5.0 Land-based Source Modules

5.1 Purpose and Scope

The Land-based Source Modules simulate partitioning and emission of constituents from land-based waste management units (WMUs). Three Land-based Source Modules were developed for the 3MRA modeling system to represent the major management practices where wastes are put into or on the land for recycling, recovery, reuse, treatment, or disposal. These modules simulate waste management practices in the following types of WMUs:

- **Landfills,** which are a common disposal unit for many nonliquid industrial wastes;
- **Waste piles,** which are temporary storage areas on the ground for nonliquid industrial waste, such as ash or slag; and
- **Land application units (LAUs),** which are used to reuse, treat, or dispose of industrial waste in liquid, semiliquid, or solid form. Some wastes are used as a soil amendment, which is a reuse practice; some wastes are applied to land for treatment through biological degradation; and some wastes are applied to land as a disposal method.

The three Land-based Source Modules were designed to provide estimates of annual average constituent concentrations in surface soil and constituent mass emission rates to air, surface water, and ground water, and to maintain mass balance between the source and all release routes. The emission rate estimates are then used in the 3MRA modeling system, which links source modules with environmental fate and transport modules. Figure 5-1 shows the relationship and information flow among the Land-based Source Modules in the 3MRA modeling system.

Each of the three Land-based Source Modules provides some similar and some different features in terms of the ways constituents of concern can be released to the environment. All three modules have the potential to release constituents to the air by volatilization or particle entrainment, and to the subsurface and ground water by leaching. Waste piles, because they are elevated and have more surface area exposed, are assumed to have a greater potential for air emissions than the other two source types. Waste piles and LAUs have the additional release mechanism of erosion and runoff to the surrounding watershed and the nearest stream or other waterbody. Landfills are assumed to be below grade and, thus, do not release constituents through erosion or runoff.

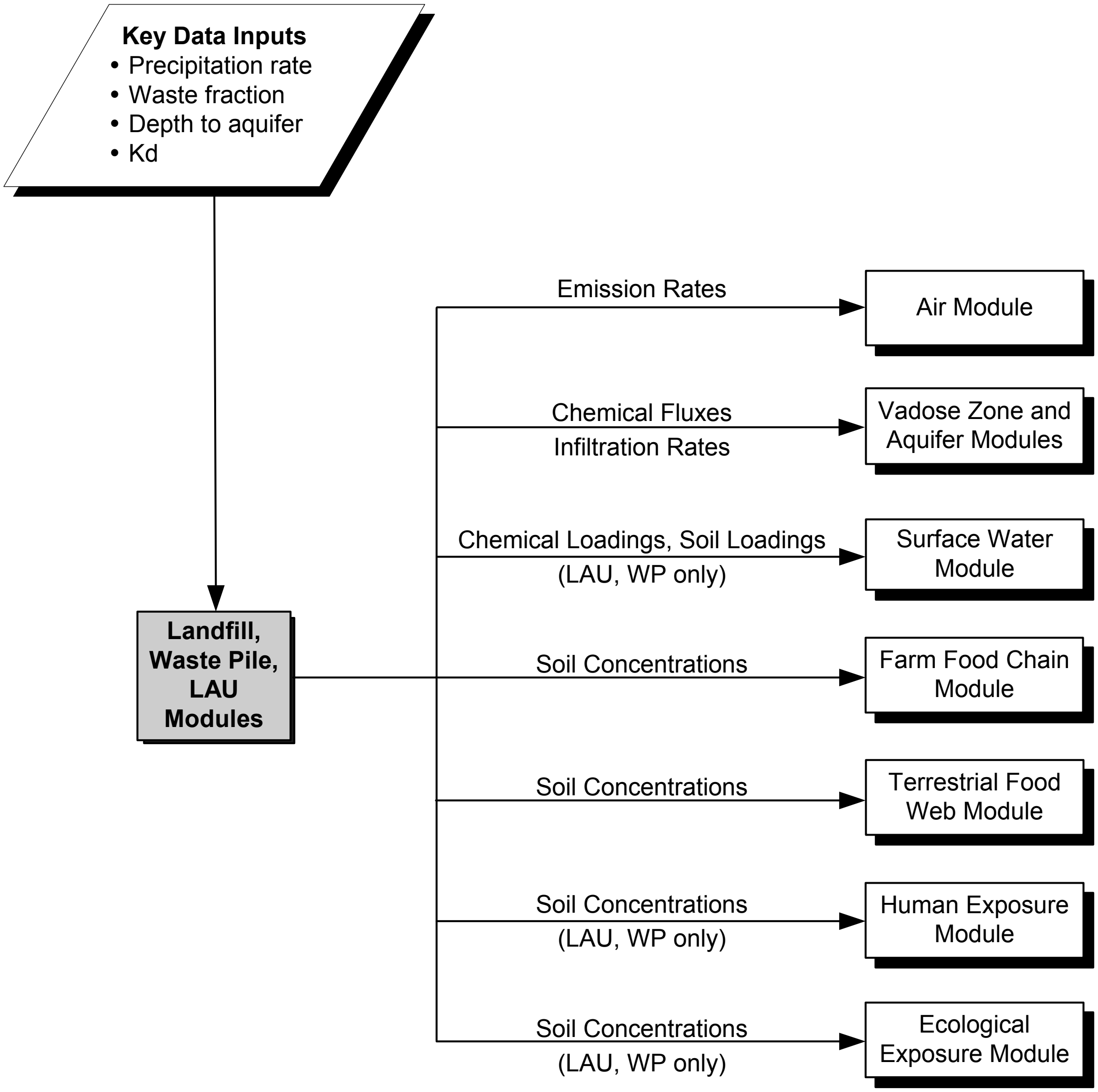

Figure 5-1. Information flow for the Land-based Source Modules in the 3MRA modeling system.

The Land-based Source Modules contain the following three models:

1. **The Generic Soil Column Model (GSCM)** was developed to describe the constituent fate and transport in a porous medium, such as soil or waste. It provides the vertical concentration profile in the soil/waste column at various times. The GSCM provides the following outputs:

   – Annual average constituent concentrations in surficial soil (top 1 cm), as well as depth-averaged concentrations over greater depths in the WMU

   – Annual average constituent concentrations in surficial soils, as well as depth-averaged concentrations over greater depth in the buffer zone located downslope from the WMU (LAU and waste pile only)

- Annual average constituent fluxes in leachate draining from the WMU into the vadose zone
- Annual average leachate flow rates (infiltration rates) draining from the WMU into the vadose zone
- Annual average constituent fluxes volatilizing from the WMU surface into the atmosphere.

2. **The Local Watershed Model** (for LAUs and waste piles) is based on mass balances of solids and constituents in the runoff and the top layer of the soil column modeled by the GSCM. The "local watershed" comprises the land area between the waterbody and the top of the hillside containing the WMU and may include an upslope area, the WMU, and a downslope or buffer area between the WMU and the waterbody. The Local Watershed Model provides the following outputs:

   - Annual average constituent loadings in surface runoff and erosion that enter the nearest surface waterbody downslope of the WMU
   - Annual average eroded soil loadings in surface water runoff that enter the nearest surface waterbody downslope of the WMU
   - Annual average runoff that enters the nearest surface waterbody downslope of the WMU.

3. **The Particulate Emissions Model** was designed to provide estimates of the annual average emission rate of constituent mass adsorbed to particulate matter less than 30 μm in diameter. The release mechanisms considered differ for each WMU, but may include wind erosion, vehicular activity, unloading operations, tilling, and spreading/compacting operations. The Particulate Emissions Model provides the following outputs:

   - Annual average particulate constituent fluxes emitted into the atmosphere from the WMU surface sorbed to soil particles via wind erosion or other surface disturbances
   - Annual average particulate fluxes (the particles themselves) emitted into the atmosphere from the WMU surface via wind erosion or other surface disturbances.
   - Particle size distributions for airborne soil particles.

