

US EPA ARCHIVE DOCUMENT

**SOURCE MODULES FOR NONWASTEWATER  
WASTE MANAGEMENT UNITS  
(LAND APPLICATION UNITS,  
WASTEPILES, AND LANDFILLS)**

**BACKGROUND AND IMPLEMENTATION FOR  
THE MULTIMEDIA, MULTIPATHWAY, AND  
MULTIRECEPTOR RISK ASSESSMENT (3MRA)  
FOR HWIR99**

Work Assignment Manager  
and Technical Direction:

Stephen M. Kroner  
David A. Cozzie  
U. S. Environmental Protection Agency  
Office of Solid Waste  
Washington, DC 20460

Prepared by:

Research Triangle Institute  
P. O. Box 12194  
3040 Cornwallis Road  
Research Triangle Park, NC 27709-2194  
Under Contract No. 68-W-98-085, WA B-15

U.S. Environmental Protection Agency  
Office of Solid Waste  
Washington, DC 20460

October 1999

## ACKNOWLEDGMENTS

A number of individuals have been involved in the development of the methodologies and computer programs described herein. Stephen Kroner of the U.S. EPA, Office of Solid Waste, provided overall technical direction and review throughout this work.

Philip Lawless of the Research Triangle Institute (RTI) developed the original, semi-analytical solution technique on which the Generalized Soil Column Module (GSCM) is based. Paula Labieniec, under contract to RTI, extended, modified, and implemented the GSCM for the Landfill, Wastepile, and Land Application Unit source modules. She was the lead modeler on much of this work. Keith Little of RTI was primarily responsible for the surface water hydrology algorithms, and developed the conceptual framework and coupling algorithms for the “local watershed” construct that implements the GSCM in a watershed context. Terry Pierson of RTI, along with Keith Little, provided day-to-day management and technical direction. Randall Williams of RTI was the primary programmer.

## DISCLAIMER

The work presented in this document has been funded by the United States Environmental Protection Agency. Mention of trade names or commercial products does not constitute endorsement or recommendation for use by the Agency.

## Table of Contents

Section	Page
Figures .....	v
Tables .....	v
1.0 Introduction .....	1-1
2.0 Generic Soil Column Module (GSCM) .....	2-1
2.1 Assumptions .....	2-1
2.2 Governing Mass Balance Equation .....	2-3
2.3 Parameter Estimation Methodologies .....	2-4
2.4 Solution Technique .....	2-4
2.5 Limitations Related to Use of the GSCM .....	2-12
3.0 Local Watershed/Soil Column Module (LAU, Wastepile) .....	3-1
3.1 Introduction .....	3-1
3.2 Hydrology .....	3-4
3.2.1 Overview .....	3-4
3.2.2 Runoff .....	3-4
3.2.3 Evapotranspiration .....	3-7
3.2.4 Infiltration (Recharge) .....	3-9
3.3 Soil Erosion .....	3-9
3.4 Chemical Fate and Transport .....	3-15
3.4.1 Runoff Compartment .....	3-15
3.4.2 Soil Compartment .....	3-21
3.5 Implementation .....	3-26
3.5.1 Overview .....	3-26
3.5.2 Simulation Stopping Criteria .....	3-27
3.5.3 Leachate Flux Processing .....	3-28
3.5.4 End-of-Simulation Mass Balance Check .....	3-28
3.6 Output Summary .....	3-32
3.7 Wastepile Module Specifics .....	3-34
3.7.1 Introduction .....	3-34
3.7.2 Additional Assumptions .....	3-34
3.7.3 Initial Conditions .....	3-37
3.8 Land Application Unit .....	3-37
3.8.1 Introduction .....	3-37
3.8.2 Additional Assumptions .....	3-37
3.8.3 Initial Conditions .....	3-40

## Table of Contents (continued)

Section	Page
4.0	Landfill Module . . . . . 4-1
4.1	Introduction . . . . . 4-1
4.2	Additional Assumptions . . . . . 4-1
4.3	Landfill Cell Simulation—First Year . . . . . 4-4
4.3.1	Boundary Conditions . . . . . 4-4
4.3.2	Initial Conditions . . . . . 4-4
4.4	Landfill Cell Simulation—After First Year . . . . . 4-5
4.4.1	Boundary Conditions . . . . . 4-5
4.4.2	Initial Conditions . . . . . 4-6
4.5	Calculation of Landfill Results . . . . . 4-6
4.6	Implementation Algorithm . . . . . 4-6
4.6.1	Overview . . . . . 4-6
4.6.2	Simulation Stopping Criteria . . . . . 4-6
4.6.3	Leachate Flux Processing . . . . . 4-7
4.6.4	End of Simulation Mass Balance Check . . . . . 4-7
4.7	Output Summary . . . . . 4-10
5.0	References . . . . . 5-1
<b>Appendices</b>	
A	Particulate Emission Equations . . . . . A-1
B	Determination of $H'$ , $D_a$ , and $D_w$ for Organic Compounds . . . . . B-1
C	List of Symbols, Units, and Definitions . . . . . C-1

## Figures

<b>Number</b>		<b>Page</b>
2.4.1-1a	Development of diffusive spreading from a point source with time, corresponding to times of 0.01, 0.05, and 0.4 .....	2-6
2.4.1-1b	Diffusive spreading from a point source with a constant velocity to the right at times of 0.01, 0.05, and 0.4 .....	2-6
2.4.1-2a	Development of diffusive spreading from a layer source with time, corresponding to times of 0.01, 0.05, and 0.4 .....	2-7
2.4.1-2b	Diffusive spreading from a layer source with a constant velocity to the right at times of 0.01, 0.05, and 0.4 .....	2-7
3.1-1	Local watershed containing WMU .....	3-2
3.1-2a	Local watershed .....	3-3
3.1-2b	Cross section view .....	3-3
3.4-1	Runoff quality conceptual module .....	3-16
3.5-1a	Overview of algorithm for combined local watershed/soil column module .....	3-30
3.5-1b	Detail on calculation of first order losses in surface layer .....	3-31
3.7.1-1	Illustration of wastepile in local watershed .....	3-34
3.8.1-1	Illustration of LAU in local watershed .....	3-38
4.1-1	Illustration of Landfill with 6 cells & 3 waste layers .....	4-2
4.6-1a	Landfill module flowchart for an active cell (year 1) .....	4-8
4.6-1b	The landfill module flowchart for a closed cell (year 2+) .....	4-8

## Tables

<b>Number</b>		<b>Page</b>
3.2.2-1	Antecedent Moisture Classes for the SCS Curve Number Methodology .....	3-5
3.5.4-1	Variables Summarizing Contaminant Mass Losses .....	3-29
3.6-1	Output Summary for the WP and LAU Modules .....	3-32
4.7-1	Output Summary for the LF Module .....	4-10



## 1.0 Introduction

Source term modules were developed for wastepiles (WPs), land application units (LAUs), and landfills (LFs), i.e., nonwastewater waste management units (WMUs), to provide estimates of annual average surface soil constituent concentrations and constituent mass emission rates to air and ground water. These estimates are then used in an integrated, multipathway module linking source term modules with environmental fate and transport and exposure/risk modules. Additionally, LAU and WP source emission modules have been combined with a local watershed module (a “local” watershed is a sheet-flow-only watershed containing the WP or LAU) to provide estimates of constituent mass flux rates from runoff and erosion to a downslope waterbody, as well as surface soil constituent concentrations in downslope buffer areas. Because the LAU and WP sources are assumed here to interact hydrologically with the local watershed of which they are an integral part, they are termed “land-based” WMUs.

A soil column module was developed to describe the dynamics of constituent mass fate and transport within nonwastewater WMUs and near-surface soils in watershed subareas. Because it is applied in all the WMU source emission modules described here, it is referred to as the Generic Soil Column Module (GSCM). (The term “soil” is used loosely here to refer to a porous medium, whether it is waste in the WMU or near-surface soil in a watershed subarea.) Governing equations for the GSCM are similar to those used by Jury et al. (1983, 1990) and Shan and Stevens (1995). However, the analytical solution techniques used by these authors were not applicable to the source emission modules developed here because of the need to consider the periodic addition of constituent mass and enhanced constituent mass loss rates in the surface soil (e.g., due to runoff, erosion, wind, and mechanical processes). A new solution technique has been developed for use in HWIR that is computationally efficient and sufficiently flexible to allow consideration of the unique design and operational aspects of each WMU under consideration. Use of the GSCM described here allows:

- # Constituent mass balance
- # Waste additions/removals to simulate active facilities
- # Joint estimation of constituent mass losses due to a variety of mechanisms, including:
  - Volatilization of gas-phase constituent mass from the surface to the air
  - Leaching of aqueous-phase constituent mass by advection or diffusion from the bottom of the WMU or vadose zone



- First-order losses, which can include:
  - Abiotic and biodegradation
  - Suspension of constituent mass adsorbed to surface particles due to wind action and vehicular activity
  - Suspension of constituent mass adsorbed to surface particles due to water erosion (LAU and WP only)
  - Surface runoff of aqueous-phase constituent mass (LAU and WP only).

Section 2 provides a description of the GSCM assumptions, governing equations, boundary conditions, and solution technique. Section 3 describes the application of the GSCM to the land-based WMUs (WP and LAU) and its integration within the holistic local watershed module, including hydrology, soil erosion, and runoff water quality. Sections 4 and 5 describe the specifics of the application and integration for the WP and LAU, respectively. Section 6 describes the specifics of the application of the GSCM to the Landfill. As described in that section, the Landfill module differs from the LAU and WP modules in that it is not integrated into a local watershed construct. Appendix A lists and defines all symbols used in Sections 2 through 6. Appendixes B and C provide supplementary information on determination of  $H'$ ,  $D_a$ , and  $D_w$  for organic compounds and particulate emission equations.

## 2.0 Generic Soil Column Module

### 2.1 Assumptions

The following assumptions were made in the development of the Generic Soil Column Module used in all the nonwastewater source term modules:

- # The contaminant partitions to three phases: adsorbed (solid), dissolved (liquid), and gaseous (as in Jury et al., 1983, 1990).

$$C_T = \rho_b C_S + \theta_w C_L + \theta_a C_G \quad (2-1)$$

where

- $C_T$  = total contaminant concentration in soil (g/m<sup>3</sup> of soil)
- $\rho_b$  = soil dry bulk density (g/cm<sup>3</sup>)
- $C_S$  = adsorbed phase contaminant concentration in soil ( $\mu\text{g/g}$  of dry soil)
- $\theta_w$  = soil volumetric water content (m<sup>3</sup> soil water/m<sup>3</sup> soil)
- $C_L$  = aqueous-phase contaminant concentration soil (g/m<sup>3</sup> of soil water)
- $\theta_a$  = soil volumetric air content (m<sup>3</sup> soil air/m<sup>3</sup> soil)
- $C_G$  = gas-phase contaminant concentration in soil (g/m<sup>3</sup> of soil air).

- # The contaminant undergoes reversible, linear equilibrium partitioning between the adsorbed and dissolved phases (as in Jury et al., 1983, 1990).

$$C_S = K_d C_L \quad (2-2)$$

where  $K_d$  is the linear equilibrium partitioning coefficient (cm<sup>3</sup>/g). For organic contaminants:

$$K_d = foc \cdot K_{oc} \quad (2-3)$$

where  $foc$  is the organic carbon fraction in soil and  $K_{oc}$  is the equilibrium partition coefficient, normalized to organic carbon. Alternatively,  $K_d$  can be specified as an input parameter for inorganic contaminants. (It is implicit in this linear equilibrium partitioning assumption that the sorptive capacity of the soil column

solids is considered to be infinite with respect to the total mass of contaminant over the duration of the simulation, i.e., the soil column sorptive capacity does not become exhausted.)

- # Contaminant in the dissolved and gaseous phases is assumed to be in equilibrium and to follow Henry's law (as in Jury et al., 1983, 1990).

$$C_G = H' C_L \quad (2-4)$$

where  $H'$  is the dimensionless Henry's law coefficient.

- # The total contaminant concentration in soil can also be expressed in units of  $\mu\text{g}$  of contaminant mass per g of dry soil ( $\mu\text{g/g}$ ):

$$C'_T = \frac{C_T}{r_b} \quad (2-5)$$

- # Using the linear equilibrium approximations in Equations 2-2 through 2-5,  $C_T$  can be expressed in terms of  $C_L$ ,  $C_S$ , or  $C_G$ :

$$C_T = K_{TL} C_L = \frac{K_{TL}}{K_d} C_S = \frac{K_{TL}}{H'} C_G \quad (2-6)$$

where

$$K_{TL} = r_b K_d + q_w + q_a H' \quad (2-7)$$

$K_{TL}$  is the dimensionless equilibrium distribution coefficient between the total and aqueous-phase constituent concentrations in soil.

- # The total water flux or infiltration rate ( $I$ , m/d) is constant in space and time (as in Jury et al., 1983, 1990) and greater than or equal to zero. It is specified as an annual average.
- # Material in the soil column (including bulk waste) can be approximated as unconsolidated homogeneous porous media whose basic properties ( $\rho_b$ ,  $f_{oc}$ ,  $\theta_w$ ,  $\theta_a$ ,  $\eta$ ) are average annual values, constant in space.
- # Contaminant mass may be lost from the soil column due to one or more first-order loss processes.

- # The total chemical flux is the sum of the vapor flux and the flux of the dissolved solute (as in Jury et al., 1983, 1990).
- # The chemical is transported in one dimension through the soil column (as in Jury et al., 1983, 1990).
- # The vapor-phase and liquid-phase porosity and tortuosity factors obey the module of Millington and Quirk (1961) (as in Jury et al., 1983, 1990).
- # The modeled spatial domain of the soil column remains constant in volume and fixed in space with respect to a vertical reference, e.g., the water table.

## 2.2 Governing Mass Balance Equation

Under the above assumptions, the governing mass fate and transport equation can be written as follows:

$$\frac{\partial C_T}{\partial t} = D_E \frac{\partial^2 C_T}{\partial z^2} - V_E \frac{\partial C_T}{\partial z} - k C_T \quad (2-8)$$

where  $k$  (1/d) is the total first-order loss rate,  $D_E$  (m<sup>2</sup>/d) is the effective diffusivity in soil calculated as follows:

$$D_E = \frac{(\theta_a^{10/3} D_a H' + \theta_w^{10/3} D_w) 8.64}{\eta^2 K_{TL}} \quad (2-9a)$$

where  $D_a$  and  $D_w$  (cm<sup>2</sup>/s) are air and water diffusivities, respectively, and 8.64 is a conversion factor (m<sup>2</sup>-s/cm<sup>2</sup>-d).  $D_E$  can be considered to be the sum of the effective gaseous and water diffusion coefficients in soil,  $D_{E,a}$ , and  $D_{E,w}$ , respectively, where

$$D_{E,a} = \frac{\theta_a^{10/3} D_a H' 8.64}{\eta^2 K_{TL}} \quad (2-9b)$$

$$D_{E,w} = \frac{\theta_w^{10/3} D_w 8.64}{\eta^2 K_{TL}} \quad (2-9c)$$

The effective solute convection velocity ( $V_E$ , m/d) is equal to the water flux corrected for the contaminant partitioning to the water phase as follows:

$$V_E = \frac{I}{K_{TL}} \quad (2-10)$$

## 2.3 Parameter Estimation Methodologies

- # Water content ( $\theta_w$ ) is estimated as a function of the annual average infiltration rate (I, m/d) using (Clapp and Hornberger, 1978):

$$q_w = h \cdot \left( \frac{I}{0.24 K_{sat}} \right)^{1/(2SM_b+3)} \quad (2-11)$$

where  $K_{sat}$  (cm/h) is saturated hydraulic conductivity,  $SM_b$  is a unitless exponent specified by soil-type, and 0.24 (h-m/d-cm) is a unit conversion factor.

- # Volumetric air content is estimated using:

$$\theta = \eta - \theta_w \quad (2-12)$$

- #  $H'$ ,  $D_a$ , and  $D_w$  can be either estimated as a function of temperature in the soil column ( $T_{sc}$ , °C) using the methods described in Appendix B or specified directly as input parameters if preadjusted values are available, as they will be for the HWIR analysis.

## 2.4 Solution Technique

### 2.4.1 Background

A solution of the complete convective-diffusive-decay concentration module (Equation 2-8) was undertaken to evaluate, in a soil column of depth  $z_{sc}$

- # Total contaminant concentration as a function of time,  $t$ , and depth below the surface,  $z$ , for an arbitrary chemical
- # Contaminant mass fluxes across the upper ( $z = 0$ ) and lower boundaries ( $z = z_{sc}$ ) of the soil column.

A numerical solution of Equation 2-8, with zero concentration boundary condition at the surface and zero gradient lower boundary condition, was first examined as a straightforward

explicit finite difference method. This approach resulted in such a high numerical diffusion that it was impossible to distinguish diffusion effects. By subdividing each section into relatively thinner sections, the numerical diffusion could be reduced to more acceptable levels, but then smaller time steps were required, and the computation time became quite long. In addition, the numerical solution was not stable in the extremes (e.g., high/low  $V_E$  or  $D_E$ ).

An alternative, quasi-analytical approach was developed for use in HWIR that allows for relative computational speed and significantly reduces concern about numerical diffusion and lack of stability. The tradeoff is a loss of ability to evaluate short-term trends in concentration and diffusive flux profiles. The method was developed to allow estimation of long-term (i.e., annual average) contaminant concentration profiles and mass fluxes. Given concern in the HWIR analysis about computational speed, the need to evaluate a wide range of contaminants and soil/waste properties, and the interest in long-term, chronic exposure conditions, the method should be well-suited for the HWIR analysis.

The alternative approach developed consists of a superposition of analytic solutions of the three components of the governing equation (Equation 2-8) on the same grid. The solution for the simplified case where the soil column consists of one homogeneous zone, whose properties are uniform in space and time, is described below. Adaptations of the solution technique to account for variations from this simplified case (e.g., more than one homogeneous zone as for a landfill with cover soil zone atop the waste zone) are described in the module-specific sections.

#### 2.4.2 Description of Quasi-analytical Approach

A quasi-analytical approach was developed that is a step-wise solution of the three components of the governing Equation (equation 2-8) on the same grid. Boundary conditions of  $C_T=0$  at both the upper and lower boundaries of the soil column are assumed, although some flexibility exists in specifying the lower boundary condition as discussed below. That is, the following equations are solved individually:

$$\frac{\partial C_T}{\partial t} = D_E \frac{\partial^2 C_T}{\partial z^2} \quad (2-13)$$

$$\frac{\partial C_T}{\partial t} = - V_E \frac{\partial C_T}{\partial z} \quad (2-14)$$

$$\frac{\partial C_T}{\partial t} = - k C_T \quad (2-15)$$

Equations 2-13 through 2-15 each have an analytical solution that can be combined to obtain a pure diffusion solution that moves with velocity  $V_E$  through the porous medium (Jost, 1960). The solution of the general differential equation then has the form of the solution of the diffusive portion with its time dependence, translating in space with velocity  $V_E$ , and decaying exponentially with time.

The first two solutions for a point source are graphically depicted in Figures 2-1a and 2-1b for illustration. If it were possible to compute such point source solutions for each position in the soil column and each time of interest, then the contributions at each point could be added to obtain a global solution because the governing differential equations are linear. That is, each point in the soil column could be treated as if it were the only point for which there is a nonzero concentration.

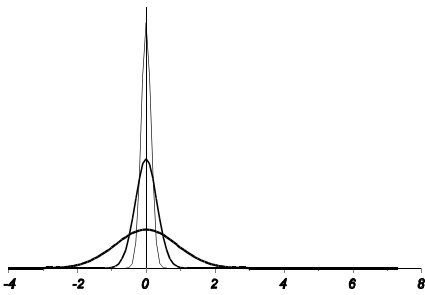


Figure 2-1a. Development of diffusive spreading from a point source with time, corresponding to times of 0.01, 0.05, and 0.4.

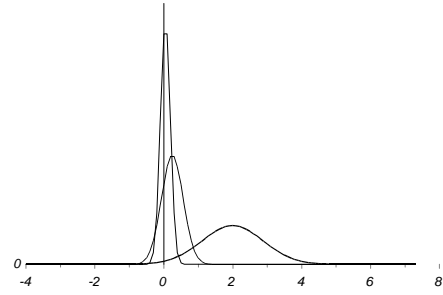


Figure 2-1b. Diffusive spreading from a point source with a constant velocity to the right at times of 0.01, 0.05, and 0.4.

To make the analysis tractable, instead of a point source, the soil column is divided into layer sources each of depth  $dz$  (i.e., a grid). A layer source can be thought of as multiple point sources packed closely together. In such a case, Equation 2-13 has a solution for one-dimensional diffusion, with the concentration at any point and any time given by

$$C_T(z', t) = \frac{C_{T0}}{2} \left[ \operatorname{erf} \left( \frac{z' + dz/2}{\sqrt{4D_E t}} \right) + \operatorname{erf} \left( \frac{dz/2 - z'}{\sqrt{4D_E t}} \right) \right] \quad (2-16)$$

for a layer of width  $dz$  centered at  $z' = 0$  (Jost, 1960). The concentration profile is assumed to be initially uniform from  $z' = -dz/2$  to  $z' = +dz/2$  and zero everywhere else. With time, the profile spreads outward and the concentration at the origin decreases, as shown in Figure 2-2a for  $dz=2$ . With a positive velocity  $V_E$ , the concentration profile also moves down the soil column as illustrated in Figure 2-2b. The use of layer solutions requires that we assume uniform average concentrations within each layer. Thus, the thickness of the layers determines the spatial resolution available.

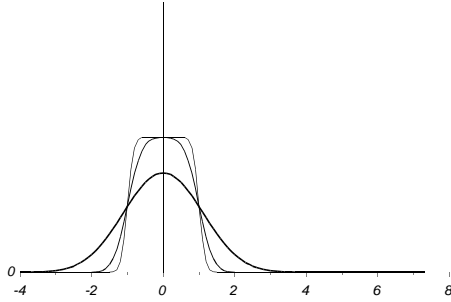


Figure 2-2a. Development of diffusive spreading from a layer source with time, corresponding to times of 0.01, 0.05, and 0.4.

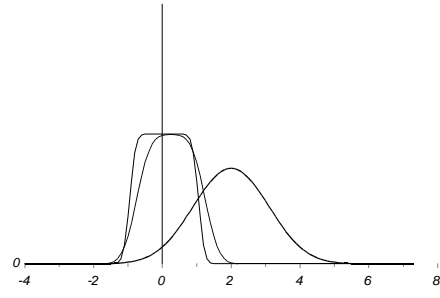


Figure 2-2b. Diffusive spreading from a layer source with a constant velocity to the right at times of 0.01, 0.05, and 0.4.

The total amount of material,  $m$ , in  $\text{g}/\text{m}^2$  that has passed any ordinate  $z'$  after time  $t$  is given by the integral of the concentration from  $z'$  to  $\infty$  with half leaving to the left (negative  $z'$  values) and half to the right (positive  $z'$  values) :

$$m(z', t) = 2 \int_{z'}^{\infty} C_T(z, t) dz \quad (2-17)$$

The integral in Equation (2-17) can be derived as

$$m(z', t) = C_{T0} \sqrt{4D_E t} \left[ \int_{(z'-dz/2)/\sqrt{4D_E t}}^{\infty} \text{erfc}(y) dy - \int_{(z'+dz/2)/\sqrt{4D_E t}}^{\infty} \text{erfc}(y) dy \right] \quad (2-18)$$

which is evaluated using the relationship (Abramowitz and Stegun, 1970):

$$\int \text{erfc}(x) dx = x \text{erfc}(x) - \frac{1}{\sqrt{p}} \exp(-x^2) + \text{constant} \quad (2-19)$$

The fraction of the original mass that diffuses past a boundary at  $z'$  in any time period 0 to  $t$ ,  $Df(z', t)$ , is one-half  $m(z', t)$  divided by the amount of mass initially present in  $\text{g}/\text{m}^2$  in the source layer ( $C_{T0} \cdot dz$ ):

$$Df(z', t) = 0.5 \cdot \frac{\sqrt{4D_E t}}{dz} \left[ \int_{(z'-dz/2)/\sqrt{4D_E t}}^{\infty} \text{erfc}(y) dy - \int_{(z'+dz/2)/\sqrt{4D_E t}}^{\infty} \text{erfc}(y) dy \right] \quad (2-20)$$



The fraction of mass that remains in the original layer of width  $dz$  after diffusion in the time period 0 to  $t$ ,  $Df_0(t)$ , is:

$$Df_0(t) = 1 - 2 \cdot Df(z' = 0.5dz, t) \quad (2-21)$$

By means of evaluations at all the layer boundaries ( $z'=0.5dz, 1.5dz, 2.5dz, \dots$ ), the amount of contaminant mass transported to any layer via diffusion after time  $t$  can be calculated as the difference between the amount outside the upstream boundary and the amount outside the downstream boundary. For example, the fraction of mass originally present in the source layer that ends up in the layer adjacent to the source layer in time  $t$  is  $Df(z'=0.5dz, t) - Df(z'=1.5dz, t)$ . The integrated amounts of material that have crossed the layer boundaries and the amount that remains in the source layer after time  $t$  are given directly by Equations 2-20 and 2-21, respectively, and only have to be computed once for fixed time steps and layer thicknesses.

