# SOURCE MODULES FOR TANKS AND SURFACE IMPOUNDMENTS

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

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Under Contract No. 68-W-98-085, WA B-15

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October 1999

## ACKNOWLEDGMENTS

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

Jeff Coburn of the Research Triangle Institute (RTI) was the lead modeler on much of this work, but received immeasurable assistance from a number of people. Keith Little of RTI assisted in the conceptual design of the two compartment model and the sediment settling, resuspension, and burial rate algorithm. Jesse Baskir of RTI spearheaded the total suspended solids (TSS) removal efficiency calculation and performed the primary technical review of the model. Jesse Baskir along with Randall Williams of RTI also provided programming support for the overall model. Zubair Saleem of the U.S. EPA OSW and Varut Guvanasen of HydroGeoLogic, Inc., provided technical support and review of the infiltration rate model and developed the sediment consolidation and clogging of native soil material and the maximum infiltration rate components of the infiltration rate model.

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# 1.0 Module Overview and Summary of Functionality

Tanks and surface impoundments (SIs) are commonly used for the treatment of wastewaters. Due to the similarities of the mass balance and transport equations for tanks and surface impoundments, a single set of equations has been developed for these basic units. Both tanks and SIs may be either aerated or quiescent, and the mass transport equations used to describe volatile contaminant losses from these units are the same. Both units may have some degree of solids settling. For aerated units, suspended solids in the influent waste will primarily pass through the system with little solids settling (depending on the degree of agitation). For quiescent units, solids settling and accumulation may be significant. When this occurs, the tank or SI will need to be cleaned or dredged to remove the accumulated solids. The primary difference between tanks and SIs is that there is no leaching from a tank.

The aerated tank (AT) and surface impoundment (SI) module functionality may be summarized as follows:

#	Mass balance approach taking into consideration contaminant removal by volatilization, biodegradation, hydrolysis, leaching, and partitioning to solids

#	Estimation of volatilization rates for both aerated and quiescent surfaces

#	Estimation of infiltration rate and contaminant leachate flux rates (for SI only)

#	Estimation of suspended solids removal (settling) efficiency

#	Estimation of temperature effects.

# 2.0 Inputs and Outputs

The aerated tank module is a source module that calculates volatile emissions flux from a simulated wastewater treatment tank. The unit has only volatile emissions (no particulates) and is assumed to have an impervious bottom so that there is no contaminant leaching. There is also no runoff and overland flow of contaminant. Therefore, the output from the AT module provides input only for calculations of air concentrations using the air module. The module is a quasi-steady-state module, and the emissions occur only while the unit operates. The volatile flux is calculated for a number of years specified either as the total number of years of the simulation or the number of years the unit is operated. The module uses data provided from the header file (hd.ssf), site layout file (sl.ssf), source module-specific file (i.e., si or at.ssf), and the monthly average meteorological data files. All SSF files are expected to be in an SSF subdirectory; the meteorological data are expected to be in a MetData subdirectory. Because the operating temperature in the unit may vary as a function of the ambient temperature and hydraulic residence time, the module also uses chemical property information calculated as a function of the unit temperature. Much of these data are provided through calls to the chemical property dll functions (which use data files stored in a chemical properties subdirectory). Some temperature correction routines are embedded within the program. The program generates a results file (sr.grf) in the grf subdirectory. The program may also generate warning messages (e.g., if the calculated unit temperature is below freezing, a warning is generated).

The surface impoundment module is a source module similar to the AT module, but the bottom of the unit is assumed to be pervious so that contaminant leaching can occur. The module, therefore, includes volatile emissions and contaminant leaching to the subsurface. The module is a quasi-steady-state module and there are no particulate emissions. There is also no runoff and overland flow of contaminant. Therefore, the output from the SI module provides input for calculations of air transport of contaminant using the air module and for ground water transport of contaminant using the ground water module. The input and output files used and their locations for the SI module are the same as for the AT module. The volatile flux is calculated for a number of years specified either as the total number of years of the simulation or the number of years the unit is operated. Ground water infiltration is assumed to be driven by the hydrostatic pressure head produced by the wastewater in the unit; when the unit ceases operation it is assumed that no additional contaminant leaches from the source. Annual liquid infiltration rates and contaminant leachate flux rates are both calculated at the base of the unit and are output for use in the ground water module.

Table 2-1 summarizes the input and output variables for the AT and SI modules.

### Table 2-1. Summary of Inputs and Outputs for AT and SI Source Modules

| Source File | Variable Name | Units | Data Type | Variable Name in Module Code | Description |
|---|---|---|---|---|---|
| HD.SSF | CPDirectory |  | String | m_pathname, pathname | Path for location of chemical properties files |
|  | MetData |  | String | MetPath | Path for location of meteorological files |
| SL.SSF | SrcArea | $m^2$ | Real | m_A_wmu, A_wmu, A_tot | Area of the waste management unit |
|  | SiteLatitude | degrees | Real | m_Lat | Latitude of the site |
|  | SiteLongitude | degrees | Real | m_Long | Longitude of the site |
|  | MetSta |  | String | m_MetSta, MetSta | ID number for meteorological station associated with site |
|  | NyrMax | years | Integer | m_NyrMax | Maximum module simulation time |
|  | SrcPh | pH units | Real | m_pH, pH | Waste pH |
|  | SrcTemp | degrees Celsius | Real | m_T_waste, T_waste | Temperature of the waste |
|  | SrcType |  | String | m_WMUType, WMUType | Type of waste management unit (AT or SI) |
|  | SrcNumLWS |  | Integer | m_SrcNumLWS, SrcNumLWS | Number of local watersheds (SI only) |
|  | SrcLWSNumSubArea |  | Integer | m_SrcLWSNumSubArea[ ] | Number of subareas in the local watershed (SI only) |
|  | SrcLWSSubAreaIndex | unitless | Integer | m_SrcLWSSubAreaIndex[ ] | Local watershed subarea containing WMU (SI only) |
|  | SrcLWSSubAreaArea | $m^2$ | Real | m_SrcLWSSubAreaArea[ ] | Area of a subarea in the local watershed (SI only) |
|  | TermFrac | fraction | Real | m_TermFrac | Peak output fraction for simulation termination |
|  | SrcDepth | m | Real | m_SrcDepth | Depth of source (0 for AT) |

*(continued)*

**Table 2-1. (continued)**

| Source File | Variable Name | Units | Data Type | Variable Name in Module Code | Description |
|---|---|---|---|---|---|
| | NumVad | | Integer | m_NumVad, NumVad | Number of vadose zones (SI only) |
| | N_stot[a] | unitless | Integer | m_N_stot, N_stot | Number of subsurface soil layers (currently hardwired to 1) (SI only)[a] |
| | VadSATK | cm/h | Real | m_hydc_s[ ], hydc_s[ ] | Saturated hydraulic conductivity in the subsurface soil layer (SI only) |
| | VadThick[a] | m | Real | m_d_s[ ][ ], d_s[ ] | Thickness of the subsurface soil layer (SI only)[a] |
| | VadALPHA | 1/cm | Real | m_alpha_s[ ], alpha_s[ ] | Alpha soil parameter for subsurface soil (SI only) |
| | VadBETA | unitless | Real | m_beta_s[ ], beta_s[ ] | Beta soil parameter for subsurface soil (SI only) |
| SI.SSF or AT.SSF | VadSATK | cm/h | Real | m_hydc_liner, hydc_liner | Hydraulic conductivity of the liner (SI only) |
| | d_liner | m | Real | m_d_liner, d_liner | Thickness of SI liner (currently hardwired to 0.5 m) (SI only) |
| | VadALPHA | 1/cm | Real | m_alpha_liner, alpha_liner | Alpha soil parameter for SI liner (SI only) |
| | VadBETA | unitless | Real | m_beta_liner, beta_liner | Beta soil parameter for SI liner (SI only) |
| | hydc_sed | m/s | Real | m_hydc_sed, hydc_sed | Hydraulic conductivity of the sediment that accumulates in the unit (SI only) |
| | bio_yield | g/g | Real | m_bio_yield, bio_yield | Biomass yield in g dry wt biomass/g CBOD |
| | CBOD | g/$cm^3$ | Real | m_CBOD, CBOD | Carbonaceous biochemical oxygen demand for the chemical |

*(continued)*

Table 2-1. (continued)

| Source File | Variable Name | Units | Data Type | Variable Name in Module Code | Description |
|---|---|---|---|---|---|
| | C_in | mg/L | Real | m_C_in, C_in | Concentration of chemical in hazardous waste |
| | EconLife | year | Integer | m_EconLife, EconLife | Economic life of the unit |
| | NumEcon | | Integer | m_NumEcon, NumEcon | Number of economic lifetimes that the unit operates |
| | d_imp | cm | Real | m_d_imp, d_imp | Diameter of the impeller used to aerate the unit |
| | dmeanTSS | cm | Real | m_m, m | Mean particle of an influent particle |
| | d_setpt | fraction | Real | m_d_setpt, d_setpt | Fraction full of sediment at which unit is dredged |
| | d_wmu | m | Real | m_d_wmu, d_wmu, d_tot | Depth of the waste management Unit |
| | F_aer | fraction | Real | m_F_aer, F_aer | Fraction of the unit surface area that is aerated |
| | focW | mass fraction | Real | m_foc, foc | Fraction of organic carbon in the waste |
| | fwmu | mass fraction | Real | m_fwmu, fwmu | Fraction of waste that is hazardous |
| | J | lb $O_2$/h-hp | Real | m_J, J | $O_2$ transfer rating of aerator |
| | kba1 | unitless | Real | m_kba1, kba1 | Ratio of biologically active solids to the total solids concentration |
| | k_dec | 1/s | Real | m_k_dec, k_dec | Anaerobic digestion/decay constant of the organic sediment |
| | u_l | g/cm-s | Real | m_mu_H2O, mu_H2O | Viscosity of water |
| | MWt_H2O | g/mol | Real | m_MWt_H2O, MWt_H2O | Molecular weight of water |

*(continued)*

**Table 2-1. (continued)**

| Source File | Variable Name | Units | Data Type | Variable Name in Module Code | Description |
|---|---|---|---|---|---|
| | n_imp | unitless | Integer | m_n_imp, n_imp | Number of impellers/aerators |
| | O2Eff | unitless | Real | m_O2eff, O2eff | $O_2$ transfer correction factor |
| | Powr | hp | Real | m_Powr, Powr | Total power to aerators/impellers |
| | Q_wmu | $m^3/s$ | Real | m_Q_wmu, Q_wmu, Q_in | Total influent flow rate into the unit |
| | rho_l | $g/cm^3$ | Real | m_rho_H2O, rho_H2O | Density of water |
| | rho_part | $g/cm^3$ | Real | m_rho_part, rho_part | Density of particles in the influent waste |
| | TSS_in | $g/cm^3$ | Real | m_TSS_in, TSS_in | Total suspended solids concentration in the influent |
| | w_imp | rad/s | Real | m_w_imp , w_imp | Rotational speed of impellers |
| CP.SSF | NumChem | | Integer | m_NumChem, | Number of chemical species |
| | ChemType | | String | m_ChemType, ChemType | Type of chemical |
| | ChemADiff | $cm^2/s$ | Real | m_Da, Da | Diffusivity of chemical in air |
| | ChemWDiff | $cm^2/s$ | Real | m_Dw, Dw | Diffusivity of chemical in water |
| | ChemHLC | $(atm\ m^3)$ / mol | Real | m_HLC, HLC | Henry’s law constant for the chemical |
| | ChemKoc | mL/g | Real | m_Koc, Koc | Soil-water partitioning coefficient for the chemical |
| | ChemAnaBioRate | 1/day | Real | m_kbiou, kbs | Biodegradation / decay rate of contaminant in sediment compartment |
| | ChemAerBioRate[b] | 1/day | Real | m_kbioa, kbm | Complex first-order biodegradation rate constant for the chemical[b] |