Figure 5-2 illustrates how these three models interact within the Land-based Source Modules. The GSCM models vertical movement of constituents within and from the waste/soil (with the exception of particulate emissions, which are modeled by the Particulate Emissions Model). The Local Watershed Model simulates lateral movement and mass balance between waste/soil and runoff. In addition to the constituent fluxes indicated in the figure, various media fluxes are also calculated (e.g., leachate flux, by the GSCM; eroded soil load, by the Local Watershed Model; and particle size distribution, by the Particulate Emissions Model). The three models interact to maintain mass balance between the compartments. The GSCM calculates the depth-averaged soil concentration in the buffer zone for several additional layers below the surficial layer only in order to maintain mass balance between the surficial layer and the deeper layers. The deeper layers represent a sink, and the soil concentrations in those layers are not used. Similarly, the GSCM calculates volatilization from the buffer zone only to maintain mass balance—the volatilization flux from the buffer zone is not used in the Air Module. The omission of volatilization and leachate flux from the buffer zone from subsequent modeling results in an underestimation of air and ground water concentrations. However, these emissions likely have a less significant impact on the results than do direct releases from the WMU.

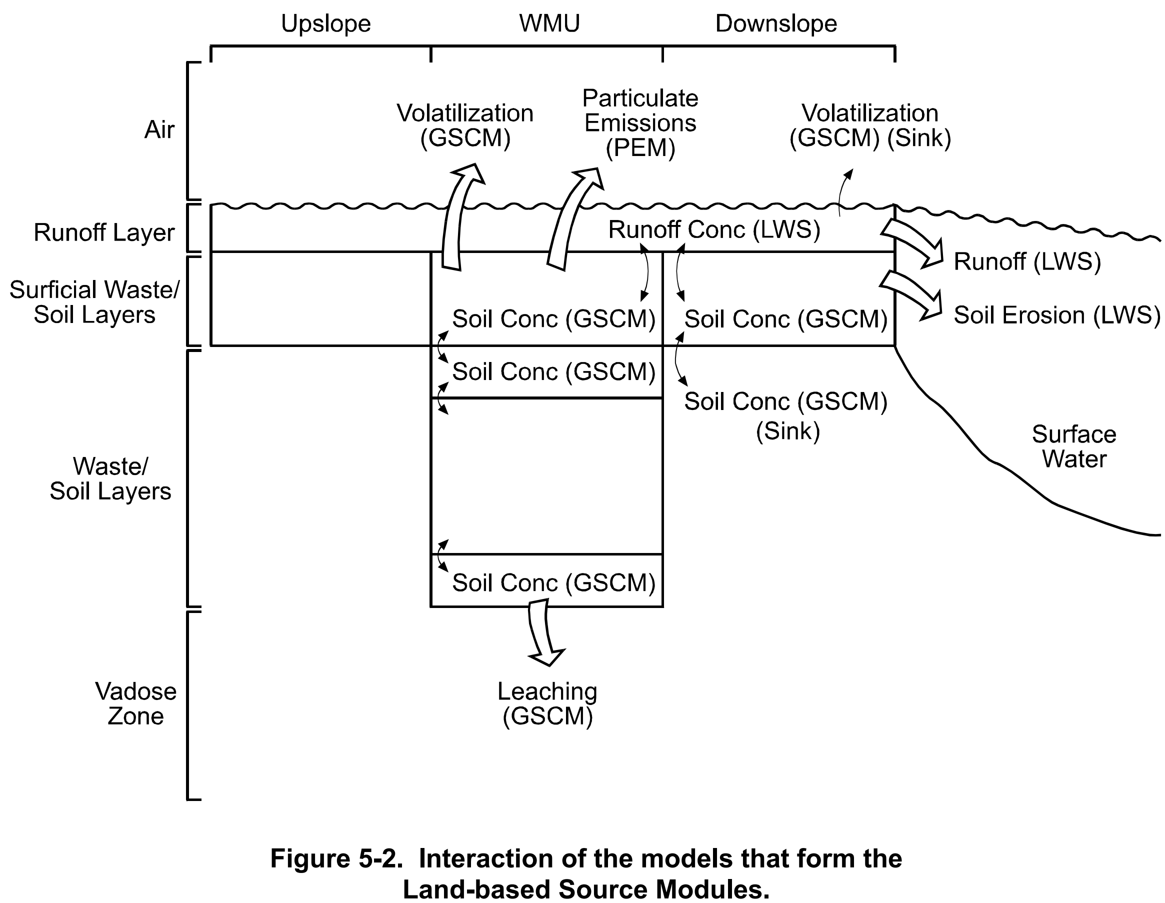

Figure 5-2. Interaction of the models that form the Land-based Source Modules.

5.2 Conceptual Approach

The physical processes modeled differ among the three land-based sources. As a result, not all of the models listed above are used for all three of the WMUs. This section first describes the three different WMUs and the processes modeled for each and then describes the three models that are contained in the Land-based Source Modules in greater detail.

5.2.1 Description of WMUs

Landfills. Figure 5-3 shows the physical processes being modeled in the 3MRA modeling system for landfill operations. The Landfill Module was developed to approximate the effects of the gradual filling of active landfills. The landfill is divided into vertical cells of equal volume 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 may be covered with a clean soil cover (this is optional). This process is repeated with the next cell and continues until the landfill reaches maximum capacity. The landfill can be sized to operate for a specified number of years (such as a 20-year operational life). Releases of a constituent to the air or ground water are modeled for up to 200 years or until the concentration in the landfill is 1 percent of the maximum concentration during the operating life of the landfill.

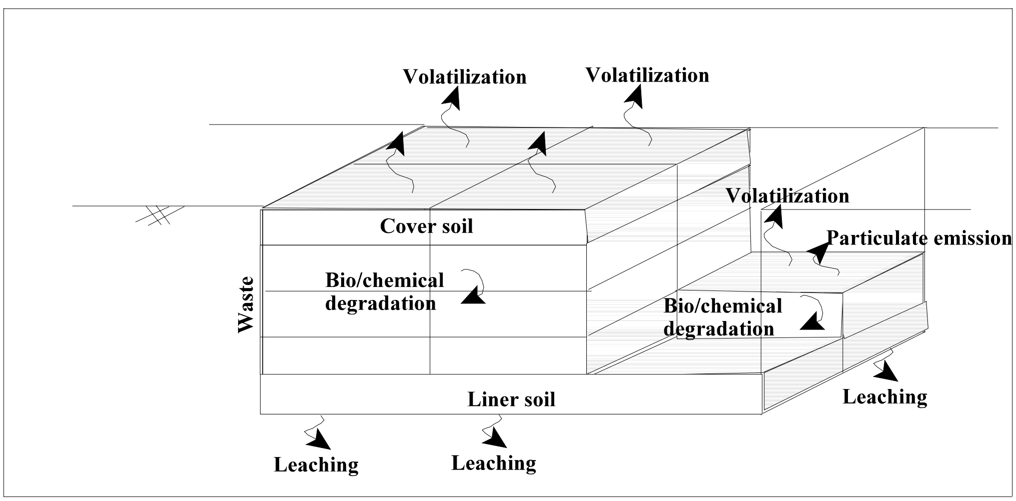

Figure 5-3. Illustration of landfill (shown with six cells and three waste layers).

The following assumptions were made in developing the Landfill Module:

- The empty landfill is approximated as an excavated volumetric rectangle. The volume is assumed to be completely below grade; therefore, it is assumed that no constituent mass is lost due to runoff or erosion.

- Each landfill cell is approximated as a soil column consisting of three homogeneous zones: soil cover, landfill waste, and subsoil. Each zone is modeled as a homogeneous porous medium whose properties are uniform in space and time within the zone. The soil cover zone and subsoil zones are optional.

- The concentration of constituents is constant in the incoming waste, and waste is added at a constant rate. The concentration of constituents in the waste can be adjusted to account for other wastes entering the landfill that do not contain the constituent of interest.

- There is no lateral transport of constituents between cells.

- Waste is added to the landfill cell in layers. A waste layer, for the purposes of the model, is simply a zone within which initial concentrations are assumed to be uniform. Waste layers are conceptualized as being formed over time by the dumping of loads of waste next to one another in the landfill cell until eventually a waste layer of uniform depth is formed. At this point, a new layer is started.