The amount of mass that diffuses from a given layer out the lower boundary of the soil column in time  $t$  can be tracked by multiplying  $Df(z', t)$ , evaluated at the point where, for that layer,  $z'$  is at the bottom of the soil column ( $z = z_{sc}$ ) by  $(C_{T0} \cdot dz)$  for that layer. Diffusive losses across the bottom boundary from all the soil column layers are summed to get the total diffusive (aqueous and gaseous phase) loss across the bottom boundary,  $M_{lchd}(t)$  ( $g/m^2$ ) in time  $t$ .

Likewise, by summing the total diffusive losses across the upper boundary from each layer, the total diffusive loss out the top of the soil column,  $M_0(t)$  ( $g/m^2$ ), is determined. The volatilization loss from the surface of the soil column,  $M_{vol}(t)$  ( $g/m^2$ ), is assumed to be due to gaseous phase diffusion only and is determined by

$$M_{vol}(t) = M_0(t) \cdot \frac{D_{E,a}}{D_E} \quad (2-23)$$

where  $(D_{E,a}/D_E)$  is the fraction of the total diffusive loss from any layer that is due to diffusion in the gaseous phase in the soil. It is assumed that mass is not lost across the top boundary due to diffusion in the aqueous phase in the soil. In order to maintain mass balance, mass calculated to be lost this way is added back into the top layer in the soil, augmenting the total contaminant concentration there by  $(M_0(t) \cdot D_{E,w}/D_E)$ . This method of obtaining  $M_{vol}(t)$  is an approximation, justified on the basis of computational efficiency. A more rigorous treatment would include a mathematical transition layer across which diffusion from the soil to the air occurs. However, use of such a transition layer would require a more computationally intensive solution technique as well as specification of the thickness of the transition layer. Without this approximation (i.e., if  $M_{vol}(t) = M_0(t)$ ),  $M_{vol}(t)$  could be greater than zero for non-volatile contaminants ( $D_a = H' = 0$ ) due to the possible contribution to  $M_0$  from the aqueous phase diffusive flux. It is believed that this method of estimating  $M_{vol}(t)$  and augmenting the total contaminant concentration in the surface layer, while not theoretically rigorous, does represent a reasonable approximation of what actually occurs. That is, contaminant mass diffuses to the surface in both the aqueous and gaseous phases. While the contaminant mass in the gas phase volatilizes out the surface of the

soil column, the contaminant mass in the aqueous phase is left behind, concentrating the contaminant mass in surface soil (approximated here as the surface soil column layer).

To account for decay, Equation 2-15 is solved readily by the technique of separation of variables (Jost,1960). It has a solution of the form

$$C_T = C_{T0} \exp(-k t) \quad (2-23)$$

As Equation 2-23 is applied to each layer, the amount of mass lost due to first-order decay in time,  $t$ ,  $M_{loss}$  ( $\text{g}/\text{m}^2$ ), can be tracked using:

$$M_{loss}(t) = (1 - \exp(-kt))C_{T0} \cdot dz \quad (2-24)$$

Where multiple first-order loss processes may occur (i.e.,  $k = \sum k_j$ ), the fraction of initial mass present lost due to each process  $j$  is determined using:

$$M_{loss,j}(t) = \frac{k_j}{k} M_{loss}(t) \quad (2-25)$$

A potential difficulty with the layer solution is that the convection of material leads to an artificial numerical diffusion because the concentration within each layer can only be expressed as an average value. This component of numerical diffusion can be avoided completely if the contents of each layer are transferred completely to the next layer at the end of each time step by making the time step equal to the layer thickness divided by the effective velocity,  $V_E$ .

$$dt = \frac{dz}{V_E} \quad (2-26)$$

The contaminant mass in the bottom layer is convected out of the lower boundary. Total mass lost due to advection in  $dt$ ,  $M_{cha}$  ( $\text{g}/\text{m}^2$ ), is simply  $C_{T0}$  in the lowest soil column layer times  $dz$ .

**2.4.2.1 Boundary Conditions.** Zero concentration is assumed at the upper boundary of the soil column. This is consistent with the assumption that the air is a sink for volatilized contaminant mass, but requires the approximate method for estimating  $M_{vol}(t)$  described above.

At the lower boundary of the soil column, the flexibility exists with this solution technique to specify a value between zero and one for the ratio (bcm) of the total contaminant concentration in the soil directly below the modeled soil column and in the soil column. A ratio of one (bcm=1) corresponds to a zero gradient boundary condition ( $dC_T/dz=0$ ). A ratio of zero (bcm=0) corresponds to a zero concentration boundary condition ( $C_T=0$ ).

When  $bcm$  is equal to zero, diffusive fluxes at the upper and lower boundaries of the soil column are calculated directly as described above. When  $bcm$  is greater than zero, a reflection of the soil column is created. The contaminant concentrations in the reflected soil column cells are set equal to  $bcm$  times the contaminant concentration in the soil column cell being reflected (i.e., the concentration in the first cell of the reflected soil column is set to  $bcm$  times the contaminant concentration in the lowest cell of the actual soil column). The upward diffusive flux from the reflected soil column cells: (1) offsets the diffusive flux out the lower boundary of the soil column, (2) increments the contaminant concentrations in the soil column, and (3) augments the diffusive flux out the upper boundary of the soil column. Hence, when  $bcm$  is equal to one (the no diffusion boundary condition), the downward diffusive flux out the bottom boundary of the soil column is completely offset by the upward diffusive flux across the same boundary from the reflected soil column cells.

**2.4.2.2 Algorithm.** The general algorithm developed for HWIR for applying the individual solutions to Equations 2-13 through 2-15 is as follows for a homogeneous soil column and an averaging time period of 1 year.

1. Specify
  - # Lower boundary condition multiplier ( $bcm$ )
  - # Initial conditions in soil column ( $C_{T0}$ )
  - # Soil column size ( $z_{sc}$ ) and properties ( $\rho_b$ ,  $foc$ ,  $\eta$ ,  $K_{sat}$ ,  $SM_b$ )
  - # First-order loss rates ( $k_j$ )
  - # Chemical properties ( $K_{oc}$ ,  $H'$ ,  $D_a$ ,  $D_w$ )
  - # Upper and lower averaging depths ( $z_{ava}$ ,  $z_{avb}$ ).
2. Calculate/read  $K_d$ .  $K_d$  is internally calculated for organics, and read as a user input for metals.
3. Subdivide the soil column into multiple layers of depth,  $dz$ , that are an integral fraction of  $z_{sc}$ . Calculate the total number of layers,  $N_{dz} = z_{sc}/dz$ .
4. Get annual average infiltration rate ( $I$ ) for the year.
5. Calculate  $\theta_w$ ,  $\theta_a$ ,  $K_{TL}$ ,  $D_E$ ,  $V_E$ .
6. Calculate the time to cross a single layer at velocity  $V_E$  (Equation 2-26). This is the convection-based computing time step,  $dt$ . See also note below.
7. Evaluate the fraction of mass that remains in a layer (Equation 2-23) and that diffuses across layer boundaries  $z' = 0.5dz$ ,  $1.5dz$ ,  $2.5dz$ ,... (Equation 2-22) at  $t=dt$ . (These fractions are constant for a fixed  $dt$ .)
8. Calculate the amount of mass present in the soil column at the beginning of the year ( $M_{coll}$ ,  $g/m^2$ ).

9. Initialize cumulative mass loss variables ( $M_{vol}$ ,  $M_{lchd}$ ,  $M_{lcha}$ ,  $M_{loss,j}$ ).
10. Diffusion. Adjust the concentration profile to reflect diffusive fluxes for one time step. This redistributes material throughout the whole soil column. Increment  $M_{vol}$  and  $M_{lchd}$ .
11. First-order losses: Allow the concentration profile to decay in each layer (Equation 2-25) for one time step. Increment mass lost due to all applicable first-order loss processes,  $j$ ,  $M_{loss,j}$  (Equation 2-23).
12. Convection: Propagate the concentration profile one layer downstream. Increment  $M_{lcha}$ .
13. Repeat Steps 10 through 12 until it is time to add and/or remove contaminant mass (go to Step 14) or until the end of the year (go to Step 15).
14. To account for the addition of contaminant mass, update the contaminant concentrations in the affected layers. Track total mass added ( $M_{add}$ ,  $g/m^2$ ) and/or removed ( $M_{rem}$ ,  $g/m^2$ ). Begin the algorithm again at Step 10.
15. At end of the year, calculate/report:

- # Total mass in the soil column ( $M_{col2}$ ,  $g/m^2$ )
- # Mass balance error for the year ( $M_{err}$ ,  $g/m^2$ ):

$$M_{err} = M_{col2} - M_{col1} - M_{add} + M_{rem} + M_{vol} + M_{lcha} + M_{lchd} + \sum_j M_{loss,j} \quad (2-27)$$

- # Annual average total concentration in surface layer
- # Annual, depth-weighted average total concentration ( $z_{ava} \leq z \leq z_{avb}$ )
- # Annual average volatilization flux ( $J_{vol}$ ,  $g/m^2/d$ )

$$J_{vol} = \frac{M_{vol}}{365} \quad (2-28)$$

- # Annual average leaching flux ( $J_{lch}$ ,  $g/m^2/d$ ):

$$J_{lch} = \frac{M_{lchd} + M_{lcha}}{365} \quad (2-29)$$

16. Begin the algorithm again at Step 4 until mass is no longer added to the soil column and mass has been depleted from the soil (i.e.,  $M_{col2} = 0$ ).

Note that the convection time step cannot be any greater than the length of time between mass additions or removals (e.g., waste applications in an LAU). For example, if contaminant mass is added every 30 days, this is the maximum time step, regardless of how small the velocity is. When  $dt$  is limited in this fashion, the number of time steps required before a convective transfer can take place is determined, and the convective transfer step is performed on an “as-needed” basis. If the calculated convective time step is 60 days, in this example, the convective transfer would occur every other time step. This will result in a temporal distortion of the concentrations within the layers, but over several steps and, by the end of the year, preliminary module runs show that the effects average out.

The primary means by which the performance of the solution algorithm is checked is via the annual mass balance check (Equation 2-27) to ensure that the change in mass in the system over the year is equal to the difference between mass additions and losses. If  $M_{err}$  is greater than  $10^{-8}$  g/m<sup>2</sup>, a message is written to the warning file.

## 2.5 Limitations Related to Use of GSCM

The following limitations are noted for the GSCM:

- # The GSCM was developed originally for organic contaminants, and assumes that the partition efficient,  $K_d$ , is linear and is estimated as the product of  $K_{oc}$  and  $f_{oc}$ . Partitioning for metals involves complex chemistry, including the dynamic effects of aqueous-phase contaminant concentration, precipitation, dissolution, adsorption/desorption, and the geochemistry of media (e.g., oxidation-reduction conditions) on the value of  $K_d$  and the fate and transport behavior of metals in general. This complexity is not modeled by the GSCM for metals partitioning; rather,  $K_d$  is externally provided as a randomly sampled value by the chemical properties processor (CPP).
- # With organic contaminants, the GSCM is not applicable if nonaqueous phase liquid (NAPL) is present. Similarly, with metals, the presence of a precipitate is not allowed. The presence of NAPL (precipitate) is determined by comparing  $C_T$  to the theoretical maximum contaminant concentration in soil without NAPL (precipitate), determined by the aqueous solubility, saturated soil-gas concentration of the contaminant, and the sorptive capacity of the soil. The limit on  $C_T$  is estimated using

$$C_T < K_{TL} C_L^{sol} \quad (2-30)$$

where  $C_L^{sol}$  (g/m<sup>3</sup>) is the aqueous solubility. This is not expected to be a significant limitation in applying the module to develop HWIR exit levels. It is expected that in most circumstances exit levels will be sufficiently low that the presence of NAPL (precipitate) would be precluded.

- # The algorithm is being applied to develop source release estimates on an annual average basis, to support estimation of chronic (long-term average) risk estimates. Some of the inputs used (e.g., infiltration) are long-term annual average estimates, while others are annual average. Accordingly, the outputs are not strictly applicable to individual years.
- # The module allows consideration of only one contaminant at a time and does not simulate fate and transport of reaction products in its current form. With further module development, it would be possible to track the production of reaction products in each soil column layer and use basically the same algorithm that is used for the parent compound to model the fate of reaction products.
- # The solution technique used, sequential solutions to the three-component differential equations of the governing differential equation, allows computational efficiency. However, systematic errors could result from the choice of the order in which these solutions are applied. The size of the error would be dependent on the relative loss rates associated with the three processes. For example, if the first-order loss rate due to degradation were high and losses due to degradation were calculated first, then less contaminant mass would be available for diffusive and advective losses. The current algorithm prioritizes diffusive losses since the diffusion equation is solved first. This is followed by first-order losses and advection in that order.
- # As discussed, a boundary condition at the soil/air interface of  $C_T = 0$  was assumed in developing this solution technique. This is consistent with the assumption that the air is a sink for volatilized contaminant mass. However, as discussed in Section 2.4.1, because the diffusion coefficient used in the governing equation (Equation 2-8) includes diffusion in both the air and aqueous phases of the soil, contaminant mass that is transported upward in the soil column via diffusion can include mass in both the air and aqueous phases. While this is appropriate within the soil where the ratio of air to water is relatively constant, the assumption breaks down at the soil/air interface itself. To account for the fact that contaminant mass in the aqueous phase should not be lost out of the surface of the soil column—which, for example, would lead to nonzero volatilization fluxes for nonvolatile contaminants ( $D_a = H' = 0$ )—the volatilization flux at the surface is assumed to include only the diffusive flux due to gas-phase diffusion. Mass estimated to be lost from the surface due to aqueous-phase diffusion is added back into the surface soil column layer, augmenting the contaminant concentration there and maintaining mass balance. This is an approximation, justified on the basis of computational efficiency; nonetheless, the approximation should be in reasonable agreement with what actually occurs in nature.



## 3.0 Local Watershed/Soil Column Module (LAU, Wastepile)

### 3.1 Introduction

As a component of the overall HWIR multimedia exposure/risk module, the WP and LAU source emissions modules are required to provide annual average contaminant mass flux rates from the surface of the WMU and its subsurface interface with the vadose zone, total contaminant concentration in the surface material, and contaminant mass emission rate due to particulate emissions. In addition, because these WMUs are on the land surface, they are integral land areas in their respective watersheds and, consequently, are not only affected by runoff and erosion from upslope land areas, but also affect downslope land areas through runoff and erosion. Indeed, after some period of time during which runoff and erosion has occurred from a WMU, the downslope land areas will have been contaminated and their surface concentrations could approach (or conceivably even exceed long after WMU operation ceases) the residual chemical concentrations in the WMU at that time. Thus, after extensive runoff and erosion from a WMU, the entire downslope surface area can be considered a “source” and it becomes important to consider these “extended source” areas in the risk assessment. It is for this reason that a holistic modeling approach has been taken with the WP and LAU source modules to incorporate them into the watershed of which they are a part.

The watershed including an LAU or WP is termed here the “local” watershed, and is illustrated in Figure 3-1. A local watershed is defined as that drainage area that just contains the WMU (or a portion thereof — there can be multiple local watersheds) in the lateral (perpendicular to runoff flow) direction, and in which runoff occurs as overland flow (sheet flow) only. Thus, a local watershed extends downslope only to the point that runoff flows and eroded soil loads would enter a well-defined drainage channel, e.g., a ditch, stream, lake, or some other waterbody. The sheet-flow-only restriction is based on the assumption that any subareas downslope of the WMU subarea are subject to chemical contamination from the WMU through overland runoff and soil erosion.

Figure 3-2 illustrates how the local watershed is conceptualized for the combined Local Watershed/Soil Column Module, that is, as a two-dimensional, two-medium system. The dimensions are longitudinal, i.e., downslope or in the direction of runoff flow, and vertical, i.e., through the soil column. The media are the soil column and, during runoff events, the overlying runoff water column. The local watershed is assumed to be made up of, in the longitudinal direction, an arbitrary number of land subareas that may have differing surface or subsurface characteristics, e.g., land uses, soil properties, and chemical concentrations. For example,



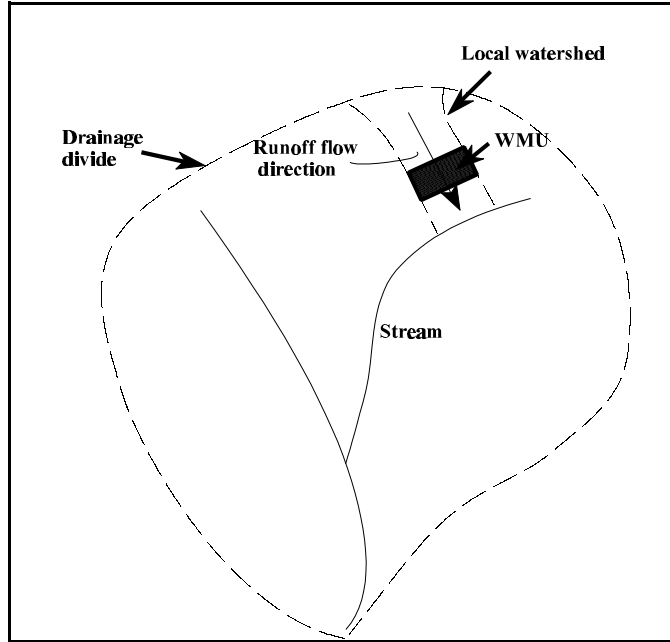


Figure 3-1. Local watershed containing WMU.

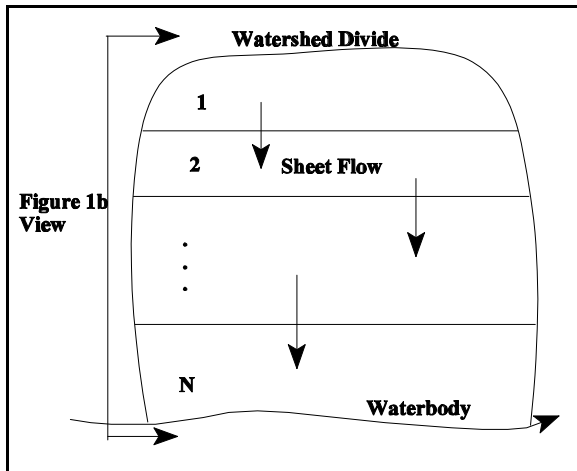


Figure 3-2a. Local watershed.

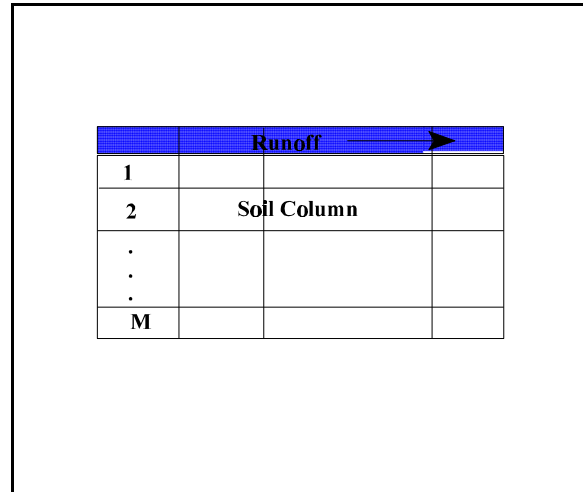


Figure 3-2b. Cross-section view.

subarea 2 might be a WMU, subarea 1 would then represent an upslope area, and subareas 3 through N would be downslope buffer areas extending to the waterbody.

## 3.2 Hydrology

### 3.2.1 Overview

Hydrologic modeling is performed to simulate watershed runoff and ground water recharge (termed here “infiltration”). The hydrology module is based on a daily soil moisture water balance performed for the root zone of the soil column. At the end of a given day,  $t$ , the soil moisture in the root zone of an arbitrary watershed subarea,  $i$ , is updated as

$$SM_{i,t} = SM_{i,t-1} + P_t + RO_{i-1,t} - RO_{i,t} - ET_{i,t} - IN_{i,t} \quad (3-1)$$

where

$SM_{i,t}$	=	soil moisture (cm) in root zone at end of day $t$ for subarea $i$
$SM_{i,t-1}$	=	soil moisture (cm) in root zone at end of previous day for subarea $i$
$P_t$	=	total precipitation (cm) on day $t$
$RO_{i-1,t}$	=	storm runoff (cm) on day $t$ coming onto subarea $i$ from $i-1$
$RO_{i,t}$	=	storm runoff (cm) on day $t$ leaving subarea $i$
$ET_{i,t}$	=	evapotranspiration (cm) from root zone on day $t$ for subarea $i$
$IN_{i,t}$	=	infiltration (ground water recharge) on day $t$ (cm) for subarea $i$ .

Precipitation is undifferentiated between rainfall and frozen precipitation; that is, frozen precipitation is treated as rainfall. Runoff, evapotranspiration, and infiltration losses from the root zone are discussed in subsequent sections. The equations presented in these sections refer to “day  $t$  and subarea  $i$ ” in accordance with the above water balance equation (3-1).

### 3.2.2 Runoff

**3.2.2.1 Governing Equations.** Daily runoff is based on the Soil Conservation Service’s (SCS) widely used “curve number” procedure (USDA, 1986) and is a function of current and antecedent precipitation and land use. Land use is considered empirically by the curve numbers, which are catalogued by land use or cover type (e.g., woods, meadow, impervious surfaces), treatment or practice (e.g., contoured, terraced), hydrologic condition, and hydrologic soil group.

Runoff depth is calculated by the SCS procedure as

$$RO = \frac{(P-Ia)^2}{P-Ia + S} \quad \text{for } P \geq Ia \quad (3-2)$$

where

- RO = runoff depth (cm)  
 P = precipitation depth (cm)  
 Ia = initial abstraction (threshold precipitation depth for runoff to occur) (cm)  
 S = watershed storage (cm).

By experimentation with over 3,000 soil types and cover crops, the SCS developed the following relationships for watershed storage as a function of CN and initial abstraction as a function of storage.

$$S = \frac{2540}{CN} - 25.4 \quad (3-3)$$

$$Ia = 0.2S \quad (3-4)$$

Combining Equations 3-2 and 3-3 results in

$$RO = \frac{(P-0.2S)^2}{P + 0.8S} \quad \text{for } P \geq 0.2S \quad (3-5a)$$

$$RO = 0 \quad \text{for } P < 0.2S \quad (3-5b)$$

where S is given by Equation 3-3. For impervious surfaces (CN = 100), it can be seen that RO = P.

Three antecedent moisture classes (AMCs) have been defined for use in adjusting the SCS curve numbers as shown in Table 3-1. The growing season is assumed to be June through August (Julian Day 152 to 243) throughout the country.

**Table 3-1. Antecedent Moisture Classes for SCS Curve Number Methodology**

AMC Class	Total 5-day Antecedent Rainfall (cm)	
	Dormant Season	Growing Season
I	< 1.3	< 3.6
II	1.3 to 2.8	3.6 to 5.3
III	> 2.8	> 5.3

Source: U.S. EPA et al. (1985).

Curve numbers are typically presented in the literature assuming average antecedent moisture conditions (AMC II) and can be adjusted for drier (AMC I) or wetter (AMC III) conditions as (Chow et al., 1988)

$$CN(I) = \frac{4.2CN(II)}{10-0.058CN(II)} \quad (3-6)$$

$$CN(III) = \frac{23CN(II)}{10+0.13CN(II)} \quad (3-7)$$

These adjustments have the effect of increasing runoff under wet antecedent conditions and decreasing runoff under dry antecedent conditions, relative to average conditions.

**3.2.2.2 Implementation.** Recall the conceptual module for the local watershed (Figure 3-2), where the subareas may have different land uses and different curve numbers for each subarea. Equation 3-5 is nonlinear in the curve number; therefore, the method by which the SCS procedure is applied to multiple subareas can make a significant difference in the resulting cumulative runoff values for downslope subareas. There are essentially two options for implementing the procedure. The first is based on runoff **routing** from each subarea to the next downslope subarea. That is, the runoff depth from subarea 1 would first be calculated from Equation 3-5. The cumulative runoff depth from subareas 1 and 2 would then be calculated by applying Equation 3-5 to subarea 2 and adding (routing) the runoff depth from subarea 1. This would be repeated for all subareas. This method is **not** appropriate for the sheet flow assumption of the local watershed and can give much higher cumulative runoff depths (volumes) than would actually occur under the sheet flow assumption. (The implicit assumption of the routing method is that the subareas are not hydrologically connected, e.g., runoff from subarea 1 is captured in a drainage system (non-sheet-flow) and diverted directly to the watershed outlet without passing through/over downslope subareas.)