*(continued)*

**Table 2-1. (continued)**

| Source File | Variable Name | Units | Data Type | Variable Name in Module Code | Description |
|---|---|---|---|---|---|
| | ChemHydRate | 1/day | Real | m_k_hyd, k_hyd | Hydrolysis rate for the chemical |
| | ChemSol | mg/L | Real | m_Sol, Sol | Chemical solubility |
| | ChemCASID | | String | m_CAS, CAS | Chemical CAS ID number |
| | ChemName | | String | m_ChemName, ChemName | Chemical name |
| | ChemKd | L/kg | Real | m_Kds, Kds | Solid/water partition coefficient |
| Met data file | --- | °C | Real | m_AvgTemp[ ][ ] | Average monthly temperature |
| | --- | m/s | Real | m_um[y][z] | Monthly average windspeed |
| | --- | m/d | Real | m_AvgPpt[ ][ ] | Average monthly precipitation |
| | --- | m/d | Real | m_E[ ][ ] | Average monthly evaporation |
| | --- | | Integer | NyrMet | Number of years of meteorological data |
| SR.GRF | VENY | | Integer | VENumOut | number of years in VE outputs |
| | VEYR | year | Integer | VEOutYear[ ] | Year associated with VE output |
| | VE | $g/m^2/d$ | Real | E_wmu_t[ ] | Volatile emission rate |
| | LeachFluxNY | | Integer | LeachFluxNumOut[ ] | Number of years in leach flux outputs (SI only) |
| | LeachFluxYR | year | Integer | LeachFluxOutYear[ ][ ] | Year associated with leach flux output (SI only) |
| | LeachFlux | $g/m^2/d$ | Real | L_wmu_t[ ] | Leachate contaminant flux (SI only) |
| | NyrMet | year | Integer | nyrs | Number of years in the available met record (set equal to number of year unit operates) |

*(continued)*

**Table 2-1. (continued)**

| Source File | Variable Name | Units | Data Type | Variable Name in Module Code | Description |
|---|---|---|---|---|---|
| | AnnInfil | m/d | Real | Infil_t[ ] | Annual average leachate infiltration rate (SI only) |
| | SrcOvl | | Logic | l_SrcOvl | Flag for overland flow presence |
| | SrcSoil | | Logic | l_SrcSoil | Flag for soil presence |
| | SrcLeachSrc | | Logic | l_SrcLeachSrc | Flag for leachate presence when leachate is not met-driven (unit is active) |
| | SrcLeachMet | | Logic | l_SrcLeachMet | Flag for leachate presence when leachate is met-driven |
| | SrcVE | | Logic | l_SrcVE | Flag for volatile emissions presence |
| | SrcCE | | Logic | l_SrcCE | Flag for chemical sorbed to particulates emissions presence |
| | SrcH2O | | Logic | l_SrcH2O | Flag for surface water presence |

[a] The module currently assumes there is one native soil layer and that the thickness of the underlying soil layer is assumed to be a minimum of 1 meter thick. If the regional vadose zone thickness is less than $1+d_{wmu}$, then the impoundment is assumed to be built up (via an earthen berm) so that there is 1 meter of soil between the bottom of the SI and the ground water.

[b] Note: If normalized biodegradation rate constants are unavailable, normalized biodegradation rates constants are estimated from first-order biodegradation rate constants developed for soil systems by assuming the effective biomass in the soil system is $2.0\times10^{-6}$ Mg/m$^3$. This value was developed by RTI as an interim estimate until a more rigorously developed value for this parameter is available from EPA.

# 3.0 Assumptions and Limitations

The general module construct used for the AT and SI modules includes losses due to volatilization from aerated and/or quiescent surfaces, biodegradation, hydrolysis, solids settling/accumulation, and leaching (for SIs). This general module construct can be useful for a wide variety of tank and SI waste management unit (WMU) applications. Certain applications of tanks and SIs, such as chemical precipitation, however, may not be well moduleed with this module construct. However, with judicious selection of the input parameters, the general module construct can provide accurate fate estimates for most tank and SI waste applications. For example, if the precipitation rate for chemical precipitation is known, the input parameters used for "biomass" growth could be manipulated to simulate the solids generation rate caused by precipitation (rather than biomass growth).

The following assumptions are used in the development of the AT and SI module solution:

- # Two-compartment module: "mostly" well-mixed liquid compartment and a well-mixed sediment compartment, which includes a temporary accumulating solids compartment
- # First-order kinetics for volatilization in liquid compartment
- # First-order kinetics for hydrolysis in both liquid and sediment compartment
- # First-order kinetics for biodegradation with respect to both contaminant concentration and biomass concentration in liquid compartment
- # First-order kinetics for biodegradation in sediment compartment
- # Darcy's law for calculating the infiltration rate
- # First-order kinetics for solids settling
- # First-order biomass growth rate with respect to total biological oxygen demand (BOD) loading
- # First-order biomass decay rate within the accumulating sediment compartment
- # No contaminant in precipitation/rainfall

- Linear contaminant partitioning among adsorbed solids, dissolved phases, and vapor phases

Due to the simplicity of the biodegradation rate module employed and the use of Henry's law partitioning coefficients, the module is most applicable to dilute aqueous wastes. At higher contaminant concentrations, biodegradation of toxic constituents may be expected to exhibit zero-order or even inhibitory rate kinetics. For waste streams with high contaminant or high total organic concentrations, vapor phase contaminant partitioning may be better estimated using partial pressure (Raoult's law) rather than Henry's law. Also, because daughter products are not included in the module, any contaminant emissions or leachate generated as a reaction intermediate or end product from either biodegradation or hydrolysis are not included in the module output.

# 4.0 Theory and Algorithms

The AT or SI is divided into two primary compartments: a "liquid" compartment and a "sediment" compartment. Mass balances are performed on these primary compartments at time intervals small enough that the hydraulic retention time in the liquid compartment is not significantly impacted by the solids settling and accumulation. Figure 4-1 provides a general schematic of a module construct for an SI; the AT module construct is similar except there is no infiltration (leachate to ground water loss mechanism) in the AT.

In the liquid compartment, there is flow both in and out of the waste management unit. There is also a leachate flow to the sediment compartment and out the bottom of the WMU for surface impoundments. Within the liquid compartment, there is contaminant loss through volatilization, hydrolysis, biodegradation (presumably aerobic), and particle burial (net sedimentation). The sediment compartment has contaminant losses due to (anaerobic) biodegradation and hydrolysis. Some contaminant mixing between the liquid and sediment compartments occurs due to contaminant diffusion and due to particle sedimentation and resuspension.

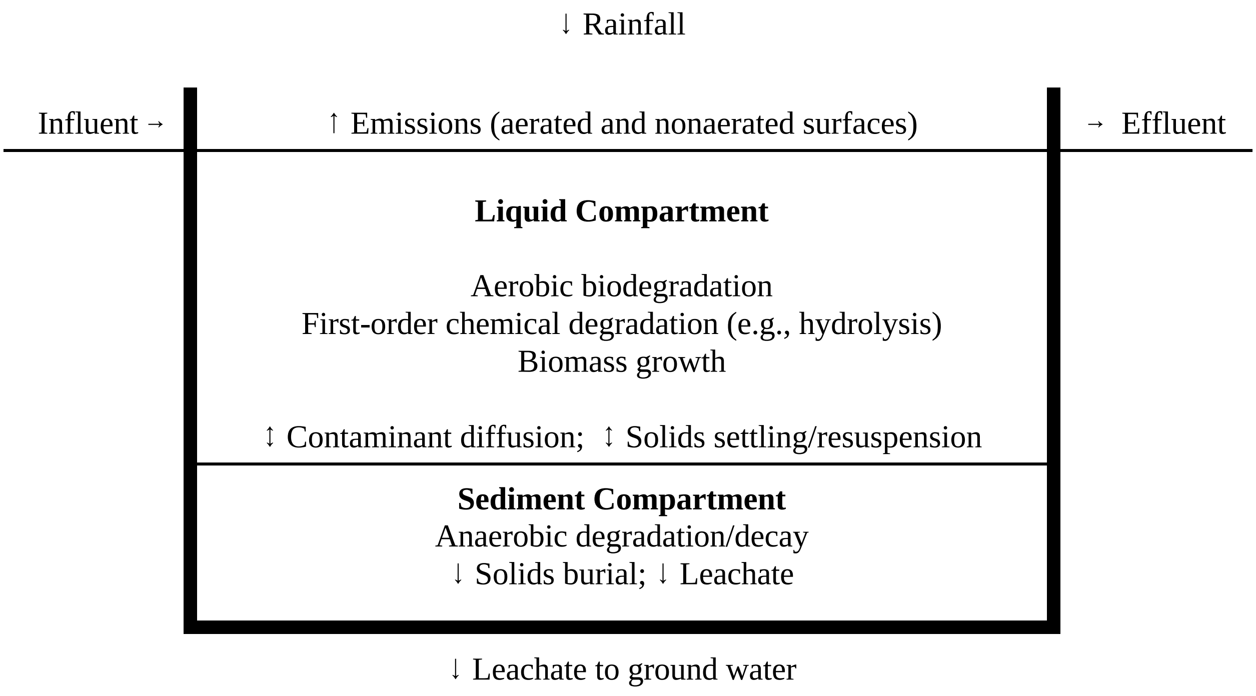

**Figure 4-1. Schematic of general module construct for tanks and surface impoundments.**

Solids generation occurs in the liquid compartment due to biological growth; solids destruction occurs in the sediment compartment due to sludge digestion. Using a well-mixed assumption, the suspended solids concentration within the WMU is assumed to be constant throughout the WMU. 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 tank is assumed to be a function of the WMU's TSS removal efficiency rather than equal to the effluent TSS concentration. The liquid (dissolved) phase contaminant concentration within the tank, however, is assumed to be equal to the effluent dissolved phase concentration (i.e., liquid is well mixed). Consequently, the term "mostly well mixed" is used in this document to describe the liquid compartment.

The primary output of the AT and SI module is the annual average volatilization rate. The SI module also outputs the average annual infiltration rate and the average annual leachate contaminant flux rate from the SI.

## 4.1 Mass Balance Equations and General Solution

### 4.1.1 Constituent Mass Balance for Liquid Compartment

In the liquid compartment, there is flow both in and out of the WMU. There is also a leachate flow to the sediment compartment and out the bottom of the WMU for surface impoundments. Within the liquid compartment, there is contaminant loss through volatilization, hydrolysis, and biodegradation. Additionally, contaminant is transported across the liquid/sediment compartment interface by solids settling and resuspension and by contaminant diffusion. At steady state, the constituent mass balance for the liquid compartment is:

$$\begin{aligned} Q_{infl}\, C_{tot,infl} = {} & Q_{out}\, C_{tot,out} + Q_{leach}\, C_{tot,1} + (K_{OL}\, A + k_{hyd}\, V_1\, \theta_{liq1,1})\, C_{liq,1} \\ & + V_1\, (k_{bm}\, k_{ba}\, [TSS]_1)\, C_{tot,1} + v_{sed}\, A\, [TSS]_1\, C_{sol,1} \\ & - v_{res}\, A\, [TSS]_2\, C_{sol,2} - v_{diff}\, A\, (C_{liq,2} - C_{liq,1}) \end{aligned} \tag{4-1}$$

where

$Q_{infl}$ = volumetric flow rate of influent ($m^3/s$)

$C_{tot,infl}$ = total contaminant concentration in influent stream ($mg/L = g/m^3$)

= $C_{in} \times f_{wmu}$ (assumes density of hazardous waste and other influent wastes are equal)

$C_{in}$ = contaminant concentration in hazardous waste ($mg/L = g/m^3$)

$f_{wmu}$ = mass fraction influent waste that is hazardous (Mg/Mg).