- At the start of the landfill cell simulation, one waste layer is assumed to be present. After each time period, another waste layer is laid down until the landfill cell is full. At that time, it may be covered with clean soil or left exposed.

- The first-order constituent and biological loss processes modeled for the entire landfill (including cover soil, waste, and liner material) are anaerobic biodegradation and hydrolysis.

- The first-order loss rate due to particulate emissions from an active landfill cell includes losses due to wind erosion, vehicular activity, and spreading and compacting. Only losses due to wind erosion are modeled from inactive landfill cells.

Waste Piles. Figure 5-4 shows the physical processes modeled in the 3MRA modeling system for waste piles, which may manage ash, slag, or other similar types of waste. The waste pile has a constant height and constant area equal to the footprint of the waste pile. At the start, the waste pile is filled to capacity. After each period of time, such as 1 year, the entire waste pile is removed and instantaneously refreshed (i.e., replaced with fresh waste). In reality, waste is added and removed from a waste pile incrementally; the assumption that the waste is instantaneously refreshed is made to simplify modeling. Because the waste surface is not refreshed between placements of new waste, the Waste Pile Module may underestimate volatile losses relative to a model where waste is built up gradually. This is unlikely to affect emission estimates for nonvolatile constituents.

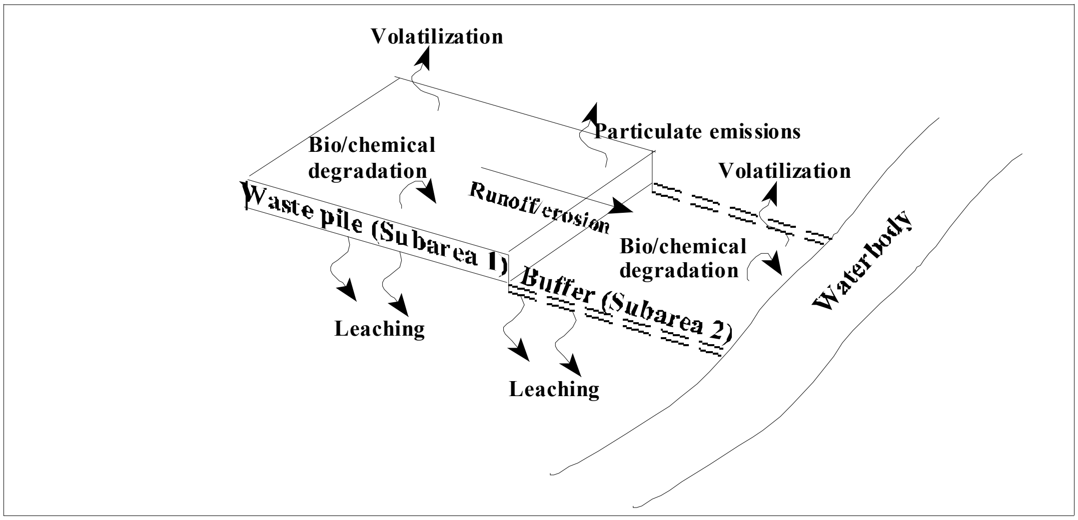

Figure 5-4. Illustration of a waste pile in local watershed.

The following assumptions were made in developing the Waste Pile Module:

- The waste pile site is used for a finite number of years, after which it is assumed that the final waste pile is removed and clean soil is placed on the surface where the waste pile was.

- The first-order constituent and biological loss processes modeled for the waste pile are aerobic biodegradation and hydrolysis in the surface waste layer, and anaerobic biodegradation and hydrolysis in all subsurface layers of the waste pile.

- The first-order loss rate due to particulate emissions from an active waste pile is applied only to the surface layer and includes losses due to wind erosion, vehicular activity, and spreading and compacting operations from an active waste pile.

- For purposes of modeling runoff and erosion processes, the following assumptions were made:

  - The waste pile is conceptualized as having side slopes (from which increased runoff and erosion would occur) that are insignificant (i.e., the sloped surface area is small relative to the surface area of the top of the waste pile).

  - The top surface of the waste pile has the same slope as the average slope of the local watershed.

  - No run-on occurs to the waste pile subarea from upslope subareas in the local watershed.

– Following removal of the waste pile, there is no subsequent runoff/erosion transport pathway from the waste pile subarea of the local watershed downslope to the surface water, only from the buffer subarea. That is, there is assumed to be no remaining surficial contamination in the subarea that contained the waste pile because clean soil is assumed to be placed there after waste pile removal.

■ The topmost layer of waste serves as the "soil" compartment in the runoff and erosion algorithms used in the local watershed model. For the purposes of applying these algorithms, it is assumed that the surface layer is 0.01 m deep.

Land Application Unit. Figure 5-5 shows the physical processes being modeled in the 3MRA system for LAUs. Such units are used to manage liquid, semi-solid, and solid wastes. Certain types of waste can be used to amend agricultural soils, thus constituting a reuse of the waste.

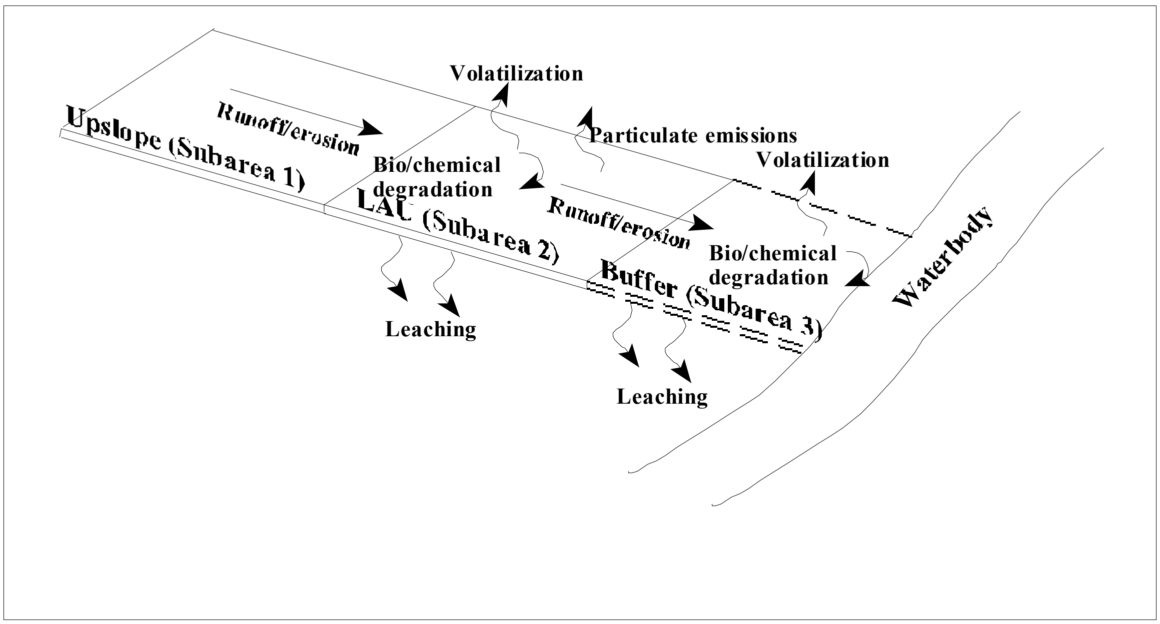

Figure 5-5. Illustration of LAU in local watershed.

The following assumptions were made in developing the LAU Module:

■ Waste is applied to the soil surface periodically at even intervals (e.g., quarterly) and then tilled into the soil to a specified depth, such as 0.2 m.

■ The till zone is completely mixed upon each application of waste to soil.

■ The modeled surface layer consists of one homogeneous zone—the till zone—which consists of a soil/waste mixture. The till zone properties can be estimated as the depth-weighted average of the soil and waste properties according to the depth of soil and waste in the till zone.

- The water contained in the wet waste added to the LAU increases the annual average infiltration rate.

- The constituent 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.