A different, nonrouting method is appropriate for implementing the SCS procedure for the local (sheet flow) watershed. The method is based on determining composite curve numbers and is analogous to the nonsoil routing implementation of the Universal Soil Loss Equation (USLE) soil erosion module presented in Section 3.3. The methodology used for implementing this method is illustrated by the following pseudo-code.

```
FOR i = 1,...,N (subareas)
  CNeffi = area-weighted composite CNi for all subareas j, j=1,...,i
  Calculate Si from equation (3.2.2-2) using CNeffi
  Calculate ROi from equation (3.2.2-1) using Si. (ROi is the average runoff depth
  over all upslope subareas j, j=1,...,i).
  Calculate Qi = ROi*WSAi where Qi is cumulative runoff volume and WSAi is
  cumulative area.
  IF i = 1 THEN
```

```

H1i = ROi where H1i is subarea-specific runoff depth for subarea i, i.e. ROi - ROi-1
ELSE
H1i = (Qi - Qi-1)/Ai where Ai is subarea-specific surface area
IF H1i < 0 THEN H1i = 0
END IF
NEXT i

```

### 3.2.3 Evapotranspiration

Potential evapotranspiration (PET) is the demand for soil moisture from evaporation and plant transpiration. When soil moisture is abundant, actual evapotranspiration (ET) equals PET. When soil moisture is limiting, ET will be less than PET. The extent to which it is less under limiting conditions has been expressed as a function of PET, available soil water (AW), and available soil water capacity (AWC) as (Dunne and Leopold, 1978)

$$ET = PET * f\left(\frac{AW}{AWC}\right) \quad (3-8)$$

where

$$AW = (SM - WP) \frac{DRZ}{100} \quad (3-9)$$

$$AWC = (FC - WP) \frac{DRZ}{100} \quad (3-10)$$

and

- f = a functional relationship of the arguments.
- WP = soil wilting point (% volume), which is the minimum soil moisture content that is available to plants. (Plants can exert a maximum suction of approximately 15 atmospheres. The wilting point is that moisture that would not be available at 15 atmospheres.)
- FC = soil field capacity (% volume), which is the maximum soil moisture content that can be held in the soil by capillary or osmotic forces. Soil moisture above the field capacity is readily drained by gravity.
- DRZ = depth of the root zone (cm).

The functional relationship in Equation 3-8 is assumed here to be linear, so that ET (cm) is calculated as

$$ET = \min[PET, PET(\frac{SM-WP}{FC-WP})] \quad (3-11)$$

PET is estimated as described below.

The more theoretically based modules for daily evapotranspiration (e.g., the Penman-Monteith equation [Monteith, 1965]) rely on the availability of significant daily meteorological data, including temperature gradient between surface and air, solar radiation, windspeed, and relative humidity. For HWIR purposes, it is assumed that all of these variables will not be readily available for all application sites. Therefore, a less data-demanding module, the Hargreaves equation (Shuttleworth, 1975), is proposed. As compared with the most theoretical modules, some accuracy will be sacrificed. Nonetheless, the Hargreaves method, which is primarily temperature-based, has been shown to provide reasonable estimates of evaporation (Jensen, 1990)—presumably because it also includes an implicit link to solar radiation through its latitude parameter (Shuttleworth, 1993).

The Hargreaves equation is

$$PET = 0.0023S_0\Delta_T^{0.5}(T+17.8)*0.1 \quad (3-12)$$

where

PET = potential evapotranspiration (cm/d)

T = mean daily air temperature (° C)

$\Delta_T$  = difference in mean monthly maximum and mean monthly minimum air temperature

$S_0$  = water equivalent of extraterrestrial radiation (mm/d) and is given as (Duffie and Beckman, 1980)

$$S_0 = 15.392d_r(\omega_s \sin \phi \sin \theta + \cos \phi \cos \theta \sin \omega_s) \quad (3-13)$$

where

$$d_r = 1 + 0.033 \cos(\frac{2\pi}{365} J) \quad (3-14)$$

and

J = Julian day  
 $\omega_s$  = sunset hour angle (radians) given by

$$\omega_s = \text{Arccos}(-\text{Tan } \phi \text{ Tan } \theta) \quad (3-15)$$

$\phi$  = site latitude (positive for northern hemisphere, negative for southern)

$\theta$  = solar declination (radians) given by

$$\theta = 0.4093 \text{Sin} \left( \frac{2\pi}{365} J - 1.405 \right) \quad (3-16)$$

### 3.2.4 Infiltration (Recharge)

Soil moisture in excess of the soil's field capacity (FC), if not used to satisfy ET, is available for gravity drainage from the root zone as infiltration to subroot zones (Dunne and Leopold, 1978). This infiltration rate will, however, be limited by the root zone soil's saturated hydraulic conductivity. Accordingly, infiltration is calculated as

$$IN = \min[K_{sat}, (SM - FC) \frac{DRZ}{100}] \quad (3-17)$$

where

IN = infiltration rate (cm/d)  
 K<sub>sat</sub> = saturated hydraulic conductivity (cm/d).

In the event that infiltration is limited by K<sub>sat</sub>, the hydrology algorithm includes a feedback loop that increases the previously calculated runoff volume by the amount of excess soil moisture, i.e., the water above the field capacity that exceeds K<sub>sat</sub>. This adjustment is made to preserve water balance and is based on the assumption that the runoff curve number method, which is only loosely sensitive to soil moisture (through the antecedent precipitation adjustment) has admitted more water into the soil column than can be accommodated by ET, infiltration, and/or increased soil moisture. After the runoff is increased for this excess, the ET, infiltration, and soil moisture are updated to reflect this modification and preserve the water balance.

## 3.3 Soil Erosion

### 3.3.1 General

The Soil Erosion Module is based on the Universal Soil Loss Equation, an empirical methodology (see, e.g., Wischmeier and Smith, 1978) based on measured soil losses for experimental field-scale plots in the United States for some 40,000 storms. The USLE predicts

sheet and rill erosion from hillsides upslope of defined drainage channels, such as streams. It does not predict streambank erosion. Let  $SL$  ( $\text{kg}/\text{m}^2\text{-time}$ ) denote the eroded soil flux (unit load) from a hillside area over some time period.  $SL$  is predicted by the USLE as the product of six variables:

$$SL = R \times K \times C \times P \times LS \times Sd \quad (3-18)$$

These variables are discussed below.

$R$  is the rainfall factor with units of  $1/\text{time}$ . The rainfall factor accounts for the erosive (kinetic) energy of falling raindrops, which is essentially measured by rainfall intensity. The kinetic energy of an individual storm times its maximum 30-minute intensity is sometimes called the erosivity index (EI) factor.  $R$  factors have been compiled throughout the United States on a long-term annual average basis. These  $R$  factors were developed by cumulating these individual storm EI factors.

$K$  is the soil erodibility factor with units of  $\text{kg}/\text{m}^2$ . Soil erodibility is an experimentally determined property and is a function of soil type, including particle size distribution, organic content, structure, and profile.  $K$  values are reported by soil type in the literature.

$C$  is the dimensionless “cropping management” factor that varies between 0 and 1. It accounts for the type of cover (e.g., sod, grass type, fallow) on the soil.  $C$  is used to correct the USLE prediction relative to the cover type for which the experimentally determined  $K$  values were measured (fallow).

$P$  is the dimensionless practice factor and accounts for the effect of erosion control practices, e.g., contouring or terracing.  $P$  is never negative, but could be greater than 1.0 if land practices actually encourage erosion relative to the original experimental plots on which  $K$  was measured.

$LS$  is the combined “length-slope” factor and is given by (U.S. EPA, 1985b) as

$$LS_i = (.045X_i)^b (65.41 \sin^2 \theta + 4.56 \sin \theta + .065) \quad (3-19)$$

where

$X_i$  = flow distance (m) from the point at which sheet flow originates (the upslope drainage divide) to the point of interest on the hillside.

$\theta$  = slope angle (degrees), where  $\theta$  may be calculated from percent slope,  $S$ , as

$$\theta = \arctan(S/100) \quad (3-20)$$



and  $b$ , the exponent, is determined as a function of  $S$  as:

- $b = 0.5$ , if  $S > .05$
- $b = 0.4$ , if  $.035 \leq S \leq .045$
- $b = 0.3$ , if  $.01 \leq S < .035$
- $b = 0.2$ , if  $S < .01$ .

LS increases with increasing flow distance because runoff quantity generally increases with distance. It increases with slope because runoff velocity generally increases with slope.

$S_d$  is the “sediment delivery ratio,” which estimates the fraction of onsite eroded soil that reaches a particular downslope or downstream location in the subbasin (Shen and Julien, 1993). The sediment delivery ratio is here used to account for deposition of eroded soil from the local watershed in ditches, gullies, or other depressions. Vanoni (1975) developed the sediment delivery ratio as a function of watershed drainage area. That formulation is where

$$S_d = a \times A^{-1.25} \quad (3-21)$$

- $S_d$  = sediment delivery ratio (dimensionless)
- $A$  = subbasin area ( $m^2$ )
- $a$  = normalized to give  $S_d = 1.0$  for an area of  $0.001 \text{ mi}^2$  as per Vanoni (1975). (For area in  $m^2$ ,  $a = 2.67$ .)

### 3.3.2 MUSLE Implementation

The USLE is implemented for HWIR on a storm event basis, i.e., the “modified” USLE (MUSLE) is used. This implementation requires determining an  $R$  value (with units of 1/day) for each daily storm event that specifies the erosivity of that individual storm. Let the storm-event-specific  $R$  value be denoted as  $R_t$  for storm event  $t$ , so that the pseudo-code presented above is applied for a given daily storm event. Several methods have been proposed for estimating  $R_t$  and are summarized below. Method 4 is used for HWIR.

*Method 1 —  $R_t$  as a Function of Total Daily Precipitation.* This method (Richardson et al., 1983) predicts  $R_t$  as a function of total daily precipitation by means of a two-parameter regression module (a power function). The parameters were estimated by Richardson et al. from long-term records of daily “erosivity index” (EI, which is operationally equivalent to  $R$ ) and total daily precipitation for 11 sites, all located east of the Rocky Mountains. (Western sites were not included in the data “... so that the relationships would not be influenced by the complex orographic effects of mountainous terrain.”) It was determined that one of the parameters (the exponent) was statistically invariant with respect to site, while the other parameter did vary by site. In addition, the variance of the prediction error was also found to be a predictable function of site location. Thus, tables relating the varying regression parameter and its prediction error variance were generated from the regression data by site. This method is nearly ideally suited for HWIR; except for the unfortunate fact that all of the 11 sites used for the regression module were

located east of the Rocky Mountains. Several methods were considered for correlating those 11 sites to western sites (e.g., correlation by average storm intensity), but were rejected as either too data-intensive or too uncertain.

*Method 2 —  $R_t$  as a Function of Storm Runoff.* This method (used by PRZM) predicts  $R_t$  as a function of daily storm event runoff and peak storm runoff (Williams, 1975). Although total runoff from the (daily) storm event is available to HWIR (from the SCS Curve Number module), the shape and duration of the runoff hydrograph for the storm is not calculated and, thus, the peak runoff from the storm is not available.

*Method 3 —  $R_t$  Calculated from Hourly Erosivity Index Values.* This method (Wischmeier and Smith, 1978) is the most rigorous MUSLE approach. It is not based on regression analysis of presumed correlated independent variables, but rather predicts  $R_t$  directly by aggregating hourly EI calculations over the storm's duration. The EI values are calculated from hourly average rainfall intensity data. This is the method that has been used to estimate long-term annual total R values for the classical (annual total) use of the USLE. Because hourly precipitation data are available from the SAMSON files, this method is feasible for HWIR. Method 4 below is essentially based on this method, although the method allocates the (published) long-term annual R values down to hourly R (and then up to daily  $R_t$ ) instead of building up the long-term annual R from the hourly data.

*Method 4 —  $R_t$  Allocated from Published Long-Term Annual Total R Values.* Because published values of long-term annual total R values exist in the form of isopleths across the country, it seems appropriate to use these annual total R data for HWIR and disaggregate them down to a daily basis for the MUSLE. This is the method used for HWIR. Pseudo-code to implement this method is:

Given: Long-term annual total R,  $R_{ann}$ , for a site.

Given: Number of years in the simulation, NYR.

Given: Hourly time series of precipitation amounts for the complete record of NYR years.

1. Compute cumulative R over record,  $R_{total} = R_{ann} \times NYR$
2. Compute cumulative precipitation over NYR years,  $PPT_{total}$
3. For each hourly precipitation value in the record, allocate  $R_{total}$  to that hour based on the fraction of  $PPT_{total}$  represented by the hourly precipitation. Denote an hourly allocation as  $R_{hour}$ .
4. For each day of the record, cumulate all  $R_{hour}$  values to the daily total. The result is  $R_t$  for each day of the NYR record.

### 3.3.3 Spatial Implementation

For the local watershed application, the USLE is applied spatially to a hillside that comprises N subareas (see Figure 3-2a). Pseudo-code for this application is:

LET  $CSL_i$  = cumulative soil load (kg/day) for subarea  $i$ , i.e. eroded load from subarea  $i$  and all upslope subareas  $j$ ,  $j = 1, \dots, i$

LET  $WSA_i$  = cumulative land area ( $m^2$ ) upslope of and including subarea  $i$

FOR  $i=1, \dots, N$

$K_{eff_i}$  = area-weighted  $K_i$  for all subareas  $j$ ,  $j=1, \dots, i$

$C_{eff_i}$  = area-weighted  $C_i$  for all subareas  $j$ ,  $j=1, \dots, i$

$P_{eff_i}$  = area-weighted  $P_i$  for all subareas  $j$ ,  $j=1, \dots, i$

$CSL_i = R * WSA_i * K_{eff_i} * C_{eff_i} * P_{eff_i} * LS_i * Sd_i$

NEXT  $i$

The assignment of the sheet-flow distance parameter,  $X_i$ , within the  $LS_i$  factor (see Equation 3-19) merits discussion in the context of the “local watershed” conceptual module. This local watershed construct (see Figure 3-1) was developed to simulate the downslope transport of contaminant due to storm water runoff and soil erosion from the WMU. The use of the USLE equation for estimating soil erosion (and associated chemical load) assumes that runoff is essentially sheet flow and that erosion results from sheet, or, at most, rill (very small channels) erosion; i.e., runoff does not occur in significantly defined drainage channels (e.g., ditches, swales) within the local watershed. As part of HWIR data collection, the delineation of the sheet-flow-only local watershed is accomplished by geographic information system (GIS) analysis, and a key component of this analysis with respect to the sheet-flow-only assumption is the correct generation of the waterbody network such that the waterbody delineated as lying downslope of the local watershed is in fact the first “defined drainage channel” that the runoff would encounter. That is, runoff upslope of the GIS-defined waterbody is essentially sheet flow, in accordance with the conceptual module and the underlying assumptions of the USLE. The criterion used for terminating (headwater) the GIS-delineated streams is a tributary drainage area of 700,000  $m^2$ , which has been estimated (see *Data Collection for the Hazardous Waste Identification Rule. Section 5. Watershed and Waterbody Layout*. [U.S. EPA, 1999a]) to coincide with “first-order” stream headwaters. Thus, the 700,000- $m^2$  criterion provides an upper bound on the area of a local watershed.

The issue here, however, is that within this 700,000- $m^2$  upper bound there is ample opportunity for the length of the sheet-flow path (measured in the direction of the steepest gradient) of any given local watershed to greatly exceed a distance at which one could reasonably expect to maintain sheet-flow conditions; that is, a ditch or swale (but not necessarily a first-order stream) would have been encountered. That distance is dependent on many factors such as slope, soil type, and runoff intensity, but has been estimated to be no more than approximately one-quarter of a mile (400 m) (Wischmeier and Smith, 1978). Indeed, more recent data (Lightle and Weesies, 1998) have suggested even more restrictive limits that vary nonlinearly with slope, e.g., 30.5 m for a slope of 0.5 percent, 91 m for slope of 2 percent and 15 m for slopes exceeding 17 percent. Thus, to the extent that a GIS-delineated flow path distance greatly exceeds a reasonable maximum sheet-flow-only distance, application of the sheet-flow-only module to that entire local watershed becomes inconsistent with what might actually be occurring at that site. The implications of such an inconsistency are the following:

- # Soil erosion (and associated contaminant loss) would be overestimated, because erosion is an increasing function of flow distance (see Equation 3-19).
- # Contamination in a downslope buffer would be overestimated. (The runoff/erosion may instead be channeled directly into the waterbody via a ditch or swale before it reaches the buffer area.)

The obvious solution to this issue is to further disaggregate the local watershed into a series of sublocal watersheds, each defined by a flow distance not exceeding the maximum, and apply the module sequentially to each sublocal watershed. There are a number of difficulties associated with this option, however, including:

- # The impracticality of implementation in GIS in an automated manner.
- # The increased computational burden.
- # Is soil/chemical “piped” directly to the waterbody at the outlet of each sublocal watershed or assumed to be deposited in the ditch or swale? If deposited, when would it finally be transported to the waterbody?
- # The inherent uncertainty in spatial resolution of the WMU within the local watershed in the first place.

In short, while this solution is appealing from a conceptual point of view, it is believed to be impractical in HWIR and, indeed, an inappropriate complexity given HWIR’s screening-level objective. The resolution used for HWIR is to simply limit the flow distance to a reasonable maximum when the GIS-delineated distance exceeds that maximum. The maximum is sampled from a distribution as described in the technical background document, *Data Collection for the Hazardous Waste Identification Rule. Section 5. Watershed and Waterbody Layout.* (U.S. EPA, 1999a). The conceptual module corresponding to this approach is that the runoff water itself may be diverted by swales or ditches, but the soil and chemical being eroded are maintained on the local watershed surface, to be transported downslope over time across the buffer and into the waterbody. This resolution is environmentally conservative with respect to contamination in the buffer. Depending on the actual residence time of a chemical deposited in a swale or ditch within the local watershed, it is not necessarily conservative with respect to chemical loadings to the waterbody. Nonetheless, mass balance is conserved.

## 3.4 Chemical Fate and Transport

### 3.4.1 Runoff Compartment

**3.4.1.1 Introduction.** A module of chemical and suspended solids concentrations in storm event runoff is presented in this section. The module is based on mass balances of solids and chemical in the runoff and the top soil column layer of thickness  $dz$ . The soil compartment is external to this module (see Section 3.4.2) and results from that compartment are called as needed by the software. A simplifying assumption is made that solids and chemical

concentrations in the runoff are at instantaneous steady-state during each individual runoff event, but can vary among runoff events, i.e. a quasi-dynamic approach is used. While assumption of instantaneous steady-state for each storm event is not strictly accurate, it was felt appropriate for the following reasons:

- # Run time considerations (i.e., maximize the numerical time step).
- # Data will not be available at the temporal scale to accurately track within-storm event conditions (e.g., rainfall hyetographs).
- # Because of the anticipated relatively small surface areas of the watershed subareas and the associated relatively small runoff volumes, the actual time to steady-state may not differ significantly from the one day or less implicitly assumed here. (A sensitivity analysis was performed using a dynamic form of the runoff compartment module that suggested relatively little difference in soil concentrations as a function of the steady-state versus dynamic assumption.)
- # To the extent that the actual time to steady-state would be greater than 1 day, the module is biased toward overestimating downslope concentrations and waterbody loads (i.e., it is risk-conservative).

Figure 3-3 presents the conceptual Runoff Quality Module showing the two compartments and the fate and transport processes considered. Development of mass balance equations for solids and chemical follow. (It should be noted that hydrolysis, volatilization, and biodegradation processes are not simulated in the runoff compartment. The percentage of time that runoff is actually occurring will be sufficiently short that any additional losses from these processes should be minimal. In addition, these processes are continuously simulated in the surface layer of the soil column. To also include them in the runoff compartment would be "double-counting.")

**3.4.1.2 Solids in Runoff Compartment.** A steady-state mass balance of solids in the runoff, i.e. suspended solids from erosion, written for arbitrary local watershed subarea  $i$  is given by the following equation. (In the subsequent module development, units are presented in general dimensional format, i.e., M(ass)-L(ength)-T(ime), for simplicity of presentation.)

$$0 = Q'_{i-1}m_{1,i-1} - Q'_im_{1,i} - vS_iA_im_{1,i} + vr_iA_im_2 \quad (3-22a)$$

$$Q'_{i-1} = Q_{i-1} + \frac{CSL_{i-1}}{\rho} \quad (3-22b)$$

$$Q'_i = Q_i + \frac{CSL_i}{\rho} \quad (3-22c)$$

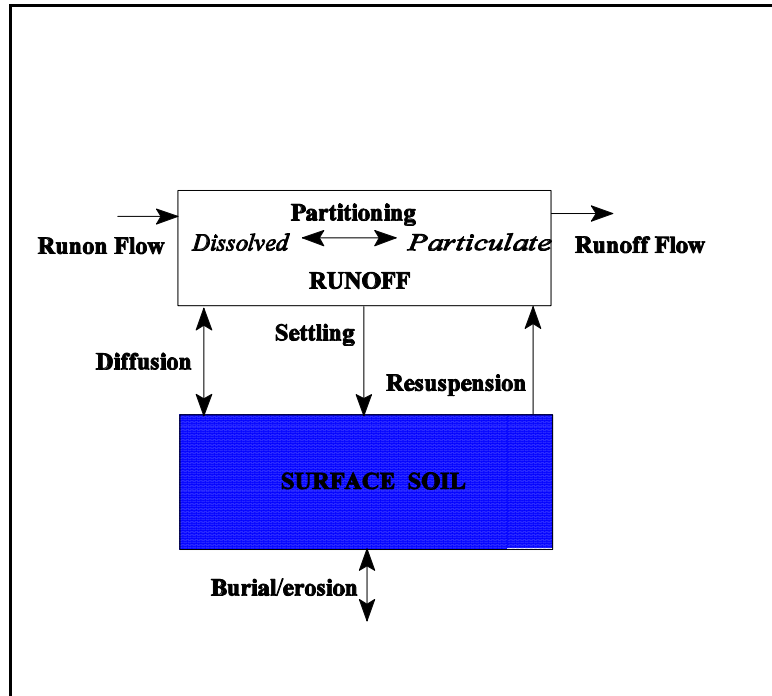


Figure 3-3. Runoff quality conceptual model.

where

$m_{1,i}$	=	solids concentration ( $M/L^3$ ) in the subarea $i$ runoff (suspended solids)
$m_2$	=	solids concentration ( $M/L^3$ ) in the top soil column layer of subarea $i$
$Q_i$	=	runoff flow ( $L^3/T$ ) leaving subarea $i$
$Q_{i-1}$	=	runon flow ( $L^3/T$ ) from subarea $i-1$
$A_i$	=	surface area ( $L^2$ ) of subarea $i$
$vs_i$	=	settling velocity ( $L/T$ )
$vr_i$	=	resuspension velocity ( $L/T$ )
$Q'_i$	=	total runoff flow volume ( $L^3/T$ ) (water plus solids) leaving subarea $i$
$CSL_i$	=	cumulative soil load leaving subarea $i$ ( $M/T$ )
$\rho$	=	particle density ( $M/L^3$ ) (i.e., $2.65 \text{ g/m}^3$ ).

(Note: subscript "1" denotes the runoff compartment while "2" denotes the top soil column layer compartment.) The first term in Equation 3-22a is the flux of soil across the upslope interface of subarea  $i$ . The second term is the flux of soil across the downslope interface. The third term is an internal sink of soil due to settling while the fourth term is an internal source due to resuspension.

**3.4.1.3 Solids in Soil Compartment.** The GSCM does not consider chemical mass transport among watershed subareas due to soil erosion, because it is based on a single subarea only. Therefore, that transport is considered here. The assumption is made that solids mass transport from or to the soil compartment of any given watershed subarea occurs only in a vertical direction, i.e., no downgradient advection of the top soil column layer itself is considered. (This is analogous to the assumption of a stationary sediment bed in stream/sediment quality modules.) The downslope mass transport of soil occurs due to vertical erosion or resuspension of soil followed by advective transport of the soil in the runoff water as suspended solids. The transport is described in terms of three parameters — settling, resuspension, and burial/erosion velocities. Under the assumption of no advective transport of the soil column layer, the steady-state mass balance equation for the surficial soil layer is

$$0 = v_s m_{1,i} A_i - v_r m_{2,i} A_i - v_b m_{2,i} A_i \quad (3-23)$$

where

$v_b$  = burial/erosion velocity (L/T).

The first term of Equation (3-23) is a source of soil mass to the surficial soil column layer due to settling from the overlying runoff water. The second term is a sink from resuspension. The third term is either a source or a sink depending on the sign of the burial/erosion velocity as described subsequently.

Consider the solids balances in the runoff and soil compartments, Equations 3-22 and 3-23, respectively. These two equations involve three parameters— $v_s$ ,  $v_r$ , and  $v_b$ —and two solids concentrations— $m_1$  and  $m_2$ . Which of these five variables is known for arbitrary subarea  $i$ ? It can be assumed that the solids concentration in the soil ( $m_2$ ) is a known value — it is simply the bulk soil density. Consider now the suspended solids concentration in subarea  $i$ ,  $m_{1,i}$ . From the Soil Erosion Module, the total solids mass fluxes moving across both the upslope and downslope interfaces of subarea  $i$  are known, and these two fluxes are, respectively, the first two terms on the right side of Equation 3-22.  $m_{1,i}$  can then be determined as

$$m_{1,i} = CSL_i / Q'_i \quad (3-24)$$

where  $CSL_i$  is the cumulative soil load leaving subarea  $i$ , as determined by the Soil Erosion Module, and  $Q'_i$  is the cumulative runoff flow volume (including solids' volume) leaving subarea  $i$ , as determined by the Runoff Quantity Model. Therefore, because the soil concentration ( $m_2$ ) is assumed to be known and the Soil Erosion and Runoff Quantity modules can be used to determine the suspended solids concentrations (the  $m_{1,i}$ ), Equations 3-22 and 3-23 can now be considered as two equations in three unknowns,  $v_s$ ,  $v_r$ , and  $v_b$ .

