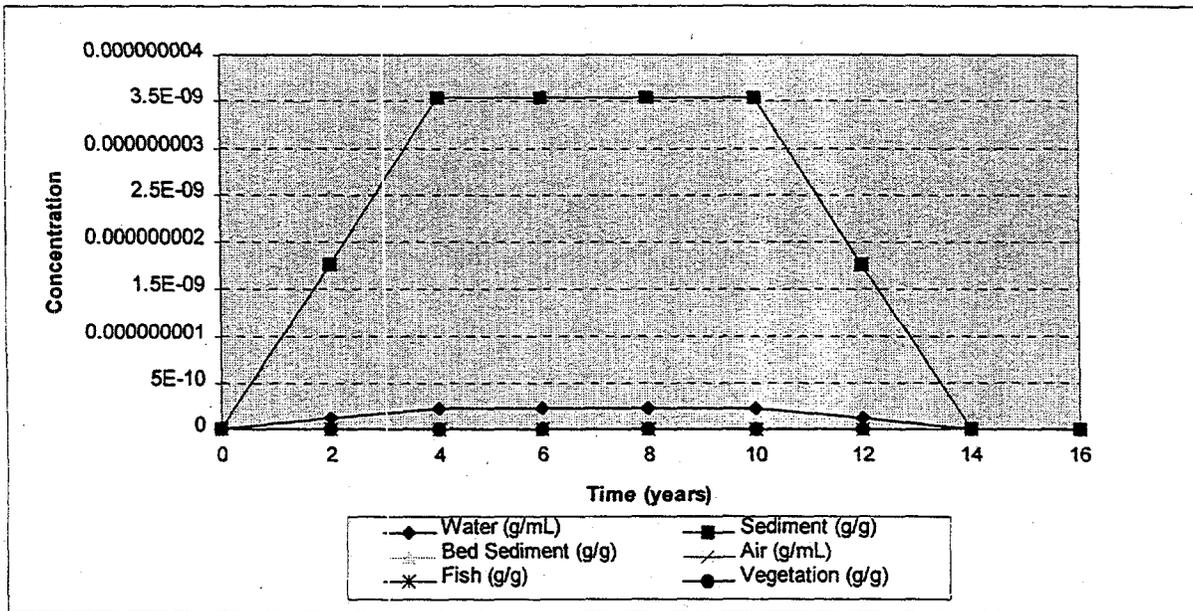


Figure 4.5. Time-Varying Contaminant Concentration for the Far-Field Receptor, in each Environmental Compartment, when $K_d = 6000 \text{ mL/g}$

5.0 SUMMARY

This approach provides a mathematical model for multimedia contaminant transport mechanisms in river water. It uses the advection-dispersion equation to model the flow and transport of the contaminants in the water. It uses compartment modeling to partition the contaminant into the water, sediment, bed sediment, air, fish, vegetation, and free product environmental compartments, and it calculates the contaminant concentrations in each environmental compartment. As long as the approach is applied with an understanding of its assumptions and limitations, it should be useful in further defining the risk associated with contaminant transport in river water.

Risk and the qualitative process of decision-making are the primary endpoints of this mathematical model. The model outlined in this paper has accomplished this by providing a preliminary assessment and/or screening tool for contaminant transport in rivers by capturing the essence of environmental partitioning without unduly burdening the analyst with data input computations and/or requirements.

The mathematical model outlined in this paper is intended as a potential replacement for the approach in existing multimedia models that assumes the contaminant is completely dissolved in the water column. Although the compartment modeling may not be necessary in all preliminary multimedia assessments, it can be very useful when key data input parameters exist for the exposure scenario. Those key data input parameters include:

1. Contaminant Characteristics
 - distribution coefficient (K_d)
 - Henry's constant (K_H)
 - biological concentration factor for fish (BCF_f')
 - biological concentration factor for vegetation (BCF_v')

- solubility limit (S)

2. River Characteristics

- sediment concentration (C_{sed})
- height of bed sediment (H_{bed})
- mass of fish (M_f)
- mass of vegetation (M_v)

If this approach is used by MEPAS or other multimedia models, it is recommended that the advection-dispersion equation be adapted to account for the losses of contaminant in the system due to volatilization, adsorption, and settling associated with the air, fish, vegetation, sediment, bed sediment and free product factors as the contaminant makes its way to the receptor. Currently, losses (except for degradation/decay) are not accounted for in the solution to the advection-dispersion equation. The approach outlined in this paper does not address these potential losses of contaminant in the advection-dispersion equation. The MEPAS model may want to use this approach only when the key input parameters are significant enough to justify the time spent partitioning the contaminant into the environmental compartments. MEPAS may also want to consider allowing the users to select which environmental compartments they want the model to use.

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Appendix A

Equation Notation/Definitions

APPENDIX A

EQUATION NOTATION/DEFINITIONS

Alphabetized list of variables and their definitions.