$Q_{out}$ = volumetric flow rate of effluent ($m^3/s$)

$C_{tot,out}$ = total contaminant concentration in effluent stream (mg/L = g/m$^3$)

$Q_{leach}$ = leachate flow rate from WMU, (m$^3$/s)

$C_{tot,1}$ = total contaminant concentration in liquid compartment [and effluent] (mg/L = g/m$^3$)

$K_{OL}$ = overall volatilization mass transfer coefficient (m/s)

$A$ = total surface area of WMU (m$^2$)

$k_{hyd}$ = hydrolysis rate (1/s)

$V_1$ = volume of liquid compartment in WMU= $d_1$ A (m$^3$ )

$d_1$ = depth of liquid compartment (m)

$\theta_{liq,1}$ = volumetric liquid content of liquid compartment (m$^3$/m$^3$)

$C_{liq,1}$ = liquid phase contaminant concentration in liquid compartment (mg/L = g/m$^3$)

$k_{bm}$ = complex first-order biodegradation rate constant (m$^3$ /Mg-s)

$k_{ba}$ = ratio of biologically active solids to the total solids concentration (i.e., $k_{ba}$ = $[MLVSS]_1/[TSS]_1$)

$[MLVSS]_1$ = concentration of biomass as mixed liquor volatile suspended solids (MLVSS) liquid compartment and in effluent (g/cm$^3$ = Mg/m$^3$)

$C_{tot,1}$ = total contaminant concentration in the WMU (mg/L = g/m$^3$)

$[TSS]_1$ = concentration of total suspended solids (TSS) in liquid compartment and in effluent (g/cm$^3$ = Mg/m$^3$)

$v_{sed}$ = solids settling or sedimentation velocity (m/s)

$C_{sol,1}$ = solid phase contaminant concentration in liquid compartment (mg/kg = g/Mg)

$v_{res}$ = solids resuspension velocity (m/s)

$[TSS]_2$ = concentration of total suspended solids in the sediment compartment (g/cm$^3$ = Mg/m$^3$).

$C_{sol,2}$ = solid phase contaminant concentration in sediment compartment (mg/kg = g/Mg)

$v_{diff}$ = mass transfer coefficient between liquid and sediment compartments (m/sec)

$C_{liq,2}$ = liquid phase contaminant concentration in sediment compartment (mg/L = g/m$^3$)

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### 4.1.2 Constituent Mass Balance for Sediment Compartment

Within the sediment compartment, there is contaminant loss through hydrolysis and biodegradation. Additionally, contaminant is transported across the liquid/sediment compartment interface by solids settling and resuspension and by contaminant diffusion. For surface impoundments, there is also leachate flow from the liquid compartment (which includes entrained sediment) and "filtered" leachate out the bottom of the WMU. At steady state, the general constituent mass balance for the sediment compartment is:

$$\begin{aligned} Q_{leach}\, C_{tot,1} = {} & Q_{leach}\, C_{liq,2} + k_{bs}\, V_2\, C_{tot,2} + \left(v_{res} + v_b\right) A\, [TSS]_2\, C_{sol,2} \\ & + V_2\, \theta_{liq,2}\, k_{hyd}\, C_{liq,2} - v_{sed}\, A\, [TSS]_1\, C_{sol,1} + v_{diff}\, A \left(C_{liq,2} - C_{liq,1}\right) \end{aligned} \qquad (4\text{-}2)$$

where

$k_{bs}$ = (anaerobic) biodegradation decay rate of contaminant (1/s)
$v_b$ = solids burial velocity (m/s)
$C_{tot,2}$ = total contaminant concentration of sediment compartment (g/m$^3$)
$\theta_{liq,2}$ = volumetric liquid content of sediment compartment (m$^3$/m$^3$).

### 4.1.3 Mass Balance for Sediment in Liquid Compartment

Sedimentation and resuspension provide a means of sediment transfer between the liquid and sediment compartments. As seen in Equations 4-1 and 4-2, sedimentation and resuspension are assumed to occur in the quiescent areas. For systems in which biodegradation occurs within the liquid compartment, there is also a production of biomass associated with the decomposition of organic constituents. At steady state, the sediment mass balance for the liquid compartment is:

$$Q_{infl}([TSS]_{infl} + \lambda \epsilon_{BOD} C_{BOD}) = Q_{out}[TSS]_{out} + Q_{leach}[TSS]_1 + v_{sed} A [TSS]_1 - v_{res} A [TSS]_2 \qquad (4\text{-}3)$$

where

$\lambda$ = biomass yield (g-biomass (dry basis)/g-BOD)
$\epsilon_{BOD}$ = biological oxygen demand removal efficiency of WMU (Mg/m$^3$)
$C_{BOD}$ = biological oxygen demand of influent (Mg/m$^3$)
$[TSS]_{out}$ = concentration of total suspended solids in the effluent (g/cm$^3$ = Mg/m$^3$).

### 4.1.4 Mass Balance for Sediment in Sediment Compartment

In the sediment compartment, as in the liquid compartment, sedimentation and resuspension provide a means of sediment transfer between the liquid and sediment compartments. In the sediment compartment, however, there is some accumulation of sediment during the time step. This sediment accumulation is also referred to as sediment burial, and the rate of sediment accumulation is determined by the burial velocity. The sediment mass balance for the sediment compartment is:

$$(Q_{leach} + v_{sed}\, A)\ [TSS]_1 - v_{res}\, A\ [TSS]_2 = v_b\, A\ [TSS]_2 \tag{4-4}$$

### 4.1.5 Equilibrium Partitioning Equations

Equations 4-1 and 4-2 are written in terms of the three contaminant concentration phases (i.e., liquid (dissolved), sorbed (particle), and total. It is, therefore, appropriate to derive expressions to convert among liquid phase, sorbed phase, and total contaminant concentrations for any given compartment, x.

For a given compartment, the total, liquid, and particle phase concentrations are related as follows:

$$C_{tot,x} = C_{liq,x} \frac{V_{liq,x}}{V_{tot,x}} + C_{sol,x}\ [TSS]_x \tag{4-5}$$

where

$V_{liq,x}$ = volume of liquid in compartment x ($m^3$)
$V_{tot,x}$ = total volume of compartment x ($m^3$).

These liquid and particle phase concentrations are defined in this manner because these are the concentrations used to define the contaminant partitioning. Specifically, the liquid-to-particle phase partitioning can be expressed as:

$$C_{sol,x} = k_{ds}\, C_{liq,x} \tag{4-6}$$

where

$k_{ds}$ = 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 total volume of compartment x is equal to the volume occupied by the liquid plus the volume occupied by the particles.

$$V_{tot,x} = V_{liq,x} + V_{tot,x}\,[TSS]_x \,/\, \rho_{TSS} \qquad (4\text{-}7)$$

or

$$\frac{V_{liq,x}}{V_{tot,x}} = \theta_{liq,x} = (1 - [TSS]_x/\rho_{TSS}) \qquad (4\text{-}8)$$

Substituting Equations 4-6 and 4-8 into Equation 4-5 and solving for the ratio of the liquid phase concentration to the total contaminant concentration yields:

$$\frac{C_{liq,x}}{C_{tot,x}} = f_{d,x} = \frac{1}{\left(\theta_{liq,x} + k_{ds}[TSS]_x\right)} \qquad (4\text{-}9)$$

Note: As defined here, the liquid concentration can exceed the total concentration when there are high TSS concentrations and little contaminant adsorption (small $k_{ds}$).

In Equations 4-1 and 4-2, the solid (particle phase) concentrations are always used in conjunction with the TSS concentration so that the particle concentration can be expressed on a volumetric basis. Therefore, the fraction of the contaminant that is in the sorbed (particle) phase is expressed as follows:

$$\frac{C_{sol,x}[TSS]_x}{C_{tot,x}} = f_{p,x} = \frac{k_{ds}[TSS]_x}{\left(\theta_{liq,x} + k_{ds}[TSS]_x\right)} \qquad (4\text{-}10)$$

### 4.1.6 Prediction of TSS Concentration in Liquid Compartment

To apply Equations 4-9 and 4-10, the TSS concentration in each compartment must be determined. The TSS concentration in the sediment compartment is a direct input variable and is assumed to be a constant independent of sediment depth (i.e., a homogeneous sediment layer). The TSS concentration in the effluent is predicted by the module based on the influent TSS concentration, the size and density of the influent TSS particles, and the "upflow" velocity in the liquid compartment (the module estimation methodology is described in Sections 4.4). To account for anticipated gradients of TSS concentration with WMU length and depth, the effective TSS concentration within the WMU is estimated to be the log-mean average between the influent and effluent TSS concentrations (based on first-order sedimentation). Given the influent and effluent TSS concentrations, the effective (mean) TSS concentration in the liquid compartment is:

$$[TSS]_1 = \exp\left[\frac{(\ln[TSS]_{infl}) + \ln([TSS]_{out})}{2}\right] \tag{4-11}$$

### 4.1.7 General Solution for Contaminant Concentrations

Equations 4-9 and 4-10 are applied to Equations 4-1 and 4-2, noting that $C_{liq,1} = C_{liq,out}$ (by assumption), to develop equations that are expressed only in terms of total contaminant concentration.

$$\begin{aligned} Q_{infl}\, C_{tot,infl} = {} & [Q_{out}\, (f_{d,1}/f_{d,out}) + Q_{leach} + f_{d,1}(K_{OL}\, A + k_{hyd}\, V_1\, \theta_{liq,1})]\, C_{tot,1} \\ & + [\, V_1\, (k_{bm}\, k_{ba}\, [TSS]_1) + v_{sed}\, A\, f_{p,1} + v_{diff}\, A\, f_{d,1}]\, C_{tot,1} \\ & - (\, v_{res}\, A\, f_{p,2} + v_{diff}\, A\, f_{d,2})\, C_{tot,2} \end{aligned} \tag{4-12}$$

$$\begin{aligned} Q_{leach}\, C_{tot,1} = {} & [(Q_{leach} + V_2\, \theta_{liq,2}\, k_{hyd} + v_{diff}\, A)\, f_{d,2} + k_{bs}\, V_2]\, C_{tot,2} \\ & + (v_{res} + v_b)\, A\, f_{p,2}\, C_{tot,2} - (v_{sed}\, A\, f_{p,1} + v_{diff}\, A\, f_{d,1})\, C_{tot,1} \end{aligned} \tag{4-13}$$

Combining Equations 4-12 and 4-13, a second equation can be written in terms of the influent contaminant load to the WMU as follows:

$$\begin{aligned} Q_{infl}\, C_{tot,infl} = {} & [Q_{out}\, (f_{d,1}/f_{d,out}) + f_{d,1}(K_{OL}\, A + k_{hyd} V_1\, \theta_{liq,1}) + V_1\, (k_{bm} k_{ba} [TSS]_1)]\, C_{tot,1} \\ & + [(Q_{leach} + V_2\, \theta_{liq,2}\, k_{hyd})\, f_{d,2} + k_{bs}\, V_2 + v_b\, A\, f_{p,2}]\, C_{tot,2} \end{aligned} \tag{4-14}$$

Equations 4-12 and 4-14 can then be solved simultaneously to derive expressions for the contaminant concentration in the liquid and sediment compartments. For simplicity, the following "constants" are defined:

$$\begin{aligned} K_{c1} = {} & Q_{out}\, (f_{d,1}/f_{d,out}) + Q_{leach} + f_{d,1}(K_{OL}\, A + k_{hyd}\, V_1\, \theta_{liq,1} + v_{diff}\, A) \\ & + V_1\, (k_{bm}\, k_{ba}\, [TSS]_1) + v_{sed}\, A\, f_{p,1} \end{aligned} \tag{4-15}$$

$$K_{c2} = Q_{out}\, (f_{d,1}/f_{d,out}) + f_{d,1}(K_{OL}\, A + k_{hyd}\, V_1\, \theta_{liq,1}) + V_1\, (k_{bm}\, k_{ba}\, [TSS]_1) \tag{4-16}$$

$$K_{c3} = v_{res}\, A\, f_{p,2} + v_{diff}\, A\, f_{d,2} \tag{4-17}$$

Using these "constants," Equations 4-12 and 4-14 can be rewritten as:

$$K_{c4} = (Q_{leach} + V_2 \, \theta_{liq,2} \, k_{hyd}) \, f_{d,2} + k_{bs} \, V_2 + v_b \, A \, f_{p,2} \tag{4-18}$$

$$Q_{infl} \, C_{tot,infl} = K_{c1} \, C_{tot,1} - K_{c3} \, C_{tot,2} \tag{4-19}$$

$$Q_{infl} \, C_{tot,infl} = K_{c2} \, C_{tot,1} + K_{c4} \, C_{tot,2} \tag{4-20}$$

Equations 4-19 and 4-20 can be solved simultaneously by rearranging Equation 4-19 in terms of $C_{tot,1}$ as follows:

$$C_{tot,1} = \frac{Q_{infl} \, C_{tot,infl} + K_{c3} \, C_{tot,2}}{K_{c1}} \tag{4-21}$$

$$C_{tot,2} = \frac{(K_{c1} - K_{c2}) \, (Q_{infl} \, C_{tot,infl})}{(K_{c2} \, K_{c3} + K_{c1} \, K_{c4})} \tag{4-22}$$

Therefore, once the four "constants" are determined, Equations 4-21 and 4-22 can be used to determine the pseudo-steady-state concentrations in each of the compartments. The following sections describe the methodologies and equations used to estimate the mass transfer coefficients, first-order rate constants, and other terms that are included in these "constants" that are not direct module inputs.