The settling ( $v_s$ ) and resuspension ( $v_r$ ) parameters reflect processes internal to subarea  $i$ , while the burial/erosion parameter ( $v_b$ ) reflects net changes across subarea  $i$  and is completely determined by the difference in the soil fluxes entering and leaving subarea  $i$ . This can be seen

by adding the right-hand-sides of Equations 3-22 and 3-23 and setting the result to zero. All terms involving  $v_s$  and  $v_r$  cancel, and the burial/erosion velocity is then given by

$$vb_i = \frac{CSL_{i-1} - CSL_i}{A_i m_2} \quad (3-25)$$

where  $CSL_{i-1}$  and  $CSL_i$  denote the soil fluxes into and out of subarea  $i$ , respectively, as discussed above. From Equation 3-25 it can be seen that, if the soil load entering subarea  $i$  ( $CSL_{i-1}$ ) is greater than the soil load leaving ( $CSL_i$ ), then the burial/erosion velocity is positive and soil is being deposited (buried). Conversely, as will typically be the case, if the load leaving is greater than the load entering, then the burial/erosion velocity will be negative and erosion is occurring in an upward direction.

Consider now  $v_s$  and  $v_r$ . With the net soil flux across the subarea having been determined, Equations 3-22 and 2-23 are in fact the same equation—the burial velocity term is explicitly shown in Equation 3-23 and implicitly shown in Equation 3-22. Thus, either Equation 3-22 or 3-23 represents one equation in two unknowns,  $v_s$  and  $v_r$ . If one of these is known, the other can be solved for. Of the two, the resuspension velocity would be very difficult to obtain estimates for, while the settling velocity could be assumed similar to, for example, hindered or compaction settling in sludge thickeners. Accordingly,  $v_r$  as a function of  $v_s$  (and  $vb_i$ , which is determined as per Equation 3-25) is given for subarea  $i$  by

$$vr_i = vs_i \frac{m_{1,i}}{m_2} - vb_i \quad (3-26)$$

The settling velocity,  $v_s$ , is assigned values for HWIR99 from a uniform random distribution between the range 0.05 and 1.0 m/d, based on observed settling velocities for “mineral” sludges in sludge thickening experiments (U.S. EPA, 1999b).

In summary, because  $m_2$  is assumed known and  $m_1$  is calculated from results of the Soil Erosion and Runoff modules, the solids mass balance equations are used to determine the burial/erosion and resuspension parameters for subsequent use in the chemical (contaminant) model.

**3.4.1.4 Contaminant in Runoff Compartment.** As illustrated in Figure 3-3, a steady-state mass balance of contaminant in the runoff results in the equation

$$0 = Q'_{i-1}c_{1,i-1} - Q'_i c_{1,i} - vs_i A_i Fp_{1,i} c_{1,i} + vr_i A_i Fp_{2,i} Er_i c_{2,i} + vd_i A_i \left( \frac{Fd_{2,i}}{\Phi_2} c_{2,i} - \frac{Fd_{1,i}}{\Phi_{1,i}} c_{1,i} \right) \quad (3-27)$$

where



- $c_{1,i}$  = total contaminant concentration (particulate + dissolved) in runoff in subarea i (M/L<sup>3</sup>)  
 $c_{2,i}$  = total contaminant concentration in soil (M/L<sup>3</sup>)  
 $V_{1,i}$  = subarea-specific (not cumulative) runoff volume for subarea i (L<sup>3</sup>)  
 $Fp_{1,i}$  = fraction particulate in runoff  
 $Fd_{1,i}$  = fraction dissolved in runoff (1- $Fp_{1,i}$ )  
 $vd_i$  = diffusive exchange velocity (L/T)  
 $Er_i$  = enrichment ratio  
 $\Phi_{1,i}$  = is the porosity of the runoff, calculated as

$$\Phi_{1,i} = 1 - \frac{m_{1,i}}{\rho} \quad (3-28)$$

where  $\rho$  is the density (M/L<sup>3</sup>) of suspended solids (e.g., 2.65 g/cm<sup>3</sup>).

- $\Phi_2$  = soil porosity, calculated as

$$\Phi_2 = 1 - \frac{m_2}{\rho} \quad (3-29)$$

Note that  $\phi_2$  is equivalent to porosity ( $\eta$ ) in the GSCM.

Equation (3-27) can be used to express  $c_{1,i}$  as a function of  $c_{1,i-1}$  and  $c_{2,i}$  as

$$c_{1,i} = \frac{Q'_{i-1}c_{1,i-1} + [vr_i A_i Fp_{2,i} Er_i + vd_i A_i (Fd_{2,i} / \Phi_2)] c_{2,i}}{Q'_i + vs_i A_i Fp_{1,i} + vd_i A_i (Fd_{1,i} / \Phi_{1,i})} \quad (3-30)$$

where  $c_{2,i}$  is determined by the GSCM as described in Section 2. Determination of the individual terms constituting this equation are described below.

$Fp_{1,i}$  is calculated as (Thomann and Mueller, 1987)

$$Fp_{1,i} = \frac{(k_d/\Phi_{1,i})m_{1,i}}{1 + (k_d/\Phi_{1,i})m_{1,i}} \quad (3-31)$$

where

$k_d$  = chemical-specific partition coefficient ( $L^3/M$ ) (Note:  $k_d$  is divided by porosity to attain the porosity-corrected  $k_d$  with units of mass per total [liquid plus solids] volume.)

$Fp_{2,i}$  is similarly calculated as

$$Fp_{2,i} = \frac{(k_d/\Phi_2)m_2}{1 + (k_d/\Phi_2)m_2} \quad (3-32)$$

where it can be seen that  $Fp_2$  (and  $Fd_2$ ) will be constant among all subareas  $i$ .

$Fd_{1,i}$  and  $Fd_{2,i}$  are then determined as

$$Fd_{1,i} = 1 - Fp_{1,i} \quad (3-33)$$

$$Fd_{2,i} = 1 - Fp_{2,i} \quad (3-34)$$

Under the assumption that resistance to vertical diffusion is much greater in the soil than in the runoff, the diffusive exchange velocity,  $vd_i$ , can be expressed as (Thomann and Mueller, 1987, p. 548)

$$vd_i = \frac{Dw}{\Phi_2 Lc} \quad (3-35)$$

where

$Dw$  = water diffusivity ( $L^2/T$ ).  
 $Lc$  = characteristic mixing length ( $L$ ) over which a concentration gradient exists; assumed to be the depth of the runoff including the solids ( $H1'$ ):

$$Lc = HI'_i = \frac{Q'_i}{A_i} \quad (3-36)$$

The enrichment ratio,  $Er_i$ , is used to account for preferential erosion of finer soil particles — with higher specific surface areas and more sorbed chemical per unit area — as

rainfall intensity decreases. That is, large (highly erosive) runoff events may result in average eroded soil particle sizes and associated sorbed chemical loads that do not differ much from the average sizes/loads in the surficial soil column layer. However, less intense runoff events will erode the finer materials and resulting chemical loads could be significantly higher than represented by the average soil concentration. U.S. EPA et al. (1985) give the storm event-specific enrichment ratio as a power function of sediment discharge flux ( $M/L^2$ ). This formulation results in:

$$Er_i = \frac{a}{(CSL_i/WSA_i)^{0.2}} \quad (3-37)$$

where  $a = 7.39$  for  $CSL_i/WSA_i$  in kg/ha (U.S. EPA et al., 1985). ( $CSL_i$  is the event soil load leaving subarea  $i$  and  $WSA_i$  is the local watershed surface area from the drainage divide down to and including subarea  $i$ .) It should be noted that the enrichment ratio is greater than or equal to 1.0. Should specific values of the sediment discharge (the denominator) result in an enrichment ratio less than 1.0, it is reset to 1.0 in the code.

### 3.4.2 Soil Compartment

The GSCM (see Section 2.2) is coupled to the Runoff Compartment Module (see Section 3.4.1) in this section and applied to the several subareas that constitute the sheet flow local watershed of which the LAU or wastepile is an integral part. Continuing the chemical concentration indexing scheme (i.e., subscript "1" denoting runoff compartment, and subscript "2" denoting surficial soil compartment), let the total (dissolved, particulate, and gaseous phase) chemical concentration in the surficial soil column layer of any local watershed subarea  $i$  be denoted as  $C_{2,i}$ . ( $C_{2,i}$  is equivalent to  $C_T$  in the GSCM description.) From Section 2.2 (GSCM), the governing differential equation for the surface soil layer of subarea  $i$  is

$$\frac{\partial C_{2,i}}{\partial t} = D_E \frac{\partial^2 C_{2,i}}{\partial z^2} - V_E \frac{\partial C_{2,i}}{\partial z} - \sum k_j C_{2,i} + ss_i \quad (3-38)$$

where  $k_j$  represents first-order rate constant due to process  $j$  not including runoff/erosion processes, i.e., biological decay and hydrolysis and wind/mechanical action. The last term,  $ss_i$ , is a source/sink term representing the net effect of runoff and erosion processes on  $C_{2,i}$  as illustrated in Figure 3-3. This term is given by

$$ss_i = \frac{vs_i Fp_{1,i} C_{1,i} - vr_i Fp_{2,i} Er_i C_{2,i} - vd_i \left( \frac{Fd_{2,i}}{\Phi_2} C_{2,i} - \frac{Fd_{1,i}}{\Phi_{1,i}} C_{1,i} \right) - vb_i Fp_2 C_{2,i}}{dz} \quad (3-39)$$

where  $vs_i$ ,  $vr_i$ ,  $vb_i$ , and  $vd_i$  denote, respectively, the settling, resuspension, burial/erosion and diffusive exchange velocities for subarea  $i$  as described in the Runoff Compartment model. Thus, the terms comprising  $ss_i$  are, respectively, a source of chemical due to settling from the

overlying runoff water, a sink of chemical due to resuspension, and a source or sink (depending on the relative values of  $C_{1,i}$  and  $C_{2,i}$ ) due to chemical diffusion from/to the runoff.

(The burial/erosion mechanism introduces a minor mass balance error into the model. The module for surface soil/runoff water fate and transport [Section 3.4.1] is based on a conceptual module originally developed for use in a stream/sediment application [e.g., Thomann and Mueller, 1987] where the sediment compartment location relative to a reference point below the surface can move vertically [“float”] as burial and erosion occur. In that moving frame of reference, burial/erosion of contaminant does not introduce a mass balance error because, with respect to the modeled sediment, this sink/source of contaminant is **exogenous** to the modeled system, i.e., it is coming from/going to outside of the modeled system. There is internal [endogenous] mass balance consistency within the modeled system. However, in this HWIR99 application, the frame of reference is not allowed to float, but is fixed by the elevation of the lower boundary, e.g. top of the vadose zone. Thus, if sorbed chemical is eroded from the surface cell, that surface cell, which is vertically fixed, must have a “source” that is internal to the modeled soil column to compensate for this sink or its internal mass balance is not maintained. The magnitude of this mass balance error is equal to the mass of eroded soil from the surface over the duration of the simulation times its average sorbed chemical concentration. In most cases, this error as a percentage of the total chemical mass in the modeled WMU will be quite small, and that has been confirmed in multiple executions of the module. Conceptually at least, the GSCM could be designed so that, after each runoff event, the surficial soil compartment could decrease or increase in size to accommodate the event’s erosion/burial magnitude, while maintaining a fixed vertical reference. This degree of complexity, however, falls outside the scope of the “screening level” approach to the HWIR99 analysis.)

Grouping coefficients of  $C_{1,i}$  and  $C_{2,i}$ , Equation 3-39 can be rewritten as

$$ss_i = a_i C_{1,i} - b_i C_{2,i} - k_{bu,i} C_{2,i} \quad (3-40a)$$

where

$$a_i = \frac{vs_i Fp_{1,i} + vd_i \frac{Fd_{1,i}}{\Phi_{1,i}}}{dz} \quad (3-40b)$$

$$b_i = \frac{vr_i Fp_{2,i} Er_i + vd_i \frac{Fd_{2,i}}{\Phi_2}}{dz} \quad (3-40c)$$

$$k_{bu,i} = \frac{vb_i Fp_{2,i}}{dz} \quad (3-40d)$$

and  $k_{bu,i}$  is the first-order rate constant (1/T) associated with the burial/erosion process.

Using Equation 3-40, Equation 3-38 can be rewritten as

$$\frac{\partial C_{2,i}}{\partial t} = D_E \frac{\partial^2 C_{2,i}}{\partial z^2} - V_E \frac{\partial C_{2,i}}{\partial z} - \sum_j k_j C_{2,i} + a_i C_{1,i} - b_i C_{2,i} - k_{bu,i} C_{2,i} \quad (3-41)$$

From Equation 3-41, it can be seen that  $C_{2,i}$  is a function of  $C_{1,i}$ . Similarly, from Equation 3-30 of the Runoff Compartment Module, it can be seen that  $C_{1,i}$  is a function of  $C_{2,i}$ . Thus,  $C_{2,i}$  and  $C_{1,i}$  are jointly determined at any time  $t$  by simultaneous solution of their two respective equations.

$C_{2,i}$  at time  $t$  can be determined by substitution for  $C_{1,i}$ . From the Runoff Compartment module (Equation 3-30).  $C_{1,i}$  can be expressed as

$$C_{1,i} = \frac{Q'_{i-1} C_{1,i-1}}{d_{2,i}} + \frac{d_{1,i}}{d_{2,i}} C_{2,i} \quad (3-42a)$$

where

$$d_{1,i} = vr_i A_i F p_{2,i} E r_i + vd_i A_i \frac{F d_{2,i}}{\Phi_2} \quad (3-42b)$$

Substituting for  $C_{1,i}$  from Equation 3-42 into Equation 3-41, the differential equation for  $C_{2,i}$  is now

$$d_{2,i} = Q'_{i-1} + vs_i A_i F p_{1,i} + vd_i A_i \frac{F d_{1,i}}{\Phi_{1,i}} \quad (3-42c)$$

expressed implicitly as a function of  $C_{1,i}$  as

$$\frac{\partial C_{2,i}}{\partial t} = D_E \frac{\partial^2 C_{2,i}}{\partial z^2} - V_E \frac{\partial C_{2,i}}{\partial z} - (\sum_j k_j + b_i + k_{bu,i} - \frac{a_i d_{1,i}}{d_{2,i}}) C_{2,i} + \frac{a_i Q'_{i-1} C_{1,i-1}}{d_{2,i}} \quad (3-43)$$

Once  $C_{2,i}$  at time  $t$  is determined by solution of Equation 3-43, the associated value for  $C_{1,i}$  can be found from Equation 3-42, thus completing the simultaneous solution. (The value for  $C_{1,i-1}$ , i.e., the runoff concentration in the immediately upslope subarea, will have been determined previously during the simultaneous solution for the  $i-1$  subarea at time  $t$ .)

To implement the simultaneous solution, Equation 3-43 can be simplified to

$$\frac{\partial C_{2,i}}{\partial t} = D_E \frac{\partial^2 C_{2,i}}{\partial z^2} - V_E \frac{\partial C_{2,i}}{\partial z} - k'_i C_{2,i} + ld_{i-1} \quad (3-44a)$$

where

$$k'_i = \sum k_j + k_{ev,i} + k_{bu,i} \quad (3-44b)$$

$$k_{ev,i} = b_i - a_i \frac{d_{1,i}}{d_{2,i}} \quad (3-44c)$$

$k_{ev,i}$  is the storm event (or runoff and erosion) first-order loss rate,  $k'_i$  is the lumped first-order loss rate which includes the effects of abiotic hydrolysis (j=hy), aerobic biodegradation (j=ae), and wind/mechanical activity (j=wd), in addition to runoff and erosion.  $k_{hy}$  and  $k_{ae}$  are inputs to the module

$$ld_{i-1} = \frac{a_i}{d_{2,i}} Q'_{i-1} C_{1,i-1} \quad (3-44d)$$

and  $k_{wd}$  is calculated using the methodologies detailed in Appendix A. The last term,  $ld_{i-1}$  is the run-on load from upslope subareas in  $g/m^3/d$ .

Recall that in the GSCM, the governing equation is broken up into three component equations—diffusion, convection, and first-order losses (Equations 2-13 through 2-15), each solved individually on a grid. In the subsurface layers, the solution technique described in Section 2 is applied directly. However, for the surface soil column layer, the first two-component equations remain the same, while the third is revised to:

$$\frac{\partial C_{2,i}}{\partial t} = -k'_i C_{2,i} + ld_{i-1} \quad (3-45)$$

which has the following analytical solution for  $C_{2,i} = C_{2,i}^0$  at  $t = 0$ :

$$C_{2,i} = \begin{cases} C_{2,i}^0 \exp(-k'_i t) + ld_{i-1} \left[ \frac{1 - \exp(-k'_i t)}{k'_i} \right] & k'_i > 0 \\ C_{2,i}^0 + ld_{i-1} t & k'_i = 0 \end{cases} \quad (3-46)$$

To track mass losses, the total mass added to the soil column in subarea *i* in any time period zero to *t* due to settling from runoff water,  $M_{add,i}$  ( $M/L^2$ ), is evaluated using

$$M_{add,i} = l d_{i-1} t \, dz \quad (3-47)$$

A mass balance on the soil column in time *t* gives:

$$\Delta M_i = M_{add,i} - M_{loss,i} \quad (3-48)$$

where  $\Delta M_i$  ( $M/L^2$ ) is the change in mass in the soil column in subarea *i* as given by  $((C_{2,i} - C_{2,i}^0) \cdot dz)$  and  $M_{loss,i}$  ( $M/L^2$ ) is the total mass lost from the subarea *i* soil column in any time period zero to *t*. By substituting Equation 3-46 for  $C_{2,i}$  and Equation 3-47 for  $M_{add,i}$  and rearranging, the following equation for  $M_{loss,i}$  was derived for  $k'_i > 0$ . For  $k'_i = 0$ ,  $M_{loss,i} = 0$ .

$$M_{loss,i} = [C_{2,i}^0 (1 - \exp(-k'_i t)) + l d_{i-1} \left( \frac{k'_i t + \exp(-k'_i t) - 1}{k'_i} \right)] dz \quad (3-49)$$

The total mass lost in any time period zero to *t* from subarea *i* soil column can be attributed to specific first-order loss processes, *j*,  $M_{j,i}(t)$  ( $M/L^2$ ) using

$$M_{j,i} = M_{loss,i} \frac{k_j}{k'_i} \quad (3-50)$$

where

- j* = hy for hydrolysis,
- j* = ae for aerobic degradation,
- j* = wd for losses due to wind/mechanical activity,
- j* = ev for runoff/erosion events, and
- j* = bu for burial/erosion.

Equation 3-42a provides the contaminant concentration in the runoff water at time *t*. The average contaminant concentration in the runoff water ( $\bar{C}_{1,i}$ ) over time 0 to *t* is determined using:

$$\bar{C}_{1,i} = \frac{Q'_{i-1} \bar{C}_{1,i-1}}{d_{2,i}} + \frac{d_{1,i}}{d_{2,i}} \bar{C}_{2,i} \quad (3-51)$$

where  $C_{2,i}$  is the time-weighted average contaminant concentration in the soil compartment over the same time period. Given the short time step (i.e., 1 day) used in the integration of the Local Watershed/Soil Column Module,  $C_{2,i}$  is approximated using:

$$\bar{C}_{2,i} = \frac{C_{2,i}^0 + C_{2,i}}{2} \quad (3-52)$$

where the 0 superscript denotes concentration at the beginning of the day.

## 3.5 Implementation

### 3.5.1 Overview

An overview of the algorithm implementing the combined Local Watershed/Soil Column Modules is provided in Figure 3-4a and b. Some additional differences from the GSCM general algorithm (Section 2.4.1) are noted. In the GSCM, it is assumed that infiltration is constant and convection events occur at regular intervals throughout the entire simulation. (With a convection event, soil column concentrations are propagated downward and  $M_{\text{cha}}$  is incremented.) In the Local Watershed/Soil Column Modules, the infiltration rate ( $I$ ) is allowed to vary from year to year. As a result, convection events do not occur at regular intervals. To determine the appropriate time to initiate a convection event, at the end of every time step a variable ( $\text{fadv}$ ) tracking the fraction of mass in the bottom soil column layer that would have convected is incremented by  $(dt \cdot V_E / dz)$ . If  $\text{fadv}$  is sufficiently close to 1, a convection event is initiated and  $\text{fadv}$  is reset to zero. At the end of the simulation (year =  $\text{NyrMax}$ ), if  $\text{fadv}$  is greater than zero,  $M_{\text{cha}}$  is incremented by  $\text{fadv}$  times  $dz$  times  $C_T$  in the lowest layer and  $C_T$  in the lowest layer is adjusted accordingly. Leachate flux for the final year is then calculated using Equation 2-29.

### 3.5.2 Simulation-Stopping Criterion

For a given local watershed,  $i$ , the simulation is stopped in each successive subarea when the amount of contaminant mass in local watershed  $i$  and all upslope subareas  $j$  ( $j < i$ ) is determined to be insignificant. "Insignificance" is defined by the input parameter  $\text{TermFrac}$ , and this simulation criterion is implemented as follows:

1. During the years before the end of the operating life of the WMU, the year-end cumulative subarea contaminant mass in each subarea is determined. Here, cumulative subarea mass ( $\text{samass}_j$ ) refers to the sum of the contaminant mass in subarea  $i$  and all upslope subareas  $j$  ( $j < i$ ). The maximum cumulative subarea contaminant mass ( $\text{max\_samass}_j$ ) is stored for each subarea.
2. After WMU operation ceases, the year-end cumulative subarea contaminant mass in each subarea is compared to the stored maximum for that subarea. The simulation in subarea  $i$  is stopped when



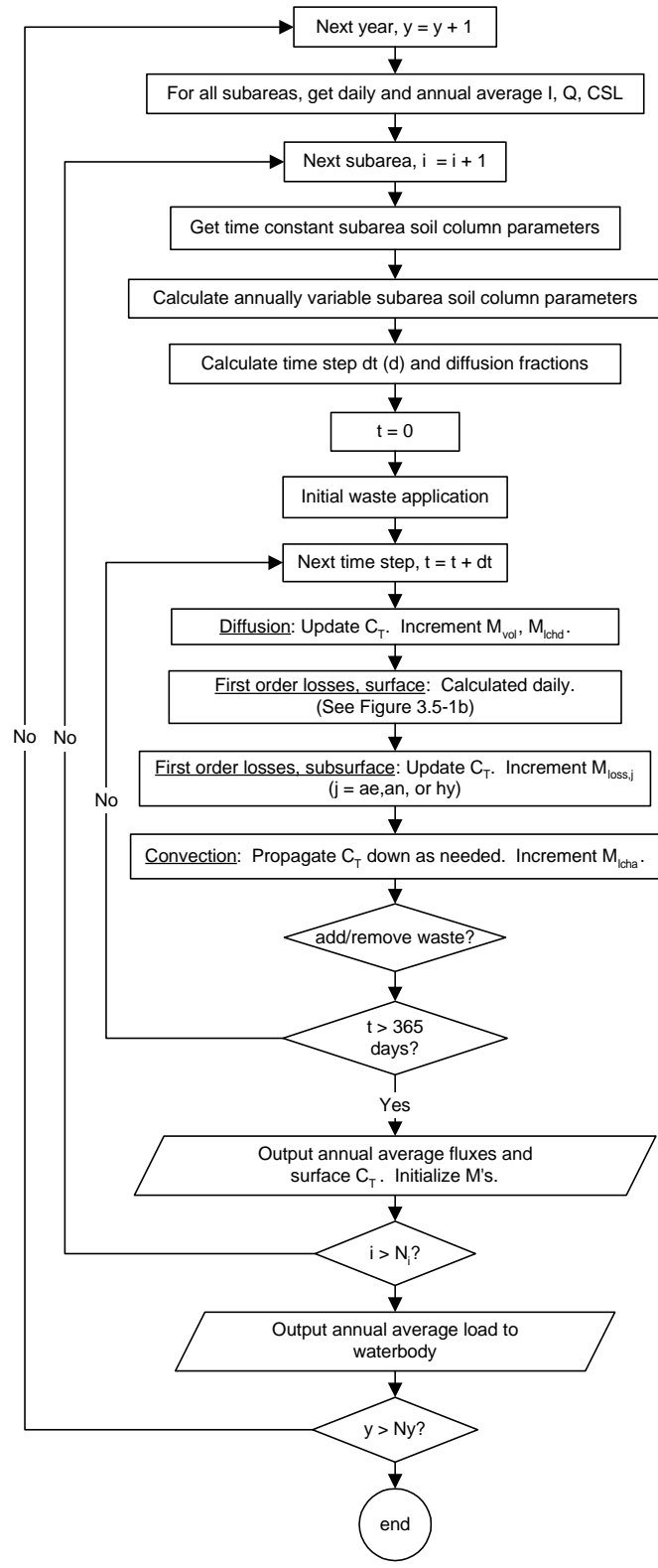


Figure 3-4a. Overview of algorithm for combined local watershed/soil column module.