$(1 - n)$ = total porosity fraction (fraction)

$\beta_{d(\text{bed})}$ = bulk density of bed sediment (g/m^3 ; mass of sediment/volume of water)

$\beta_{d(\text{clay})}$ = bulk density of clay portion of bed sediment (g/m^3 ; mass of clay/volume of water)

$\beta_{d(\text{fish})}$ = bulk density of fish (g/m^3 ; mass of fish/volume of water)

$\beta_{d(\text{sand})}$ = bulk density of sand portion of bed sediment (g/m^3 ; mass of sand/volume of water)

$\beta_{d(\text{silt})}$ = bulk density of silt portion of bed sediment (g/m^3 ; mass of silt/volume of water)

$\beta_{d(\text{veg})}$ = bulk density of vegetation (g/m^3 ; mass of vegetation/volume of water)

γ = specific weight of water

γ_s = specific weight of sediment

λ = degradation/decay constant (s^{-1})

ρ_{clay} = density of clay portion of sediment (g/m^3 ; mass of clay/volume of clay)

ρ_f = density of fish (g/m^3 ; mass of fish/volume of fish)

ρ_{OM} = density of organic matter portion of sediment (g/m^3 ; mass of organic matter/volume of organic matter)

ρ_{sand} = density of sand portion of sediment (g/m^3 ; mass of sand/volume of sand)

ρ_{silt} = density of silt portion of sediment (g/m^3 ; mass of silt/volume of silt)

ρ_v = density of vegetation (g/m^3 ; mass of vegetation/volume of fish)

A = function of $10^5 v^{1/3}/10 U_*'$ as given in Figure 2.10

B = width of river (m)

BCF_f' = biological concentration factor for fish (m^3/g ; volume of water/mass of fish)

BCF_v' = biological concentration factor for vegetation (m^3/g ; volume of water/mass of fish)

C_{clay} = concentration of clay in water compartment (g/m^3 or Ci/m^3 ; mass of clay/volume of water)

C_{OM} = concentration of organic matter in water compartment (g/m^3 or Ci/m^3 ; mass of organic matter/volume of water)

C_{sand} = concentration of sand in water compartment (g/m^3 or Ci/m^3 ; mass of sand/volume of water)

C_{sed} = sediment concentration in the sediment compartment (g/m^3 ; mass of sediment/volume of water)

C_{silt} = concentration of silt in water compartment (g/m^3 or Ci/m^3 ; mass of silt/volume of water)

$C_{C(\text{air})}$ = contaminant concentration in the air compartment (g/m^3 or Ci/m^3 ; mass of contaminant/volume of air)

$C_{C(\text{bed})}$ = contaminant concentration in the bed sediment compartment (g/g or Ci/g ; mass of contaminant/mass of bed sediment)

$C_{C(\text{fish})}$ = contaminant concentration in the fish compartment (g of contaminant/g of fish or Ci/g ; mass of contaminant/mass of fish)

$C_{C(\text{sed})}$ = adsorbed contaminant concentration in the sediment compartment (g/g or Ci/g; mass of contaminant/mass of sediment)

$C_{C(\text{veg})}$ = contaminant concentration in the vegetation compartment (g/g or Ci/g; mass of contaminant/mass of vegetation)

$C_{C(\text{w})}$ = contaminant concentration in the water compartment (g/m³ or Ci/m³; mass of contaminant/volume of water)

C_i = concentration

clay = fraction of clay in sediment (fraction)

C_{Li} = concentration in lower zone

C_{Mi} = concentration in middle zone

C_{n-1} = contaminant concentration for the previous receptor (g/m³ or Ci/m³; mass of contaminant/volume of water)

C_T = total contaminant concentration in stream due to advection & dispersion (g/m³ or Ci/m³; mass of contaminant/volume of water)

$C_{T(n)}$ = contaminant concentration for the current receptor (g/m³ or Ci/m³; mass of contaminant/volume of water)

C_{Ui} = concentration in upper zone

d = depth of river (m)

d_{50} = mean particle size (mm)

d_{si} = sand size (ft)

d_{si} = mean size fraction of sediment (ft)

D_y = dispersion coefficient in the y-direction (m²/s)

f_b' = Darcy-Weisbach bed friction factor

f_n = fraction of the source term upstream of the current receptor (fraction)

f_{n-1} = fraction of the source term upstream of the previous receptor (fraction)

g = acceleration due to gravity

g_s = sediment discharge (tons/day/ft or lbs/s/ft)

g_{sbi} = bed load sediment discharge (tons/day/ft)

g_{si} = sediment discharge as a function of V, d, and d_{50} (tons/day/ft)

g_{si} = total sediment discharge (tons/day/ft)

g_{ss} = sediment mass flux rate (g/s)

g_{ssLi} = suspended sediment load discharge in lower zone (tons/day/ft)

g_{ssMi} = suspended sediment load discharge in middle zone (tons/day/ft)

g_{ssUi} = suspended sediment load discharge in upper zone (tons/day/ft)

h = depth of river (m)