## 4.2 Mass Transfer Rate Equations

The overall mass transfer coefficient that determines the rate of volatilization is determined based on a two-resistance module: a liquid phase mass transfer resistance and a gas phase mass transfer resistance. The liquid and gas phase mass transfer resistances are very different for turbulent surfaces compared to quiescent (laminar flow) surfaces. Therefore, the overall mass transfer coefficient is a composite of the overall mass transfer coefficient for the turbulent surface area and the overall mass transfer coefficient for the quiescent surface area based on an area weighted average as follows:

$$K_{OL} = \frac{K_{OL,t} \, A_t + K_{OL,q} \, A_q}{A} \tag{4-23}$$

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
$K_{OL,q}$ = overall mass transfer coefficient for quiescent surface areas (m/s)
$A_q$ = quiescent surface area = (1-$f_{aer}$) A, $m^2$ (Note: $A_t + A_q$ must equal A).

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

$$K_{OL,t} = \left( \frac{1}{k_{l,t}} + \frac{1}{H' \, k_{g,t}} \right)^{-1} \tag{4-24}$$

where

$k_{l,t}$ = liquid phase mass transfer coefficient for turbulent surface areas (m/s)
$H'$ = dimensionless Henry's law constant = $H/RT_H$
H = Henry's law constant (atm-$m^3$/mol)
R = ideal gas law constant = 0.00008205 (atm-$m^3$/mol-K)
$T_H$ = temperature at which Henry's law constant was evaluated = 298 K.
$k_{g,t}$ = gas phase mass transfer coefficient for turbulent surface areas (m/s)

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

$$K_{OL,q} = \left( \frac{1}{k_{l,q}} + \frac{1}{H' \, k_{g,q}} \right)^{-1} \tag{4-25}$$

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 in this module to estimate the individual mass transfer coefficients are the same as those used in the WATER8 and CHEMDAT8 emission modules developed by EPA. The documentation of these mass transfer correlations can be accessed from EPA's Internet site (http://www.epa.gov/ttn/chief/software.html, then select "Water8 and Chemdat8"). Only the basic equations are provided here. For a more detailed discussion of these mass transfer correlations, the reader is referred to Chapter 5 of the CHEMDAT8 module documentation (U.S. EPA, 1994).

### 4.2.1 Liquid Phase Mass Transfer Coefficient for Turbulent Surfaces

The liquid phase, turbulent surface mass transfer coefficient is calculated as

$$k_{l,t} = \left( \frac{8.22\times10^{-3} \times J \times P_{tot} \times 1.024^{(T-20)} \times O_{cf} \times MW_l}{10.76 \times A_t \times \rho_l} \right) \left( \frac{D_{i,l}}{D_{O2,l}} \right)^{0.5} \tag{4-26}$$

where

$J$ = oxygen transfer factor (lb/h/hp)
$P_{tot}$ = total power to the impellers (hp)
$T$ = liquid temperature in WMU (°C)
$O_{cf}$ = oxygen correction factor
$MW_l$ = molecular weight of liquid (water) (g/mol)
$\rho_l$ = density of liquid (water) (g/cm$^3$ = Mg/m$^3$)
$D_{i,l}$ = diffusivity in liquid (water) (cm$^2$/s)
$D_{O2,l}$ = diffusivity of oxygen in liquid (water) (cm$^2$/s).

### 4.2.2 Gas Phase Mass Transfer Coefficient for Turbulent Surfaces

The gas phase, turbulent surface mass transfer coefficient is calculated as

$$k_{g,t} = 1.35 \times 10^{-7} \times Re_g^{1.42} \times p^{0.4} \times Sc_g^{0.5} \times Fr^{-0.21} \times D_{i,a} \times MW_a \times d_{imp}^{-1} \tag{4-27}$$

where

$Re_g$ = gas phase Reynolds number = $(d_{imp}^2 \; w \; \rho_g)/\mu_g$
$\rho_g$ = density of gas (air) (g/cm$^3$)
$\mu_g$ = viscosity of gas (air) (g/cm-s)
$p$ = power number = $0.85 \, (550 \, P_{tot}/N_{aer}) \, g_{c,2} \, / \, [(62.428\rho_l) w^3 \, (d_{imp}/30.48)^5 \, ]$
$g_{c,2}$ = gravitational constant = 32.17 lb$_m$-ft/s$^2$-lb$_f$ = 0.03283 $g_c$
$N_{aer}$ = number of aerators
$w$ = rotational speed (rad/s)
$Sc_g$ = gas phase Schmidt number = $\mu_g/(\rho_g \, D_{i,g})$
$Fr$ = Froud number = $[w^2 \, (d_{imp}/30.48) \, ]/ \, g_{c,2}$
$D_{i,a}$ = diffusivity of constituent in air (cm$^2$/s)
$MW_a$ = molecular weight of air (g/mol)
$d_{imp}$ = impeller diameter (cm)
$g_c$ = gravitational constant = 980 cm/s$^2$.

### 4.2.3 Liquid Phase Mass Transfer Coefficient for Quiescent Surfaces

The appropriate correlation to use to estimate the liquid phase mass transfer coefficient is dependent on the windspeed and the fetch-to-depth ratio of the impoundment. The fetch is the linear distance across the WMU, and it is calculated from the WMU's surface area assuming a circular shape for the WMU. That is,

$$F = \left( \frac{4\ A}{\pi} \right)^{0.5} \tag{4-28}$$

where

F = fetch of the WMU (m)

For windspeeds less than 3.25 m/s, the following correlation is used regardless of the fetch-to-depth ratio ($F/d_{liq}$):

$$k_{l,q} = 2.78 \times 10^{-6} \left( \frac{D_{i,l}}{D_{ether}} \right)^{\frac{2}{3}} \tag{4-29}$$

where

$k_{l,q}$ = liquid phase, quiescent surface mass transfer coefficient, m/s
$D_{i,l}$ = diffusivity of constituent in liquid (water), $cm^2/s$
$D_{ether}$ = diffusivity of ether in water = $8.5 \times 10^{-6}$ $cm^2/s$.

For windspeeds greater than or equal to 3.25 m/s, the appropriate correlation is dependent on the fetch-to-depth ratio as follows:

$$For\ \frac{F}{d_{liq}} < 14 \quad k_{l,q} = 1.0 \times 10^{-6} + (a \times 10^{-4})\ (U^{*})^{b}\ Sc_{liq}^{-0.5} \tag{30}$$

where

a = equation constant, a = 34.1 for U* > 0.3 m/s; a = 144 for U* < 0.3 m/s
$U^*$ = friction velocity, m/s = $0.01U\ (6.1 + 0.63U)^{0.5}$
b = equation constant, b = 1 for U* > 0.3 m/s; b = 2.2 for U* < 0.3 m/s
$Sc_{liq}$ = liquid phase Schmidt number = $\mu_l/(\rho_l\ D_{i,l})$
$\mu_l$ = viscosity of water (g/cm-s)
$\rho_l$ = density of water ($g/cm^3$)

$$For \quad 14 \leq \frac{F}{d_{liq}} \leq 51.2$$

$$k_{l,q} = \left[ 2.605 \times 10^{-9} \left( \frac{F}{d_{liq}} \right) + 1.277 \times 10^{-7} \right] U^{2} \left( \frac{D_{i,l}}{D_{ether}} \right)^{\frac{2}{3}} \qquad (4\text{-}31)$$

$$For \quad \frac{F}{d_{liq}} > 51.2 \quad k_{l,q} = 2.611 \times 10^{-7} \; U^{2} \left( \frac{D_{i,l}}{D_{ether}} \right)^{\frac{2}{3}} \qquad (4\text{-}32)$$

### 4.2.4 Gas Phase Mass Transfer Coefficient for Quiescent Surfaces

The gas phase mass transfer coefficient for quiescent surface areas is estimated as follows:

$$k_{g,q} = (4.82 \times 10^{-3}) \; U^{0.78} \; Sc_{g}^{-0.67} \; F^{-0.11} \qquad (4\text{-}33)$$

### 4.2.5 Estimating the Effective Diffusion Velocity

The effective diffusion velocity between the liquid and sediment compartments is estimated based on the liquid phase mass transfer coefficient for quiescent surfaces as calculated in Section 4.2.3 and the porosity of the sediment compartment using the following two-resistance module:

$$v_{diff} = \left( \frac{1}{k_{l,q}} + \frac{1}{k_{eff,2}} \right)^{-1} \qquad (4\text{-}34)$$

where

$k_{l,q}$ = 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 effective liquid diffusion rate is first calculated from the porosity of the sediment layer using a Millington-Quirk (Millington and Quirk, 1961) tortuosity module as follows:

$$D_{eff,2} = \theta_{liq,2}^{\frac{4}{3}} \times D_{i,l} \tag{4-35}$$

where

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

In most cases, the sediment accumulating at the bottom of the WMU will not be a rigid mass of particles, but more of a viscous sludge layer. As such, the top layer of sediment is expected to be impacted 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. As the liquid phase quiescent mass transfer coefficient is primarily a function of the liquid diffusivity raised to the two-thirds power, the effective liquid mass transfer coefficient for the sediment layer is estimated from the liquid compartment as follows:

$$k_{eff,2} = k_{l,q} \left( \frac{D_{eff,2}}{D_{i,1}} \right)^{\frac{2}{3}} = k_{l,q} \; \theta_{liq,2}^{\frac{8}{9}} \tag{4-36}$$

Substituting Equation 4-36 into Equation 4-34 and simplifying yields:

$$v_{diff} = \frac{k_{l,q} \; \theta_{liq,2}^{0.89}}{1 + \theta_{liq,2}^{0.89}} \tag{4-37}$$

## 4.3 Estimation of Leachate and Effluent Flow Rates

### 4.3.1 General Infiltration Rate Module Construct

The leachate flow rate is zero for tanks. For surface impoundments, the leachate flow rate is estimated from liquid depth and from the hydraulic conductivities and thicknesses of the sediment compartment, the clogged native soil layer, and the underlying soil layer. The procedure used to determine the leaching rate follows the method outlined in the EPA Composite Module for Leachate Migration with Transformation Products (EPACMTP) background document (U.S. EPA, 1996). There are two important differences: (1) the liquid depth is known and (2) there is a sediment layer between the liquid and the liner. Figure 4-2 presents a schematic of the leaching module construct.