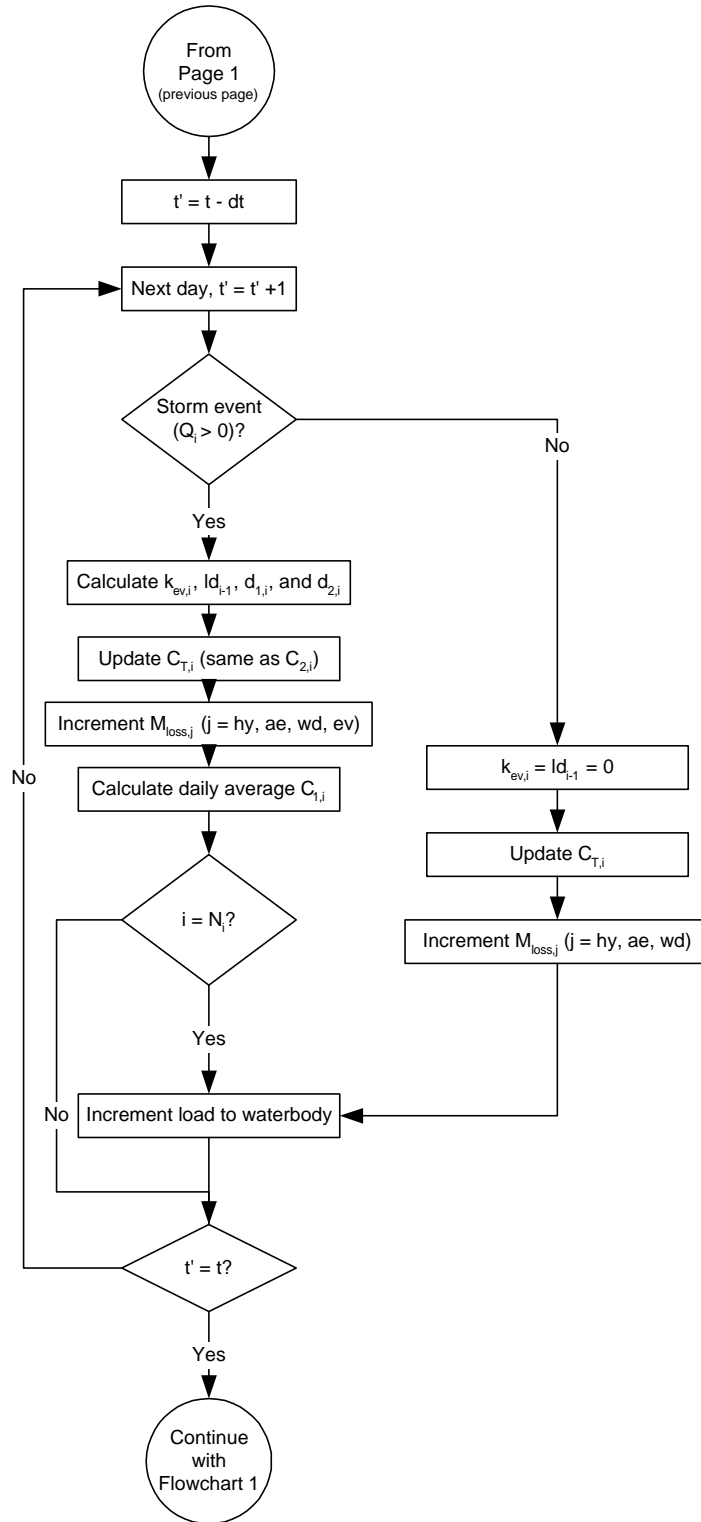


Figure 3-4b. Detail on calculation of first-order losses in surface layer.

$$samass_i \leq TermFrac * maxsamass_i$$

where “TermFrac” is the user-specified fraction ranging from 0 to 1.0 (unless the NyrMax parameter is reached first, at which point the simulation is automatically stopped). The year the simulation ceases in each local watershed and subarea is stored in an internal two-dimensional array dimensioned on local watershed and subarea.

(Note: As of this writing, computer memory requirements have resulted in an inability to make full use of the above-described TermFrac stopping criterion for highly persistent chemicals. Time series outputs are kept in random access memory [RAM] for postprocessing. When the length of the time series becomes excessive with respect to array sizes and available RAM, memory-caching occurs with a concomitant drastic slowdown in run time. To mitigate this problem, it was determined that the length of the time series would be determined by the TermFrac criterion, as described above, or 200 years, whichever comes first.)

### 3.5.3 Leachate Flux Processing

Preliminary module runs indicated that there are many cases where the convective transfer step will occur less than once per year, sometimes even less than once in the entire simulation period. In these cases the leachate flux will be nonzero in the years when a convection event occurs and zero in years when it did not. This is a limitation of the solution technique. In reality, leaching occurs more or less continuously over the time between the modeled convection events. To mitigate this limitation, a leachate flux postprocessing algorithm was developed. The entire simulation ( $0 < j \leq NyrMax$ ) is split into three time periods, where  $j$  is used here as the year index:

1. WMU operating years ( $0 \leq j \leq y_{op}$ )
2. Non-operating years ( $y_{op} < j \leq LeachFluxNY$ )
3. No leachate flux years ( $LeachFluxNY < j \leq NyrMax$ )

where LeachFLuxNY is the last year there is a positive leachate flux. The processed leachate fluxes ( $J_{lchp}$ ,  $g/m^2/d$ ) in time periods 1 and 2 are calculated from  $J_{lch}$  in each year,  $j$ , using:

$$J_{lchp,j} = \frac{I_j}{\bar{I} (b-a+1)} \sum_{j=a}^{j=b} J_{lch,j} \quad (3-53)$$

where, in time period 1,  $a = 0$  and  $b = y_{op}$ . In time period 2,  $a = y_{op}$  and  $b = LeachFluxNY$ . The first term in Equation (3-53) is an infiltration-based weight where  $I_j$  is the annual average infiltration rate in year  $j$  and  $\bar{I}$  is the average infiltration rate between years  $a$  and  $b$ . In time period 3,  $J_{lchp}$  is zero.

With use of Equation 3-53 to estimate the leachate flux, mass is conserved. That is, the total mass lost due to leaching over the course of the simulation is the same using the processed and unprocessed leachate fluxes. However, with the processed leachate flux, a smoother function of leachate flux over time is provided.

### 3.5.4 End-of-Simulation Mass Balance Check

At the end of the simulation, a system-wide mass balance check is performed in the code. The system, in the Local Watershed/Soil Column Modules, includes the WMU subarea and all other subarea “soil columns.” The mass balance error ( $fMerr$ ) is computed as a fraction of the total contaminant mass added to the system from the mass balance equation

$$fMerr = 1 - (fMrem + fMlost) \quad (3-54)$$

where  $fMrem$  is the fraction of total contaminant mass added that remains in the system at the end of the simulation.  $fMlost$  is the fraction of the contaminant mass added that was estimated to have been lost from the system by the end of the simulation.  $fMlost$  is the sum of the variables listed and defined in Table 3-2.

**Table 3-2. Variables Summarizing Contaminant Mass Losses**

Variable	Definition: Fraction of the total mass added lost due to:
fMvol_wmu	Volatilization from the WMU
fMlch_wmu	Leaching from the WMU
fMwnd_wmu	Wind/mechanical action on the WMU surface
fMdeg_wmu	Abiotic and biodegradation within the WMU
fMrmv_wmu <sup>a</sup>	Removal from the WMU
fMvol_sa	Volatilization from the non-WMU subarea soil columns
fMlch_sa	Leaching from the non-WMU subarea soil columns
fMdeg_sa	Abiotic and biodegradation in the non-WMU subarea soil columns
fMswl	Runoff/erosion from the most downslope subarea
fMbur <sup>b</sup>	Burial/erosion in all subareas (see $k_{bu}$ in Equation 3-44d)

<sup>a</sup> Applies only to the WP, which is removed and refreshed regularly. See Section 3.7 for details.

<sup>b</sup>  $fMbur$  is the only variable listed that can be negative (indicating a mass gain). This results from the inclusion of a burial/erosion term in linking the runoff and soil compartments. See Figure 3-3 and the discussion of the meaning of the burial/erosion term in Section 3.4.2.

Time series outputs to the various other HWIR99 modules are reported as follows:

- # *Outputs to Air Module.* All annual time series outputs to the Air Module are reported up to and including the last year that there is nonzero VE or CE. Thus, the annual time series outputs to the Air Module are all the same length. After this, all outputs to the Air Module will be zero and are not reported.
- # *Outputs to the Vadose Module.* The annual time series of LeachFlux for each local watershed is reported up to and including the last year that there is a nonzero LeachFlux in any local watershed. This results in the same reported LeachFlux time series length for all local watersheds. After this, all LeachFlux values for all local watersheds will be zero and are not reported. AnnInfil is reported from year one to the last year that meteorological data are available.

### 3.6 Output Summary

Table 3-3 summarizes the outputs of the combined Local Watershed/Soil Column Module.

**Table 3-3. Output Summary for the WP and LAU Modules**

Variable Name <sup>a</sup>		Definition	Units
Documentation	Code		
I	AnnInfil	Leachate infiltration rate (annual avg., WMU subarea(s) only)	m/d
J <sub>vol</sub>	VE	Volatile emission rate	g/m <sup>2</sup> /d
	VEYR	Year associated with output	Year
	VENY	Number of years in outputs	Unitless
CE30	CE	Constituent mass emission rate-PM30	g/m <sup>2</sup> /d
	CEYR	Year associated with output	Year
	CENY	Number of years in outputs	Unitless
E30	PE30	Eroded solids mass emission rate-PM30	g/m <sup>2</sup> /d
	PE30YR	Year associated with output	Year
	PE30NY	Number of years in outputs	Unitless
pmf	PMF	Particulate emission particle size distribution	Mass frac.
	PMFYR	Year associated with output	Year
	PMFNY	Number of years in outputs	Unitless

(continued)

**Table 3-3. (continued)**

Variable Name <sup>a</sup>		Definition	Units
Documentation	Code		
Q	Runoff	Runoff flow to waterbody	m <sup>3</sup> /d
J <sub>lch</sub>	LeachFlux	Leachate contaminant flux	g/m <sup>2</sup> /d
	LeachFluxYR	Year associated with output	Year
LeachFluxNY	LeachFluxNY	Number of years in outputs	Unitless
	SWLoadChem	Chemical load to waterbody	g/d
	SWLoadChemYr	Year associated with output	year
	SWLoadChemNY	Number of years in outputs	Unitless
CSL	SWLoadSolid	Total suspended solids load to waterbody	g/d
C1	SWConcTot	Total chemical concentration in surface water runoff	mg/L
	SWConcTotYR	Year associated with output	Year
	SWConcTotNY	Number of years in outputs	Unitless
C <sub>T</sub>	CTss	Soil concentration in surface soil layer	µg/g
	CTssYR	Year associated with output	Year
	CTssNY	Number of years in outputs	Unitless
C <sub>T</sub>	CTda	Depth-weighted average soil concentration (from zava to zavb)	µg/g
	CTdaYR	Year associated with output	Year
	CTdaNY	Number of years in outputs	Unitless
	SrcSoil	Flag for soil presence (true)	Logical
	SrcOvl	Flag for overland flow presence (true)	Logical
	SrcLeachMet	Flag for leachate presence when leachate is met-driven (true)	Logical
	SrcLeachSrc	Flag for leachate presence when leachate is not met-driven (false)	Logical
	SrcVE	Flag for volatile emissions presence (true)	Logical
	SrcCE	Flag for chemical sorbed to particulates emissions presence (true)	Logical
	SrcH2O	Flag for surface water presence for eco-exposure (false)	Logical
	NyrMet	Number of years in the available met record	Unitless

<sup>a</sup>Where the variable name is used in the code but not in the documentation, the first column is left blank.

- # *Outputs to the Surface Water Module.* The annual time series of SWLoadChem are reported up to and including the last year that there is nonzero SWLoadChem in any local watershed. This results in the same reported SWLoadChem time series length for all local watersheds. SWLoadSolid and Runoff are reported for all local watersheds up to the last year that meteorological data are available.
- # *Outputs to Exposure Modules (Human and Ecological).* The annual time series of CTda is reported to the the last year of nonzero CTda in each local watershed and subarea. Thus, the length of the reported time series for CTda in each local watershed and subarea may differ. The same is true for CTss.

### 3.7 Wastepile Module Specifics

#### 3.7.1 Introduction

Section 3.4 presents the Local Watershed/Soil Column Module as common to both the wastepile and the LAU. This section discusses wastepile-specific issues in implementation. Figure 3-5 illustrates the wastepile in the local watershed conceptual module.

#### 3.7.2 Additional Assumptions

- # The wastepile has a constant height equal to  $h$  (m) (i.e.,  $z_{sc} = h$ ) and constant area ( $A$ ,  $m^2$ ) equal to the footprint of the wastepile.
- # At time zero, the wastepile is filled to capacity. After each period of time equal to  $t_{bet}$ , the entire wastepile is removed and instantaneously refreshed (i.e., replaced with fresh waste). The time between fresh wastepiles is determined by:

$$t_{bet} = \frac{r_{b,w} \cdot A \cdot h}{L'} \cdot 365 \frac{d}{yr} \quad (3-55)$$

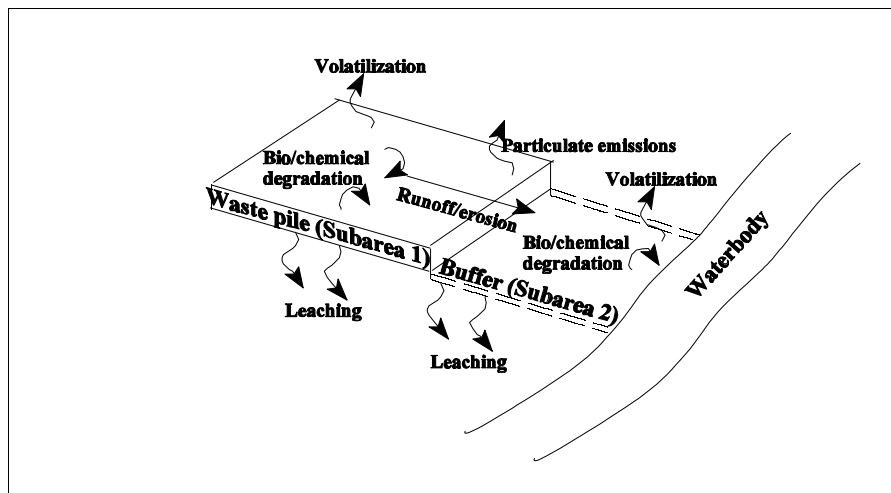


Figure 3-5. Illustration of wastepile in local watershed.

where  $\rho_{b,w}$  (g/cm<sup>3</sup>) is the dry bulk density of the waste and  $L'$  (Mg/yr) is the annual waste (dry) loading rate, adjusted for waste losses during the process of unloading raw waste:

$$L' = L - E30un \cdot A \cdot \frac{365}{10^6} \quad (3-56)$$

$E30un$  (g/m<sup>2</sup>) is the mass lost due to particulate emission during the unloading of raw waste. The methodology used for calculating  $E30un$  is presented in Appendix A.

In reality, waste is added and removed from a wastepile incrementally. The assumption that the waste is instantaneously refreshed is made to simplify modeling. As such, for volatile contaminants, the wastepile module may underestimate volatile losses since the waste surface is not refreshed in between the placement of new waste relative to a module where waste is built up gradually. For nonvolatile contaminants, this is unlikely to affect emission estimates.

- # Total porosity for the wastepile is specified rather than calculated (as it is for the LAU).
- # The wastepile site is used for a finite number of years ( $y_{op}$ , yr), after which it is assumed that the final wastepile is removed.
- # The first-order chemical and biological loss processes include aerobic biodegradation ( $k_{ae}$ , 1/d) and hydrolysis ( $k_{hy}$ , 1/d) in the surface soil column layer, and anaerobic bio-degradation ( $k_{an}$ , 1/d) and hydrolysis in all subsurface layers of the wastepile.
- # The first-order loss rate due to wind and other surface activities ( $k_{wd}$ , 1/d) is applied to the surface soil column layer only and is calculated each year as an annual average with consideration of losses due to wind erosion, vehicular activity, spreading/compacting operations from an active wastepile, and wind erosion only from an inactive wastepile. Appendix A outlines the estimation procedures for annual average  $k_{wd}$ .
- # For purposes of runoff and erosion processes, the following assumptions apply:
  - ▶ The wastepile is conceptualized as having side slopes (from which increased runoff and erosion would occur) that are insignificant in terms of surface area in comparison to the top surface of the wastepile.
  - ▶ The top surface of the wastepile has the same slope as the average slope of the local watershed.



- ▶ No run-on to the wastepile subarea from upslope subareas in the local watershed occurs.
  - ▶ Following removal of the wastepile, there is no subsequent runoff/erosion transport pathway from the wastepile subarea of the local watershed downslope to the surface water, only from the buffer subarea. That is, there is assumed to be no remaining contamination in the subarea that contained the wastepile. The only remaining contamination is in the buffer. This is an implicit assumption imposed by the modeling boundary between the WP and Vadose Modules. The WP Module considers the soil surface to be its lower boundary for the WP subarea. However, for the downslope, buffer subarea, a surficial soil layer is modeled (see Figure 3-5). Once the WP has been removed at the end of its operating life, the WP subarea effectively ceases to be part of the local watershed, because there is no residual contamination (from the perspective of the WP Module). Any such residual contamination is in the underlying vadose zone, which is modeled by the Vadose Module and which does not have the runoff/erosion pathway functionality. The “missing” chemical in the WP subarea post-removal does not imply a mass balance error between the WP and Vadose Modules, however. That chemical is being simulated in the Vadose Module, only no surface water pathway is considered.
- # The annual average infiltration rate ( $I$ , m/d) is determined using the method described in section 3.2.4 (note that  $I$  is the same as  $I_N$  in section 3.2.4) with consideration of the properties of the waste only.
- # As described in Section 3.4, the topmost soil column layer in the GSCM developed for the wastepile serves as the soil compartment in the watershed/soil column algorithm (see Figure 3-3). For the purposes of applying the watershed/soil column algorithm, it is assumed that the appropriate depth for the soil column surface layer ( $dz$ ) is 0.01 m. To achieve computational savings, yet provide the spatial resolution in the wastepile surface that is required by the watershed/soil column algorithm, the wastepile is subdivided into two homogeneous zones with identical properties, but different layer thicknesses ( $dz$ ). The upper wastepile zone consists of the top 0.1 m of the wastepile and uses  $dz = 0.01$  m. The lower wastepile zone has a thickness equal to  $(h - 0.1)$  m, and  $dz$  is determined in the code as a function of  $(h - 0.1)$ , a limit on the maximum number of layers equal to 100, and an initial value for  $dz = 0.01$  m. (For example, if  $h = 5$  m, the upper zone consists of 10 x 0.01 m soil column layers; the lower zone consists of 98 x 0.05 m cells).

Within each homogeneous zone, the solutions can be obtained in the manner described in Section 2.4. The method used to propagate the material (numerically) across the boundary dividing the two zones is as follows. At the boundary between two zones, contaminant mass from layers in the upstream (higher) zone will be considered to diffuse into the uppermost layer of the downstream (lower) zone. A counter-diffusion of material from all the layers in the

downstream zone to the bottom layer of the upstream zone will also take place. All of the material in the bottom layer of the upstream zone will be carried into the top layer of the downstream zone after one convection-based time step in the upstream zone.

### 3.7.3 Initial Conditions

The simulation starts immediately following placement of the initial wastepile on clean soil. The same initial conditions are reestablished each time the wastepile is refreshed. For  $t < y_{op} * 365$ :

$$C_T \Big|_{z,t=j \cdot t_{bet}; j=0,1,2,\dots} = C'_{T,w} \cdot r_{b,w} \cdot f_{wmu} \quad (3-57)$$

where  $C'_{T,w}$  ( $\mu\text{g/g}$ ) is the mass-based contaminant concentration in the HWIR99 waste of concern and  $f_{wmu}$  is the fraction of the HWIR99 waste of concern in waste disposed of in the wastepile.

## 3.8 Land Application Unit

### 3.8.1 Introduction

Section 3.4 presented the Local Watershed/Soil Column Module as common to both the wastepile and the LAU. This section discusses LAU-specific issues in implementation. Figure 3-6 illustrates the LAU in the local watershed conceptual module.

### 3.8.2 Additional Assumptions

- # Waste is applied to the soil surface periodically at even intervals (e.g., quarterly) and then tilled into the top layer of soil to a depth of  $z_{till}$  (m).
- # Till zone ( $z = 0$  to  $z_{till}$ ) is completely mixed upon each application of waste to soil.
- # The modeled soil column consists of one homogeneous zone, the till zone, consisting of a soil/waste mixture. The till zone properties ( $\rho_{b,till}$ ,  $f_{oc,till}$ ) can be estimated as the depth-weighted average of the soil ( $\rho_{b,s}$ ,  $f_{oc,s}$ ) and waste properties ( $\rho_{b,w}$ ,  $f_{oc,w}$ ) according to the depth of soil ( $d_s$ , m) and waste ( $d_w$ , m) in the till zone. To illustrate, an example using  $\rho_b$  is presented below.

$$\rho_{b,till} = \rho_{b,s} \frac{d_s}{z_{till}} + \rho_{b,w} \frac{d_w}{z_{till}} \quad (3-58)$$

$$d_s = z_{till} - d_w \quad (3-59)$$

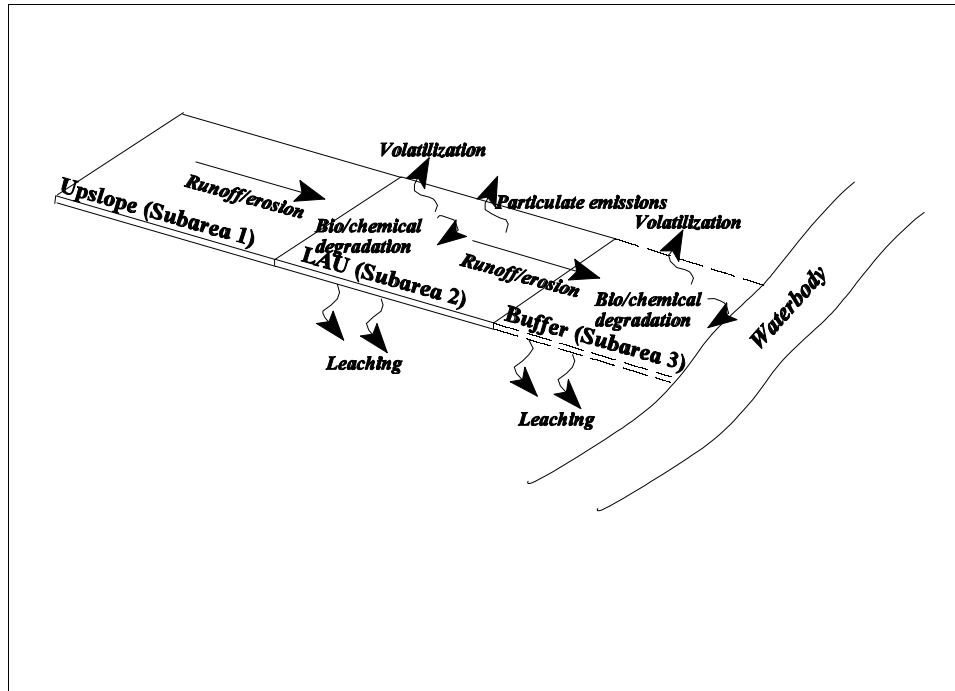


Figure 3-6. Illustration of LAU in local watershed.

where  $W$  is the wet waste mass loading for a single application, determined as

$$d_w = \frac{W}{\rho_{b,w}} \quad (3-60)$$

$$W = \frac{R_{appl} \cdot sd/100}{N_{appl}} \quad (3-61)$$

where  $R_{appl}$  is the wet waste application rate ( $\text{Mg}/\text{m}^2\text{-y}$ ),  $sd$  is the weight percent solids in the waste,  $N_{appl}$  is the number of waste applications per year,  $\rho_{b,s}$  ( $\text{g}/\text{cm}^3$ ) is the dry bulk density of the soil estimated from  $\eta_s$  using Equation (3-63), and  $\rho_{b,w}$  ( $\text{g}/\text{cm}^3$ ) is the dry bulk density.

