4.0   Wastewater Source Modules

4.1   Purpose and Scope

The Wastewater Source Modules simulate wastewater management. Two Wastewater Source Modules were developed for the 3MRA modeling system to represent the common management practices for industrial wastewaters. These management practices include flow equalization, storage, treatment (typically biological treatment or neutralization), and solids settling (clarification). The two waste management units (WMUs) for wastewaters are

- ■   **Surface Impoundments**, which may be either aerated or quiescent and are used to treat, store, or dispose of many industrial wastewaters; and

- ■   **Aerated Tanks**, which are aerated or mixed tanks used to treat or store many industrial wastewaters.

The two Wastewater Source Modules use a common set of algorithms with similar mass balance and transport equations. Both modules estimate volatile emissions to air. Leaching losses from the bottom of the unit are modeled only for surface impoundments; tanks are assumed to have impervious bottoms. Both modules simulate degradation and solids settling, although solids settling and accumulation are more significant for quiescent units.

The two Wastewater Source Modules were designed to provide estimates of annual average volatilization rates to air, which are used by the Air Module. In addition, the Surface Impoundment Module outputs annual average infiltration rates and leachate constituent flux rates, which are used by the Vadose Zone and Aquifer Modules, and annual average surface impoundment water concentrations, which are used by the Ecological Exposure Module to estimate exposure to wildlife receptors that may drink or consume organisms from the impoundment. Figure 4-1 shows the relationship and information flow between the Wastewater Source Modules and the 3MRA modeling system.

The Wastewater Source Modules have six major functions, as follows:

1.   **Calculate constituent concentrations within the unit.** The Wastewater Source Modules use a mass-balance, temperature-adjusted approach to estimate constituent concentrations in the WMU. This approach considers constituent diffusion between wastewater and sediments, and constituent removal by volatilization, biodegradation, hydrolysis, partitioning to solids, solids settling, and, for surface impoundments only, infiltration through the bottom of the unit.
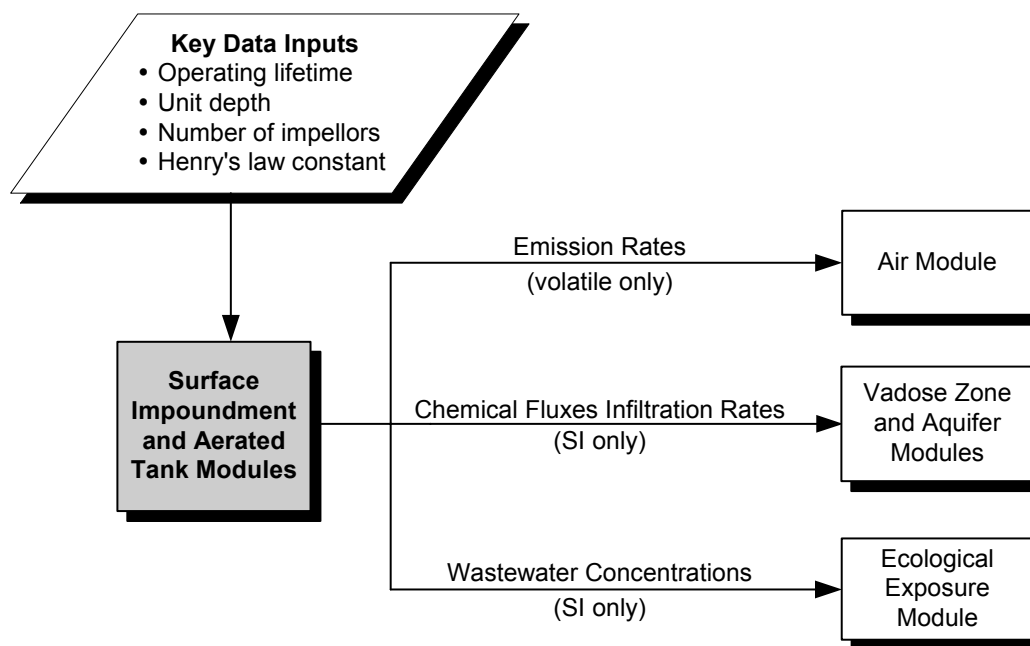
Figure 4-1. Information flow for the Wastewater Source Module in the 3MRA modeling system.

2. **Calculate solids concentrations within the unit.** The Wastewater Source Modules use a mass-balance approach to estimate solids concentrations in the WMU.

3. **Calculate volatile emission rates.** The modules calculate volatile emission rates for both aerated and quiescent surfaces.

4. **Estimate resuspension, sedimentation, and burial velocities within the units.**

5. **Estimate constituent release in leachate.** The Surface Impoundment Module calculates infiltration rates and constituent leachate flux rates for use in the Vadose Zone and Aquifer Modules. The Aerated Tank Module does not calculate leachate release, as tanks are assumed to have impervious bottoms.

6. **Adjust for temperature effects.** The modules account for the effect of temperature on air viscosity and density, water viscosity, chemical properties, and sediment biodegradation rates.

4.2 Conceptual Approach

This section first describes the two different WMUs and the processes modeled for them, and then describes the major model functions listed above.

4.2.1   Description of Waste Management Units

The Aerated Tank Module was developed to model tanks that are aerated or mixed; thus, it uses a well-mixed, steady-state mass balance solution. Tanks are assumed to have an impervious bottom; therefore, leaching is not modeled for tanks.

The Surface Impoundment Module was developed to model both aerated and quiescent impoundments using either a well-mixed, steady-state mass balance solution for well-mixed impoundments or a time-dependent mass balance solution for plug flow, batch, or disposal impoundments.

The following assumptions were made in developing both modules:

■   The WMU is divided into three distinct compartments: impoundment liquid, unconsolidated sediment, and consolidated sediment. Each compartment has a fixed volume for a given monthly solution and volumes are readjusted to account for solids accumulation. The three-compartment model is described in more detail later in this section.

■   Aerated tanks are well mixed; surface impoundments may be well mixed or have plug or batch flow. For well-mixed units, a steady-state mass balance solution is used. For plug or batch flow impoundments, a time-dependent mass balance solution is used.

■   Volatilization in the liquid compartment follows first-order kinetics.

■   Hydrolysis in both the liquid and sediment compartments follows first-order kinetics.

■   Aerobic biodegradation in the liquid compartment follows first-order kinetics with respect to both constituent concentration and biomass concentration.

■   Biomass growth rate follows Monod kinetics with respect to total biological oxygen demand loading.

■   Solids settling follows first-order kinetics.

■   Anaerobic biodegradation of constituent in the sediment compartments follows first-order kinetics.

■   The biomass decay rate within the accumulating sediment compartment is first-order.

■   There is no constituent in precipitation (i.e., rain or snow).

■   Constituent partitioning among adsorbed solids, dissolved phases, and vapor phases is linear.

■ A moisture-dependent infiltration rate is calculated using Darcy's law and Van Genuchten moisture relationships.

Figure 4-2 illustrates the model construct for both Wastewater Source Modules, which are divided into three primary compartments:

■ The **liquid compartment** includes the influent and effluent wastewater streams and the aqueous liquid layer above the sediment at the bottom of the unit. Liquid enters the compartment via the influent waste stream and rainfall, and leaves the compartment via evaporation and the effluent waste stream. Processes modeled in this compartment include volatilization, aerobic biodegradation, constituent hydrolysis, biomass solids growth, and solids settling and resuspension.

■ The **unconsolidated sediment compartment** is a layer of loose sediment immediately below the liquid compartment. Processes modeled in this layer include anaerobic biological degradation and burial of solids into the consolidated sediment compartment.