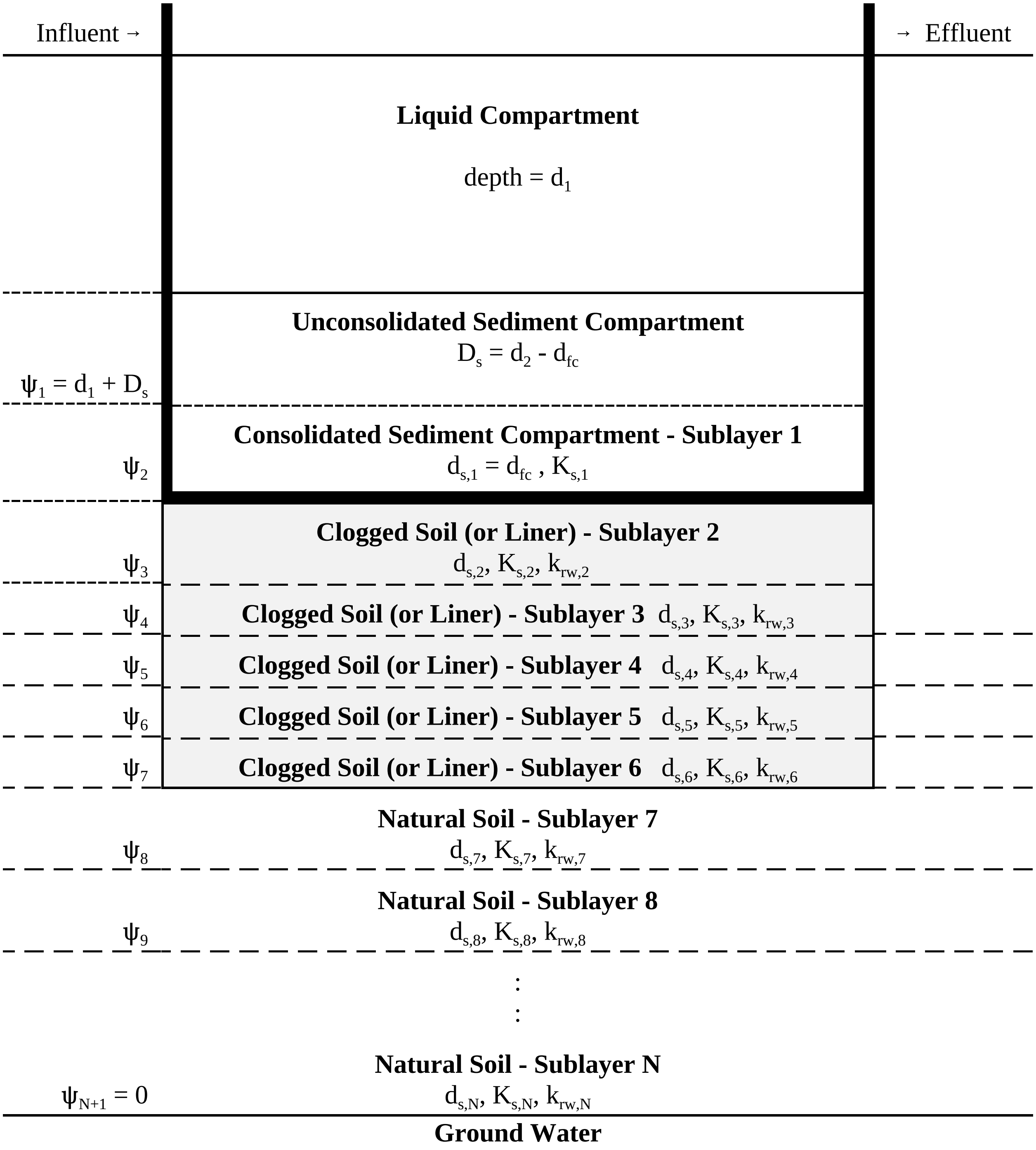

**Figure 4-2. Schematic of general module construct for leaching from surface impoundments.**

The unconsolidated sediment layer is treated as free liquid so that the pressure head on the consolidated sediment layer is known ($\Psi_1 = d_1 + D_s$). The general solution algorithm is to guess the infiltration rate, calculate the pressure profile in the underlying soil, and compare the calculated pressure head at the ground water surface with the boundary condition (i.e., $\Psi_{N+1} = 0$). Successive estimates of the infiltration rate are made until the boundary conditions are met.

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

$$I_n = K_{s,n} k_{rw,n} \left( \frac{\psi_n - \psi_{n+1}}{d_{s,n}} + 1 \right) \tag{4-38}$$

where

$K_{s,n}$ = hydraulic conductivity of the nth soil sublayer (m/d)
$k_{rw,n}$ = relative permeability of the nth soil sublayer, dimensionless
$\Psi_n$ = pressure head at top of the nth soil sublayer (m)
$\Psi_{n+1}$ = pressure head at base of the nth soil sublayer (m).

The relative permeability is a function of the effective saturation and can be expressed by soil class parameters as follows (U.S. EPA, 1996):

$$if \ \psi \geq 0 \qquad k_{rw,n} = 1 \tag{4-39a}$$

$$if \ \psi < 0 \qquad k_{rw,n} = \frac{(1 - (-\alpha_n \psi_n)^{\beta_n - 1}[1 + (-\alpha_n \psi_n)^{\beta_n}]^{-\gamma_n})^2}{(1 + (-\alpha_n \psi_n)^{\beta_n}]^{\gamma_n/2}} \tag{4-39b}$$

where

$\alpha_n$ = first soil retention module parameter for nth soil sublayer (1/m)
$\beta_n$ = second soil retention module parameter for nth soil sublayer, dimensionless
$\gamma_n$ = third soil retention module parameter for nth soil sublayer = $1 - 1/\beta_n$.

The EPACMTP employs a weighting factor for determining the average or "effective" pressure head, $\psi_{eff,n}$, for the soil layer based on the pressure head at both the top and bottom of the soil layer, but recommends using the effective pressure head for a soil layer as the pressure head at the top of that soil layer (termed an "upstream-weighted approximation"). The sediment layer is assumed to be saturated so that no discretization is needed for the sediment layer. The liner or clogged soil layer and each subsequent soil layer is divided into five sublayers following the guidance provided in the EPACMTP. For a given soil layer, the top sublayer is one-half the total depth of that layer, the second layer is one-quarter the total depth, the third layer is one-eighth the total depth, and the fourth and fifth layers are one-sixteenth the total depth. The diagram shows the nomenclature for the discrete sublayers, but not the relative depths.

### 4.3.2 **Effective Hydraulic Conductivity of Consolidatable Filter Cake** (HydroGeoLogic, 1999).

As sediment accumulates at the base 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 nonconsolidated sediment. Shown in Figure 4-3 is a snapshot of a compartmentalized surface impoundment with stratified sediment. It is assumed that the system has attained a pseudo-steady-state condition and all sediment layer thicknesses are near stationary and approximately constant. The initial depth of the sediment layer for the surface impoundment is set at 20 cm to account for sediment and compaction created during the excavation of the impoundment. Note that the tank module, which assumes no infiltration, assumes that there is no sediment layer ($d_2$ = 0 cm) at the start of the module simulation.

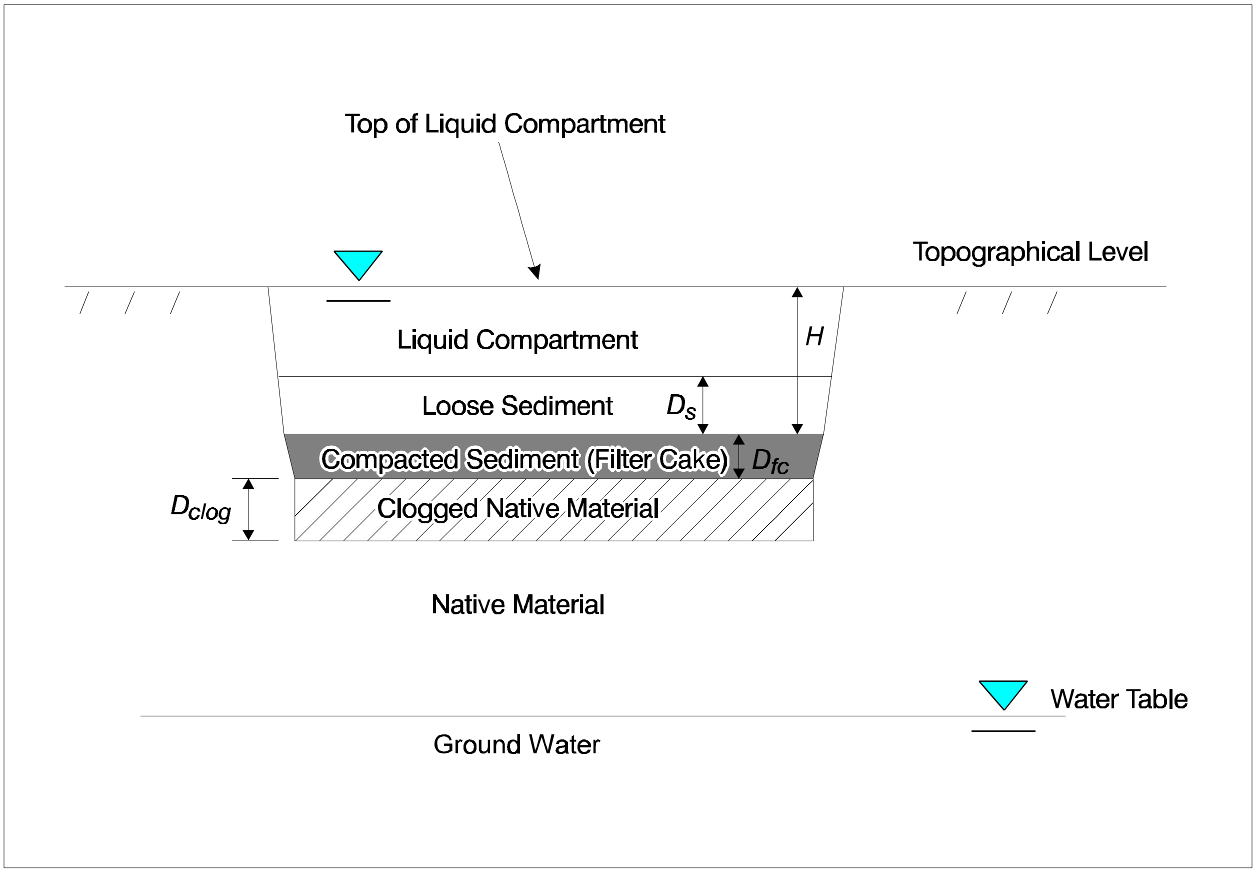

**Figure 4-3.** Definition sketch of the filter cake and clogged native material components to the surface impoundment infiltration rate module. Shown in the figure are, in descending order: the liquid compartment, the sediment compartment (with loose and compacted sediments), and the vadose zone (with clogged and unaffected native materials).

Assume that initially the effective stress in the sediment is nonexistent. The final stress in the consolidatable sediment after the deformation and dissipation of fluid pressure is given by

$$\begin{aligned}\sigma_{vf} &= (H - D_s - D_{fc})\,\rho_w g + (1-\theta)\,\rho_s g D_s + \theta\,\rho_w g D_s \\ &+ (1-\theta)\,\rho_s g z + \theta \rho_w g z - [(H - D_{fc})\,\rho_w g - \frac{z}{D_{fc}}(H - D_{fc})\rho_w g]\end{aligned} \tag{4-40}$$

where

$\sigma_{vf}$ = vertical effective stress in the z-direction, Mg/m-s$^2$
H = total depth of a given SI unit (height from bottom) (m)
$D_s$ = thickness of unconsolidatable sediment (m)
$D_{fc}$ = thickness of filter cake or consolidatable sediment (height from bottom) (m)
$\rho_w$ = water density (Mg/m$^3$)
g = gravitational acceleration (m/s$^2$)
$\rho_s$ = sediment grain density (Mg/m$^3$)
$\theta$ = porosity, volume fraction
z = vertically downward distance from the top of the consolidatable sediment (m).