H_{air} = height of the air compartment (m)

H_{bed} = height of contamination in bed sediment (m)

k_1 = water temperature correction factor (° F)

k_2 = presence of fine sediment correction factor

k_3 = sediment size correction factor

k_4 = correction factor from Figure 2.10

$K_{d(\text{clay})}$ = contaminant distribution coefficient for clay (m³/g; volume of water/mass of clay)

$K_{d(OM)}$ = contaminant distribution coefficient for organic matter (m^3/g ; volume of water/mass of organic matter)
 $K_{d(sand)}$ = contaminant distribution coefficient for sand (m^3/g ; volume of water/mass of sand)
 $K_{d(silt)}$ = contaminant distribution coefficient for silt (m^3/g ; volume of water/mass of silt)
 K_H = Henry's constant ($atm\ m^3/mole$)
 K_H' = Henry's constant (dimensionless)
 L = unit length of control volume (m)
 $l_{m(n)}$ = lateral mixing length at the current receptor location (m)
 $l_{m(n-1)}$ = lateral mixed length at the previous receptor location (m)
 M_{bed} = mass of bed sediment in the contaminated portion of the bed (g; mass of sediment)
 Mc_a = mass of contaminant in air compartment (g or Ci; mass of contaminant)
 Mc_{bed} = mass of contaminant in the bed sediment compartment (g or Ci; mass of contaminant)
 $Mc_{bed(clay)}$ = mass of contaminant in clay portion of the bed sediment compartment (g; mass of contaminant)
 $Mc_{bed(OM)}$ = mass of contaminant in organic matter portion of the bed sediment compartment (g; mass of contaminant)
 $Mc_{bed(sand)}$ = mass of contaminant in sand portion of the bed sediment compartment (g; mass of contaminant)
 $Mc_{bed(silt)}$ = mass of contaminant in silt portion of the bed sediment compartment (g; mass of contaminant)
 Mc_{clay} = mass of contaminant on clay portion of the sediment compartment (g or Ci; mass of contaminant)
 Mc_f = mass of contaminant in fish compartment (g or Ci; mass of contaminant)
 Mc_{fp} = mass of contaminant in free product compartment (g or Ci; mass of contaminant)
 Mc_{OM} = mass of contaminant on organic matter portion of the sediment compartment (g or Ci; mass of contaminant)
 Mc_{sand} = mass of contaminant on sand portion of the sediment compartment (g or Ci; mass of contaminant)
 Mc_{sed} = mass of contaminant in sediment compartment (g or Ci; mass of contaminant)
 Mc_{silt} = mass of contaminant on silt portion of the sediment compartment (g or Ci; mass of contaminant)
 Mc_t = total contaminant mass (g or Ci; mass of contaminant)
 Mc_v = mass of contaminant in aquatic vegetation compartment (g or Ci; mass of contaminant)
 Mc_w = mass of contaminant in water compartment (g or Ci; mass of contaminant)
 M_f = mass of fish in water (g)
 M_{sed} = sediment mass (g; mass of sediment)
 M_v = total mass of vegetation in water (g; mass of vegetation)
 n = number of receptors (dimensionless)
 OM = fraction of organic matter in sediment (fraction)
 p_i = fraction by weight of fraction of bed with mean size d_{si}
 Q = water discharge rate (m^3/s)
 Q_c = contaminant flux at the source (g/s or Ci/s)
 Q_n = river discharge at the current receptor location (m^3/s)

Q_{n-1} = river discharge at the previous receptor location (m^3/s)
 r = depth of stream (ft)
 R = universal gas constant [8.2057×10^{-5} (atm m^3)/(mole K)]
 r_b = depth of bed (ft)
 S = solubility limit (g/m^3 or Ci/m^3 ; mass of contaminant/volume of water)
 S = slope of stream (ft/ft)
sand = fraction of sand in sediment (fraction)
silt = fraction of silt in sediment (fraction)
 T = temperature ($^{\circ}F$ or Kelvin)
 u = average flow velocity (m/s)
 U = flow velocity at distance y above bed (ft/s)
 U_*' = shear velocity (ft/s)
 V = mean velocity (ft/s)
 w_i = fall velocity
 x = downstream distance to receptor (m)
 y = distance above sediment bed (ft)
 V_a = volume of air (m^3)
 V_{bed} = volume of bed sediment (m^3)
 V_{clay} = volume of clay in water compartment (m^3 ; volume of clay)
 V_f = volume of fish (m^3)
 V_{OM} = volume of organic matter in water compartment (m^3 ; volume of organic matter)
 V_{sand} = volume of sand in water compartment (m^3 ; volume of sand)
 V_{sand} = volume of sand in bed sediment (m^3)
 V_{silt} = volume of silt in water compartment (m^3 ; volume of silt)
 V_v = volume of vegetation (m^3)
 V_w = volume of water (m^3)

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