■ The **consolidated sediment compartment** is a layer of compacted sediment at the bottom of the unit. Processes modeled in this compartment include anaerobic degradation and removal of solids by cleaning and dredging and by decomposition due to anaerobic digestion.
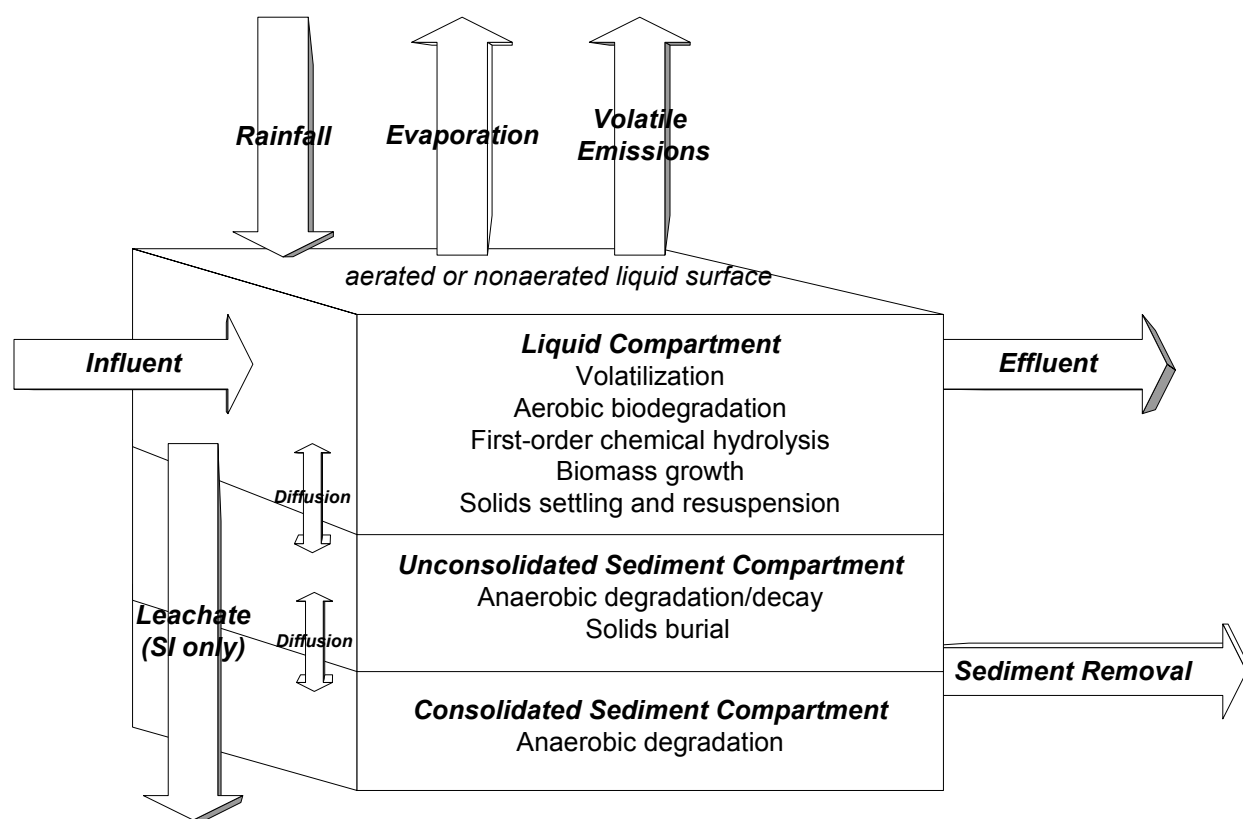

Figure 4-2. Conceptual model schematic for Wastewater Source Modules.

As shown in Figure 4-2, sediment is deposited and resuspended across the boundary between liquid and unconsolidated sediment, but only deposition (burial) occurs between the unconsolidated to consolidated sediment compartments. The modules also allow constituents to diffuse between adjacent compartments. In addition, the Surface Impoundment Module models leachate loss from the liquid layer through the sediment layers to the underlying soil.

For each compartment, the Wastewater Source Modules perform mass balances at time intervals small enough that the hydraulic retention time in the liquid compartment is not significantly affected by the solids settling and accumulation. In the liquid compartment, there is flow both in and out of the WMU, with constituent loss through volatilization, constituent decay (hydrolysis), aerobic biodegradation, and particle settling and burial (net sedimentation).

The following processes are modeled in the liquid compartment:

- ■   Volatilization using a two-film model and mass transfer correlations from *Air Emissions Models for Waste and Wastewater* (U.S. EPA, 1994).

- ■   Constituent loss due to hydrolysis and biodegradation using first-order rate constants for natural soil systems. These are adjusted to WMU conditions by assuming an effective system biomass concentration of 2.0×10^{-6} Mg/m.[3]

- ■   Particle removal using particle settling velocities to estimate the projected sediment removal efficiency of the unit.

The modules estimate solids generation in the liquid compartment according the relationship of biological growth to the decomposition of organic chemicals (as biological oxygen demand) in the influent. These solids settle in the liquid to form the two underlying sediment compartments.

The following processes are modeled in the sediment compartments:

- ■   Constituent loss due to hydrolysis and (anaerobic) biodegradation using first-order degradation rate constants. Hydrolysis and biodegradation rate constants are assumed to apply to the total constituent concentration (both dissolved and sorbed constituent) in each compartment.

- ■   Constituent mixing between the compartments through constituent diffusion as well as particle sedimentation and resuspension.

- ■   Solids destruction due to sludge digestion. It is assumed that solids decomposition is limited to the fraction of solids that are biologically active.

- ■   Sediment compaction in the consolidated compartment, estimated by calculating the vertical effective stress across the consolidated sediment. Sediment compaction impacts the depth, volumetric water fraction, and the effective hydraulic conductivity of the consolidated sediment compartment.

Using the well-mixed assumption, the model assumes that the suspended solids concentration within the WMU is constant throughout the unit. However, some stratification of sediment is expected across the length and depth of the WMU so that the effective total suspended solids concentration within the unit is assumed to be a function of the WMU's total suspended solids removal efficiency rather than equal to the effluent total suspended solids concentration. The liquid (dissolved) phase constituent concentration within the unit, however, is assumed to be equal to the effluent dissolved phase concentration for the well-mixed model solution.

4.2.2   Calculate Constituent Concentrations within the Unit

The governing constituent mass balance equations used to calculate the constituent concentrations in the liquid and sediment compartments of the impoundment or tank are presented in the box starting on the next page. Detailed equations and solutions used by the Surface Impoundment and Aerated Tank Modules can be found in U.S. EPA (1999), including all assumptions and algorithms used in the modules.

The following sections describe the calculations for each of the three compartments, and the calculations for diffusion between the liquid and sediment compartments.

4.2.2.1   Liquid Compartment. The change in the constituent mass in the liquid compartment is a function of the constituent loss through volatilization, aerobic biodegradation, hydrolysis, and infiltration (denoting liquid flow of both liquid and entrained solids) into the sediment compartment. In addition, constituent is transported across the liquid/sediment compartment interface by constituent diffusion and by solids settling and resuspension. These processes are affected by whether the unit is aerated or nonaerated, and by constituent-specific properties.

For the time-dependent solution, the initial liquid compartment concentration is equal to the influent waste concentration.

4.2.2.2   Unconsolidated Sediment Compartment. The change in constituent mass within the unconsolidated sediment compartment is dependent on constituent infiltration from the liquid compartment (which includes entrained sediment), "filtered" leachate out the bottom of the compartment, and constituent loss through hydrolysis and anaerobic biodegradation. In addition, constituent is transported across the liquid/sediment compartment interface by constituent diffusion and by solids settling and resuspension. Constituent is transported across the unconsolidated/ consolidated compartment interface by constituent diffusion.

For aerated tanks, the initial sediment depth is zero. For surface impoundments, the initial sediment depth is 20 cm (unconsolidated). When the simulation begins, this initial sediment mass is partitioned equally into the unconsolidated and consolidated sediment compartments. The sediment mass is fixed for each month. At the end of the month, the gross mass of sediment accumulated during the month is calculated and the mass of sediment that is decomposed is calculated, resulting in a net mass of accumulated sediment. This net mass of accumulated sediment is partitioned equally into the unconsolidated and consolidated sediment compartments prior to simulation of the next month.

Aerated Tank and Surface Impoundment Constituent Mass Balance Equations
(variables listed on next page)

Liquid Compartment

Time-dependent constituent mass balance (surface impoundments only):

$$-\frac{\partial\left(V_1 C_{tot,1}\right)}{\partial t} = Q_{leach} C_{tot,1} + f_{d,1} K_{OL} A\, C_{tot,1} + V_1\left(k_{bm} k_{ba}[TSS]_1 + k_{hyd}\right)\, C_{tot,1}$$

$$+ v_{sed} A\, f_{p,1} - v_{res} A\, f_{p,2}\, C_{tot,2} - v_{diff\,12} A\, \theta_{liq,2}\left(f_{d,2}\, C_{tot,2} - f_{d,1}\, C_{tot,1}\right)$$

Well-mixed model solution:

$$Q_{\inf l} C_{tit,\inf l} - Q_{out} C_{tot,out} = Q_{leach} C_{tot,1} + f_{d,1} K_{OL} A\, C_{tot,1} + V_1\left(k_{bm} k_{ba}[TSS]_1 + k_{hyd}\right)\, C_{tot,1}$$

$$+ v_{sed} A\, f_{p,1} - v_{res} A\, f_{p,2}\, C_{tot,2} - v_{diff\,12} A\, \theta_{liq,2}\left(f_{d,2}\, C_{tot,2} - f_{d,1}\, C_{tot,1}\right)$$

Unconsolidated Sediment Compartment

Time-dependent constituent mass balance (surface impoundments only):

$$-\frac{\partial(V_2\, C_{tot,2})}{\partial t} = Q_{leach}\, f_{d,2}\, C_{tot,2} - Q_{leach}\, C_{tot,1} + (k_{bs} + k_{hyd})\, V_2\, C_{tot,2}$$

$$+ (v_{res} + v_b)\, A\, f_{p,2}\, C_{tot,2} - v_{sed}\, A\, f_{p,1}\, C_{tot,1}$$

$$+ v_{diff12}\, A\, \theta_{liq,2}\, (f_{d,2}\, C_{tot,2} - f_{d,1}\, C_{tot,1})$$

$$+ v_{diff23}\, A\, \theta_{liq,3}\, (f_{d,2}\, C_{tot,2} - f_{d,3}\, C_{tot,3})$$

For the well-mixed model solution, the left-hand side of the time-dependent mass balance equation is set to zero.