The following limits are imposed on the filter cake thickness

$$D_{fcMin} \le D_{fc} = f_D(D_s + D_{fc}) \le D_{fcMax} \le H \tag{4-41}$$

where

$D_{fcMin}$ = minimum permissible thickness of filter cake, m = 0.1 m
$f_D$ = fraction of total sediment depth that is consolidatable = 0.5
$D_{fcMax}$ = maximum permissible thickness of filter cake, m = 0.6 m.

The compressibility of the consolidatable sediment is determined from

$$a_v = \frac{0.435 C_c}{\frac{1}{2}\sigma_{vf}\,\big|_{z=\frac{1}{2}D_{fc}}} \tag{4-42}$$

where

$C_c$ = compression index = 1.02

From

$$\Delta e = -a_v \Delta\sigma_{vf} \tag{4-43}$$

where

e = void ratio

we can determine the change in void ratio by

$$e' = e_0 + \Delta e \tag{4-44}$$

where

$e_0$ = initial void ratio (based on initial hydraulic conductivity at no stress condition)
= 2.0

or

$$e' = e_0 - a_v \Delta\sigma_{vf} \tag{4-45}$$

From a number of laboratory observations (see Lambe and Whitman, 1969), we can express hydraulic conductivity, K, of the sediment as a function of void ratio, thus:

$$\log(e) = \log(A) + b\ \log(K) \tag{4-46}$$

or

$$\left(\frac{e}{A}\right)^{\frac{1}{b}} = K \tag{4-47}$$

where A, b are constants and

A = 1,120
b = 0.337

Using Equations 4-40, 4-42, 4-45, and 4-47, we can write:

$$\begin{aligned} K(e') = {} & [(e_0 - a_v((H - D_s - D_{fc})\rho_w g + (1-\theta)\rho_s g D_s + \theta\rho_w g D_s \\ & + (1-\theta)\rho_s g z + \theta\rho_w g z - [(H - D_{fc})\rho_w g - \frac{z}{D_{fc}}(H - D_{fc})\rho_w g]))\frac{1}{A}]^{\frac{1}{b}} \end{aligned} \tag{4-48}$$

or simply

$$K(e') = (C_1 + C_2 z)^{\frac{1}{b}} \tag{4-49}$$

where

$C_1$, $C_2$ = constants.

The effective hydraulic conductivity of the consolidatable sediment is

$$\frac{1}{K_{FcEff}} = \frac{1}{D_{fc}} \int_0^{D_{fc}} \frac{1}{(C_1 + C_2 z)^{\frac{1}{b}}} dz \tag{4-50}$$

Integrating Equation 4-50, one obtains:

$$\frac{1}{K_{FcEff}} = \frac{1}{D_{fc}(1 - \frac{1}{b})C_2} \left( (C_1 + C_2 D_{fc})^{1-\frac{1}{b}} - (C_1)^{1-\frac{1}{b}} \right) \tag{4-51}$$

### 4.3.3 Effective Hydraulic Conductivity of Clogged Native Material (HydroGeoLogic, 1999)

The values of saturated hydraulic conductivity of the clogged zone are commonly lower than that of the pristine native material, or

$$K_{clogged} = C_{fact} K_{sat} \tag{4-52}$$

where

$C_{fact}$ = clogging factor = 0.1
$K_{sat}$ = saturated hydraulic conductivity of the native vadose zone material (m/d).

The following conditions are imposed on the hydraulic conductivity of the clogged native material:

$$K_{fc} \leq K_{Clogged} \leq K_{sat} \tag{4-53}$$

Penetration depth of up to about 0.45 m has been observed; the depth of the clogged layer is assumed to be fixed at 0.5 m.

### 4.3.4 Estimating Leachate Flow Rate

The following equations and nomenclature are based on **sublayers** as illustrated in Figure 4-2 using the upstream-weighted approximation (specifically, $\psi_{eff,n} = \psi_n$).

The unconsolidated sediment layer is assumed to be loose (fluid) so that the effective pressure head for the consolidated sediment layer is simply the liquid depth ($d_1$) plus the depth of the unconsolidated sediment ($D_s$). It is assumed that the system is at steady state. Therefore, a water balance dictates that the infiltration rate is the same for all sublayers. Assuming the pressure head at the ground water interface is zero, the general solution for the infiltration rate becomes, from Equation 4-38:

$$I = \frac{(d_1 + D_s + \sum d_{s,sn})}{\sum \left( \frac{d_{s,n}}{K_{s,n} k_{rw,n}} \right)} \tag{4-54}$$

where

I = saturated infiltration rate (m/d)
$K_{5,2}$ = saturated hydraulic conductivity of the sediment layer (m/d)
$d_{s,n}$ = thickness of the nth soil (or liner) sublayer (m).

The relative permeabilities ($k_{rw}$) of the clogged native material and native soil sublayers are a function of whether the previous sublayer is saturated (i.e., $\psi_n \geq 0$). There are two potential initial assumptions that can be made to provide an initial guess for the leaching rate. For the first initial approximation, the clogged native material is assumed to be the primary flow restriction (at small sediment depths), and the pressure head at the base of Sublayer 3 is assumed to be zero (i.e., $\psi_4 = 0$). Equation 4-54 then reduces to

$$I_{g1} = \frac{(d_1 + D_s + d_{s,1} + d_{s,2} + d_{s,3})}{\left[ \frac{d_{s,1}}{K_{s,1}} + \frac{d_{s,2}}{K_{s,2}} + \left( \frac{d_{s,3}}{K_{s,3} k_{rw,3}} \right) \right]} \tag{4-55}$$

To solve Equation 4-55, one first needs an estimate of $\psi_3$ to subsequently calculate $k_{rw,3}$ using Equation 4-39b. By setting the infiltration rate for the sediment and the first two sublayers equal to each other (steady-state water balance), the pressure head at the top of the second sublayer corresponding to the assumptions for Equation 4-55 is

$$\psi_3 = \frac{\left(\frac{d_{s,3}}{K_{s,3}k_{rw,3}}\right)\left(d_1 + D_s + d_{s,1} + d_{s,2}\right) - d_{s,3}\left(\frac{d_{s,1}}{K_{s,1}} + \frac{d_{s,2}}{K_{s,2}}\right)}{\left[\frac{d_{s,1}}{K_{s,1}} + \frac{d_{s,2}}{K_{s,2}} + \left(\frac{d_{s,3}}{K_{s,3}k_{rw,3}}\right)\right]} \tag{4-56}$$

Equation 4-56 is solved for $\psi_1$ by first assuming $k_{rw,2}$ is equal to 1. Then $k_{rw,2}$ is calculated using Equation 4-39a or 4-39b, as appropriate, and Equation 4-56 is resolved for $\psi_1$. Using a limited number of successive iterations on $\psi_1$, a value of $k_{rw,2}$ is estimated for use in Equation 4-55.

For the second potential initial approximation, it is assumed that all of the soil layers are saturated. The infiltration rate estimate is then calculated as follows:

$$I_{g2} = \frac{(d_1 + D_s + \sum d_{s,n})}{\left[\sum\left(\frac{d_{s,n}}{K_{s,n}}\right)\right]} \tag{4-57}$$

The infiltration rate is then set equal to the smallest of the initial approximations as

$$I^{\,i} = \min(I_{g1},\ I_{g2}) \tag{4-58}$$

Given the infiltration rate, Equation 4-38 can be rearranged to solve for the base pressure head of any soil (or the liner) sublayer as follows:

$$\psi_{n+1} = \psi_n - d_{s,n}\left(\frac{I^{\,i}}{K_{s,n}k_{rw,n}} - 1\right) \tag{4-59}$$

The solution algorithm starts at the consolidated sediment layer, where $\psi_1 = d_1 + D_s$. The relative permeability, $k_{rw,n}$, is based on $\psi_n$ (upstream weighted relative permeability calculation) and is calculated using Equation 4-39a or 4-39b, as appropriate. Equation 4-59 is then used to calculate successively values for $\psi_2$ through $\psi_{N+1}$. The final value of $\psi_{N+1}$ is then compared to the boundary condition at the ground water interface of $\psi_{N+1} = 0$. Based on that result, a new estimate of the infiltration rate is made ($I^i$), and Equation 4-59 is again solved to calculate the pressure profile in the underlying soil. This process is repeated until the boundary condition at the ground water interface is met within a 0.001-m tolerance.

For certain SI input operating conditions, very small changes in the infiltration rate caused large changes in the calculated pressure head at the ground water interface. As such, convergence on the ground water interface boundary condition was difficult. Therefore, when incremental estimates of the infiltration rate were different by less than 0.01 percent, convergence on the infiltration rate was considered to be completed. Under this circumstance, the final pressure profile was recalculated using this infiltration rate and an upstream calculational algorithm for the pressure profile. That is, the pressure at the ground water interface was set equal to zero ($\psi_{N+1} = 0$). The value for $\psi_N$ was then estimated and Equation 4-59 was solved for $\psi_{N+1}$. Iterative estimates of $\psi_N$ were made until the value of $\psi_{N+1}$ calculated from Equation 4-59 matched the boundary condition (($\psi_{N+1} = 0$). Successive estimates of the upstream pressure head were made using the following chord-slope convergence algorithm

$$\psi_n^{i+1} = \psi_n^i + (\psi_n^i - \psi_n^{i-1}) \left( \frac{\psi_{n+1} - \psi_{n+1}^i}{\psi_{n+1}^i - \psi_{n+1}^{i-1}} \right) \tag{4-60}$$

where

i = iteration number

$\Psi_n^i$ = $i^{th}$ estimate of the pressure head at top of the $n^{th}$ soil sublayer (m)

$\Psi_{n+1}$ = known pressure head at bottom of the $n^{th}$ soil sublayer (m)

$\Psi_{n+1}^i$ = pressure head at bottom of the $n^{th}$ soil sublayer calculated from Equation 4-59 for the $i^{th}$ iteration of $\Psi_n$ (m).

Convergence is assumed when $\Psi_{n+1} - \Psi_{n+1}^i$ is within a 0.001-m tolerance. At this point, $\psi_N$ is "known" and the solution proceeds to the next higher soil sublayer ($\psi_{N-1}$), and so on until the entire pressure profile is calculated up to all of the $\psi_1$. At this point, $\psi_1$ is compared to $d_1 + D_s$ to confirm pressure profile (and infiltration rate) convergence.

The volumetric leachate flow rate is then calculated from the infiltration rate as follows:

$$Q_{leach}\ (m^3/s) = \frac{I \times A}{24 \times 3600} \tag{4-61}$$

### 4.3.5 Limitations on Maximum Infiltration Rate

If the infiltration rate calculated using the equations in Section 4.3.4 exceed the rate at which the saturated zone can transport the ground water, the ground water level will rise into the unsaturated zone, and the assumption of zero pressure head at the base of the unsaturated zone is violated. This ground water "mounding" will reduce the effective infiltration rate. The maximum infiltration rate is estimated as the one that does not cause the ground water mound to rise to the bottom elevation of the SI unit. The maximum allowable infiltration rate may be approximated by (HydroGeoLogic, 1999):

$$I_{Max} \leq \frac{2K_{aqsat}D_{aqsat}(D_{vadose} - H)}{R_0^2 \ \ln\frac{R_\infty}{R_0}} \tag{4-62}$$

where

$\mathrm{I_{Max}}$ = infiltration rate (m/d)

$\mathrm{K_{aqsat}}$ = hydraulic conductivity of the saturated zone (m/d)

$\mathrm{D_{aqsat}}$ = depth of the saturated zone (m)

$\mathrm{D_{vadose}}$ = vadose zone thickness (m)

$\mathrm{R_0}$ = equivalent source radius (m)

$\mathrm{R_\infty}$ = length between the center of the source and the downgradient boundary where the boundary location has no perceptible effects on the heads near the source (m).