- Waste applications do not result in significant buildup of the soil surface, nor does erosion significantly degrade the soil surface (i.e., the vertical distance from the site surface). As a result, there is no naturally occurring limit to the modeled concentration of constituents in the soil other than the limit for nonaqueous-phase liquids (NAPLs). As a result, the modeled concentration in the till zone could exceed the concentration in the waste. 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 LAU is operated for a specified number of years (e.g., 40 years).

- The first-order constituent and biological loss processes in the till zone include aerobic biodegradation and hydrolysis.

- The first-order loss rate due to particulate emissions from an active LAU is applied to the surface layer of the till zone only and includes losses 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.

- The topmost waste/soil layer serves as the soil compartment in the runoff and erosion algorithms used in the Local Watershed Model. For the purposes of applying these algorithms, it is assumed that the surficial soil layer is 0.01 m deep.

5.2.2 The Generic Soil Column Model

The GSCM was developed to describe the dynamics of constituent mass fate and transport within land-based WMUs and near-surface soils in watersheds. Figure 5-6 illustrates the processes modeled by the GSCM. The GSCM solves the 1-D partial differential equation describing constituent fate and transport in a porous medium in space and time. This solution represents the vertical concentration profile in the soil/waste column at various times, where the soil/waste column can represent either the top portion of the vadose zone of a land application site (LAU Module), the waste pile (Waste Pile Module), a landfill cell (Landfill Module), or the top portion of the vadose zone of an entire watershed subbasin (Watershed Module). In addition to describing vertical constituent concentration gradients in the soil column, the GSCM is coupled with a runoff/erosion model (either the Local Watershed Model, described in Section 5.2.3, or the Watershed Module, described in Section 7) that describes constituent

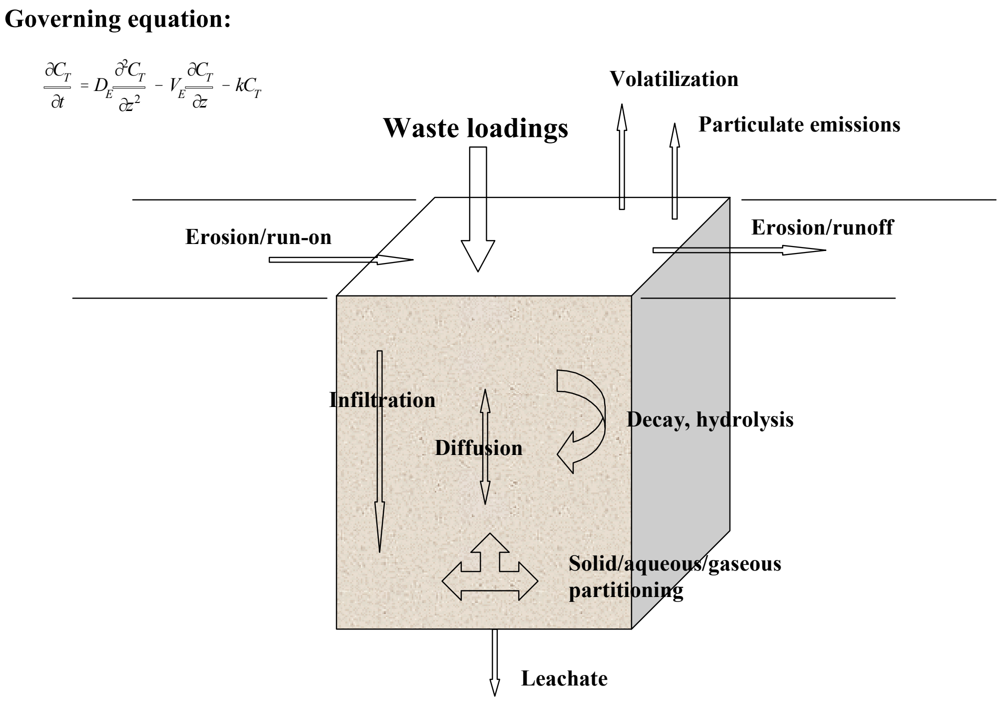

Figure 5-6. Conceptual diagram of the Generic Soil Column Model (GSCM).

concentration in surface runoff across the soil column's surface and interactions between this runoff compartment and the soil compartment.

The GSCM was originally designed for the 3MRA modeling system to make some modest improvements to the well-known Jury model (Jury et al., 1983, 1990), which had been used historically to simulate constituent fate and transport in land-based sources. Similar to the GSCM, the Jury model describes vertical concentration gradients over time of total (sorbed, dissolved, and gaseous) constituent concentration. The Jury model was limited for 3MRA purposes for two reasons. First, it assumes an infinitely deep soil column. The 3MRA Land-based Source Modules output leachate fluxes to the Vadose Zone Module, so the infinite depth assumption is inappropriate. Second, the Jury model's initial conditions cannot accommodate the vertical gradient resulting from periodic waste loadings, such as from repeated land application of waste, over all or a portion of the soil column depth. The governing equations for the GSCM are similar to those used by Jury et al. (1983, 1990) and Shan and Stephens (1995), but have been applied in a manner that avoids these limitations. Use of the GSCM allows

- Constituent mass balance;
- Waste additions and removals to simulate active facilities; and

- Joint estimation of
  - 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,
  - Concentrations of constituents within the soil or waste column, and
  - First-order losses, which can include hydrolysis and anaerobic and aerobic biodegradation.

The following assumptions were made in the development of the GSCM for use in all of the Land-based Source Modules:

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

$$C_T = \rho_b C_s + \theta_w C_L + \theta_a C_G \tag{5-1}$$

where

C_T = total constituent concentration in soil (g/m^3 of soil)
ρ_b = soil dry bulk density (g/cm^3)
C_s = adsorbed-phase constituent concentration in soil (µg/g of dry soil)
θ_w = soil volumetric water content (m^3 soil water/m^3 soil)
C_L = aqueous-phase constituent concentration in soil (g/m^3 of soil water)
θ_a = soil volumetric air content (m^3 soil air/m^3 soil)
C_G = gas-phase constituent concentration in soil (g/m^3 of soil air).

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

$$C_s = K_d \times C_L \tag{5-2}$$

where

K_d = linear equilibrium partitioning coefficient (cm^3/g).

For organic constituents,

$$K_d = f_{oc} \times K_{oc} \tag{5-3}$$

where

f_{oc} = organic carbon fraction in soil or waste (unitless)
K_{oc} = equilibrium partition coefficient, normalized to organic carbon (cm^3/g).

Alternatively, K_d can be specified as an input parameter for inorganic constituents.

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 constituent over the duration of the simulation, i.e., the soil column sorptive capacity does not become exhausted.

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

$$C_G = H' \times C_L \tag{5-4}$$

where

H′ = dimensionless Henry's law coefficient.

The Henry's law coefficient is adjusted for seasonal variations in temperature.

- The total constituent concentration in soil can also be expressed in units of mass of constituent per mass of dry soil (µg/g) by dividing by the soil dry bulk density.

- Using the linear equilibrium approximations in Equations 5-2 through 5-4, C_T can be expressed in terms of C_L, C_S, or C_G as follows:

$$C_T = K_{TL} \times C_L = \frac{K_{TL}}{K_d} \times C_S = \frac{K_{TL}}{H'} \times C_G \tag{5-5}$$

where

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

- The total water flux or infiltration rate 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 (i.e., one whose basic properties, which include dry bulk density, fraction organic carbon, soil volumetric water content, soil volumetric air content, and total soil porosity, are uniform in space). Waste/soil properties are specified as annual average values.

- Constituent mass may be lost from the soil column through one or more first-order loss processes.

- The total constituent flux is the sum of the vapor flux and the flux of the dissolved solute (as in Jury et al., 1983, 1990).

- The constituent is transported in one dimension through the soil column (as in Jury et al., 1983, 1990).

- The effective diffusivity in soil may be calculated by the model 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, such as the water table.

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

$$\frac{\partial C_T}{\partial t} = D_E \frac{\partial^2 C_T}{\partial z^2} - V_E \frac{\partial C_T}{\partial z} - k C_T \qquad (5\text{-}6)$$

where

t	=	time
k	=	total first-order loss rate (1/d)
D_E	=	effective diffusivity in soil (m^2/d)
z	=	verticle direction (m), depth
V_E	=	effective solute convection velocity (m/d).