# The water added to the LAU contained in the wet waste increases the annual average infiltration rate ( $I$ ) by:

$$+ \frac{R_{appl} (1 - sd/100)}{365 \rho_{H_2O}} \quad (3-62)$$

- # The contaminant mass is concentrated in the solids portion of the waste and is re-partitioned among the solid, aqueous, and gas phases in the soil column.
- # The waste added to the till zone does not significantly affect the hydraulic properties of the till zone. Thus, the hydraulic properties of the soil ( $K_{sat}$ ,  $SM_b$ ) are used in Equation 2-11 to determine the water content of the till zone. Although the waste may affect the hydraulic properties of the till zone, there is no way of determining this effect theoretically.
- # Total porosity of the till zone ( $\eta_{till}$ ) is estimated using the following relationship for porous media (Freeze and Cherry, 1979):

$$h = 1 - \frac{r_b}{2.65} \quad (3-63)$$

- # Waste applications do not result in significant buildup of the soil surface, nor does erosion significantly degrade the soil surface (i.e., the distance from the site surface ( $z = 0$ ) to a fixed point below the surface is constant). As a result, there is no naturally occurring limit to the modeled  $C_T$  other than the limit for NAPLs. In other words, the modeled contaminant concentration in the till zone could exceed the contaminant concentration in the waste. Indeed, this is physically possible for highly immobile constituents if the waste matrix is organic and decomposes, leaving behind the constituent to concentrate over multiple applications.
- # The land application unit is operated for  $y_{op}$  years.
- # The first-order chemical and biological loss processes in the till zone include aerobic biodegradation ( $k_{ae}$ , 1/d) and hydrolysis ( $k_{hy}$ , 1/d).
- # The first-order loss rate due to wind erosion and other surface disturbances ( $k_{wd}$ , 1/d) is applied to the surface layer of the till zone only and is calculated each year as an annual average with consideration of losses from an active LAU due to wind erosion, vehicular activity on the surface of the LAU, and tilling operations. The particulate emission loss rate from an inactive LAU includes wind erosion only. Appendix A outlines the estimation procedures for  $k_{wd}$ .
- # The annual average infiltration rate ( $I$ , m/d) is determined using the method described in Section 3.2.4 (note that  $I$  is the same as  $IN$  in Section 3.2.4) with consideration of the properties of the till zone only.
- # As described in Section 3.4, the topmost soil column layer in the GSCM developed for the LAU serves as the soil compartment in the watershed/soil column algorithm (see Figure 3-3). For the purposes of applying the watershed/soil column algorithm, it is assumed that the appropriate depth for the soil column

surface layer (dz) is 0.01 m. In the LAU module, dz = 0.01 m is used for the entire till zone.

### 3.8.3 Initial Conditions

The simulation starts immediately following the first application of waste, at which time the till zone is well-mixed. Initial conditions are

$$C_T|_{z,t=0} = \frac{W \cdot C'_{T,w} \cdot f_{wmu}}{z_{till}} \quad (3-64)$$

where  $C'_{T,w}$  is the initial total contaminant concentration in the dry waste, calculated by dividing the total mass-based concentration in the wet waste (input by the user as Cw in FRAMES or CTPwaste in the LAU code) by sd/100.

During the operating lifetime of the LAU ( $t \leq 365y_{op}$ ), with each application of waste the initial condition in the till zone is reset to account for the contaminant mass added as well as any contaminant mass remaining in the till zone from previous applications.

$$C_T|_{z,t=j \cdot t_{bet}} = \frac{W \cdot C'_{T,w} \cdot f_{wmu}}{z_{till}} + \bar{C}_T^z(z_{till}, j \cdot t_{bet}) \quad (3-65)$$

where j is the waste application counter index = 1,2,3...,  $C_T^z(z,t)$  (g/m<sup>3</sup>) is the depth-weighted average total contaminant concentration at time t averaged over a depth of z, and  $t_{bet}$  is the time between applications:

$$t_{bet} = \frac{365}{N_{appl}} \quad (3-66)$$

## 4.0 Landfill Module

### 4.1 Introduction

The landfill module was developed to approximate the effects of the gradual filling of active landfills. The landfill is divided into equal-volume vertical cells running from the site surface to the bottom of the landfill, each sized so that they require 1 year to fill. Waste mass is added gradually, forming layers of waste. After 1 year, the cell is full and the waste is covered with a clean soil cover (optional). Then the next cell begins to full, and so on until the landfill reaches maximum capacity. The landfill module is computationally efficient because only a single cell is simulated and results are stored. Results for the landfill as a whole are then obtained by aggregating stored results for a single cell to account for the time that each cell in the landfill came on-line. For example, the results for the landfill at the end of year 3 account for the fact that the first cell is at year 3 in the single cell simulation, the second cell filled is at year 2, and the third, at year 1.

### 4.2 Additional Assumptions

- # Landfill (empty) can be approximated as an excavated volumetric rectangle. Since it is assumed to be below grade, it is also assumed that no contaminant mass is lost due to runoff and erosion. (The runoff curve number parameter, CN, is set to approximately 0 to ensure no runoff.)
- # Landfill waste, cover, and subsoil (or liner) below are divided into vertical cells running from the site surface ( $z = 0$ ) to the bottom of the subsoil zone at  $z = z_s + z_w + z_c$  where  $z_s$ ,  $z_w$ , and  $z_c$  are the thicknesses of the subsoil, waste, and cover soil zones.
- # Each landfill cell can be approximated as a soil column consisting of three homogeneous zones, as shown in Figure 4-1: soil cover, landfill waste, and subsoil. Each zone can be approximated as having homogeneous porous media whose properties are uniform in space and time within the zone but may differ between zones. The soil cover zone and subsoil zones are optional. The subsoil zone can be treated as the unsaturated zone or as a landfill liner layer with properties consistent with those of a homogeneous porous media (i.e., impermeable liners are not considered). (Note: As of this writing, it has been decided for HWIR99 purposes that no liner shall be included in the Landfill module.)

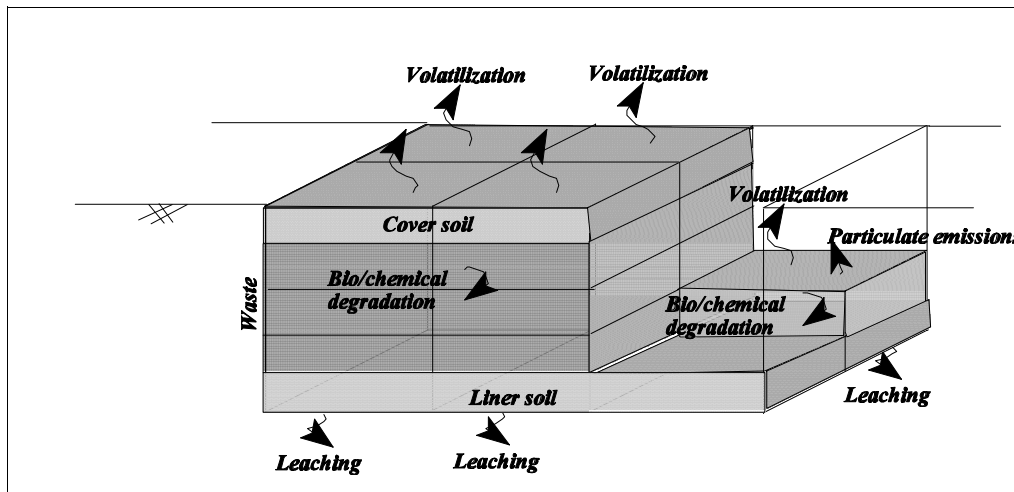


Figure 4-1. Illustration of landfill with six cells and three waste layers.

- # It takes 1 year (365 days) to fill a landfill cell. The area of a landfill cell ( $A_{cell}$ ,  $m^2$ ) is calculated as follows:

$$A_{cell} = \frac{L'}{z_w \cdot \rho_{b,w}} \quad (4-1)$$

where  $L'$  (Mg/yr) is the dry bulk waste mass loading rate adjusted for losses during the process of unloading waste as in Equation 3-59, and  $\rho_{b,w}$  ( $g/cm^3$ ) is the dry bulk density of waste. The number of full cells is determined by:

$$N_{cell} = \left[ \frac{A}{A_{cell}} \right]_{truncate} \quad (4-2)$$

where  $A$  ( $m^2$ ) is the area of the landfill.

- # It is assumed that a fractional cell would contribute little to the total mass flux rates. Therefore, the landfill area used in the simulation is ( $N_{cell} \times A_{cell}$ ).
- # Landfill cells are filled sequentially.
- # Incoming HWIR99 waste is at constant contaminant concentration ( $C'_{T,w}$ ,  $\mu g/g$ ) and added at a constant rate ( $L$ , Mg/yr).  $C'_{T,w}$  can be adjusted by  $f_{wmu}$  to indicate

that the waste entering the landfill consists also of other wastes not containing the contaminant of interest.

- # There is no transport laterally between cells.
- # Waste is added to the landfill cell in layers. A waste layer, for the purposes of the module, is simply a zone wherein initial concentrations are assumed uniform. Waste layers are conceptualized as being formed over time by the dumping of loads (e.g., via dump truck) of waste next to one another in the LF cell until eventually a waste layer of uniform depth is formed. At this point, a new layer is started. The time required to lay down a layer ( $t_{ly}$ , d) is simply  $365/N_{ly}$  where  $N_{ly}$  is the user-specified number of waste layers in a landfill cell. The depth of a waste layer ( $d_{ly}$ , m) is determined by  $(z_w/N_{ly})$ .
- # At the start of the landfill cell simulation, one waste layer is assumed present. After each time period,  $t_{ly}$ , another waste layer is laid down until there are  $N_{ly}$  waste layers and the landfill cell is full. At this time, it is optionally covered with clean soil.
- # The first-order chemical and biological loss processes in the entire landfill including cover soil, waste, and liner material include anaerobic biodegradation ( $k_{an}$ , 1/d) and hydrolysis ( $k_{hy}$ , 1/d).
- # The first-order loss rate due to wind erosion and other surface disturbances ( $k_{wd}$ , 1/d) is calculated with consideration of losses due to wind erosion, vehicular activity, and spreading and compacting from an active landfill cell and with consideration of losses due to wind erosion only from an inactive landfill cell. Appendix A outlines the estimation procedures for  $k_{wd}$ .
- # The annual average infiltration rate ( $I$ , m/d) is determined using the method described in Section 3.2.4 (note that  $I$  is the same as  $IN$  in Section 3.2.4) with consideration of the properties of the landfill waste only.  $I$  is assumed unaffected by the possible existence of cover and liner soil (i.e., cover and subsoil are permeable).
- # The long-term annual average of the infiltration rate and meteorological parameters used in the calculation of the  $k_{wd}$  (e.g., windspeed) are determined from the respective time series of annual averages, and the scalar long-term averages are used in the simulation. This results in significant computational savings. With constant infiltration rate and  $k_{wd}$  each year, the annual time series results for all the landfill cells are the same relative to the time they began filling. As described below, this allows simulation results for a single landfill cell to be stored and aggregated to get results for the landfill as a whole. It obviates the need to simulate each landfill cell individually.



- # The thickness of the “soil column” layers ( $dz$ ) in each homogeneous zone (cover soil, waste, and subsoil) in a landfill cell are determined in the code as a function of zone thickness, a limit on the maximum number of “soil column” layers of 100, and an initial value for  $dz = 0.01$  m.

### 4.3 Landfill Cell Simulation—First Year

In each filled cell there are three distinct zones, the optional soil cover, the waste zone, and the optional subsoil zone, where the  $z$  axis is considered fixed with  $z=0$  at the landfill surface (i.e., the cover soil surface, if it exists, or the filled waste zone surface). During the first year, there is no cover soil zone. There is a subsoil zone and a growing waste zone. By the end of the first year, the waste zone is full. The location of the upper boundary is moving as waste layers are added. An alternative  $z$ -dimension,  $z''$ , is defined to identify the position of the upper boundary relative to the  $z$ -axis where  $z''=0$  at  $z = z_c + (N_{ly} - i) d_{ly}$ , where  $i=1,2,\dots,N_{ly}$ , the total number of waste layers. The location  $z$  can be determined from  $z = z'' + z_c + (N_{ly} - i) d_{ly}$ .

#### 4.3.1 Boundary Conditions

**4.3.1.1 Upper and Lower Boundaries.** A boundary condition of  $C_T=0$  is applied at the surface of the waste. At the lower boundary (the bottom of the waste zone or subsoil zone, if a subsoil zone exists), the user-specified boundary condition multiplier (bcm) can be used to specify the boundary condition as discussed in Section 2.4.

**4.3.1.2 Inner Waste/Subsoil Boundary.** At the inner waste/subsoil boundary, under the assumption that the sorptive capacity of the subsoil has been exhausted and that partitioning is no longer applicable, a boundary condition where the aqueous-phase contaminant concentration gradient is zero ( $dC_L/dz = 0$ ) should be applied to ensure that dissolved concentrations cannot increase across the subsoil. Such an increase could occur if mass is allowed to diffuse into the subsoil from the waste zone. Since diffusive flux occurs in the aqueous and gas phases only,  $dC_L/dz = 0$  implies no diffusive flux across this boundary. This boundary condition is approximated in the landfill module by: (1) setting the boundary condition equal to  $dC_T/dz=0$  at the bottom of the waste zone, which prevents diffusive flux from waste to subsoil, and (2) modeling only advection and decay in the subsoil zone.

With use of these approximations, the existence of a subsoil zone simply shifts the leachate flux profile by the amount of time required for the contaminant to travel from the top to the bottom of the subsoil zone. The delay can be calculated in years using  $(z_s K_{TL,s}/I/365)$  where  $z_s$  (m) is the subsoil zone thickness,  $K_{TL,s}$  is the dimensionless total/aqueous phase partition coefficient in the subsoil, and  $I$  (m/d) is the long-term average infiltration rate. In addition, with long delays, if the first-order chemical and biological decay rate (determined from  $k_{an} + k_{by}$ ) is substantial, the peak leachate flux rate will be reduced due to decay in the subsoil zone.

#### 4.3.2 Initial Conditions

At  $t = 0$ , the waste zone has one waste layer at initial concentration and the subsoil zone is clean:

$$C_T|_{z'',t=0} = \begin{cases} C'_{TW} \cdot r_{b,w} \cdot f_{wmu} & 0 < z'' \leq d_{ly} \\ 0 & d_{ly} < z'' \leq d_{ly} + z_s \end{cases} \quad (4-3)$$

With the addition of subsequent waste layers at  $t = i \times t_{ly}$ , where  $i$  is the number of layers, the surface of the waste zone shifts up. Initial concentration in the new waste layer is established by the bulk waste concentration, and initial concentration in the remainder of the waste zone as well as the subsoil zone are the modeled concentrations, reassigned to reflect the  $d_{ly}$  increment in waste zone size and the update to  $z''$ .

$$C_T|_{z'',t=i \cdot t_{ly}, i=1,2,\dots,N_{ly}-1} = \begin{cases} C'_{TW} \cdot r_{b,w} \cdot f_{wmu} & 0 < z'' \leq d_{ly} \\ C_T(z'' - d_{ly}, i \cdot t_{ly}) & d_{ly} < z'' \leq i \cdot d_{ly} + z_s \end{cases} \quad (4-4)$$

## 4.4 Landfill Cell Simulation — After First Year

At the start of the second year, the waste zone is full and the optional cover soil is added.

### 4.4.1 Boundary Conditions

**4.4.1.1 Upper and Lower Boundaries.** A boundary condition of  $C_T=0$  is applied at the surface of the waste (or cover soil, if it exists). At the lower boundary (the bottom of the waste zone or subsoil zone, if a subsoil zone exists), the user-specified boundary condition multiplier (bcm) can be used to specify the boundary condition as discussed in Section 2.4.

**4.4.1.2 Inner Waste/Subsoil Boundary.** The waste/subsoil boundary is treated the same as for the first year (see Section 4.3.1).

**4.4.1.3 Inner Cover Soil/Waste Boundary.** To be rigorous, at the inner cover soil/waste boundary, a boundary condition should be applied where the sums of the advective and diffusive fluxes on either side of the boundary are equal. However, using the current solution technique, it is not possible to implement such a rigorous boundary condition. As an approximation, at the bottom of the cover soil zone, a no diffusive flux ( $dC_T/dz = 0$ ) boundary condition is applied. At the top of the waste zone, a zero concentration ( $C_T = 0$ ) boundary condition is applied. The diffusive flux from the waste into the cover soil zone is added to the bottom-most soil column layer in the cover soil zone.

This set of boundary conditions allows diffusive transfer of contaminant mass from the waste to the cover soil. Conversely, advective, but not diffusive, transfer of contaminant mass from the cover soil to the waste zone is allowed. Use of these conditions would tend to overestimate contaminant mass losses from the waste zone into the cover soil zone and overestimate the volatile emissions.

## 4.4.2 Initial Conditions

The landfill cell is full and optionally covered. The  $z$  dimension and final  $z''$  dimension are related by  $z'' = z - z_c$ . The initial conditions reflect a clean soil cover and the waste and subsoil zone concentrations are modeled concentrations that have been reassigned to reflect the updated  $z$  dimension as follows:

$$C_T|_{z,t=365} = \begin{cases} 0 & 0 < z \leq z_c \\ C_T(z - z_c, t) & z_c < z \leq z_s \end{cases} \quad (4-5)$$

## 4.5 Calculation of Landfill Results

The results for the landfill as a whole are obtained by aggregating the results for the landfill cell with consideration of the year that each cell came on line. Fluxes are averaged over the whole landfill area, even when the landfill is not yet full. Soil concentrations are averaged over the filled cells only.

## 4.6 Implementation Algorithm

### 4.6.1 Overview

An overview of the algorithm implementing the Landfill module is provided in Figure 4-2. As for the local watershed modules, a variable ( $fadv$ ) is used to track the fraction of mass in the bottom soil column layer that would have convected each computational time step. (For example, if the computational time step is half of a year and the convection-based time step is 2 years, a convection event will occur every 4 computational time steps. At the end of each computational time step,  $fadv$  will be incremented by 0.25). A convection event will occur when  $fadv$  is equal to 1 and, when it does,  $fadv$  is reset to zero. At the end of the simulation ( $year = NyrMax$ ), if  $fadv$  is greater than zero,  $M_{lcha}$  is incremented by  $fadv$  times  $dz$  times  $C_T$  in the lowest layer and  $C_T$  in the lowest layer is adjusted accordingly to conserve mass. Leachate flux for the final year is then calculated using Equation 2-31. Thus, even if the convection-based time step in years is greater than  $NyrMax$ , a leachate flux will be generated in the final year.

### 4.6.2 Simulation-Stopping Criteria

As with the LAU/WP implementation, the single landfill cell simulation is stopped when the contaminant mass in the landfill cell is significantly depleted as defined by the TermFrac input parameter. At the end of the year in which the contaminant mass in the landfill cell is less than or equal to TermFrac times the maximum contaminant mass in the cell, the simulation is stopped. (Unless the NyrMax parameter is reached first, at which point the simulation is automatically stopped.) The maximum contaminant mass in the cell is assumed to occur at the end of the first year when the landfill cell is full and no further contaminant mass will be added to that cell. (Note: As of this writing, the NyrMax computer memory constraint corresponding to 200 years discussed previously also applies to the LF.)

### 4.6.3 Leachate Flux Processing

As for the Local Watershed/Soil Column Modules, a leachate flux postprocessing algorithm for the landfill was developed to account for the fact that leaching occurs gradually over the time between convective events. The algorithm developed for the landfill differs from that developed for the local watershed modules to take advantage of the fact that in the landfill cell, convective events occur at regular intervals since a constant, long-term average infiltration rate is used every year (versus the variable annual average infiltration rate used in the local watershed modules).

During the landfill cell simulation, if the convection-based time step in the waste zone is greater than 1 year, each time a convection event occurs, the mass leached is distributed back over the appropriate number of years.

(Note: As of this writing, the leachate flux processing algorithm is applicable only when there is no subsoil zone as currently planned for HWIR99. The algorithm has not yet been adapted to allow a subsoil zone.)

### 4.6.4 End-of-Simulation Mass Balance Check

An end-of-simulation mass balance check is performed on the entire landfill results using procedure similar to that described for the Local Watershed/Soil Column Modules (see Section 3.5.4). The difference is that, in the landfill module, the system includes the landfill (and associated cover and subsoil zones, if present). There are no buffer subareas since the local watershed is not modeled. Therefore the term  $fM_{lost}$  in Equation 3-57 includes only the first four variables listed in Table 3-2.

Time series outputs to the various other HWIR99 modules are reported as follows:

- # *Outputs to Air Module.* All annual time series outputs to the Air Module are reported up to and including the last year that there is nonzero VE or CE. Thus, the annual time series outputs to the Air Module are all the same length. After this, all outputs to the Air Module will be zero and are not reported.
- # *Outputs to Vadose Module.* The annual time series of LeachFlux is reported up to and including the last year that there is a nonzero LeachFlux. AnnInfil is reported from year 1 to the last year that meteorological data are available.
- # *Outputs to Exposure Modules (Human and Ecological).* The annual time series of CTda is reported to the last year of nonzero CTda. The same is true for CTss.

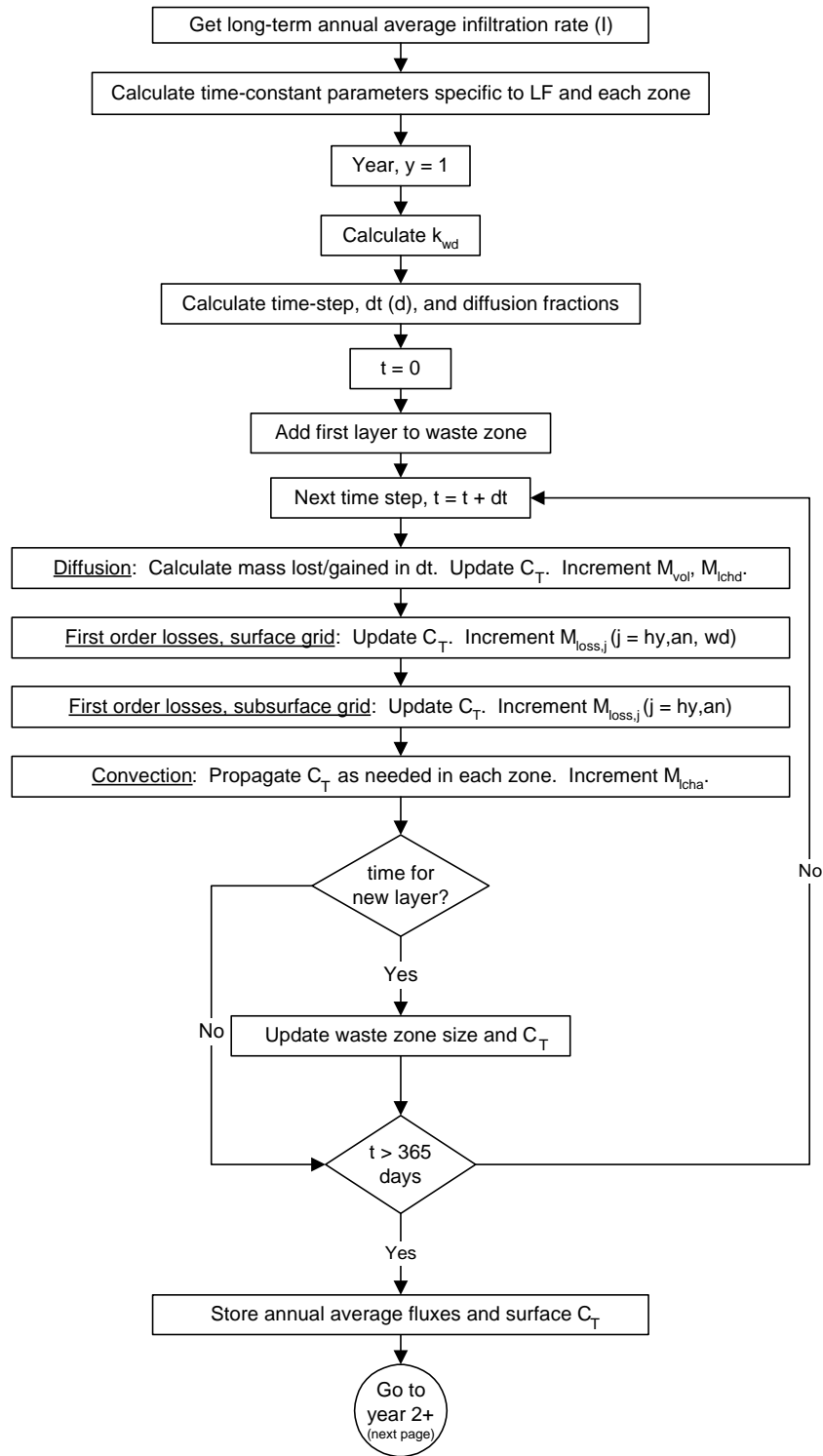


Figure 4-2a. Landfill module flowchart for an active cell (year 1).