The equivalent source radius may be calculated from (HydroGeoLogic, 1999):

$$R_0 = \sqrt{\frac{A}{\pi}} \tag{4-63}$$

where

A = source area, $\mathrm{m^2}$.

If Equation 4-62 is used to limit the infiltration (leachate flow) rate, the program will output a warning message stating that the infiltration rate is being capped to prevent ground water mounding.

Under certain conditions of high soil-saturated hydraulic conductivity and long residence time in the SI, the leachate flow rate may exceed the influent flow rate. That is, given a porous underlying soil layer and high WMU residence time, the steady-state water depth may be less than the assumed depth of the liquid compartment as calculated as $d_{wmu} - d_2$. Rather than reiterating the infiltration rate calculation with liquid depth as a variable, the leachate rate is set equal to 99 percent of the influent flow rate as follows:

$$Q_{leach} = 0.99\ Q_{infl} \tag{4-64}$$

This equation is based on a volumetric balance on the WMU and an assumption that $Q_{out}$ equals 1 percent of $Q_{in}$. If Equation 4-64 is used to calculate the leachate flow rate, the program will output a warning message stating that the infiltration (leachate flow) rate is being capped by the influent flow rate.

### 4.3.6 Estimating Effluent Flow Rate

A volumetric water balance on the WMU can be arranged to calculate the effluent flow rate as follows:

$$Q_{out} = Q_{infl} - Q_{leach} + A\ (P_{rain} - P_{evap}) \tag{4-65a}$$

Under certain conditions of influent flow rate, impoundment dimensions, infiltration, precipitation, and evaporation, there may be months that Equation 4-65a predicts a negative or zero effluent rate, which would violate the pseudo-steady-state assumption. Therefore, if Equation 4-65a produces an effluent flow rate of less than 1 percent of the influent flow rate, the effluent flow rate is calculated as

$$Q_{out} = 0.01\ Q_{infl} \tag{4-65b}$$

As the infiltration rate is capped at 99 percent of the influent rate (Equation 4-64), Equation 4-65b would only be triggered if the evaporation rate exceeds the precipitation rate. Depending on the various rates, Equation 4-65b can be triggered even if Equation 4-64 is not, but the impact of Equation 4-65b, in any event, is to limit (or cap) the evaporation rate to prevent a zero or negative effluent rate. If Equation 4-65b is triggered, a warning message is output stating that the precipitation rate was capped to prevent the impoundment from drying out.

## 4.4 Sediment Deposition, Resuspension, and Burial

The sediment movement between the liquid and sediment compartment is expected to 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 based on the theoretical TSS mass removal efficiency given a vertical flow ("upflow") velocity. The resuspension velocity is determined by the sediment transport created by the upflow velocity and the sedimentation velocity is adjusted to achieve the calculated TSS mass removal efficiency.

### 4.4.1 Estimating Resuspension Velocity and Design Sediment Removal Efficiency

The WMU quiescent surface area and flow rate are used to calculate the upflow velocity of the impoundment as follows:

$$v_{upflow} = \frac{Q_{infl}}{A_q} \tag{4-66}$$

where

$v_{upflow}$ = upflow velocity (m/s).

Note: Comments were received from reviewers regarding the appropriateness of Equation 4-66 and whether the upflow velocity should be based on the effluent flow rate rather than the influent flow rate. A sensitivity analysis is being conducted to determine if the flow rate selected for calculating the upflow velocity makes a significant impact on the overall sediment removal efficiency calculated by the module. For example, at high residence times where $Q_{out} << Q_{infl}$, is the overall sediment removal efficiency capped at 99.99 percent removal.

The upflow velocity acts on the liquid compartment and effects an upward flux of particles. The resuspension velocity acts on the sediment compartment, and it is assumed to effect 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:

$$v_{res} = v_{upflow} \frac{[TSS_1]}{[TSS_2]} \tag{4-67}$$

The sediment removal efficiency of the WMU is estimated from WMU characteristics (flow rate and surface area) and the particle size distribution characteristics (mean particle size and relative standard deviation) by considering the terminal settling velocity of the particles. If a particle has a terminal settling velocity greater than the upflow velocity, it is assumed to settle within the WMU. If a particle has a terminal velocity less than this upflow velocity, it is assumed to be entrained in the effluent.

The suspended solids are assumed to be spherical for calculating the terminal velocity (or critical particle diameter) and the mass to volume ratio of the particles. The terminal velocity of the suspended solids is dependent on the friction factor (or drag coefficient) and the particle Reynolds number. For a sphere falling at terminal velocity the friction factor is

$$f = \frac{4}{3} \frac{g_c \, d_{part}}{v_{part}^2} \left( \frac{\rho_{part} - \rho_l}{\rho_l} \right) \tag{4-68}$$

where

$f$ = friction factor for sphere at terminal velocity
$d_{part}$ = mean diameter of suspended particles (cm)
$v_{part}$ = particle velocity (cm/s)
$\rho_l$ = density of water (g/cm$^3$).

There are three possible correlations that may be used to describe the correlation between the friction factor and the Reynolds number depending on the value of the Reynolds number (Bird et al., 1960, Figure 6.3-1, p. 192). The three possible correlations between the friction factor and the Reynolds number are:

$$\text{For} \quad Re_p < 0.1 \qquad f = \frac{24}{Re_p} \tag{4-69a}$$

$$\text{For} \quad 0.1 \le Re_p \le 500 \qquad f = \frac{24}{Re_p^{0.6}} \tag{4-69b}$$

$$\text{For} \quad Re_p > 500 \qquad f = 0.44 \tag{4-69c}$$

where

$Re_p$ = Reynolds number for particle = $d_{part}\, v_{part}\, \rho_l / \mu_l$
$\mu_l$ = viscosity of water, g/cm-s

By substituting in the expressions for both the friction factor and the Reynolds number into Equations 4-69(a-c), these equations can be solved in terms of the particle diameter associated with a given terminal velocity as follows:

$$\text{Assuming} \quad Re_p < 0.1 \qquad d_{part} = \left( \frac{18 \, v_{part} \, \mu_l}{g_c \, (\rho_{part} - \rho_l)} \right)^{0.5} \tag{4-70a}$$

$$\text{Assuming} \quad 0.1 \le Re_p \le 500 \qquad d_{part} = \left[ \frac{3}{4} \frac{v_{part}^{1.4}}{g_c} \left( \frac{18.5 \, \mu_l^{0.6} \, \rho_l^{0.4}}{(\rho_{part} - \rho_l)} \right) \right]^{\frac{1}{1.6}} \tag{4-70b}$$

$$\text{Assuming} \quad Re_p > 500 \qquad d_{part} = \frac{3}{4} v_{part}^2 \frac{0.44 \, \rho_l}{g_c \, (\rho_{part} - \rho_l)} \tag{4-70c}$$

The evaluation of the critical particle diameter is determined by an iterative calculation assuming $v_{part} = v_{upflow}$. First, Equation 4-70a is used to estimate $d_{part}$, then the resulting $d_{part}$ is used to calculate the Reynolds number to see if the assumption for the Reynolds number was correct. If the Reynolds number value fits the assumed range, the calculation is complete. If not, Equation 4-70b is employed to estimate $d_{part}$. Again the assumption for the Reynolds number is checked. If the Reynolds number falls within the assumed range, the calculation is complete; otherwise, Equation 4-70c is used to estimate $d_{part}$.

Once $d_{part}$ is estimated, the mass sediment removal efficiency of the WMU is calculated by the particle size distribution (assumed to be lognormally distributed) and a mass to diameter weighting ratio (based on spherical particles). The lognormal distribution density function is:

$$\phi(d_{part}) = \frac{1}{d_{part}\ \sigma\ (2\pi)^{½}} \times \exp\left(\frac{-[\ln(d_{part}/d_{mean})]^2}{2\sigma^2}\right) \qquad (4\text{-}71)$$

where

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

The mass to diameter weighting factor is

$$WtFactor_{part} = \frac{\pi}{6}\ d_{part}^{3} \qquad (4\text{-}72)$$

The "design" mass solids removal efficiency is then calculated as follows:

$$\epsilon_{TSS,o} = \frac{\int_{d_{crit}}^{+\infty} [\phi(d_{part}) \times WtFactor_{part}]}{\int_{0}^{+\infty} [\phi(d_{part}) \times WtFactor_{part}]} \qquad (4\text{-}73)$$

where

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

Due to 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 99.99 percent. That is, if $\epsilon_{TSS,o}$ >0.9999 from Equation 4-73, $\epsilon_{TSS,o}$ is set equal to 0.9999.

### 4.4.2 Estimating Burial Velocity

The suspended solids burial (or accumulation) rate is determined from the predicted sediment removal efficiency, which is the design mass removal efficiency corrected for a decrease in sediment removal efficiency as sediment accumulates in the WMU. As constructed, the design sediment removal efficiency is independent of WMU depth. 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. In attempts 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

$$k_{sed} = \frac{-\ln\ (1 - \epsilon_{TSS,o})}{\dfrac{(1.2\ m)\ A}{Q_{infl}}} \tag{4-74}$$

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

$$\epsilon_{TSS} = \epsilon_{TSS,o} \left(1 - e^{\frac{-k_{sed}\ d_1\ A}{Q_{infl}}}\right) \tag{4-75}$$

From a mass balance of sediment in the liquid compartment, the total suspended solids concentration in the effluent can be calculated as

$$[TSS]_{out} = \frac{Q_{infl}}{Q_{out}} \left([TSS]_{infl} + \lambda\ \epsilon_{BOD}\ C_{BOD}\right)\ (1 - \epsilon_{TSS}) \tag{4-76}$$

The second term of this equation accounts for new biomass solids that grow within the WMU and is based on the total mass of food (as BOD) consumed across the WMU. The BOD removal efficiency is estimated from the food-to-microorganism ratio (F/M) in the WMU. Typical design values for F/M for activated sludge systems range from 0.2 to 0.6 g BOD/g

MLVSS-d (Eckenfelder et al., circa 1984), but F/M ratios of 0.2 to 1.2 g BOD/g MLVSS-d have been observed in practice (Hermann and Jeris, 1992). A value of 0.6 g BOD/g MLVSS-d was selected to estimate the BOD removal capacity of the unit as follows:

$$BOD_{rem} = 0.6\ g/g\text{-}d \times k_{ba}\ [TSS]_{est} \times A_{wmu}\ d_{liq1} \tag{4-77}$$

where

$BOD_{rem}$ = BOD removal capacity of the unit, g BOD/d
$[TSS]_{est}$ = estimated TSS concentration, $Mg/m^3$
= $[TSS]_{in}$ for first time step and $[TSS]_1$ from past time step for all other times.

The BOD removal efficiency is then calculated as

$$\epsilon_{BOD} = \frac{BOD_{rem}}{C_{BOD}\ Q_{infl}} \tag{4-78}$$

The BOD removal efficiency as calculated using Equation 4-78 can be greater than 1. Therefore, a maximum limit was placed on the BOD removal efficiency. BOD removal efficiencies are generally up to 95 percent for a variety of biological wastewater systems (Eckenfelder et al., 1985), although reports of BOD removal efficiencies as high as 99 percent have been cited (Weber et al., 1985 and Bryant, 1985). Consequently, the cap for the BOD removal efficiency was set at 0.99. Note, a BOD removal efficiency cap of 0.95 would decrease the total projected biomass growth by less than 5 percent compared to the selected cap of 0.99.