Consolidated Sediment Compartment

Time-dependent constituent mass balance (surface impoundments only):

$$-\frac{\partial(V_3\, C_{tot,3})}{\partial t} = Q_{leach}\, f_{d,3}\, C_{tot,3} - Q_{leach}\, f_{d,2}\, C_{tot,2} + (k_{bs} + k_{hyd})\, V_3\, C_{tot,3}$$

$$+ v_{diff23}\, A\, \theta_{liq,3}\, (f_{d,3}\, C_{tot,3} - f_{d,2}\, C_{tot,2})$$

For the well-mixed model solution, the left-hand side of the time-dependent mass balance equation is set to zero.

<div align="right">*(continued)*</div>

Constituent mass balance equation variables
(x denotes the compartment: 1 = liquid, 2 = unconsolidated sediment, 3 = consolidated sediment)

$C_{tot,x}$	=	total constituent concentration in compartment x (mg/L = g/m^3)
$C_{tot,infl}$	=	total constituent concentration in influent (mg/L = g/m^3)
$C_{tot,out}$	=	total constituent concentration in effluent (mg/L = g/m^3)
Q_{leach}	=	leachate flow rate from WMU (m^3/s)
Q_{infl}	=	influent flow rate into WMU (m^3/s)
Q_{out}	=	effluent flow rate out of WMU (m^3/s)
K_{OL}	=	overall volatilization mass transfer coefficient (m/s)
A	=	total surface area of WMU (m^2)
V_1	=	volume of liquid compartment in WMU= d_1 A (m^3)
V_2	=	volume of unconsolidated sediment compartment in WMU (m^3)
V_3	=	volume of consolidated sediment compartment in WMU (m^3)
d_1	=	depth of liquid compartment (m)
k_{hyd}	=	hydrolysis rate (1/s)
k_{bm}	=	complex first order biodegradation rate constant (m^3/Mg-s)
k_{ba}	=	ratio of biologically active solids to the total solids concentration (i.e., k_{ba} = [MLVSS]$_1$/[TSS]$_1$)
k_{bs}	=	anaerobic biodegradation decay rate of constituent (1/s)
[TSS]$_x$	=	concentration of total suspended solids (TSS) in compartment x (g/cm^3 = Mg/m^3)
[MLVSS]$_1$	=	concentration of biomass as mixed liquor volatile suspended solids (MLVSS) liquid compartment (g/cm^3 = Mg/m^3)
v_{sed}	=	solids settling or sedimentation velocity (m/s)
v_{res}	=	solids resuspension velocity (m/s)
v_b	=	solids burial velocity (m/s)
v_{diff12}	=	mass transfer coefficient between liquid compartment (1) and unconsolidated sediment compartment (2) (m/s)
v_{diff23}	=	mass transfer coefficient between unconsolidated sediment compartment (2) and consolidated sediment compartment (3) (m/s)
$f_{d,x}$	=	dissolved constituent fraction in compartment x:

$$f_{d,x} = \frac{C_{liq,x}}{C_{tot,x}} = \frac{1}{\left(\theta_{liq,x} + k_{ds}[TSS]_x\right)}$$

$f_{p,x}$	=	particulate constituent fraction in compartment x:

$$f_{p,x} = \frac{C_{sol,x}[TSS]_x}{C_{tot,x}} = \frac{k_{ds}[TSS]_x}{\left(\theta_{liq,x} + k_{ds}[TSS]_x\right)}$$

$\theta_{liq,x}$	=	volumetric liquid fraction of compartment x (m^3/m^3)
$C_{liq,x}$	=	liquid-phase constituent concentration in compartment x (mg/L = g/m^3)
$C_{sol,x}$	=	solid-phase constituent concentration in compartment x (mg/kg = g/Mg)
k_{ds}	=	solid-water partition coefficient (m^3/Mg) = $K_{oc} \times f_{oc}$ for organics
K_{oc}	=	soil-water partitioning (m^3/Mg)
f_{oc}	=	fraction organic carbon in the waste (mass fraction).

The initial sediment compartment concentrations are calculated by assuming the sediment compartments' void space is filled with waste at the influent concentration and that the initial sediment particles do not contain any contaminant. For each subsequent month, the initial sediment compartment constituent concentration (for either sediment compartment) is estimated based on the previous month's sediment compartment concentration. For a plug-flow unit, it is estimated as the log mean average sediment compartment concentration across the unit from the previous month. For batch units, it is the final sediment compartment concentration at the end of the previous month.

4.2.2.3 Consolidated Sediment Compartment. The change in the constituent mass within the consolidated sediment compartment is a function of "filtered" leachate flow from the unconsolidated sediment compartment and out the bottom of the unit, and constituent loss through hydrolysis and biodegradation. In addition, constituent is transported across the unconsolidated/consolidated compartment interface by constituent diffusion.

4.2.2.4 Diffusion between Liquid and Sediment. The models estimate effective diffusion velocity between the liquid and sediment compartments using the following two-resistance model based on the liquid phase mass transfer coefficient for quiescent surfaces and the porosity of the sediment compartment:

$$v_{diff} = \left(\frac{1}{k_{l,q}} + \frac{1}{k_{eff,2}} \right)^{-1} \tag{4-1}$$

where

v_{diff} = effective diffusion velocity between liquid and sediments

$k_{l,q}$ = liquid phase mass transfer coefficient for quiescent surface areas as calculated in Section 4.2.3 (m/s)

$k_{eff,2}$ = effective liquid mass transfer coefficient in sediment compartment (m/s).

To determine the effective liquid mass transfer coefficient in the sediment compartment, the models first calculate the effective liquid diffusion rate from the porosity of the sediment layer using the Millington-Quirk tortuosity model (Millington and Quirk, 1961):

$$D_{eff,2} = \theta_{liq,2}^{\frac{4}{3}} \times D_{i,l} \tag{4-2}$$

where

$D_{eff,2}$ = effective liquid diffusion rate (cm^2/s)

$\theta_{liq,2}$ = volumetric porosity (assumed to be liquid filled) of sediment compartment = $1 - [TSS]_2 / \rho_{TSS}$, where ρ_{TSS} = density of total suspended solids

$D_{i,l}$ = diffusivity in liquid (water) (cm^2/s).

In most cases, the sediment accumulating at the bottom of the WMU will be more of a viscous sludge layer than a rigid mass of particles. Therefore, the top layer of sediment is expected to be affected by the bulk currents within the WMU (caused by wind shear, aeration, or mixing) similar to the liquid phase mass transfer coefficient for quiescent surfaces. The liquid phase quiescent mass transfer coefficient is primarily a function of the liquid diffusivity raised to the two-thirds power; therefore, the models estimate the effective liquid mass transfer coefficient from the liquid compartment to the sediment layer as follows:

$$k_{eff,2} = k_{l,q} \left(\frac{D_{eff,2}}{D_{i,1}} \right)^{\frac{2}{3}} = k_{l,q} \, \theta_{liq,2}^{\frac{8}{9}} \qquad (4\text{-}3)$$

4.2.3   Calculate Solids Concentrations within the Unit

The time-dependent solution for estimating total solids concentration within the unit is based on the assumption of constant total suspended solids (TSS) concentration. In reality, the solids concentration varies, either increasing as a result of biomass production from the consumption of organic material in the waste stream or decreasing as a result of solids settling. The solids mass balance for the liquid compartment is

$$\frac{- \partial (V_1 [TSS]_1)}{\partial t} = r_{BOD} \lambda \, k_{ba} [TSS]_1 V_1 + v_{res} [TSS]_2 A - Q_{leach} [TSS]_1 - v_{sed} A [TSS]_1 \qquad (4\text{-}4)$$

where

$[TSS]_1$	=	concentration of total suspended solids in liquid compartment (g/cm^3 = Mg/m^3)
V_1	=	volume of liquid compartment (m^3)
r_{BOD}	=	normalized biodegradation rate of BOD_5 (g-BOD/g-biomass/sec)
λ	=	biomass yield (g-biomass (dry basis)/g-BOD consumed)
k_{ba}	=	ratio of biologically active solids to the total solids concentration (i.e., $k_{ba} = [MLVSS]_1/[TSS]_1$)
v_{res}	=	solids resuspension velocity (m/s)
$[TSS]_2$	=	concentration of total suspended solids in unconsolidated sediment compartment (g/cm^3 = Mg/m^3)
A	=	total surface area of WMU (m^2)
Q_{leach}	=	leachate flow rate from WMU (m^3/s)
v_{sed}	=	solids settling or sedimentation velocity (m/s).