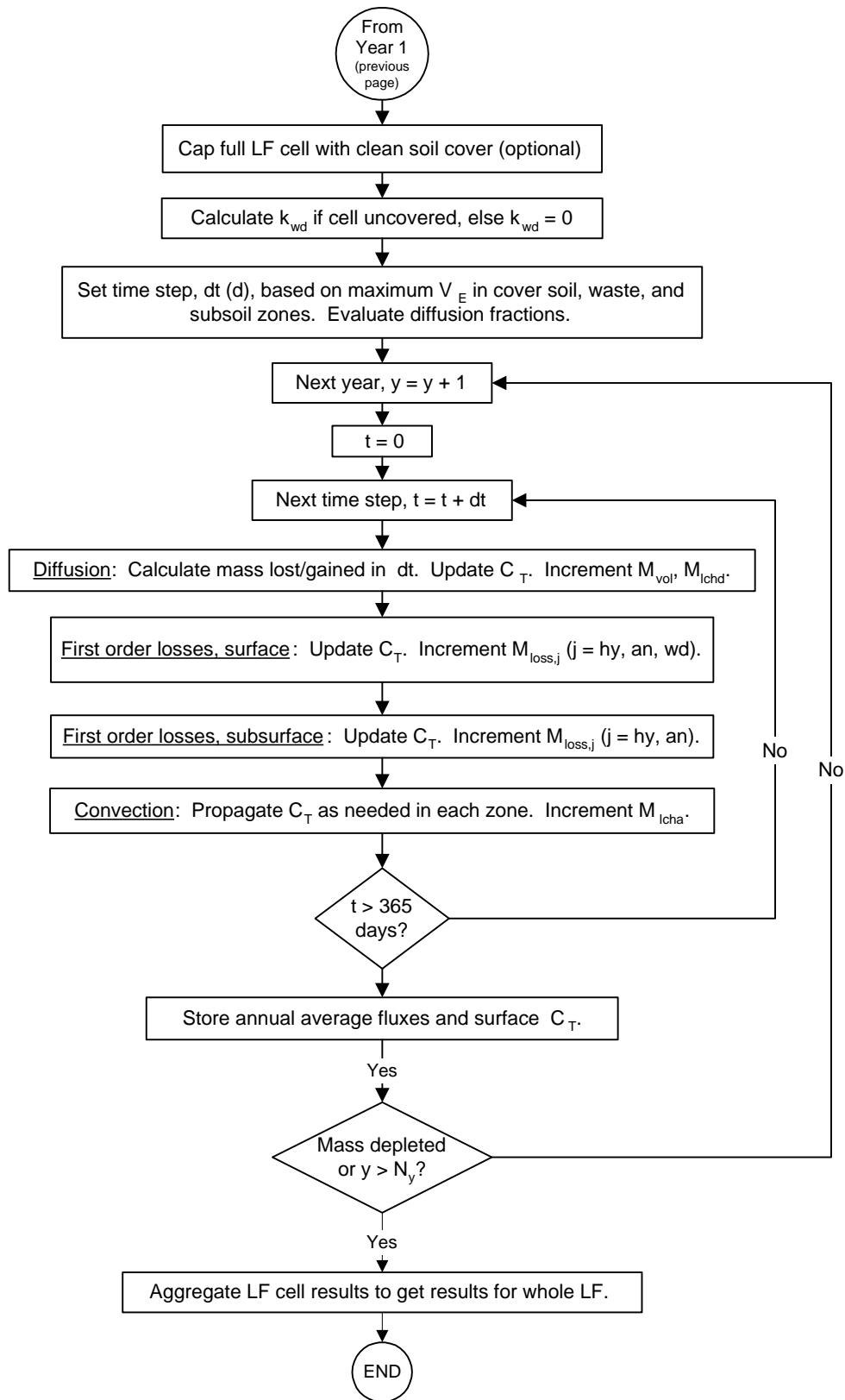


Figure 4-2b. The landfill module flowchart for a closed cell (year 2+).

## 4.7 Output Summary

Table 4-1 summarizes the outputs of the Landfill Module.

**Table 4-1. Output Summary for the LF Module**

Variable Name <sup>a</sup>			
Documentation	Code	Definition	Units
I	AnnInfil	Leachate infiltration rate (annual avg., WMU subarea(s) only)	m/d
J <sub>vol</sub>	VE	Volatile emission rate	g/m <sup>2</sup> /d
	VEYR	Year associated with output	Year
	VENY	Number of years in outputs	Unitless
CE30	CE	Constituent mass emission rate-PM <sub>30</sub>	g/m <sup>2</sup> /d
	CEYR	Year associated with output	Year
	CENY	Number of years in outputs	Unitless
E30	PE30	Eroded solids mass emission rate-PM <sub>30</sub>	g/m <sup>2</sup> /d
	PE30YR	Year associated with output	Year
	PE30NY	Number of years in outputs	Unitless
pmf	PMF	Particulate emission particle size distribution	Mass frac.
	PMFYR	Year associated with output	Year
	PMFNY	Number of years in outputs	Unitless
J <sub>ich</sub>	LeachFlux	Leachate contaminant flux	g/m <sup>2</sup> /d
	LeachFluxYR	Year associated with output	Year
	LeachFluxNY	Number of years in outputs	Unitless
C <sub>T</sub>	CTss	Soil concentration in surface soil layer	µg/g
	CTssYR	Year associated with output	Year
	CTssNY	Number of years in outputs	Unitless
C <sub>T</sub>	CTda	Depth-weighted average soil concentration (from zava to zavb)	µg/g
	CTdaYR	Year associated with output	Year
	CTdaNY	Number of years in outputs	Unitless
	SrcSoil	Flag for soil presence (true)	Logical
	SrcOvl	Flag for overland flow presence (false)	Logical
	SrcLeachMet	Flag for leachate presence when leachate is met-driven (true)	Logical
	SrcLeachSrc	Flag for leachate presence when leachate is not met-driven (false)	Logical
	SrcVE	Flag for volatile emissions presence (true)	Logical
	SrcCE	Flag for chemical sorbed to particulates emissions presence (true)	Logical
SrcH2O	Flag for surface water presence for eco-exposure (false)	Logical	
	NyrMet	Number of years in the available met record	Unitless

<sup>a</sup> Where the variable name is used in the code but not in the documentation, the first column is left blank.

## 5.0 References

- Abramowitz, M. and I. A. Stegun (eds.). 1970. *Handbook of Mathematical Functions*. Dover Publications, Inc., New York, NY.
- Chow, Ven Te, David R. Maidment, and Larry W. Mays. 1988. *Applied Hydrology*. McGraw-Hill, Inc., New York, NY.
- Clapp, R.B., and G.M. Hornberger. 1978. Empirical equations for some soil hydraulic properties. *Water Resources Research*, 14: 601-605.
- Cowherd, C., G. E. Muleski, P. J. Englehart, and D. A. Gillette. 1985. *Rapid Assessment of Exposure to Particulate Emissions from Surface Contamination Sites*. EPA/600/8-85/002. U.S. Environmental Protection Agency, Office of Research and Development, Office of Health and Environmental Assessment, Washington, DC. February.
- Duffie, John A., and William A. Beckman. 1980. *Solar Engineering of Thermal Processes*. John Wiley & Sons, Inc., New York, NY.
- Dunne, Thomas, and Luna B. Leopold. 1978. *Water in Environmental Planning*. W.H. Freeman and Company, New York.
- Freeze, R. Allan, and John A. Cherry. 1979. *Groundwater*. Prentice-Hall, Inc., Englewood Cliffs, NJ.
- Jensen, M.E., R.D. Burman, and R.G. Allen. 1990. Evapotranspiration and irrigation water requirements. *ASCE Manual* 70:332.
- Jost, W. 1960. *Diffusion in Solids, Liquids, Gases*. Academic Press, Inc., New York, NY. Third Printing (with Addendum).
- Jury, W. A., W. F. Spencer, and W. J. Farmer. 1983. Behavior assessment model for trace organics in soil: I. Model description. *Journal of Environmental Quality*, 12(4):558-564. October.
- Jury, William A., David Russo, Gary Streile, and Hesham El Abd. 1990. Evaluation of volatilization by organic chemicals residing below the soil surface. *Water Resources Research*, 26(1):13-20. January.



- Lightle, D. T. and Glenn Weesies. 1998. Default slope parameters. Memorandum to Scott Guthrie (RTI) from D. T. Lightle and Glenn Weesies (USDA, Natural Resources Conservation Service), West Lafayette, IN. June 8.
- Millington, R. J., and J. P. Quirk. 1961. Permeability of porous solids. *Transactions of the Faraday Society*, 57(7):1200-1207. July.
- Monteith, J. L. 1965. Evaporation and Environment. In: *Syposia of the Society for Experimental Biology: Number XIX*. pp. 205-234, Academic Press, Inc., Publishers, New York, NY.
- Richardson, C. W., G. R. Foster, and D. A. Wright. 1983. Estimation of erosion index from daily rainfall amount. *Transactions of the ASAE*, 26(1):153-156.
- Shan, Chao, and Daniel B. Stephens. 1995. An analytical solution for vertical transport of volatile chemicals in the vadose zone. *Journal of Contaminant Hydrology*, 18:259-277.
- Shen, Hsieh Wen, and Pierre Y. Julien. 1993. Chapter 12: Erosion and sediment transport. In: *Handbook of Hydrology*, David R. Maidment (ed.). McGraw-Hill, Inc., New York, NY. pp. 12-12.
- Shuttleworth, W. James. 1993. Chapter 4: Evaporation. In: *Handbook of Hydrology*, David R. Maidment (ed.). McGraw-Hill, Inc., New York, NY. pp. 4-4.
- Thomann, Robert V., and John A. Mueller. 1987. *Principles of Surface Water Quality Modeling and Control*. Harper & Row, Publishers, Inc., New York, NY.
- USDA (Department of Agriculture). 1986. *Urban Hydrology for Small Watersheds*. TR-55. U.S. Department of Agriculture, Engineering Division, Soil Conservation Service, Washington, DC. pp. 2-5. June.
- U.S. EPA (Environmental Protection Agency). 1985a. *Compilation of Air Pollutant Emission Factors. Volume I: Stationary Point and Area Sources (Fourth Edition)*. AP-42. U.S. Environmental Protection Agency, Office of Air and Radiation and Office of Air Quality Planning and Standards, Research Triangle Park, NC. September.
- U.S. EPA (Environmental Protection Agency). 1985b. *Water Quality Assessment. A Screening Procedure for Toxic and Conventional Pollutants in Surface and Ground Water-Part I*. (Revised). EPA/600/6-85/002a. Office of Research and Development, Environmental Research Laboratory, Athens, GA. September.
- U.S. EPA (Environmental Protection Agency). 1999a. *Data Collection for the Hazardous Waste Identification Rule. Section 5. Watershed and Waterbody Layout*. U.S. Environmental Protection Agency, October.

- U.S. EPA (Environmental Protection Agency). 1999b. *Data Collection for the Hazardous Waste Identification Rule. Section 6. Surface Water Data*. U.S. Environmental Protection Agency, October.
- Vanoni, Vito A. (ed.). 1975. *Sedimentation Engineering*. American Society of Civil Engineers, New York, NY.
- Williams, Jimmy R. 1975. Sediment-yield prediction with universal equation using runoff energy factor. In: *Present and Prospective Technology for Predicting Sediment Yields and Sources*. ARS-S-40, 1972, U.S. Department of Agriculture, Washington, DC.
- Wischmeier, W. H., and D. D. Smith. 1978. Predicting rainfall erosion losses. A guide to conservation planning. In: *Agricultural Handbook*. 537 Edition. U.S. Department of Agriculture, Washington, DC.



## **Appendix A**

### **Symbols, Units, and Definitions**



## Appendix A

### Symbols, Units, and Definitions

(Symbols listed in Tables in Appendix A, Particulate Emission Equations are not repeated here.)

**Table A-1. Symbols, Units, and Definitions**

Symbol	Units	Definition
$\eta_j$	---	total porosity where j is a subscript indicating waste, w; waste/soil mixture in the till zone, till; and soil, s.
$\eta$	---	total porosity
$\theta_a$	---	soil volumetric air content
$\theta_{a,j}$	---	soil volumetric air content where j is a subscript indicating waste, w; waste/soil mixture in the till zone, till; and soil, s.
$\theta_w$	---	soil volumetric water content
$\theta_{w,j}$	---	soil volumetric water content where j is a subscript indicating waste, w; waste/soil mixture in the till zone, till; and soil, s.
$\rho_b$	g/cm <sup>3</sup>	soil dry bulk density. Same as m2. (Note: g/cm <sup>3</sup> = Mg/m <sup>3</sup> )
$\rho_{b,j}$	g/cm <sup>3</sup>	dry bulk density where j is a subscript indicating waste, w; waste/soil mixture in the till zone, till; and soil, s.
$\rho_{b,w}^{\text{wet}}$	g/cm <sup>3</sup>	wet bulk density of LAU waste
$A$	m <sup>2</sup>	area of WMU
$A_{\text{cell}}$	m <sup>2</sup>	surficial area of vertical landfill cell
$a_i$	1/d	calculated parameter (equation 3.4.2-3b) for subarea i
$bcm$	---	lower coil column boundary condition multiplier

(continued)

Table A-1. (continued)

Symbol	Units	Definition
$b_i$	1/d	calculated parameter (equation 3.4.2-3c) for subarea i
$C'_T$	$\mu\text{g/g}$	total mass-based contaminant concentration in dry soil
$C'_{T,W}$	$\mu\text{g/g}$	total mass-based contaminant concentration in incoming dry waste
$C_{2,i}$	$\text{g/m}^3$	contaminant concentration in surface soil grid space in subarea i (equivalent to $C_T$ )
$C_G$	$\text{g/m}^3$	contaminant concentration in gaseous phase in soil
$C_L$	$\text{g/m}^3$	contaminant concentration in aqueous phase in soil
$C_L^{sol}$	$\text{g/m}^3$	contaminant aqueous solubility
$CN$	unitless	SCS runoff module Curve Number parameter
$C_S$	$\mu\text{g/g}$	contaminant concentration in adsorbed phase in soil
$CSL_{i,t}$	kg	cumulative soil load leaving subarea i, day t
$C_T$	$\text{g/m}^3$	total volume-based contaminant concentration in soil
$C_{T0}$	$\text{g/m}^3$	initial total volume-based contaminant concentration in soil
$d_{1,i}$	$\text{m}^3/\text{d}$	calculated parameter (equation 3.4.2-5b) for subarea i
$d_{2,i}$	$\text{m}^3/\text{d}$	calculated parameter (equation 3.4.2-5c) for subarea i
$D_a$	$\text{cm}^2/\text{s}$	diffusivity in air
$D_E$	$\text{m}^2/\text{d}$	effective diffusivity in soil
$D_{E,a}$	$\text{m}^2/\text{d}$	effective diffusivity in soil air
$D_{E,w}$	$\text{m}^2/\text{d}$	effective diffusivity in soil water
$Df$	---	fraction of original mass in soil column grid space that diffuses past a boundary in time, t.
$Df_0$	---	fraction of original mass in soil column grid space that remains after time, t.
$d_{ly}$	m	thickness of one LF waste layer in LF cell
$DRZ$	cm	depth of the root zone
$d_s$	m	thickness of soil in unmixed LAU till zone
$dt$	d	length of time step in GSCM solution algorithm
$d_w$	m	thickness of waste in unmixed LAU till zone

(continued)

Table A-1. (continued)

Symbol	Units	Definition
$D_w$	cm <sup>2</sup> /s	diffusivity in water
$dz$	m	soil column grid size in GSCM solution algorithm
$ER_i$	unitless	erosion chemical enrichment ratio for subarea i
$ET_{i,t}$	cm/day	evapotranspiration from root zone on day t for subarea i
$FC_i$	cm	soil moisture field capacity for subarea i
$foc$	---	organic carbon fraction in soil
$foc_j$	---	organic carbon fraction where j is a subscript indicating waste, w; waste/soil mixture in the till zone, till; and soil, s.
$fwmu$	---	fraction of HWIR99 waste of concern disposed in WMU
$h$	m	height of wastepile
$H'$	---	dimensionless Henry's Law constant
$I$	m/d	average annual water infiltration rate
$IN_{i,t}$	cm/day	daily infiltration for subarea i, day t
$J_{lch}$	g/m <sup>2</sup> /d	annual average leachate flux at lower soil column boundary
$J_{vol}$	g/m <sup>2</sup> /d	annual average volatilization flux at upper soil column boundary
$k$	1/d	total first-order loss rate
$k_{bu,i}$	m/d	first order rate constant due to burial/erosion for subarea i
$K_d$	cm <sup>3</sup> /g	soil-water partition coefficient
$k_j$	1/d	annual average first order loss rate due to process j, where j indicates hydrolysis, h; aerobic biodegradation, ae; anaerobic biodegradation, an; storm events in subarea i, ev,i; and wind/mechanical activity, wd.
$K_{oc}$	cm <sup>3</sup> /g	equilibrium partition coefficient normalized to organic carbon
$K_{sat}$	cm/hr	saturated hydraulic conductivity
$K_{TL}$	---	equilibrium distribution coefficient between the total (g/m <sup>3</sup> ) and aqueous phase (g/m <sup>3</sup> ) contaminant concentrations in soil
$L$	Mg/yr	bulk waste mass loading rate into WMU
$ld_{i-1}$	g/m <sup>3</sup> /d	run-on load to subarea i from subarea i-1
$L'$	Mg/yr	bulk waste loading rate adjusted for mass losses due to unloading

(continued)



Table A-1. (continued)

Symbol	Units	Definition
$mI_i$	g/m <sup>3</sup>	suspended solids concentration in runoff water, subarea i
$m$	g/m <sup>2</sup>	total amount of material from soil column grid space that has passed a boundary at time, t
$M_{col1}$	g/m <sup>2</sup>	total mass in soil column at start of year
$M_{col2}$	g/m <sup>2</sup>	total mass in soil column at end of year
$M_i$	g/m <sup>2</sup>	annual contaminant mass loss due to process i, where i is a subscript indicating: # total diffusive loss at the surface, 0; # gas phase diffusive losses (volatilization) at the surface, vol; # aqueous phase leaching due to diffusion, lchd; # aqueous phase leaching due to advection, lcha; # first order loss process j where j is as defined in k <sub>j</sub> .
$M_{add}$	g/m <sup>2</sup>	annual mass added to soil column
$M_{rem}$	g/m <sup>2</sup>	annual mass removed from soil column
$N_{appl}$	1/y	number of LAU applications per year
$N_{cell}$	--	total number of annual cells in a LF
$N_{dz}$	---	total number of grid spaces of depth dz in soil column
$N_{ly}$	---	assumed number of waste layers in LF cell
$PET_i$	cm/day	potential evapotranspiration for day t
$P_t$	cm	total precipitation on day t
$Q_{i,t}$	m <sup>3</sup> /day	runoff flow volume (water only) leaving subarea i, day t
$Q'_{i,t}$	m <sup>3</sup> /day	total runoff flow volume (including solids) leaving subarea i, day t
$R_{appl}$	Mg/m <sup>2</sup> -y	LAU waste application rate
$Sd$	unitless	sediment delivery ratio for subarea/watershed i
$RO_{i,t}$	cm	stormwater runoff depth leaving subarea i, day t
$sd$	w/w, %	weight percent of solids in raw waste applied to LAU
$SM_b$	---	unitless soil-specific exponent in equation (2.3-1)
$SM_{i,t}$	cm	soil moisture in root zone at end of day t for subarea i
$t$	d	time since start of simulation

(continued)

Table A-1. (continued)

Symbol	Units	Definition
$t_{bet}$	d	time between WP refresh or LAU waste application
$t_{ly}$	d	time required to lay down one layer in LF cell
$vb_i$	m/d	burial/erosion velocity for subarea i
$vd_i$	m/d	diffusive exchange velocity between runoff and surficial soil
$vr_i$	m/d	stormwater runoff resuspension velocity for subarea i
$C_T^z$	g/m <sup>3</sup>	depth-weighted average $C_T$ at time, t
$V_E$	m/d	effective solute velocity in soil
$W$	Mg/m <sup>2</sup>	average mass of waste added per LAU application
$WP_i$	cm	soil moisture wilting point for subarea i
$Y_{op}$	yr	last year of operation of LAU or WP
$z$	m	distance down from soil surface
$z_c$	m	thickness of LF cover soil
$z_s$	m	thickness of LF subsoil or liner
$z_{sc}$	m	total depth of soil column
$z_{till}$	m	distance from soil surface to bottom of LAU till (mixing) zone
$z_w$	m	total thickness of LF waste zone (at capacity)



## Appendix B

### Determination $H'$ , $D_a$ , and $D_w$ for Organic Compounds



## Appendix B

# Determination $H'$ , $D_a$ , and $D_w$ for Organic Compounds and Outputs

### B.1 Introduction

For organic compounds, the dimensionless Henry's law coefficient ( $H'$ ) and air and water diffusivities ( $D_a$  and  $D_w$ ,  $\text{cm}^2/\text{s}$ , respectively) are calculated as a function of system temperature given user-input reference values and temperatures.  $H'$  is determined from the dimensionless Henry's Law Coefficient ( $H^r$ ) at temperature  $T_{H^r}$  (K).  $D_a$  and  $D_w$  are determined from air ( $D_a^r$ ) and water ( $D_w^r$ ) diffusivities ( $\text{cm}^2/\text{s}$ ) at temperature  $t_D$  ( $^\circ\text{C}$ ). The methodologies used are described in this Appendix. Here, the convention is used where  $T$  is temperature in Kelvin and  $t$  is temperature in degrees centigrade.

### B.2 Air Diffusivity ( $D_a$ )

The reference air diffusivity ( $D_a^r$ ) is adjusted using the following equation which was derived from the Fuller, Schettler, and Giddings (FSG) Method for estimating air diffusivities of organic compounds in Lyman et al. (1990, Eq. 17-12):

$$D_a = D_a^r \left[ \frac{T}{T_D^r} \right]^{1.75} \quad (\text{B.2-1})$$

In the module,  $D_a$  is converted from  $\text{cm}^2/\text{s}$  to  $\text{m}^2/\text{d}$  by multiplying by 8.64.

### B.3 Water Diffusivity ( $D_w$ )

The reference water diffusivity ( $D_w^r$ ) is adjusted using the following equation which was derived from the Hayduk and Laudie Method for estimating water diffusivities of organic compounds in Lyman et al. (1990, Eq. 17-24):

$$D_w = \frac{\eta_w(t_D^r)}{\eta_w(t)} D_w^r \quad (\text{B.3-1})$$

where  $\eta_w$  (cp) is the viscosity of water as a function of temperature,  $t$ , in degrees centigrade,  $t^r$  is the temperature for which  $D_w^r$  was specified. Values for  $\eta_w$  are provided in the program and were obtained from Lyman et al. (1990, Table 17-7) for  $t=0$  to  $30^\circ\text{C}$  in one degree increments. In the module,  $D_w$  is converted from  $\text{cm}^2/\text{s}$  to  $\text{m}^2/\text{d}$  by multiplying by 8.64.

#### B.4 Dimensionless Henry's Law Coefficient ( $H'$ )

The algorithm used to adjust the dimensionless Henry's law coefficient,  $H'$ , as a function of temperature,  $T$ , is based on the Clausius-Clayperon equation and consideration of temperature effects on solubility (Dzombak et al., 1993) and is presented below:

$$H' = H'^r \cdot \exp \left[ \frac{\Delta H_v(T_H^r)}{R T_H^r} - \frac{\Delta H_v(T)}{R T} \right] \quad (\text{B.4-1})$$

where  $H'^r$  is the dimensionless Henry's law coefficient at reference temperature  $T_{H^r}$  (K),  $R$  is the gas constant (1.9872 cal/mol-K), and  $\Delta H_v(T)$  (cal/mol) is the molar heat of vaporization as a function of temperature  $T$  (K).  $\Delta H_v(T)$  is estimated using Eq. 13-21 and Table 13-7 in Lyman et al. (1990):

$$\Delta H_v = \Delta H_{vB} \left[ \frac{1-T/T_c}{1-T_b/T_c} \right]^n \quad (\text{B.4-2a})$$

where

$$n = \begin{cases} 0.30 & \frac{T_b}{T_c} < 0.57 \\ 0.74 \left( \frac{T_b}{T_c} \right) - 0.116 & 0.57 \leq \frac{T_b}{T_c} \leq 0.71 \\ 0.41 & \frac{T_b}{T_c} > 0.71 \end{cases} \quad (\text{B.4-2b})$$

where  $T_c$  (K) is the critical temperature and  $T_b$  (K) is the boiling point of the compound of interest  $\Delta H_{VB}$  (cal/mol) is the molar heat of vaporization at the normal boiling point and is estimated using the method of Haggmacher (Lyman et al., 1990, Section 13-5):

$$\Delta H_{VB} = \frac{2.303 B R T_b^2 (z_g - z_l)}{(t_b + C)^2} \quad (\text{B.4-3a})$$

where

$$z_g - z_l = \sqrt{1 - \frac{1/P_c}{(T_b/T_c)^3}} \quad (\text{B.4-3b})$$

where  $T_c$  (K) is the critical temperature,  $P_c$  (atm) is the critical pressure,  $B$  ( $^{\circ}\text{C}$  or K) and  $C$  ( $^{\circ}\text{C}$ ) are Antoine's constants. Antoine's constants have been calculated for many compounds, especially hydrocarbons, and are tabulated in the literature (e.g., Reid et al., 1977). Some caution is required in specifying values for the Antoine's constants, because in some tabulations, the conversion factor to natural log (2.303) is included in the value of  $B$ . To check, if the value for methane is 405.42 ( $^{\circ}\text{C}$  or K) use the values for  $B$  directly. If it is about 930 ( $^{\circ}\text{C}$  or K), divide all values given for  $B$  by 2.303. Also, if Antoine's constants are presented in the literature in K,  $B$  should not be changed and  $C$  should be converted to  $^{\circ}\text{C}$  by adding 273.2. Note that this is not the usual way to convert from K to  $^{\circ}\text{C}$ , but is necessary to maintain the constancy of the term  $B/(t+C)$  in Antoine's relationship since temperature,  $t$ , is assumed to be in  $^{\circ}\text{C}$ .