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.

$$v_b = \frac{Q_{infl}\ ([TSS]_{infl} + \lambda\ \epsilon_{BOD}\ C_{BOD}) - Q_{out}\ [TSS]_{out}}{A\ [TSS]_2} \tag{4-79}$$

### 4.4.3 Estimating Sedimentation Velocity

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

$$v_{sed} = (v_{res} + v_b)\ \frac{[TSS]_2}{[TSS]_1} - \frac{Q_{leach}}{A} \tag{4-80}$$

where $[TSS]_1$ is calculated from $[TSS]_{infl}$ and $[TSS]_{out}$ using Equation 4-11.

### 4.4.4 Estimating 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 contaminant reduction associated with the sediment) by digestion can be included without significantly complicating the module. The net accumulation of sediment over a time step is estimated as:

$$\Delta d_2 = v_b \, \Delta t \left[ 1 - k_{ba} \left( 1 - e^{-k_{dec} \, \Delta t} \right) \right] \tag{4-81}$$

where

$k_{ba}$ = 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, $\Delta d_2$ 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/dredging action is compared to the input cleaning/dredging parameters (either fraction of the WMU that can be filled with sediment before the WMU is cleaned or dredged or a set frequency, e.g., once every 4 years). 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, but this removal acts as a sink from the overall system.

## 4.5 Temperature Effects

Temperature can impact a number of the different module parameters, such as the air density and diffusivity, the biodegradation rate, liquid viscosity, and Henry's law constant. Some of the equations employed 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 ambient air temperature is used to estimate the air-side properties (air diffusivity, air density, etc.). The liquid-side properties (liquid diffusivity, liquid viscosity, etc.) are evaluated at the liquid temperature within the tank.

### 4.5.1 Estimating Temperature in the Waste Management Unit

A simplified energy balance is used around the WMU to estimate the liquid temperature in the tank given the liquid temperature of the influent, the ambient air temperature, and the liquid residence time in the WMU. The simplified energy balance is

$$4.18\times10^{-6}\ \rho_l\ C_{p,liq}\ Q_{infl}\ T_{infl} = 4.18\times10^{-6}\ \rho_l\ C_{p,liq}\ Q_{infl}\ T_l + h_{ave}\ A\ (T_l - T_{air}) \qquad (4\text{-}82)$$

where

$\rho_l$ = liquid density (g/cm$^3$)
$C_{p,liq}$ = specific heat of liquid (cal/g-°C)
$T_{infl}$ = influent waste temperature (°C)
$4.18\times10^{-6}$ = unit conversion, 4.186 (kg-m$^2$/s$^2$)/cal × 1E6 cm$^3$/m$^3$
$T_l$ = liquid waste temperature in WMU (°C)
$h_{ave}$ = average overall heat transfer coefficient (W/m$^2$-°C = kg/s$^3$-°C)
$T_{air}$ = ambient air temperature (°C).

The specific heat capacity of water is 1 cal/g-°C and its density is 1 g/cm$^3$. Kreith and Black report ranges for convective heat transfer coefficients for free and forced convection for both water and air (Kreith and Black, 1980). To estimate the average overall heat transfer coefficient, it is assumed 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. For forced convection of air, the reported range is 10 to 200 W/m$^2$-°C, and a general value of 50 W/m$^2$-°C was selected. For free convection of water, the reported range is 20 to 100 W/m$^2$-°C, and a general value of 50 W/m$^2$-°C was selected. For forced convection of water, the reported range is 50 to 10,000 W/m$^2$-°C, and a general value of 1,000 W/m$^2$-°C was selected. Using thermal resistance theory, the overall quiescent heat transfer coefficient is estimated to be 25 W/m$^2$-°C, and the overall turbulent heat transfer coefficient is estimated to be 50 W/m$^2$-°C. Using the relative aerated and quiescent surface areas, the average overall heat transfer coefficient is estimated to be 25(1+$f_{aer}$) W/m$^2$-°C. Therefore, assuming the liquid waste is essentially water, Equation 4-82 can be rearranged to estimate the liquid temperature within the tank as follows:

$$T_l = \frac{T_{infl} + \left(\dfrac{25\ (1 + f_{aer})\ A}{4.18E6\ Q_{infl}}\right) T_{air}}{1 + \left(\dfrac{25\ (1 + f_{aer})\ A}{4.18E6\ Q_{infl}}\right)} \qquad (4\text{-}83)$$

Note that this equation does not take into account the heat of fusion (i.e., ice formation). As such, Equation 4-83 can yield liquid temperatures of less than 0°C. When this happens, the liquid temperature is set to 0.1°C and the amount of ice formed is estimated using the previous assumptions for the specific heat capacity and density of water (1 cal/g-°C and 1 g/cm$^3$, respectively) and using a heat of fusion of 80 cal/g and a density of ice of 0.9 g/cm$^3$. The additional heat loss in taking the water from 0°C to $T_l$ (when $T_l < 0$) is translated into a mass of ice formation, and the volume or depth of ice formed is estimated using the following equation:

$$d_{ice} = \frac{A_{wmu} \times d_{wmu} \times (-T_l)}{80\ (0.9)\ A_{wmu}} \tag{4-84}$$

where

$d_{ice}$ = depth of ice layer formed, m.

Equation 4-84 is expected to be a high estimate of ice formation because convective heat transfer from the surrounding soil was not included in the heat balance as expressed in Equation 4-82. Furthermore, a small amount of ice formation will not significantly impact the emission estimates and other parameters estimated by the module. However, if a solid crust of ice develops over the entire impoundment for a prolonged period of time, the emission estimates, which do not consider volatilization through an ice layer, are expected to overstate the potential for volatile emissions. Therefore, when the depth of the ice layer, as estimated using Equation 4-84, is 10 cm or more for 3 consecutive months, the module generates a warning message that significant ice formation is projected.

### 4.5.2 Estimating Temperature Effects on Air-Side Properties

The air-side properties are among the most temperature sensitive of the input properties. The density at any given temperature can be estimated using the ideal gas law as

$$\rho_{air}^{Tair} = \rho_{air}^{Tr} \left( \frac{273 + T_r}{273 + T_{air}} \right) \tag{4-85}$$

where

$\rho_{air}^{Tair}$ = density of air at air temperature $T_{air}$ (g/cm$^3$)
$\rho_{air}^{Tr}$ = density of air at reference temperature (g/cm$^3$)
$T_{air}$ = module simulation air temperature (°C)
$T_r$ = reference temperature, (°C, assumed to be 25°C).

The temperature dependence of the constituent's diffusivity in the gas phase is estimated by the chemical properties processor (Pacific Northwest National Laboratory, 1998).

The viscosity of air is only slightly impacted by temperatures in the temperature range of interest, and little error is introduced in ignoring its temperature dependency (ranges from

1.75×10$^{-4}$ to 2.17×10$^{-4}$ g/cm-s as temperatures range from 0°C to 100°C, Kreith and Black, 1980). Alternatively, the CHEMDAT8 module documentation (U.S. EPA, 1994) presents the following equation that can be used for a temperature-dependent estimate of air viscosity:

$$\mu_{air}^{T2}\ (g/cm{-}s) = 4.568\times10^{-7}\ T_{air}(^{\circ}C) + 1.7209\times10^{-4} \tag{4-86}$$

### 4.5.3 Estimating Temperature Effects on Liquid-Side Properties

The density of water is basically insensitive to temperature (no temperature adjustments are used).

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 following correlation was developed (using a log-log least squares linear regression as suggested by Liley and Gambill 1973, p. 3-246) for the temperature-dependent viscosity of water between 0°C to 100°C:

$$\mu_{liq}^{Tl}\ (g/cm{-}s) = \frac{3.45\times10^{12}}{(273 + T_l)^{5.884}} \tag{4-87}$$

The values for the viscosity of water calculated from Equation 4-87 agree well with the values estimated using the figure/coordinates reported by Liley and Gambill (1973, pp. 3-212 and 3-213) for temperatures between 0°C and 100°C.

The temperature dependence of the constituent's diffusivity in the liquid phase is estimated by the chemical properties processor (Pacific Northwest National Laboratory, 1998).

### 4.5.4 Estimating Temperature Effects on Vapor-Liquid Partitioning

Temperature impacts both the gas phase and liquid phase activity coefficients so that developing a temperature correction factor for Henry's law constants is not straightforward. For example, the Henry's law constant is often estimated for sparingly soluble constituents as the constituent vapor pressure divided by the solubility. Although the vapor pressure will increase with increasing temperature, the solubility of the constituent may either increase or decrease, depending on the constituent. Consequently, the combined impact of temperature on the vapor-liquid partitioning coefficient may be small or large depending on the constituent. The temperature dependence of the constituent's Henry's law constants is estimated by the chemical properties processors (Pacific Northwest National Laboratory, 1998).

### 4.5.5 Estimating Temperature Effects on Biodegradation Rates

The temperature dependence of the constituent's aerobic and anaerobic biodegradation rates ($k_{bm}$ and $k_{bs}$) is estimated by the chemical properties processors (Pacific Northwest National

Laboratory, 1998). The sediment decay rate ($k_{dec}$) is assumed to be relatively unaffected by temperatures over a reasonably wide range of temperatures. At temperatures above 50°C and at temperatures near freezing, the sediment decay rate is assumed to drop rapidly. A simple temperature correction factor for the sediment decay rate was developed based on these assumptions and is illustrated in Figure 4-4. As seen in Figure 4-4, the biodegradation rate temperature correction factor is assumed to be 1 at temperatures between 7°C and 40°C. At temperatures below 3°C and above 60°C, the temperature correction factor is 0, and a linear extrapolation is used to determine the temperature correction factor between 3°C and 7°C and between 40°C and 60°C.

At this point, all of the variables needed to calculate the "constants" in Equations 4-15 through 4-18 (i.e., $K_{c1}$, $K_{c2}$ , $K_{c3}$, $K_{c4}$) have been determined, and Equations 4-21 and 4-22 can be solved for the contaminant concentration in each compartment.

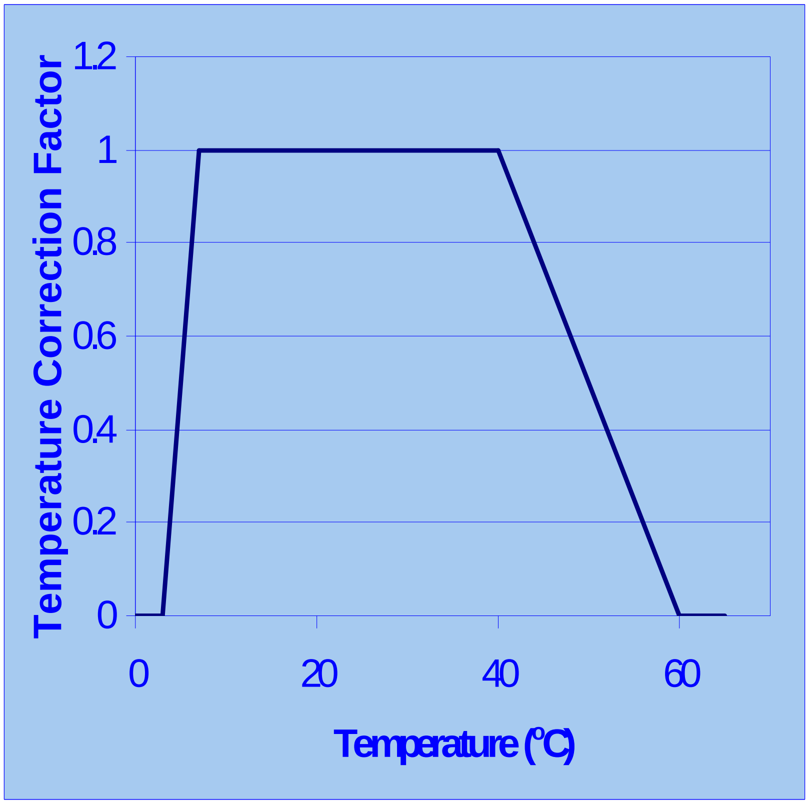

**Figure 4-4. Illustration of temperature correction factor used for biological degradation rates.**

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