The normalized BOD_5 biodegradation rate is estimated using the Monod equation as follows:

$$r_{BOD} = \frac{K_{bmax} \, C_{BOD}}{(K_{b2} + C_{BOD})} \qquad (4\text{-}5)$$

where

$C_{BOD,infl}$ = BOD_5 concentration in the influent to the WMU (g/cm^3 or Mg/m^3)

$C_{BOD,1}$ = BOD_5 concentration in the liquid compartment (g/cm^3 or Mg/m^3)

K_{bmax} = maximum BOD_5 biodegradation rate (g-BOD/g-biomass/sec or Mg/Mg/sec)
= $6.94 \times 10^{-6} \times T_{corr}$ (the value of 6.94×10^{-6} comes from the maximum rate of 0.6 g-BOD/g-biomass/hr ÷ 86,400 sec/hr)

K_{b2} = half-saturation constant = 0.00005 (g/cm^3 or Mg/m^3)

T_{corr} = temperature correction factor for biodegradation rate constants (see Section 4.2.7.5).

The models estimate the maximum BOD_5 degradation rate constant based on a typical design value for F/M (a 0.6 food-to-biomass ratio) for activated sludge systems based on values in Eckenfelder et al. (circa 1984) and Hermann and Jeris (1992). The model uses a typical half-saturation rate constant (K_{b2}) of 50 mg/L (0.00005 g/cm^3) selected from values reported in the literature (Tabak et al., 1989; Gaudy and Kincannon, 1977; Goldsmith and Balderson, 1989; Rozich et al., 1985) .

The integration period time steps in the overall time-dependent solution depend on how quickly the total suspended solids and BOD_5 concentrations vary. The model selects an initial time step based on the initial concentrations of TSS and BOD_5 so that BOD_5 concentrations are effectively constant. The TSS concentration is calculated at the end of the first time step and compared to the starting total suspended solids concentration; if it changes by more than a factor of 5, additional time steps are added until the starting and ending TSS concentrations differ by less than a factor of 5. This allows the model to determine an effective average TSS concentration across a given time step that can be used as a constant value in the constituent mass balance solution equations.

For well-mixed systems, the model calculates the effluent TSS concentration from the predicted solids removal efficiency of the unit (see Section 4.2.5) and the predicted BOD_5 removal efficiency. The TSS mass balance for the liquid compartment can be written as

$$[TSS]_{out} = \frac{Q_{infl}}{Q_{out}} (1 - \epsilon_{TSS}) ([TSS]_{infl} + \lambda \, \epsilon_{BOD} \, C_{BOD,infl}) \qquad (4\text{-}6)$$

where

ϵ_{TSS} = total suspended solids mass removal efficiency in WMU (unitless)
λ = biomass yield (g-biomass (dry basis)/g-BOD)
ϵ_{BOD} = biological oxygen demand removal efficiency of WMU (unitless)
$C_{BOD,infl}$ = biological oxygen demand of influent (Mg/m^3)
$[TSS]_{infl}$ = concentration of total suspended solids in the influent (g/cm^3 = Mg/m^3).

$[TSS]_{out}$ = concentration of total suspended solids in the effluent ($g/cm^3 = Mg/m^3$).
Q_{infl} = influent flow rate into WMU (m^3/s)
Q_{out} = effluent flow rate out of WMU (m^3/s).

Although the liquid compartment is assumed to be well mixed, solids removal and growth are not expected to be instantaneous. To account for gradients of TSS concentration along the WMU length and depth, the model estimates the effective TSS concentration within the WMU as the log-mean average between the influent and effluent total suspended solids concentrations (based on first-order sedimentation). Given the influent and effluent total suspended solids concentrations, the effective (mean) total suspended solids concentration in the liquid compartment is

$$[TSS]_1 = \exp\left[\frac{(\ln[TSS]_{infl}) + \ln([TSS]_{out})}{2}\right] \qquad (4\text{-}7)$$

The model calculates BOD_5 removal efficiency based on the BOD_5 biodegradation rate using the same biodegradation rate model used for the time-dependent solution. Because the model uses BOD_5 degradation rate primarily to determine the production rate of biological solids within the impoundment, it neglects decreases in BOD_5 concentrations due to dilution by precipitation (i.e., the influent flow rate is assumed to be equal to the effluent flow rate plus the leachate flow rate). With this simplification, the BOD_5 removal efficiency can be written as follows:

$$\epsilon_{BOD} = \frac{r_{BOD}\, k_{ba}\, [TSS]_1\, V_1}{Q_{infl}\, C_{BOD,infl}} \qquad (4\text{-}8)$$

Because BOD_5 removal efficiency depends on the effective TSS concentration, the model calculates the effective TSS concentration using iterative calculations between estimating the BOD_5 removal efficiency and the effective TSS concentration.

4.2.4   Calculate Volatile Emission Rates

The Wastewater Source Modules use an overall mass transfer coefficient that determines the rate of volatilization based on a two-resistance model: a liquid-phase mass transfer resistance and a gas-phase mass transfer resistance. The liquid- and gas-phase mass transfer resistances for turbulent surfaces are very different from those for quiescent (laminar flow) surfaces. Therefore, the overall mass transfer coefficient is a composite of the coefficients for the turbulent surface area and the quiescent surface area. The overall coefficient is based on an area-weighted average, as follows:

$$K_{OL} = \frac{K_{OL,t}\, A_t + K_{OL,q}\, A_q}{A} \qquad (4\text{-}9)$$

where

K_{OL} =   overall mass transfer coefficient for the WMU (m/s)
$K_{OL,t}$ =   overall mass transfer coefficient for turbulent surface areas (m/s)
A_t =   turbulent surface area = $f_{aer} A (m^2)$
f_{aer} =   fraction of total surface area affected by aeration (unitless)
A   =   total surface area (m^2)
$K_{OL,q}$ =   overall mass transfer coefficient for quiescent surface areas (m/s)
A_q =   quiescent surface area (m^2) = $(1-f_{aer}) \times A$ (Note: $A_t + A_q$ must equal A).

The overall mass transfer coefficient for turbulent surface areas based on the two-resistance model is

$$K_{OL,t} = \left(\frac{1}{k_{l,t}} + \frac{1}{H' \, k_{g,t}} \right)^{-1} \tag{4-10}$$

where

$k_{l,t}$ =   liquid-phase mass transfer coefficient for turbulent surface areas (m/s)
H' =   dimensionless Henry's law constant = H/RT_H
$k_{g,t}$ =   gas-phase mass transfer coefficient for turbulent surface areas (m/s).

Similarly, the overall mass transfer coefficient for quiescent surface areas is

$$K_{OL,q} = \left(\frac{1}{k_{l,q}} + \frac{1}{H' \, k_{g,q}} \right)^{-1} \tag{4-11}$$

where

$k_{l,q}$ =   liquid-phase mass transfer coefficient for quiescent surface areas (m/s)
$k_{g,q}$ =   gas-phase mass transfer coefficient for quiescent surface areas (m/s).

The mass transfer correlations used to estimate the liquid- and gas-phase mass transfer coefficients for turbulent and quiescent surfaces are the same as those used in the WATER8 and CHEMDAT8 emission models developed by EPA. Basic equations are provided in U.S. EPA (1999) with a more detailed treatment in Chapter 5 of the CHEMDAT8 model documentation (U.S. EPA, 1994).

4.2.5   Estimate Resuspension, Sedimentation, and Burial Velocities

To solve the constituent and sediment mass balance equations, the Wastewater Source Modules must estimate the transfer rate of the sediment (and its associated constituent content) between the liquid and sediment compartments in the WMU. Key parameters in this calculation include

■ Sedimentation velocity, which establishes the rate at which particles in the liquid compartment enter the unconsolidated sediment compartment;

■ Resuspension velocity, which establishes the rate at which particles in the unconsolidated sediment compartment enter the liquid compartment; and

■ Burial rate, which is the net accumulation rate of sediment in the two sediment compartments.