D_E can be considered to be the algebraic sum of the effective gaseous and water diffusion coefficients in soil. V_E is equal to the water flux corrected for the constituent partitioning to the solid phase (m/d).

A solution of the complete convective-diffusive-decay concentration model (Equation 5-6) was undertaken to evaluate, in a soil/waste column,

- Total constituent concentration as a function of time and depth below the surface, and

- Constituent mass fluxes across the upper and lower boundaries of the soil column.

A quasi-analytical approach was developed that allows for relative computational speed and significantly reduces concern about numerical diffusion and lack of stability associated with fully numerical solution techniques. 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) constituent concentration profiles and mass fluxes.

The solution for the simplified case, in which 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 of the 1999 background documents at www.epa.gov/epaoswer/hazwaste/id/hwirwste/risk.htm.

The quasi-analytical approach is a step-wise solution of the three components of the governing equation (Equation 5-6) on the same grid. That is, the following equations are solved individually and then added (under the principle of superposition for linear differential equations) to yield the complete solution:

$$\frac{\partial C_T}{\partial t} = D_E \frac{\partial^2 C_T}{\partial z^2} \tag{5-7}$$

$$\frac{\partial C_T}{\partial t} = -V_E \frac{\partial C_T}{\partial z} \tag{5-8}$$

$$\frac{\partial C_T}{\partial t} = -k\,C_T \tag{5-9}$$

Equations 5-7 through 5-9 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 following boundary conditions are assumed:

- Zero concentration is assumed at the upper boundary of the soil column.[1] This is consistent with the assumption that the air is a sink for volatilized constituent mass, but requires the approximate method for estimating the mass flux of volatile emissions.

- At the lower boundary of the soil column, the flexibility exists with this solution technique to specify a value between 0 and 1 for the ratio of the total constituent concentration in the soil directly below the modeled soil column and in the soil column. A ratio of 1 corresponds to a zero gradient boundary condition. A ratio of 0 corresponds to a zero concentration boundary condition. For the 3MRA modeling system, a boundary condition of 0 was assumed.

[1] The $C_T = 0$ "boundary condition" is not a boundary condition in the usual sense of it determining the functional form of the resulting analytical solution to the underlying diffusion differential equation (Equation 5-7). That solution is based on an implicit boundary condition of $C_T = 0$ at +/- infinity, similar to heat transfer in an infinitely long plate. The $C_T = 0$ boundary condition is here intended to reflect the fact that there is no *back*-diffusion from the overlying air column into the soil column, i.e., the concentration in the overlying air column is assumed to be zero so that no back-diffusion results.

5.2.3 Local Watershed Model

The Local Watershed Model is a holistic model used in the Waste Pile and LAU Modules to incorporate them into the watershed of which they are a part. These WMUs are on the land surface, so they are integral land area components of 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. After some period of operation during which runoff and erosion have occurred from these WMUs, the downslope land areas will have been contaminated and their surface concentrations could approach the residual constituent concentrations in the WMU itself (or conceivably even exceed them long after the WMU ceases operation). 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 model.

As stated earlier, the watershed that includes the LAU or waste pile is termed here the "local watershed" (see Figures 5-4 and 5-5). A local watershed is defined as the drainage area that contains the WMU (or a portion thereof) in the lateral direction (perpendicular to runoff flow) and the area 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 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 constituent contamination from the WMU through overland runoff and soil erosion.

The local watershed is conceptualized as a 2-D, 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 (in the longitudinal direction) of an arbitrary number of land subareas[2] that may have differing surface or subsurface characteristics (e.g., land uses, soil properties, and constituent concentrations).

The Local Watershed Model comprises the following three components:

- A hydrology model,
- A soil erosion model, and
- A constituent fate and transport model.

These are described below.

Hydrology Model. Hydrologic modeling is performed to simulate watershed runoff and ground water recharge (termed here "infiltration"). The hydrology model is based on a daily soil water balance performed for the root zone of the soil column as shown in Figure 5-7.

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[2] The conceptual approach allows for an arbitrary number of subareas, but in the implementation of the 3MRA modeling system, that number has been limited to a maximum of 3: upslope, WMU, and downslope/buffer.

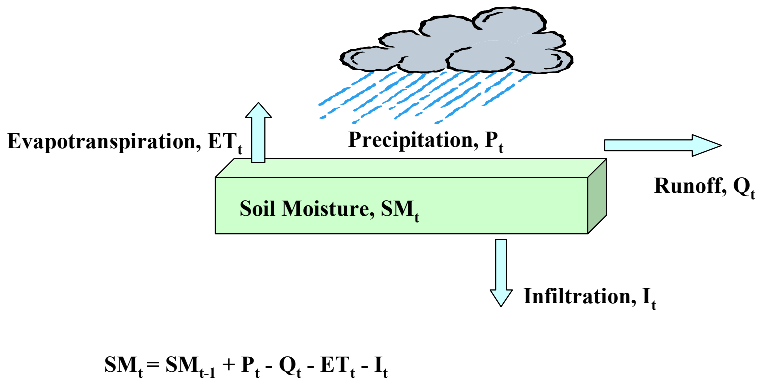

Figure 5-7. Daily water balance model.

At the end of a given day, the soil moisture in the root zone of an arbitrary watershed subarea is given as

$$SM_t = SM_{t-1} + P_t - Q_t - ET_t - I_t \tag{5-10}$$

where

SM_t	=	soil moisture in root zone at end of day *t* for subarea *i* (cm)
SM_{t-1}	=	soil moisture in root zone at end of previous day for subarea *i* (cm)
P_t	=	total precipitation on day *t* (cm)
Q_t	=	net of storm runoff on day *t* leaving the subarea and storm runoff entering the subarea (cm)
ET_t	=	evapotranspiration from root zone on day *t* for subarea *i* (cm)
I_t	=	infiltration (ground water recharge) on day *t* for subarea *i* (cm) .

Precipitation is undifferentiated between rainfall and frozen precipitation; that is, frozen precipitation is treated as rainfall.

The daily runoff estimate is based on the Soil Conservation Service's (SCS's) widely used "curve number" procedure (USDA, 1986) and is a function of land use and current and antecedent precipitation. Land use is considered empirically by application of 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.

Curve numbers are typically presented in the literature assuming average antecedent moisture conditions (AMC II), but can be adjusted for drier (AMC I) or wetter (AMC III) conditions (Chow et al., 1988). These three categories are used in the hydrology model; a distinction is made within them between the dormant season and the growing season. The growing season is assumed to be June through August (Julian Day 152 to 243) throughout the country. These adjustments have the effect of increasing runoff under wet antecedent conditions and decreasing runoff under dry antecedent conditions, relative to average conditions.

Potential evapotranspiration (PET) is the demand for soil moisture from evaporation and plant transpiration. When soil moisture is abundant, actual evapotranspiration equals the PET. When soil moisture is limiting, actual evapotranspiration 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, and available soil water capacity (Dunne and Leopold, 1978).

The more theoretically based models 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 3MRA, it is assumed that all of these variables will not be readily available for all applications. Therefore, a less data-demanding model, the Hargreaves equation (Shuttleworth, 1985), is used. The Hargreaves method, which is primarily temperature-based, has been shown to provide reasonable estimates of evaporation (Jensen, et al., 1990)—presumably because it also includes an implicit link to solar radiation through its latitude parameter (Shuttleworth, 1993).

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

In the event that infiltration is limited by the saturated hydraulic conductivity (rather than evapotranspiration), the hydrology model includes a mechanism to increase the previously calculated runoff volume by the amount of excess soil moisture (i.e., the soil water volume in excess of the field capacity). 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 evapotranspiration, infiltration, and/or increased soil moisture. After the runoff is increased by this excess, the evapotranspiration, infiltration, and soil moisture are updated to reflect this modification and preserve the water balance.