In the code, if  $T_c$  is unavailable,  $T_c$  is estimated as  $1.5T_b$  (Lyman et al., 1990, p. 14-13). If  $P_c$  is unavailable, but  $B$  and  $C$  are available,  $(z_g - z_l)$  is approximated as one (Lyman et al., 1990, Table 14-6). If  $B$  and  $C$  are unavailable, Trouton's rule is used to estimate  $\Delta H_{VB}$  (Lyman et al. (1990):

$$\Delta H_{VB} = 21 \frac{\text{cal}}{\text{mole-K}} T_b \quad (\text{B.4-4})$$



## B.5 References

- Dzombak, D. A., Fang, H., and Roy, S. B. (1993). ASDC: A microcomputer-based program for air stripper design and costing (CE Report No. 92-204). Department of Civil Engineering, Carnegie Mellon University, Pittsburgh, PA.
- Lyman, W. J., Reehl, W. F., and Rosenblatt, D. H. (1990). Handbook of Chemical Property Estimation Methods . Washington, DC: American Chemical Society.
- Reid, R. C., & Sherwood, T. K. (1977). The Properties of Liquids and Gases, 3rd Ed. New York: McGraw-Hill Book Co.

## Appendix C

### Particulate Emission Equations



## Appendix C

### Particulate Emission Equations

#### C.1 Introduction

The nonwastewater source modules have been designed to provide estimates of the annual average, area-normalized emission rate of contaminant mass adsorbed to particulate matter less than 30  $\mu\text{m}$  in diameter,  $\text{CE}_{30}$  (g of contaminant/ $\text{m}^2/\text{d}$ ), as well as annual average particle size distribution information in the form of the mass fractions of the total particulate emissions in four aerodynamic particle size categories—30 to 15  $\mu\text{m}$ , 15 to 10  $\mu\text{m}$ , 10 to 2.5  $\mu\text{m}$ , and <2.5  $\mu\text{m}$ .

A variety of release mechanisms are considered. The inventory of release mechanisms considered is different for each WMU, but includes, in general, wind erosion, vehicular activity, unloading operations, tilling, and spreading/compacting operations. The mechanisms considered for each WMU are summarized in Table C-1.

This appendix describes the algorithms and assumptions used to estimate annually for each mechanism of release:

- #  $\text{E}_{30_i}$  (g of particulates  $\leq 30 \mu\text{m}$  in diameter/ $\text{m}^2/\text{d}$ ), the annual average  $\text{PM}_{30}$  emission rate due to release mechanism  $i$ , where mechanisms of release considered for each WMU are summarized in Table C-1
- # Particle size range mass fractions, the mass fractions of  $\text{E}_{30_i}$  in the aerodynamic particle size categories identified above.

For each WMU:

- #  $\Sigma \text{E}_{30_i}$  (g/ $\text{m}^2/\text{d}$ ), the total annual average  $\text{PM}_{30}$  emission rate due to all release mechanisms
- # Annual average particle size range mass fractions of the total annual average  $\text{PM}_{30}$  emission rate

**Table C-1. Summary of Mechanisms of Release of Particulate Emissions for Each WMU**

Mechanism of Release	E30 <sub>i</sub> Subscript	WMU Type <sup>a,b</sup>						Algorithm Reference
		LAU		LF cell <sup>c</sup>		WP		
		Active	Inact.	Active	Inact. <sup>d</sup>	Active	Inact.	
Wind erosion from open area	wd	X	X	X	X			Cowherd et al. (1985)
Wind erosion from wastepile	wp					X	X	U.S. EPA (1985)
Vehicular activity	ve	X		X		X		U.S. EPA (1995)
Unloading	un			X		X		U.S. EPA (1995)
Spreading/compacting or tilling	sc	X		X		X		U.S. EPA (1985)

<sup>a</sup> X = Mechanism of release is considered in modeling the WMU.

<sup>b</sup> Active = Operating WMU.

Inact. = Inactive WMU where no additional contaminant mass is being added.

<sup>c</sup> For a description of how results for whole LF are obtained from LF cell results, see Section 4.5.

<sup>d</sup> Inactive (full) and uncovered landfill cell. Assume no emissions from a covered LF cell.

# CE30 (g/m<sup>2</sup>/d), the annual average emission rate of contaminant as PM<sub>30</sub>

# Annual average first-order loss rate from the soil surface due to contaminant mass losses caused by particulate emissions, k<sub>wd</sub> (1/d).

## C.2 Particulate Emission Rate (E30<sub>i</sub>) Algorithms and Particle Size Range Mass Fractions

### C.2.1 Wind Erosion from Open Fields (E30<sub>wd</sub>)

The algorithm for the estimation of PM<sub>30</sub> emissions due to wind erosion from an open field is based on the procedure developed by Cowherd et al. (1985). It was adapted for implementation in a computer code and is presented in detail here. E30<sub>wd</sub> is estimated in the LAU and LF source emission modules. The user-specified input parameters are summarized in Table C-2.

To account for the fact that active and inactive WMUs can differ in the degree of vegetation ( $\text{veg}$ ), surface roughness height ( $z_0$ ), and frequency of disturbances per month ( $\text{fd}$ ), different values are assigned to these parameters in the equations presented below according to whether the WMU is active or inactive. The value assignments are summarized in Table C-3 where  $\text{veg}$ ,  $z_0$ , and  $\text{fd}$  are user input values.

**Table C-2. Input Parameter Units and Definitions for E30<sub>wd</sub>**

Symbol	Units	Definition
<i>asdm</i>	mm	Mode of the aggregate size distribution
<i>Lc</i>	---	Ratio of the silhouette area of roughness elements too large to be included in sieving to total base area
<i>veg</i>	---	Fraction of surface covered with vegetation (inactive WMU)
<i>z<sub>0</sub></i>	cm	Surface roughness height (inactive WMU)
<i>S</i>	w/w, %	Silt content of surface material
<i>U<sup>+</sup></i>	m/s	Observed or probable fastest mile of wind between disturbances
<i>PE</i>	---	Thornthwaite Precipitation Evaporation Index
<i>u</i>	m/s	Mean annual windspeed
<i>p</i>	d/yr	Mean number of days per year with ≥0.01 in precipitation
<i>fd</i>	1/mo	Frequency of disturbance per month where a disturbance is defined as an action that exposes fresh surface material (inactive WMU)

**Table C-3. Active/Inactive WMU Assignments for *veg'*, *z'<sub>0</sub>*, *fd'***

Symbol	Units	Active WMU	Inactive WMU
<i>veg'</i>	---	0.0	<i>veg</i>
<i>z'<sub>0</sub></i>	cm	1.0	<i>z<sub>0</sub></i>
<i>fd'</i>	1/mo	<i>fd</i>	0.0

**Step 1: Calculate  $U_{*t}$** 

Calculate the threshold friction velocity,  $U_{*t}$  (m/s), the threshold windspeed for the onset of wind erosion:

$$U_{*t} = 0.650 \cdot cf \cdot (asdm)^{0.425} \quad (C-1a)$$

where

$$cf = \begin{cases} 1.0 & Lc < 2 \times 10^{-4} \\ 1.05 + 50.18Lc - 647.89Lc^2 + 6863.50Lc^3 & 2 \times 10^{-4} \leq Lc \leq 1 \times 10^{-1} \end{cases} \quad (C-1b)$$

Table C-2 provides definitions of  $asdm$  and  $Lc$ .  $Lc$  is measured by inspection of a representative 1-m<sup>2</sup> transect of the site surface.  $Lc$  can range from zero to 0.1. High  $Lc$  ( $\geq 2 \times 10^{-4}$ ) increases the threshold friction velocity, which results in a relatively low or zero particulate emission rate due to wind erosion. Low  $Lc$  ( $< 2 \times 10^{-4}$ ) is indicative of a bare surface with homogeneous finely divided material (e.g., an agricultural field). Such surfaces have a relatively low threshold friction velocity and increased particulate emissions. Equations (C-1a) and (C-1b) were derived from Cowherd et al. (1985, Figures 3-4 and 3-5).

### Step 2: Calculate $U_t$

$U_t$  (m/s) is the threshold wind velocity at a height of 7.0 m (7.0 m is the typical weather station anemometer height). It is calculated using Cowherd et al. (1985, Equation, 4-3, with  $z = 700$  cm):

$$U_t = \frac{U_{*t}}{0.4} \ln \left( \frac{700}{z'_0} \right) \quad z'_0 < 700 \quad (C-2)$$

where  $z'_0$  is the roughness height in cm. Values for  $z'_0$  for various surface conditions are provided in Cowherd et al. (1985, Figure 3-6).

### Step 3: Calculate $E_{30_{wd}}$

$E_{30_{wd}}$  is the annual average emission rate of particulate matter less than 30  $\mu\text{m}$  in diameter per unit area of the contaminated surface. Note that the methodology developed in Cowherd et al. (1985) was developed for estimation of emission rate of particulate matter less than 10  $\mu\text{m}$  (or  $E_{10_{wd}}$ ).  $E_{30_{wd}}$  can be approximated from  $E_{10_{wd}}$  with knowledge of the ratio between  $PM_{30}$  and  $PM_{10}$  for wind erosion. Cowherd (1998) advises that a good first approximation of this ratio is provided by the particle size multiplier information presented in U.S. EPA (1995) for wind erosion from open fields where  $PM_{30}/PM_{10}$  is equal to 2. Therefore, a factor of 2 has been incorporated into Cowherd et al.'s (1985) equations for  $E_{10_{wd}}$  to allow estimation of  $E_{30_{wd}}$ .

For sites with limited erosion potential ( $U_{*t} > 0.75$  m/s)

The following equation was derived by using Cowherd et al. (1985, Equations 4-1 to 4-3), applying a factor of 2 as discussed above and converting units to  $\text{g}/\text{m}^2/\text{d}$  :

$$E30_{wd} = \begin{cases} \frac{11.12(U^+ - U_t)(1 - veg)fd' \cdot 24}{(PE/50)^2 \cdot 10^3} & U^+ \geq U_t \\ 0 & U^+ < U_t \end{cases} \quad (C-3)$$

Data for mean annual  $U^+$  and PE for locations throughout the United States can be found in climatic atlases (e.g., U.S. Department of Commerce, 1968) and Cowherd et al. (1985, Figure 4-2), respectively. Cowherd et al. (1985) advise that, in the worst case,  $fd$  should be assumed to be 30 per month.

For sites with unlimited erosion potential ( $U_{*t} \leq 0.75$  m/s)

When  $U_{*t}$  is less than 0.75 m/s, the site is considered to have unlimited erosion potential and  $E30_{wd}$  is calculated using Cowherd et al. (1985, Equation 4-4) with a factor of 2 applied as discussed above.

$$E30_{wd} = 0.072 (1 - veg) \left( \frac{u}{U_t} \right)^3 g(x) \cdot 24 \frac{h}{d} \quad (C-4a)$$

where

$$x = 0.886 \frac{U_t}{u} \quad (C-4b)$$

$$g(x) = \begin{cases} 1.91 & 0 \leq x < 0.5 \\ 2.2 - 0.6x & 0.5 \leq x \leq 1.0 \\ 2.9 - 1.3x & 1.0 < x \leq 2.0 \\ 0.18 (8x^3 + 12x) \exp(-x^2) & x > 2.0 \end{cases} \quad (C-4c)$$

where  $g(x)$  was derived from Cowherd et al. (1985, Figure 4-3). Data for  $u$  for locations throughout the United States can be found in climatic atlases (e.g., U.S. Department of Commerce, 1968).

#### Step 4: Apply Particle Size Range Mass Fractions

Particle size range mass fractions allow estimation of the fraction of the  $PM_{30}$  emitted that is in specific size fractions. As mentioned above, Cowherd (1998) suggests using the particle



size multipliers provided for wind erosion from industrial fields in U.S. EPA (1995). The U.S. EPA (1995) distribution was adapted to get the fraction of the emissions in the designated size categories as presented in Table C-4.

**Table C-4. Aerodynamic Particle Size Range Mass Fractions for E30<sub>wd</sub> and E30<sub>wp</sub>**

30 μm -15 μm	15 μm -10 μm	10 μm -2.5 μm	≤2.5 μm
0.4	0.10	0.3	0.2

### C.2.2 Wind Erosion from Wastepiles (E30<sub>wp</sub>)

The equation used in the WP module to estimate E30<sub>wp</sub> (g/m<sup>2</sup>/d), the annual average PM<sub>30</sub> emission rate per unit area of contaminated surface due to wind erosion, is an adaptation of the empirical equation developed for total suspended particulate matter (TSP) (kg/d/hta) from active sand and gravel wastepiles in U.S. EPA (1985, referred to here as AP42; see Equation 3, p. 11.2.3-5). (TSP is defined as what is measured by a high-volume sampler, and the effective cutoff commonly assigned to standard high-volume samplers is 30 μm [U.S. EPA, 1985]. Here, units are converted to g/m<sup>2</sup>/d and a dust control efficiency factor, *eff<sub>dust</sub>*, is added.

$$E30_{wp} = 1.9 \left( \frac{S_w}{1.5} \right) \left( \frac{365 - p}{235} \right) \left( \frac{fw}{15} \right) \cdot (1 - eff_{dust}) \frac{10^3 \text{ g}}{\text{kg}} \cdot \frac{\text{ha}}{10^4 \text{ m}^2} \quad (\text{C-5})$$

Parameter definitions are provided in Table C-5. It should be noted that a more recent version of AP42 (U.S. EPA, 1995) recommends the use of an event-based algorithm for estimating wind emissions from a wastepile. The updated algorithm was evaluated for use in HWIR99, but it was determined that it requires detailed site-specific information unavailable in the HWIR99 analysis. It should be noted that the algorithm used here will tend to overestimate emissions relative to the event-based algorithm (Meyers, 1998).

The particle size range mass fractions for E30<sub>wp</sub> are provided in Table C-4. These are the particle size multipliers provided in U.S. EPA for wind erosion from open industrial area. Cowherd (1998) suggests that it is an appropriate first approximation to use the same particle size multipliers for E30<sub>wp</sub> here, but cautions that the mass fraction in the ≤2.5 category is likely to be an overestimate.

**Table C-5. Parameter Units and Definitions for E30<sub>wp</sub>**

Symbol	Units	Definition
$S_w$	w/w, %	Silt content of waste <sup>a</sup>
$p$	d/yr	Mean number of days per year with 0.01 in. precipitation
$fw$	%	Mean annual percentage of time that unobstructed windspeed exceeds 5.4 m/s (12 mph) at mean pile height
$eff_{dust}$	---	Dust suppression control efficiency (0, no control; 1, total control)

<sup>a</sup> Silt is defined as particles less than 75  $\mu\text{m}$  in diameter. Silt content is determined by the percent of loose dry surface material that passes through a 200-mesh screen using the ASTM-C-136 method (U.S. EPA, 1985).

### C2.3 Vehicular Activity (E30<sub>ve</sub>)

To estimate E30<sub>ve</sub> (g/m<sup>2</sup>/d), the quantity of particulate emissions from vehicular travel on the surface of the WMU, the following equation was used:

$$E30_{ve} = 1.36 \left( \frac{S}{12} \right) \left( \frac{vs}{48} \right) \left( \frac{vw}{2.7} \right)^{0.7} \left( \frac{nw}{4} \right)^{0.5} \left( \frac{365-p}{365} \right) \cdot nv \cdot (1 - eff_{dust}) \cdot \frac{mt}{A} \quad (\text{C-6})$$

where parameter definitions are provided in Table C-6. Equation A-6 was derived from an empirical equation presented in U.S. EPA (1995; Equation 1, p. 13.2.2-1) for the kilograms of size-specific particulate emissions emitted per vehicle kilometer traveled on unpaved roads. (In this application, the EPA parameter “fraction of waste on unpaved roads” is one since travel is on the surface of the WMU.) The first six terms of Equation C-6 are equivalent to the U.S. EPA (1995) equation after application of the 0.80 particle size multiplier for PM<sub>30</sub>. EPA's equation has been adapted here to provide emissions normalized to the contaminated surface area and to account for the control of emissions with a dust control efficiency factor of  $eff_{dust}$ .

The particle size multipliers for E30<sub>ve</sub> are presented in Table C-7. These have been adapted for the size categories of interest in the HWIR99 analysis from the particle size multiplier information presented in U.S. EPA (1995).

**Table C-6. Parameter Units and Definitions for E30<sub>ve</sub>**

Symbol	Units	Definition
<i>S</i>	w/w,%	Silt content of roadway (4.3-20) <sup>a, b</sup>
<i>vs</i>	km/h	Mean vehicle speed (21-64)
<i>vw</i>	Mg	Mean vehicle weight (2.7-142)
<i>nw</i>	—	Mean number of wheels per vehicle (4-13)
<i>nv</i>	1/d	Mean annual number of vehicles per day
<i>eff<sub>dust</sub></i>	—	Dust suppression control efficiency
<i>A</i>	m <sup>2</sup>	Contaminated surface area
<i>mt</i>	m	Meters traveled per vehicle ( <i>nv</i> ) on contaminated surface
<i>p</i>	d/y	Mean number of days per year with 0.01 in precipitation

<sup>a</sup> Silt is defined as particles less than 75 μm in diameter. Silt content is determined by the percent of loose dry surface material that passes through a 200-mesh screen using the ASTM-C-136 method (U.S. EPA, 1985).

<sup>b</sup> Values in parentheses are the ranges of source conditions that were tested in developing the U.S. EPA (1995, Equation 1, p. 13.2.1-1).

**Table C-7. Aerodynamic Particle Size Range Mass Fractions for E30<sub>ve</sub>**

30 μm -15 μm	15 μm -10 μm	10 μm -2.5 μm	≤2.5 μm
0.38	0.17	0.33	0.12

#### C.2.4 Unloading Operations (E30<sub>un</sub>)

The equation for estimating E30<sub>un</sub> (g/m<sup>2</sup>/d), the PM<sub>30</sub> emission rate due to unloading operations at wastepiles and landfills, was adapted from U.S. EPA. (1995, Equation 1, p. 13.2.4-3). The EPA equation was adapted by multiplying it by the average annual loading rate (*L*, Mg/yr), normalizing the emissions for the contaminated surface area, and applying the particle size multiplier for <30 μm.

$$E30_{un} = (0.0012) \cdot \left( \frac{u}{2.2} \right)^{1.3} \cdot \frac{L}{A} \cdot \frac{10^3 \text{ g}}{\text{kg}} \cdot \frac{\text{yr}}{365 \text{ d}} \quad (\text{C-7})$$

Parameter definitions are provided in Table C-8. The particle size range mass fractions were developed from information provided in U.S. EPA (1995) and are presented in Table C-9.

**Table C-8. Parameter Units and Definitions for E30<sub>un</sub>**

Symbol	Units	Definition
<i>u</i>	m/s	Mean annual wind speed (0.6-6.7)
<i>mcW</i>	volume %	Waste moisture content (0.25-4.8)
<i>L</i>	Mg/yr	Annual average waste loading rate

Note: Values in parentheses are the ranges of source conditions that were tested in developing the U.S. EPA (1995) equation.

**Table C-9. Aerodynamic Particle Size Range Mass Fractions for E30<sub>un</sub>**

30 μm -15 μm	15 μm -10 μm	10 μm -2.5 μm	≤2.5 μm
0.35	0.18	0.32	0.15

### C.2.5 Spreading/Compacting or Tilling Operations (E30<sub>sc</sub>)

As in HWIR95, the equation for estimating E30<sub>sc</sub> (g/m<sup>2</sup>/d), the rate of PM<sub>30</sub> emissions due to spreading and compacting or tilling operations, was adapted from an equation in U.S. EPA (1985, Equation 1, p. 11.2.2-1) that was developed for estimating emissions due to agricultural tilling in units of kilogram of particulate emissions per hectare per tilling (or spreading/compacting) event. The first two terms in Equation C-8 represent the EPA equation with the particle size multiplier for <30 μm applied.

$$E30_{sc} = (1.77) S^{0.6} N_{op} \cdot \frac{10^3 \text{ g}}{\text{kg}} \cdot \frac{\text{ha}}{10^4 \text{ m}^2} \quad (\text{C-8})$$

Parameter definitions are provided in Table C-10. The particle size range mass fractions were developed from information provided in U.S. EPA (1985) and are presented in Table C-11.

### C.3 Particle Size Range Mass Fractions for Total PM<sub>30</sub> Emission Rate

Particle size range mass fractions characterizing the total annual average PM<sub>30</sub> emission rate (E30<sub>i</sub> summed over all applicable mechanisms) is determined annually by applying the mechanism-specific mass fractions to the E30<sub>i</sub> estimates to obtain size-specific emission rate

**Table C-10. Parameter Units and Definitions for E30<sub>sc</sub>**

Symbol	Units	Definition
<i>S</i>	w/w, %	Silt content of surface material (1.7-88) <sup>a, b</sup>
<i>N<sub>op</sub></i> <sup>c</sup>	1/d	Number of tilling (or spreading and compacting) operations per day
<i>fcult</i>	---	Number of cultivations per application

<sup>a</sup> Silt is defined as particles less than 75 µm in diameter. Silt content is determined by the percent of loose dry surface material that passes through a 200-mesh screen using the ASTM-C-136 method (U.S. EPA, 1985).

<sup>b</sup> Values in parentheses are the ranges of source conditions that were tested in developing the U.S. EPA (1985) equation.

<sup>c</sup> For the LAU,  $N_{op} = (N_{appl}/365 \times fcult)$ .

**Table C-11. Aerodynamic Particle Size Range Mass Fractions for E30<sub>sc</sub>**

30 µm -15 µm	15 µm -10 µm	10 µm -2.5 µm	≤2.5 µm
0.24	0.12	0.34	0.30

estimates  $E_{i,j}$  (g/m<sup>2</sup>/d) where subscript *j* identifies the particle size range (*j*= 1 indicates 30-15 µm; 2, 15-10 µm; 3, 10-2.5 µm; and 4, <2.5 µm). The total particle size range mass fraction,  $pmf_j$ , is calculated as:

$$pmf_j = \frac{\sum_i E_{i,j}}{\sum_i E30_i} \quad (A-9)$$

#### C.4 Annual Average Constituent Emission Rate (CE30) Equations

The amount of mass lost due to wind and mechanical disturbances,  $M_{loss,wd}$  (g/m<sup>2</sup>), estimated using Equation 2-24 and accumulated throughout the simulated year is used to estimate CE30 (g/m<sup>2</sup>/d), the annual average, area-normalized emission rate of contaminant mass adsorbed to particulate matter less than 30 µm in diameter.

$$CE30 = \frac{M_{loss,wd}}{365} \quad (A-10)$$

Equation A-10 is directly applicable to the LAU during both the inactive and active years, the WP during the inactive years, and the inactive (full) LF cell. For the first year of the LF cell and the active years of the WP, the raw waste losses due to particulate emissions during unloading waste are added to the CE30 estimate. The increment is equal to

$$+ E30_{un} \cdot C'_{T,W} \cdot f_{wmu} \cdot 10^{-6} \frac{g}{\mu g} \quad (A-11)$$

### C.5 Estimation of First Order Loss Rate ( $k_{wd}$ )

An equation for  $k_{wd}$  was derived by performing a mass balance on the surface layer of the “soil” column to a depth of  $dz$  (the depth of the surface soil column cell) and considering losses due to wind and mechanical activity only:

$$\frac{\partial C_T}{\partial t} = -k_{wd} C_T \quad (A-12)$$

where:

$$k_{wd} = \frac{1}{dz} \cdot \frac{K_d}{K_{TL}} \cdot \frac{g}{10^6 \mu g} \cdot \sum_i E30_i \quad i \text{ un} \quad (A-13)$$

The processes indicated by subscript  $i$  that are included for each WMU are summarized in Table C-1. Only processes acting on the surface layer are included in the summation of  $E30_i$ . Therefore, the unloading of raw waste ( $i=un$ ) is excluded.

### C.6 References

- Cowherd, C.J. 1998. Personal communication. Midwest Research Institute, Kansas City, Missouri, February 27.
- Cowherd, C.J., G.E. Muleski, P.J. Englehart, and D.A. Gillette. 1985. *Rapid Assessment of Exposure to Particulate Emissions from Surface Contamination Sites*. Office of Health and Environmental Assessment, Office of Research and Development, U.S. Environmental Protection Agency, Washington, DC.
- Meyers, R. 1998. Personal communication. Office of Air Quality and Planning, U.S. EPA, Research Triangle Park, NC, January 8.
- U.S. Department of Commerce. 1968. *Climatic Atlas of the United States*. U.S. Government Printing Office, Washington, DC.

U.S. EPA (Environmental Protection Agency). 1985. *Compilation of Air Pollutant Emission Factors Volume 1: Stationary Point and Area Sources, 4th Edition*. AP-42. PB86-124906. Office of Air Quality Planning and Standards, Research Triangle Park, NC.

U.S. EPA (Environmental Protection Agency). 1995. *Compilation of Air Pollutant Emission Factors Volume 1: Stationary Point and Area Sources, 5th Edition*. AP-42. PB95-196028INZ, Office of Air Quality Planning and Standards, Research Triangle Park, NC.