Sediment movement between the liquid and sediment compartment should vary primarily with the dimensions and flow characteristics of the WMU, and with the relative surface area affected by turbulent mixing. The general approach used to estimate the various sediment transport rates is to first estimate the suspended solids mass removal efficiency of the WMU. Given this removal efficiency, the Wastewater Source Modules estimate the resuspension, sedimentation, and burial velocities based on the characteristics of the mean-sized particles in the WMU.

4.2.5.1 Estimate Design Sediment Removal Efficiency. The WMU quiescent surface area and flow rate are used to calculate the vertical (or "upflow") velocity of the impoundment as follows:

$$v_{upflow} = \frac{Q_{infl}}{A_q}$$

(4-12)

where

v_{upflow} = upflow velocity (m/s)
Q_{infl} = influent flow rate into WMU (m^3/s)
A_q = quiescent surface area (m^2).

The upflow velocity is assumed to act on the liquid compartment to cause an upward flux of particles. The model estimates sediment removal efficiency in the WMU from WMU flow rate, surface area (i.e., the upflow velocity), and particle size distribution characteristics (mean particle size and relative standard deviation) by considering the terminal settling velocity of the particles. Particles with a terminal settling velocity greater than the upflow velocity settle within the WMU, while particles with a terminal velocity less than the upflow velocity remain suspended and are entrained in the effluent.

The model assumes that suspended solids are spherical when calculating the terminal velocity (or critical particle diameter) and the mass-to-volume ratio of the particles. The model calculates the terminal velocity of a sphere using Stoke's Law (see U.S. EPA 2001), and determines the particle diameter that has a terminal velocity equal to the upflow velocity. The mass sediment removal efficiency of the WMU is then calculated from the particle size distribution (model input parameters assuming lognormal distribution) and the mass of particles of a given diameter (based on spherical particles). The lognormal distribution density function is

$$\phi(d_{part}) \;=\; \frac{1}{d_{part}\;\sigma\;(2\pi)^{\frac{1}{2}}} \;\times\; \exp\!\left(\frac{-\,[\ln(d_{part}/d_{mean})]^2}{2\sigma^2} \right) \tag{4-13}$$

where

$\phi(d_{part})$ =   distribution density function for sediment particles
d_{part} =   particle diameter (cm)
σ =   standard deviation of $\ln(d_{part})$
d_{mean} =   geometric mean particle diameter = $\exp[\text{mean of } \ln(d_{part})]$ (cm).

The mass of the particle is proportional to its volume; therefore, the density function is evaluated based on the cube of the particle diameter (assuming spherical particles) using the following factor:

$$WtFactor_{part} \;=\; \frac{\pi}{6}\,d_{part}^3 \tag{4-14}$$

where

$WtFactor_{part}$ =   particle weighting factor (cm³)
d_{part} =   particle diameter (cm).

Note that it is assumed that all particles have the same density, regardless of size. Therefore, the design volumetric solids removal efficiency equals the design mass solids removal efficiency, which is calculated as

$$\epsilon_{TSS,o} \;=\; \frac{\int_{d_{crit}}^{+\infty} [\phi(d_{part}) \times WtFactor_{part}]}{\int_{0}^{+\infty} [\phi(d_{part}) \times WtFactor_{part}]} \tag{4-15}$$

where

$\epsilon_{TSS,o}$ =   design mass solids removal efficiency of WMU (mass fraction).

Because of the solution algorithm selected, the equations become unsteady as $\epsilon_{TSS,o}$ approaches 1. To prevent taking the logarithm of zero, the design mass solids removal efficiency is capped at 99.9 percent.

4.2.5.2 Estimate Resuspension, Sedimentation, and Burial Velocities for Time-dependent Model Solution. The time-dependent model uses the design removal efficiency to set a target effluent concentration. The sedimentation velocity is calculated as the terminal velocity for the mean particle size diameter, which is an input to the model, using Stoke's Law (see U.S. EPA, 2001). The resuspension velocity is set so that the total mass of sediment

resuspended will equal the mass settling when the average TSS concentration in the liquid compartment equals the target effluent concentration. The burial rate is then calculated for each individual time step based on the difference in the sedimentation and resuspension rates at the average liquid compartment TSS concentration for that time step. The equations for the resuspension, sedimentation, and burial velocities are

$$v_{sed} = 100 \times v_{part,mean} \tag{4-16}$$

$$v_{res} = v_{sed} \frac{[TSS]_{target}}{[TSS]_2} \tag{4-17}$$

$$v_b = \left(\frac{Q_{leach}}{A} + v_{sed} \right) \frac{[TSS]_{ave}}{[TSS]_2} - v_{res} \tag{4-18}$$

where

$v_{part,mean}$	=	particle settling velocity of a mean-diameter particle (cm/s)
$[TSS]_{target}$	=	target effluent TSS concentration = $[TSS]_{infl} (1 - \epsilon_{TSS,o})$ (g/cm^3 = Mg/m^3)
$[TSS]_{ave}$	=	average TSS concentration in the liquid compartment for a given time interval (g/cm^3 = Mg/m^3)
v_b	=	solids burial velocity (m/s).

As constructed, the time-dependent solution assumes the mass rate of sediment resuspension will equal the mass rate of sediment settling at the target or design effluent TSS concentration. The rate at which the target TSS concentration is reached is dependent on the particle characteristics as well as the growth rate of biomass (i.e., the BOD$_5$ consumption rate). The actual effluent TSS concentration predicted by the model may not reach the target TSS concentration at very low hydraulic residence times or where significant quantities of biosolids are produced. As sediment accumulates in the WMU, the corresponding change in the hydraulic residence time may also affect the predicted effluent TSS concentration.

4.2.5.3 Estimate Resuspension, Sedimentation, and Burial Velocities for Well Mixed Model Solution. In the well-mixed model, mass balance consideration of the sediment requires that the suspended solids burial (or accumulation) rate be determined from the predicted sediment removal efficiency. As constructed, the design sediment removal efficiency is independent of WMU depth, and therefore does not change as sediment accumulates in the WMU. This will generally be true for large depths, but for shallower depths, the increased lateral flow rates tend to cause "short-circuiting" flow patterns, which decrease the sediment removal efficiency of the WMU. To take this phenomenon into account, it is assumed that the sediment removal efficiency remains constant at the design efficiency (i.e., $\epsilon_{TSS} = \epsilon_{TSS,o}$) at liquid depths of 1.2 meters (4 feet) or more based on design considerations of settling chambers. As

the liquid depth becomes less than 1.2 meters, it is assumed that the sediment removal efficiency will decrease as a function of the liquid retention time. A first-order sedimentation rate constant is estimated based on the design sediment removal rate and the WMU retention time at a liquid depth of 1.2 meters. This first-order sedimentation rate constant is calculated as

$$k_{sed} = \frac{-\ln{(1 - \epsilon_{TSS,o})}}{\dfrac{(1.2\ m)\ A}{Q_{infl}}} \tag{4-19}$$

where

   k_{sed} =   apparent first-order sedimentation rate at a liquid depth of 1.2 meters (1/s).

   For liquid depths less than 1.2 meters, the removal efficiency is estimated using this first-order sedimentation rate constant and the hydraulic retention time as

$$\epsilon_{TSS} = 1 - e^{\left(\dfrac{-k_{sed}\ d_1\ A}{Q_{infl}}\right)} \tag{4-20}$$

where

   ϵ_{TSS} =   predicted mass sediment removal efficiency of the WMU as sediment accumulates (mass fraction)
   d_1 =   depth of liquid compartment.

   The predicted mass sediment removal efficiency is assumed to apply equally to influent sediment and sediment generated within the unit. The net rate of sediment transfer or burial from the liquid compartment to the sediment compartment can be calculated based on a mass balance of sediment in the liquid compartment, which can be rearranged to calculate the burial velocity (defined in terms of the sediment concentration in the sediment compartment) as follows:

$$v_b = \frac{Q_{infl}\ ([TSS]_{infl} + \lambda\ \epsilon_{BOD}\ C_{BOD})\ (1 - \epsilon_{TSS})}{A\ [TSS]_2} \tag{4-21}$$

   The resuspension velocity acts on the sediment compartment, and it is assumed to affect the same upward flux of sediment as the upflow velocity. Therefore, the resuspension velocity can be calculated from the upflow velocity and the relative concentrations of particles in the liquid and sediment compartments as follows:

$$v_{res} = v_{upflow} \frac{[TSS_1]}{[TSS_2]} \qquad (4\text{-}22)$$

The sedimentation rate is calculated from the mass balance of sediment in the sediment compartment (Equation 4-4), which can be rearranged as follows.

$$v_{sed} = (v_{res} + v_b) \frac{[TSS]_2}{[TSS]_1} - \frac{Q_{leach}}{A} \qquad (4\text{-}23)$$

where $[TSS]_1$ is calculated from $[TSS]_{infl}$ and $[TSS]_{out}$ using Equation 4-7.