Soil Erosion Model. The soil erosion model used in the Local Watershed Model is based on the Universal Soil Loss Equation (USLE), an empirical methodology (see, e.g., Wischmeier and Smith, 1978) derived from measured soil losses at small, experimental field-scale plots throughout the United States. The USLE predicts sheet and rill erosion from hillsides upslope of defined drainage channels, such as streams. It does not predict streambank erosion. The eroded soil flux from a hillside area averaged over a specific time period is predicted by the USLE as the product of the six variables discussed below.

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

The soil erodibility factor (*K*, kg/m^2) is an experimentally determined property that is a function of soil type, including particle size distribution, organic content, structure, and profile. Soil erodibility factor values are reported by soil type in the literature.

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

The practice factor (*P*, unitless) accounts for the effect of erosion control practices, e.g., contouring or terracing. The practice factor is never negative, but could be greater than 1 if land practices actually encourage erosion relative to the original experimental plots on which soil erodibility factors were measured.

The combined length-slope factor (*LS*, unitless) is given by U.S. EPA (1985b). The length-slope factor increases with increasing flow distance because runoff quantity and erosive energy generally increase with downslope distance. LS increases with slope because runoff velocity generally increases with slope.

The sediment delivery ratio (*Sd*, unitless) estimates the fraction of on-site eroded soil that reaches a particular downslope or downstream location in the subbasin (Shen and Julien, 1993). The sediment delivery ratio is used here to account for deposition of eroded soil from the local watershed in ditches, gullies, or other depressions before reaching a downslope stream or waterbody. Vanoni (1975) developed the relationship between the sediment delivery ratio and the watershed drainage area.

The USLE is implemented within the Local Watershed Model on a storm event basis, i.e., the “modified” USLE (MUSLE) is used. This implementation requires determining a rainfall factor value for each daily storm event that specifies the erosivity of that individual storm.

Constituent Fate and Transport Model. Constituent and suspended solids concentrations in storm-event runoff are simulated using a two compartment model for the soil surface layer: a runoff compartment and the soil compartment. Figure 5-8 presents the conceptual runoff /erosion model showing the two compartments and the fate and transport processes considered. Hydrolysis, volatilization, and biodegradation processes are not simulated in the runoff compartment. These processes are continuously simulated in the surface layer of the soil column by the GSCM. The percentage of time that runoff is actually occurring is sufficiently short that any additional constituent losses in the runoff water due to these processes should be minimal.

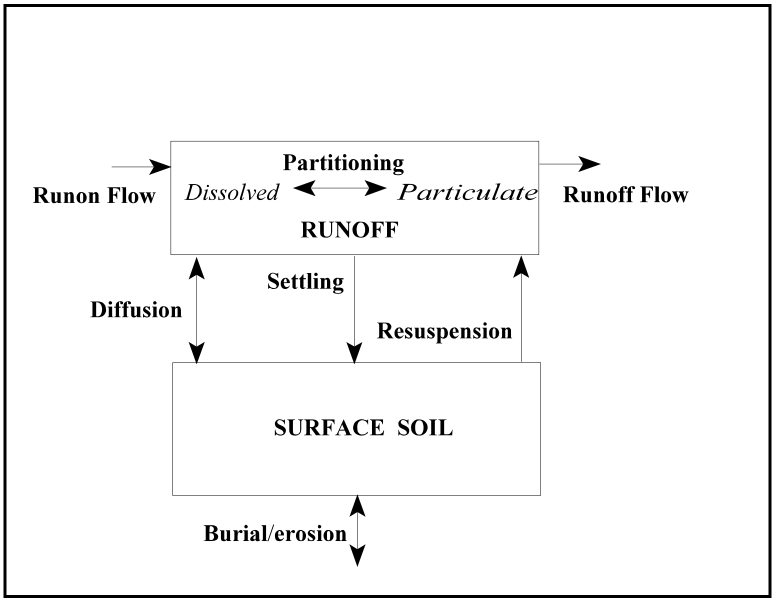

Figure 5-8. Runoff/erosion conceptual model.

Runoff Compartment. The runoff compartment model is based on mass balances of solids and constituent in the runoff water and the top soil column layer. A simplifying assumption is made that solids and constituent concentrations in the runoff are at instantaneous steady-state equilibrium 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 equilibrium for each storm event is not strictly accurate, it was deemed appropriate for the following reasons:

- Data will not generally be available at the temporal scale to accurately track within-storm event conditions (e.g., rainfall hyetographs).

- The actual time to steady-state may not differ significantly from the 1 day or less implicitly assumed here because of the anticipated relatively small surface areas of the watershed subareas and the associated relatively small runoff volumes. A sensitivity analysis was performed, using a dynamic form of the runoff compartment model, which suggested relatively little difference in calculated soil concentrations as a function of the steady-state versus dynamic assumption.

- To the extent that the actual time to steady-state is greater than 1 day, the model is biased toward overestimating downslope concentrations and waterbody loads.

A steady-state mass balance of solids in the runoff, i.e., suspended solids from erosion, is used:

$$0 = Q'_{i-1}\, m_{l,i-1} - Q'_i\, m_{1,i} - vs_i\, A_i\, m_{1,i} + vr_i\, A_i\, m_2 \qquad (5\text{-}11)$$

where

Q'_{i-1}	=	total run-on flow volume (water plus solids) from subarea *i*-1 (m^3/s) (see Equation 5-12)
Q'_i	=	total runoff flow volume (water plus solids) leaving subarea *i* (m^3/s) (see Equation 5-12)
$m_{1,i-l}$	=	solids concentration in runon from subarea *i*-l (g/m^3)
$m_{1,i}$	=	solids concentration in runoff from subarea *i* (suspended solids) (g/m^3)
m_2	=	solids concentration in the top soil column layer of subarea *i* (g/m^3)
vs_i	=	settling velocity (m/s)
vr_i	=	resuspension velocity (m/s)
A_i	=	surface area of subarea *i* (m^2).

$$Q'_i = Q_i + \frac{CSL_i}{\rho} \tag{5-12}$$

where

Q_i	=	runoff flow leaving subarea *i* (m^3/s)
CSL_i	=	cumulative soil load leaving subarea *i* (g/s)
ρ	=	particle density (g/m^3) (i.e., 2.65 g/m^3).

The first term in Equation 5-11 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, and the fourth term is an internal source due to resuspension.

Solids mass transport from or to the soil compartment within any given watershed subarea is assumed to occur only in a vertical direction, i.e., no downgradient advection of the top soil column layer itself is considered. The downslope mass transport of soil occurs because of 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

$$0 = vs_i \ m_{1,i} \ A_i - vr_i \ m_{2,i} \ A_i - vb_i \ m_{2,i} \ A_i \tag{5-13}$$

where

vb_i = burial/erosion velocity (m/s).

The first term of Equation 5-13 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.

A steady-state mass balance of constituents in the runoff is achieved, as illustrated in Figure 5-8. The governing equation for this mass balance is as follows:

$$0 = Q'_{i-1}c_{1,i-1} - Q'_i c_{1,i} - vs_i A_i Fp_{1,i} c_{1,i} + vr_i A_i Fp_{2,i} Er_i c_{2,i} + vd_i A_i \left(\frac{Fd_{2,i}}{\Phi_2} c_{2,i} - \frac{Fd_{1,i}}{\Phi_{1,i}} c_{1,i}\right) \quad (5\text{-}14)$$

where

$c_{1,i}$	=	total constituent concentration (particulate + dissolved) in runoff in subarea *i* (g/m^3)
$c_{2,i}$	=	total constituent concentration in soil (g/m^3)
$V_{1,i}$	=	subarea-specific (not cumulative) runoff volume for subarea *i* (m^3)
$Fp_{j,i}$	=	fraction of constituent sorbed to particulate in runoff in soil compartment *j* (unitless)
$Fd_{j,i}$	=	fraction of constituent sorbed to dissolved in runoff in soil compartment *j* (1-$Fp_{j,i}$)
vd_i	=	diffusive exchange velocity (m/s)
Er_i	=	enrichment ratio (unitless)
$\Phi_{1,i}$	=	porosity of the runoff (unitless)

Note that ϕ_2 is equivalent to porosity (η) in the GSCM.