4.2.5.4 Estimate Sediment Decomposition. The burial rate is the total sediment accumulation rate for the time step. To account for the reduction in solids typically associated with anaerobic digestion, a sediment decomposition rate (or sludge digestion rate) is included in the burial (accumulation) compartment. If the entire sediment compartment included this anaerobic digestion term, a more rigorous accounting of the biological (organic) versus inert solids would be required, but, ultimately, the sediment compartment will reach a steady state (i.e., biomass growth equals biomass decay). By including it only in the burial (accumulation) compartment, sediment reduction (which includes a constituent reduction associated with the sediment) by digestion can be included without significantly complicating the model. The net accumulation of sediment over a time step is estimated as

$$\Delta d_2 = v_b \, \Delta t \, [1 - k_{ba} \, (1 - e^{-k_{dec} \, \Delta t})] \qquad (4\text{-}24)$$

where

Δd_2 = change in depth of the unconsolidated sediment compartment (m)
Δt = time step (s)
k_{ba} = ratio of biologically active solids to the total solids concentration - assumed to be the same ratio as present in the liquid compartment
k_{dec} = anaerobic digestion/decay rate of the organic sediment (1/sec).

Prior to the next time step calculations, Δd_2 is added to d_2 (and subtracted from d_1). Additionally, the total amount of sediment in the tank or impoundment and the total time since the last cleaning or dredging action is compared to the input cleaning and dredging parameter (i.e., the fraction of the WMU that can be filled with sediment before the WMU is cleaned or dredged). The module will also automatically run the dredge subroutine in the event that the sediment settling for the next time step (based on the sediment settling for the current time step) would completely fill the WMU. The removed sediment and the contaminant associated with the removed sediment is recorded; this removal acts as a sink for the overall system.

4.2.6   Estimate Constituent Release in Leachate (Surface Impoundments only)

The Surface Impoundment Module estimates leachate infiltration rate from liquid depth and from the hydraulic conductivities and thicknesses of three layers: the sediment compartment, a clogged soil layer, and the underlying native soil. This procedure follows the method outlined in EPA's Composite Module for Leachate Migration with Transformation Products (EPACMTP) background document (U.S. EPA, 1996), except that the liquid depth is known and there is a sediment layer between the impoundment liquid and the underlying soil layer.

The Surface Impoundment Module treats the unconsolidated sediment layer as free liquid to calculate the pressure head on the consolidated sediment layer and underlying soil. The model calculates the infiltration rate in an iterative manner. It makes an initial estimate of the infiltration rate, calculates the associated pressure profile in the underlying soil, and compares the calculated pressure head at the ground water surface with the boundary condition (i.e., pressure head of zero). Based on this comparison, the model revises the infiltration rate estimate and iterates until the boundary conditions are met.

Based on Darcy's law, the leaching (infiltration) rate for a given soil sublayer is:

$$I_n = K_{s,n} k_{rw,n} \left(\frac{\Psi_n - \Psi_{n+1}}{d_{s,n}} + 1 \right) \tag{4-25}$$

where

I_n = infiltration rate (m/d)
$K_{s,n}$ = hydraulic conductivity of the nth soil sublayer (m/d)
$k_{rw,n}$ = relative permeability of the nth soil sublayer (unitless)
Ψ_n = pressure head at top of the nth soil sublayer (m)
Ψ_{n+1} = pressure head at base of the nth soil sublayer (m)
$d_{s,n}$ = depth of the nth soil sublayer (m).

The relative permeability is a function of the effective saturation and can be expressed by soil class parameters using relationships developed by Van Genuchten (1980) as follows:

$$if \ \psi \geq 0 \qquad k_{rw,n} = 1 \tag{4-26a}$$

$$if \ \psi < 0 \qquad k_{rw,n} = \frac{(1 - (-\alpha_n \psi_n)^{\beta_n - 1} [1 + (-\alpha_n \psi_n)^{\beta_n}]^{-\gamma_n})^2}{(1 + (-\alpha_n \psi_n)^{\beta_n}]^{\gamma_n/2}} \tag{4-26b}$$

where

α_n = soil retention model parameter alpha for n^{th} soil sublayer (1/m)
β_n = soil retention model parameter beta for n^{th} soil sublayer (unitless)
γ_n = soil retention model parameter gamma for n^{th} soil sublayer = $1 - 1/\beta_n$ (unitless).

Solution methods for these equations can be found in the EPACMTP background document (U.S. EPA, 1996). As shown in Figure 4-3, the Surface Impoundment Module applies these equations to the sediment layer, a liner or soil layer clogged with sediment particles immediately below the surface impoundment, and another soil layer under that. The sediment layer is assumed to be saturated and modeled as a single layer using Darcy's law. The underlying soil layers are partially saturated and are modeled with five sublayers using the Van Genuchten relationships and algorithms developed for EPACMTP.
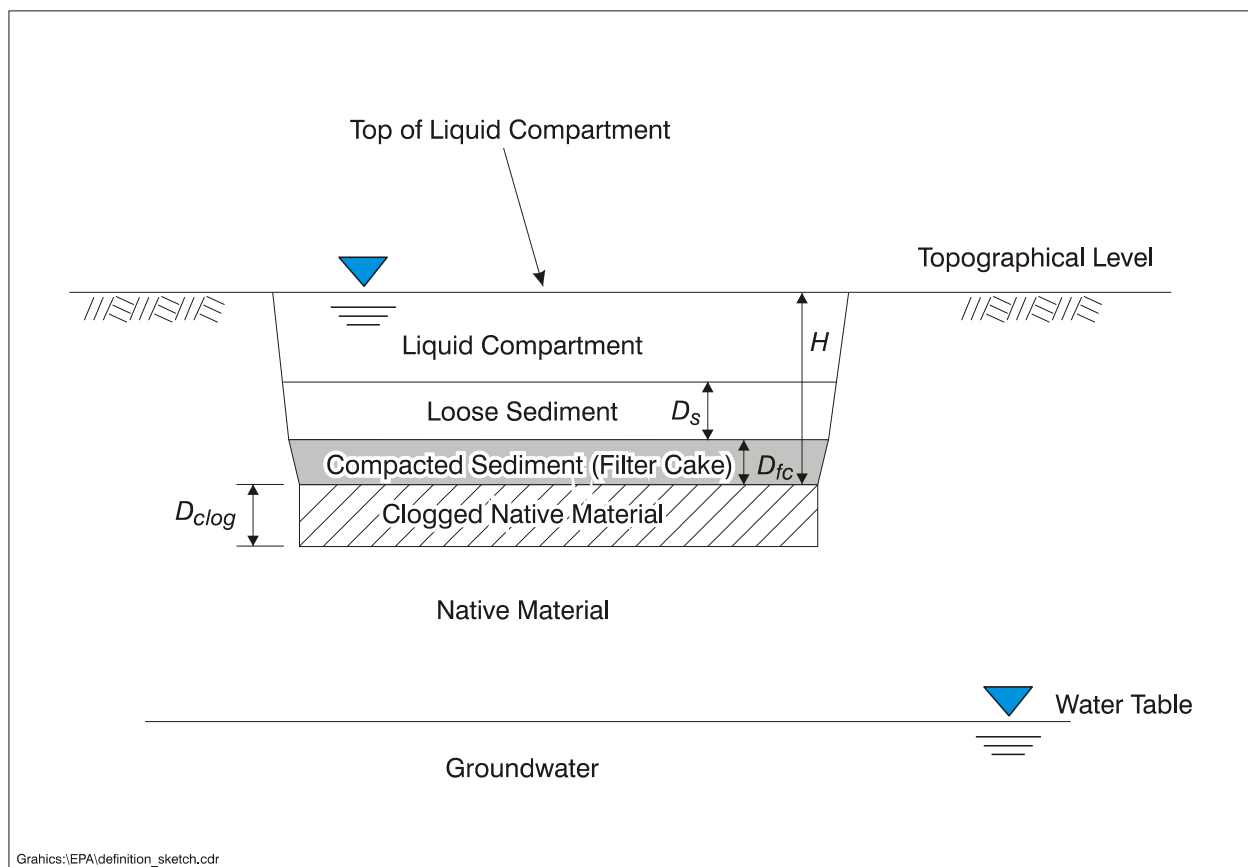

Figure 4-3. Surface impoundment cross-section showing sediment and soil layers modeled by the Surface Impoundment Module infiltration rate algorithms.

4.2.6.1 Leachate Infiltration Rate. The Surface Impoundment Module calculates a leachate infiltration rate through three compartments: consolidated sediment, clogged soil, and subsoil. Initially, the consolidated sediment is saturated and the soil layers are unsaturated. The model divides each of the soil sublayers into three sublayers. The unconsolidated sediment layer is loose (fluid) so that the effective pressure head for the consolidated sediment layer is simply the liquid depth plus the depth of the unconsolidated sediment. The model assumes that the system is at steady state; therefore, a water balance dictates that the infiltration rate is the same for all compartments and compartment sublayers. Assuming the pressure head at the ground water interface is zero, the general solution for the infiltration rate is shown in Equation 4-27.

$$I = \frac{(d_1 + D_s + \Sigma\, d_{s,n})}{\Sigma\left(\dfrac{d_{s,n}}{K_{s,n}k_{rw,n}}\right)} \tag{4-27}$$

where

I =   leachate infiltration rate (m/d)
$K_{s,n}$ =   saturated hydraulic conductivity of the nth soil sublayer (m/d)
$k_{rw,n}$ =   relative permeability of the nth soil sublayer (unitless)
$d_{s,n}$ =   thickness of the nth soil sublayer (m).

The relative permeabilities (k_{rw}) of the clogged soil and native soil sublayers are a function of whether the previous sublayer is saturated. The model uses an interative, steady-state method to solve this equation across the sediment and soil compartments, as described in U.S. EPA (1999). The infiltration rate is then set equal to the lowest of the calculated rates across the three compartments.

The Surface Impoundment Module calculates the volumetric leachate flow rate from the calculated infiltration rate as follows:

$$Q_{leach} = \frac{I \times A}{24 \times 3600} \tag{4-28}$$

where

Q_{leach} =   leachate infiltration flow rate (m^3/s)
A =   surface impoundment area (m^2).

Leachate flow rates and leachate contaminant concentrations (calculated as the liquid contaminant concentration in the consolidated sediment compartment) are output from the Surface Impoundment Module as a time series of annual-average values.

4.2.6.2 Hydraulic Conductivity of Consolidated Sediment. As sediment accumulates at the bottom of the impoundment, the weight of the liquid and upper sediments tends to compress (or consolidate) the lower sediments. This consolidated sediment acts as a filter cake, and its hydraulic conductivity may be much lower than the unconsolidated sediment. The Surface Impoundment Module assumes that the sediment compartment is at pseudo-steady-state and that all sediment layer thicknesses are nearly stationary and approximately constant. The Surface Impoundment Module sets the initial sediment depth at 20 cm to account for sediment and compaction created during the excavation of the impoundment.

The Surface Impoundment Module simulates the effective stress of the overlying liquid and unconsolidated sediment on the compacted sediment layer, and the effects of this stress on the porosity and hydraulic conductivity of the filter cake. The filter cake thickness is capped at one-half of the total sediment depth and is assumed to have a minimum thickness of 100 cm. Equations for the algorithms used to estimate sediment consolidation and the resulting hydraulic conductivity of the compacted sediment layer can be found in U.S. EPA (1999).

4.2.6.3 <u>Hydraulic Conductivity of Clogged Native Material</u>. The Surface Impoundment Module simulates the effect of sediment particles that enter and clog the soil layer immediately underlying the surface impoundment by assuming that the saturated hydraulic conductivity of the clogged soil zone is one-tenth of the hydraulic conductivity of the native soil. The model also constrains the hydraulic conductivity of the clogged layer to be less than or equal the underlying soil layer and greater than or equal to the consolidated sediment filter cake. Based on observed penetration depths of up to about 0.45 m, the depth of the clogged layer is fixed at 0.5 m.

4.2.6.4 <u>Limitations on Maximum Infiltration Rate</u>. If the surface impoundment infiltration rate exceeds the rate at which the aquifer can transport ground water, the ground water level will rise into the vadose zone, and the assumption of zero pressure head at the base of the vadose zone would be violated. This ground water "mounding" will reduce the effective infiltration rate to a maximum infiltration rate. The model estimates this maximum rate as one that does not cause the ground water mound to rise to the bottom elevation of the surface impoundment unit, using the following equation (U.S. EPA, 1999; HydroGeoLogic, 1999):

$$I_{Max} \quad \leq \quad \frac{2K_{aqsat}D_{aqsat}(D_{vadose} - H)}{R_0^2 \quad \ln\dfrac{R_\infty}{R_0}} \tag{4-29}$$

where

$$
\begin{aligned}
I_{Max} \quad &= \quad \text{maximum allowable infiltration rate (m/d)} \\
K_{aqsat} \quad &= \quad \text{hydraulic conductivity of the aquifer (m/d)} \\
D_{aqsat} \quad &= \quad \text{aquifer thickness (m)} \\
D_{vadose} \quad &= \quad \text{vadose zone thickness (m)} \\
H \quad &= \quad \text{the effective head in the WMU (see Figure 4-3)} \\
R_0 \quad &= \quad \text{equivalent source radius (m)} \\
R_\infty \quad &= \quad \text{length between the center of the source and the downgradient boundary} \\
&\qquad \text{where the boundary location has no perceptible effects on the heads near the} \\
&\qquad \text{source (m).}
\end{aligned}
$$

Under certain conditions of high soil hydraulic conductivity and long residence time in the surface impoundment, the leachate flow rate may exceed the influent flow rate. Rather than reiterating the infiltration rate calculation with liquid depth as a variable, the leachate rate is limited to 99 percent of the influent flow rate. This limit is based on a volumetric balance on the WMU and an assumption that the effluent flow is never less than 1 percent of the influent flow.

4.2.6.5 Surface Impoundment Effluent Flow Rate. The Surface Impoundment Module calculates effluent flow based on a volumetric water balance on the WMU:

$$Q_{out} = Q_{infl} - Q_{leach} + A\,(P_{rain} - P_{evap}) \qquad (4\text{-}30)$$

where

Q_{out}	=	effluent flow rate (m^3/s)
Q_{infl}	=	influent flow rate (m^3/s)
Q_{leach}	=	leachate infiltration rate (m^3/s)
A	=	surface impoundment surface area (m^2)
P_{rain}	=	precipitation rate (m/s)
P_{evap}	=	evaporation rate (m/s).

Under certain conditions of influent flow rate, impoundment dimensions, infiltration, precipitation, and evaporation, there may be months that Equation 4-30 predicts a negative or zero effluent rate, which would violate the pseudo-steady-state assumption. Therefore, if Equation 4-30 produces an effluent flow rate of less than 1 percent of the influent flow rate, the effluent flow rate is calculated as

$$Q_{out} = 0.01\,Q_{infl} \qquad (4\text{-}31)$$

When the infiltration rate is capped at 99 percent of the influent rate, the model uses this equation only if the evaporation rate exceeds the precipitation rate. Depending on the various rates, Equation 4-31 can be triggered even if the infiltration rate is not capped at 99 percent of the influent rate. The Surface Impoundment Module uses Equation 4-31 to limit (or cap) the evaporation rate to prevent a zero or negative effluent rate.

4.2.7 Adjust for Temperature Effects

Temperature can affect a number of the inputs used by the Wastewater Source Modules, including air density and diffusivity, biodegradation rate, liquid viscosity, and Henry's law constant. Some of the equations employed by the modules already include a temperature correction factor. For example, the liquid-phase, turbulent surface mass transfer coefficient includes a temperature correction term of 1.024^{T-20}. The modules use the ambient air temperature to adjust the air-side properties (air diffusivity, air density, etc.). Liquid-side properties (liquid diffusivity, liquid viscosity, etc.) are adjusted using the wastewater temperature within the tank or surface impoundment.

4.2.7.1 Estimating Temperature in the Waste Management Unit. The Wastewater Source Modules use a simplified energy balance around the aerated tank or surface impoundment to estimate the liquid temperature in the WMU from the liquid temperature of the influent, the monthly ambient air temperature, and the liquid residence time in the WMU. The model uses coefficients for free and forced convective heat transfer coefficients for both water

and air (Kreith and Black, 1980) to estimate the average overall heat transfer coefficient. The model assumes that there is forced convection on the air side (windspeed greater than 0 m/s), free convection on the quiescent liquid side, and forced convection on the turbulent liquid side. Assumptions and equations used to estimate tank and surface impoundment temperature are detailed in U.S. EPA (1999).

The surface impoundment and aerated tank temperature estimates do not take into account the heat of fusion from ice formation, and can yield liquid temperatures below 0°C. When this happens, the models set the liquid temperature to 0.1°C and estimate the amount of ice formed based on the specific heat capacity and density of water and ice. The models translate the additional heat loss in taking the water from 0°C to below 0 into a mass of ice formation, and estimate the volume or depth of ice formed using the following equation:

$$d_{ice} = \frac{A \times d_{wmu} \times (-T_l)}{80 \ (0.9) \ A} \tag{4-32}$$

where

d_{ice} = depth of ice layer formed (m)
A = area of the unit (m^2)
T_l = temperature of liquid (C).