Equation 5-14 can be used to express $c_{1,i}$ as a function of $c_{1,i-1}$ and $c_{2,i}$, as shown in Equation 5-15:

$$c_{1,i} = \frac{Q'_{i-1}c_{1,i-1} + [vr_i A_i Fp_{2,i} Er_i + vd_i A_i (Fd_{2,i}/\Phi_2)]\, c_{2,i}}{Q'_i + vs_i A_i Fp_{1,i} + vd_i A_i (Fd_{1,i}/\Phi_{1,i})} \quad (5\text{-}15)$$

where $c_{2,i}$ is determined by the GSCM, as described in Section 5.2.2.

An enrichment ratio is used to account for preferential erosion of finer soil particles—with higher specific surface areas and more sorbed constituent 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 constituent 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 constituent loads could be significantly higher than represented by the average soil concentration. U.S. EPA (1985b) gives the storm-event-specific enrichment ratio as a power function of sediment discharge flux.

Soil Compartment. From the discussion of the GSCM, the governing differential equation for the surface soil layer of subarea *i* is

$$\frac{\partial C_{2,i}}{\partial t} = D_E \frac{\partial^2 C_{2,i}}{\partial z^2} - V_E \frac{\partial C_{2,i}}{\partial z} - \Sigma k_j C_{2,t} + ss_i \quad (5\text{-}16)$$

where k_j represents first-order rate constant due to 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 the concentration in the surface soil. The term ss_i comprises the following terms respectively: a source of constituent due to settling from the overlying runoff water, a sink of constituent due to resuspension, and a source or sink (depending on the relative values of $C_{1,i}$ *and* $C_{2,i}$) due to constituent diffusion from/to the runoff.

Referring back to the governing equation for the surface soil column layer, the first two-component equations remain the same, while the third is revised to

$$\frac{\partial C_{2,i}}{\partial t} = - k'C_{2,i} + ld_{i-1} \tag{5-17}$$

With this equation, the constituent mass balance is maintained in the GSCM with the inclusion of erosion and runoff.

5.2.4 Particulate Emissions Model

The Land-based Source Modules have been designed to provide estimates of the annual average, area-normalized emission rate of constituent mass adsorbed to particulate matter less than 30 µm in diameter (PM_{30}), 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 µm, 15 to 10 µm, 10 to 2.5 µm, and <2.5 µm.

A variety of release mechanisms are considered. The release mechanisms considered differ for each WMU and may include wind erosion, vehicular activity, unloading operations, tilling, and spreading and compacting operations. Table 5-1 summarizes the mechanisms considered for each WMU.

Table 5-1. Summary of Mechanisms of Release of Particulate Emissions for Each WMU

	WMU Type[a]						
	LAU		LF		WP		
Mechanism of Release	**Active**	**Inact.**	**Active**	**Inact.**[b]	**Active**	**Inact.**	**Algorithm Reference**
Wind erosion from open area	✓	✓	✓	✓			Cowherd et al. (1985)
Wind erosion from waste pile					✓	✓	U.S. EPA (1985a)
Vehicular activity	✓		✓		✓		U.S. EPA (1995a)
Unloading			✓		✓		U.S. EPA (1995a)
Spreading and compacting or tilling	✓		✓		✓		U.S. EPA (1985a)

[a] Active = Operating WMU. Inact. = Inactive WMU where no additional constituent mass is being added.
[b] Inactive (full) and uncovered landfill cell. Assume no emissions from a covered landfill cell.

This section describes the algorithms and assumptions used to estimate the following for each mechanism of release:

- Annual average PM_{30} emission rate due to each mechanism considered for each WMU, and
- Annual particle size range mass fractions, i.e., the mass fractions of PM_{30} in the aerodynamic particle size categories identified above.

For each WMU, the following are estimated:

- The total annual average PM_{30} emission rate due to all release mechanisms,
- The annual average emission rate of constituent sorbed to PM_{30},
- Annual average particle size range mass fractions of the total annual average PM_{30} emission rate, and
- Annual average first-order loss rate from the soil surface due to constituent mass losses caused by particulate emissions.

Wind Erosion from Open Fields. The algorithm for the estimation of PM_{30} emissions due to wind erosion from an open field is based on the procedure developed by Cowherd et al. (1985). The annual average emission rate of PM_{30} per unit area of the contaminated surface is estimated in the LAU and Landfill Modules.

To account for differing degrees of vegetation, surface roughness height, and frequency of disturbances per month in active versus inactive WMUs, different values are assigned to these parameters according to whether the WMU is active or inactive.

The methodology of Cowherd et al. (1985) was originally developed to estimate the emission rate of PM_{10}. Emission rates for PM_{30} can be approximated from those for PM_{10} with knowledge of the ratio between PM_{30} and PM_{10} emissions for wind erosion. According to Cowherd (1998), 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 PM_{10} emission to allow estimation of PM_{30} emissions.

Wind Erosion from Waste Piles. The equation used in the Waste Pile Module to estimate the annual average PM_{30} 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) from active sand and gravel waste piles presented in U.S. EPA (1985a, referred to here as AP-42; see Equation 3, p. 11.2.3-5). TSP is defined as those particulates measured by a high-volume sampler, and the effective cutoff commonly assigned to standard high-volume samplers is 30 µm (U.S. EPA, 1985a). A dust-control efficiency factor is added.

A more recent version of AP-42 (U.S. EPA, 1995) recommends the use of an event-based algorithm for estimating wind emissions from a waste pile. The updated algorithm was evaluated for use in 3MRA, but it was determined that it requires detailed site-specific information, typically not available for site-based analyses. The algorithm used in the Land-based Source Modules will tend to overestimate emissions relative to the event-based algorithm (Meyers, 1998).

Vehicular Activity. To estimate the PM_{30} emissions from vehicular travel on the surface of the WMU, an algorithm 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 per kilometer traveled on unpaved roads. (In the Land-based Source Modules, the EPA parameter "fraction of waste on unpaved roads" is equal to 1 because travel is on the surface of the WMU.) EPA's equation has been adapted for the Land-based Source Modules to provide emissions normalized to the contaminated surface area and to account for the control of emissions with a dust-control efficiency factor.

Unloading Operations. The equation for estimating the PM_{30} emission rate due to unloading operations at waste piles 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, normalizing the emissions for the contaminated surface area, and applying the particle size multiplier for <30 µm.

Spreading and Compacting or Tilling Operations. The equation for estimating the rate of PM_{30} emissions due to spreading and compacting or tilling operations was adapted from an equation in U.S. EPA (1985a, Equation 1, p. 11.2.2-1) that was developed for estimating emissions due to agricultural tilling in units of kilograms of particulate emissions per hectare per tilling (or spreading and compacting) event. The particle size multiplier for <30 µm is applied in the Land-based Source Modules.

5.3 Module Discussion

5.3.1 Strengths and Advantages

Relative to other models that might have been candidates for the functionality provided by the Land-based Source Modules, the strengths and advantages of the modules include the following:

- **The GSCM extends the functionality of the Jury model.** The GSCM was developed to make modest improvements to known limitations of the Jury-type approach for the 3MRA modeling system. Specifically, the GSCM simulates changes over time in vertical soil constituent concentration profiles given (1) periodic waste applications that result in non-uniform vertical concentration profiles (this addresses the Jury limitation of uniform initial condition); and (2) a finite vertical boundary is formed by an underlying vadose zone so that the lower boundary depth is not infinite (this addresses the Jury limitation of a zero concentration boundary condition at the lower soil column boundary. (A zero concentration *gradient* boundary condition is assumed instead.)