This equation tends to overestimate ice formation because convective heat transfer from the surrounding soil is not included in the heat balance. Also, although a small amount of ice formation will not significantly impact the emission estimates and other parameters estimated by the module, if a solid crust of ice forms over the entire impoundment for a prolonged period of time, the model would overstate the potential for volatile emissions because it does not consider volatilization through an ice layer. Therefore, when the depth of the projected ice layer is 10 cm or more for 3 consecutive months, the model generates a warning message that significant ice formation is projected.

4.2.7.2 Temperature Effects on Air-Side Properties. Air-side properties include density and viscosity. The model estimates air density at a given temperature using the ideal gas law (U.S. EPA, 1999). Because the viscosity of air is only slightly affected by temperatures in the temperature range of interest, with a range from 1.75×10^{-4} to 2.17×10^{-4} g/cm-s from 0°C to 100°C (Kreith and Black, 1980), it is not adjusted for temperature in the Wastewater Source Modules.

4.2.7.3 Temperature Effects on Liquid-Side Properties. The density of water is basically insensitive to temperature and no temperature adjustments are used in the Wastewater Source Modules. The viscosity of water varies by more than a factor of 5 over the temperature range of interest (0°C to 100°C). This temperature dependency is important not only for mass transport, but also for its effect on the solids settling rate (terminal velocity) at lower Reynolds numbers. Using the data from Kreith and Black (1980), the modules use the a correlation developed using a log-log least squares linear regression to adjust the viscosity of water (U.S.

EPA, 1999). The values for the viscosity of water calculated from this equation agree well with the values reported by Liley and Gambill (1973) for temperatures between 0°C and 100°C.

4.2.7.4 Temperature Effects on Constituent-specific Properties. Air diffusivity, water diffusivity, Henry's law constant, and aerobic and anaerobic biodegradation rates are constituent-specific properties used by the Wastewater Source Modules to estimate constituent volatilization, degradation, and release to air and, for the surface impoundment, through leachate. In the 3MRA modeling system, these properties are supplied by the Chemical Properties Processor (CPP). Because the Wastewater Source Modules operate on monthly time steps, they call the CPP for these properties according to the temperature in the unit at the beginning of each month. Details on the temperature correction routines used by the CPP can be found in the documentation for the 3MRA CPP (Pacific Northwest National Laboratory, 1998).

4.2.7.5 Temperature Effects on BOD and Sediment Biodegradation Rates. The Wastewater Source Modules assume that the BOD and sediment decay rates (k_b, k_{dec}) are relatively unaffected by temperature over a reasonably wide range of temperature. At temperatures above 50°C and at temperatures near freezing, the decay rate is assumed to drop rapidly. The modules incorporate a simple temperature correction factor for these decay rates based on these assumptions: between 7°C and 40°C, the biodegradation rate temperature correction factor is assumed to be 1 (i.e., no correction). If temperatures fall below 3°C or above 60°C, the model stops biodegradation of BOD and the sediment mass by setting the temperature correction factor to 0. A linear extrapolation is used to determine the temperature correction factor between 3°C and 7°C and between 40°C and 60°C.

4.3   Module Discussion

4.3.1   Strengths and Advantages

The Wastewater Source Modules are based on sound engineering principles and algorithms, many of which have been tested and peer reviewed. Some of the strengths and advantages of these modules include the following:

- **Volatilization model.** The volatilization component of the Wastewater Source Modules employs the mass transfer correlations recommended by the Office of Air Quality Planning and Standards (OAQPS) as developed though the CHEMDAT and WATER series of models. These correlations have been developed, tested, and validated through many years of EPA research and public and industry use.

- **Leachate infiltration model.** The leachate infiltration flow rate component of the Surface Impoundment Module was adapted from the equations and algorithms developed by the Office of Research and Development (ORD) in the EPACMTP model, which has undergone peer review by SAB. The infiltration rate component also considers the effect of sediment consolidation within the impoundment and sediment impregnation (or clogging) of the underlying soil layer on the infiltration rate. These components were recommended by ORD based on their on-going research and development efforts.

■ **Solids mass balance.** The modules account for sorption using correlations for Kd and K_{oc} developed jointly by OSW and ORD. The modules also perform an explicit mass balance on the solids within the unit, including production of new solids through biomass growth, transport of solids between compartments due to infiltration (for the Surface Impoundment Module), sedimentation, resuspension and burial, and decay of sediment due to anaerobic digestion. Therefore, the modules evaluate total, dissolved, and sorbed phase concentrations needed for various potential exposure mechanisms.

■ **Loss mechanisms.** The modules account for a variety of loss mechanisms, including volatilization, sorption, hydrolysis, biodegradation, and infiltration (for the Surface Impoundment Module). Furthermore, the modules account for changes in the rates of these loss mechanisms due to monthly changes in ambient temperature, the predicted effect of these ambient temperature changes on the average wastewater temperature, and monthly evaporation and precipitation rates. Therefore, the modules can elucidate differences in constituent fate through seasonal variations. Additionally, the modules account for the accumulation and consolidation of sediment within the units, and thus can be used to predict the transient nature of the constituent fate as a unit fills with sediment (thereby reducing the hydraulic retention time and perhaps the sediment removal efficiency).

■ **Site-specific data.** The modules have a numerous input variables that allow modeling of site-specific units using detailed site-specific information. Without this site-specific data, the modules can be used with Monte-Carlo-derived inputs to derive a reasonable expectation of the expected fate of the constituent and the extremes of the potential exposure concentrations. The modules employ predominantly analytical solutions so that numerous module runs, such as those needed when performing a Monte Carlo analysis, can be completed in a short time frame.

■ **Plug-flow and batch operations.** The Surface Impoundment Module provides solution algorithms for modeling plug-flow and batch operations in addition to the well-mixed solution algorithm. The Aerated Tank Module was designed specifically for aerated or mixed tanks, and therefore assumes a well-mixed liquid compartment. However, non-aerated, quiescent tanks that operate in a plug-flow or batch mode can be effectively be modeled using the Surface Impoundment Module by setting a very low sediment hydraulic conductivity (driving the infiltration rate essentially to zero).

4.3.2 Uncertainty and Limitations

The most significant uncertainties and limitations of the Wastewater Source Modules include the following:

■ **Applicable only to dilute aqueous wastes.** By using a simple biodegradation rate model together with Henry's law partitioning coefficients, the modules are most applicable to dilute aqueous wastes. High constituent concentrations can reduce or inhibit biodegradation of toxic constituents. Also, if constituents exceed solubility

limits and free phase is present, Henry's law can overestimate volatilization (the modules output a warning when this occurs).

- **Reaction byproducts not considered.** Daughter products from hydrolysis and biological degradation of the constituents are not addressed by the modules (i.e., volatile emissions or leaching are not considered for reaction intermediates or end products).

- **No oxygen balance.** The modules assume that the liquid compartment is aerobic and contains adequate oxygen for the degradation of influent carbon (as BOD). However, high influent carbon loadings for certain low-aeration surface impoundments can result in anoxic (low oxygen) conditions that can limit biological degradation. In such cases, the modules will tend to overestimate constituent and BOD removal through biodegradation and sorption, and underestimate volatile emissions and leachate flux.

- **No delineation of organic solids.** The modules maintain suspended solids characteristics in the influent throughout the simulation. However, as influent carbon loading converts to biomass, the characteristics of the suspended solids within the WMU could change. For example, the fraction organic carbon, average particle density, and fraction of biologically active solids can change dramatically from influent solid values within a biologically active unit. Such changes can affect the solids balance (e.g., the sedimentation rate) as well as the partitioning of organic chemicals. This limitation creates uncertainty in the output variables for WMUs with high biomass generation rates relative to the influent solids loading. For units with relatively high solids loading rates and low biomass generation rates, changes in suspended solid particle characteristics due to biological growth would be limited.

- **No spatial variations in sediment depths.** For all units (well-mixed, plug-flow or batch; aerated or nonaerated), the modules assume that sediment compartment depths are uniform throughout the impoundment. For plug-flow systems, it is likely that the sediment will accumulate fastest near the influent point. For aerated units, sediment depths directly beneath high-speed aerators are expected to be less than in less agitated parts of the WMU. Because including areas of different sediment depth would greatly complicate the model construct and solution, the even distribution of sediment is a reasonable simplifying assumption. However, the modules could overestimate leachate flux for plug-flow units that have significant sediment accumulation near the influent (i.e., lower infiltration rates where the concentrations are the highest), and could underestimate leachate flux for units that have low sediment accumulation areas below mechanical aerators.

4.4 References

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