- **The "local watershed" algorithm gives the LAU and Waste Pile Modules spatial resolution appropriate for the 3MRA modeling system exposure scenarios.** The conceptual site models for both the LAU and waste pile WMUs assume that both WMUs are adjoined by a buffer area (non-WMU land area). (The landfill is not assumed to have off-site runoff or erosion, so it is not considered part of a "local watershed".) The buffer area is situated between the WMU and the nearest surface waterbody. Overland flow runoff is assumed to occur from the WMU, across the buffer area, and into the nearest surface waterbody. This set of land areas (WMU, buffer, and a possible third land area upslope of the WMU, which contributes stormwater runoff and eroded soil, but not constituent loads, to the WMU area) located on the "hillside" adjacent to a surface waterbody constitutes the "local" watershed. Because constituent concentrations over time will be different in the buffer area than in the WMU area, and receptors can be located in the buffer area, it was important for the purposes of the 3MRA modeling system to have this spatial resolution. Prior to developing the Land-based Source Modules, which contain this "local watershed" functionality, a review of candidate watershed/vadose zone models was performed, and none were found to have this spatial resolution. For example, EPA's PRZM model, widely used for pesticide contamination studies in agricultural fields, is "field-scale" only (i.e. it considers the agricultural field only and does not consider a downslope, adjacent buffer area). On the other end of the spectrum, the HSPF watershed model is "watershed-scale"(i.e., it considers entire drainage basins), so that what might be happening on a two-land-area hillside in that larger drainage area is considered by its resolution. Thus, the "hillside-scale" of the local watershed algorithm is intermediate between these two extremes and needed to be custom-developed.

- **A carefully selected hybrid of empirical and mechanistic algorithms and approaches are used to maximize overall suitability for the purposes of the 3MRA modeling system.** From a model development perspective, the 3MRA framework presented an interesting challenge with regard to selection of appropriate levels of mechanistic detail. As a general rule, the more scientifically based (mechanistic) the model, the greater potential that model has to provide realistic simulations under a variety of environmental conditions. However, that potential carries with it the price of including many parameters that must be estimated from site-specific data before these highly parameterized models reach their potential. This essentially requires site-specific model calibration. In contrast, the 3MRA modeling system is applied to many sites with limited site-specific data. Thus, site-specific model calibration was not an option and the modeling approach needed to be based on a judicious balance of theoretical and empirical methods. For example, the GSCM is based on theoretical, mass balance principles, but involves parameters that are readily available (e.g., soil properties, constituent properties), or can be assigned from national distributions. Other algorithms (e.g., the Universal Soil Loss Equation for eroded soil losses, and the "curve number" method for estimating stormwater runoff) are fundamentally empirical, yet are widely used and acknowledged to provide reasonable predictions for planning-level applications.

5.3.2 Uncertainty and Limitations

The major limitations of the Land-based Source Modules and their implications are summarized below, by model.

Limitations of the GSCM. The GSCM was originally designed for the 3MRA modeling system to make some modest improvements to the well-known Jury model, which had been used historically to simulate constituent fate and transport in land-based sources. The GSCM has the following limitations:

- **Series solution of diffusion/decay/advection processes is problematic for some constituents.** The GSCM solves the mass balance differential equation sequentially in time in the following order: diffusive transport, internal decay, advective transport. This approach is justified conceptually on the basis of linearity and the principle of superposition; however, the approach can lead to simulation errors when relatively large time steps are taken. The magnitude of the errors would depend on the relative loss rates associated with the three processes. For example, if the first-order loss rate due to degradation were high and the calculation time step were sufficiently large, then leachate flux and the mass of constituent remaining for the advection phase would be underestimated.

- **Leachate flux postprocessing algorithm is artificial.** The leachate flux postprocessing algorithm postprocesses the constituent mass in the leachate over the total period of the simulation and attempts to allocate it over the individual years in the simulation in a reasonable manner. This postprocessing is needed for persistent constituents (highly sorbed, low decay) because of the combination of choice of the GSCM state variable (total concentration) and the diffusion/decay/advection series solution methodology. Patterned after the Jury model, the GSCM's state variable is total (sorbed + dissolved + gaseous) constituent concentration. The "effective solute convection velocity," V_E, is not the actual leachate infiltration velocity, but rather (because total constituent is the state variable, not dissolved) is corrected to account for sorption. When that sorption is high (high K_d), the V_E is small and can be much smaller (slower velocity) than the true infiltration rate. "Convective transport," i.e., advection, of the constituent from one computational layer in the GSCM down to the next (or from the bottom layer out as leachate) is performed only when the constituent has traversed the depth of a computational layer (typically 1 cm) as measured by V_E, not by the actual infiltration velocity. For very small values of V_E, this travel time can become excessive, and vertical movement due to advective transport may not occur within a year; indeed, it may not occur for the duration of the simulation. In reality, dissolved constituent would be more or less continuously moving downward due to advective transport in the infiltration. The postprocessing algorithm attempts to mitigate this limitation.

- **Treatment of different zones with appropriate boundary conditions is not possible.** The GSCM solution methodology does not allow a rigorous treatment of scenarios where different zones with different sorption characteristics exist in the soil column. For example, if the landfill soil column had a liner with less sorptive capacity than the waste zone, then the liner's sorptive capacity would be exhausted relatively quickly relative to the waste zone's. At this point, since dissolved constituent drains from the waste zone into the liner, there would be no further reduction by sorption, and a boundary condition should be applied at this waste/liner interface that requires a zero concentration gradient for dissolved constituent. The GSCM cannot accommodate such a boundary condition (or an analogous waste/cover boundary condition), superficially because the GSCM is simulating total (not dissolved) constituent, but more fundamentally because the underlying solution methodology is simply not designed to deal with internal boundary conditions. This limitation has been addressed by imposing the relevant boundary condition, but it is not a mathematically rigorous treatment of the physical scenario. A more elegant solution would be to include nonlinear sorption kinetics in the algorithm, so that the relative differences in sorption among different zones are intrinsically accounted for, rather than imposed by boundary conditions.

- **Simulation of volatilization out of the surface of soil column is artificial.** The GSCM's simulation of diffusive transport over the depth of the soil column transports total constituent in accordance with the constituent's water diffusivity (corrected for sorption). This diffusion is treated as diffusion in an infinitely deep column, so that *total* constituent flux is effectively diffused across the surface of the soil column. The amount of constituent mass that is not in the gaseous phase, but has been (erroneously) diffused across the surface, is then calculated and "replaced" back into the top computational layer to better reflect reality. It is unclear to what extent this overall treatment biases the volatile emissions themselves, but the re-introduction of the escaping, nongaseous constituent into the surficial soil layer is artificial and could lead to an erroneous estimate of the vertical concentration gradient.

Limitations of the Local Watershed Model. The Local Watershed Model has the following limitations:

- **Burial/erosion introduces minor mass balance error.** The burial/erosion mechanism introduces a minor mass balance error into the model. The model for surface soil/runoff fate and transport is based on a conceptual model originally developed for use in a stream/sediment application 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 a constituent does not introduce a mass balance error. However, in this 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 constituent is eroded from the surface computational 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 multiplied by its average sorbed constituent concentration. In most cases, this error as a percentage of the total constituent mass in the modeled WMU will be quite small, and that has been confirmed in multiple executions of the model.

- **Potential hot spots in the local watershed buffer subarea are diluted.** The local watershed buffer is considered as a single, homogeneous subarea by the model to facilitate watershed delineation and decrease run time. This will result in spatial averaging of concentrations in the buffer.

- **Sheet flow is assumed across buffer subarea.** The conceptual Local Watershed Model construct assumes that runoff and erosion occur as sheet flow from the WMU across the buffer subarea to the waterbody. This implicitly assumes no short-circuiting of constituent loads directly from the WMU to the downslope waterbody, such as might actually occur in runoff/erosion-created ditches or swales. To the extent that such short-circuiting might occur, the model will underestimate waterbody constituent loadings. Mass balance is maintained; consequently, any such underestimation would come at the expense of overestimating soil concentrations in the (bypassed) buffer zone.

- **Hydrological responses are limited by the available record.** The hydrology model uses available historical records of meteorological data. When the number of years simulated exceeds the number of years in the record, the record is repeated. Thus, unusual hydrological events (e.g., major storms) are limited to those actually observed. Events not observed, but possible nonetheless, that could result in increased source releases or media transport will not be included in the simulation.

Limitations of the Particulate Emissions Model. The particulate emissions models were incorporated without changes from the sources discussed (mostly AP-42) and have the same limitations as those models, as described in the source documentation.

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