

4. SURFACE WATER AND SEDIMENT ALGORITHMS

The surface water compartment is assumed to be well-mixed and composed of three phases: water, suspended sediment particles, and algae.¹ Thus, chemicals can be dissolved in the water phase, sorbed to the sediment particles, or contained in algae. The sediment compartment is modeled as well-mixed and consisting of a benthic-solids phase and benthic pore or interstitial water. Chemicals can either be dissolved in the interstitial pore water or sorbed to the benthic sediment particles. The gas phase of the surface water and sediment compartments is considered to be negligible in terms of its impact on the movement of chemicals and is not modeled. The text box beginning on the next page provides a list of the transfer-factor algorithms developed in this chapter and defines all parameters used in those algorithms.

4.1 CONCEPTUALIZATION OF THE SURFACE WATER AND SEDIMENT COMPARTMENTS

The behavior of chemicals in surface waters is determined by three factors: the rate of input, the rate of physical transport in the water system, and chemical reactivity. Physical transport processes are dependent to a large extent on the type of water body under consideration *i.e.*, oceans, seas, estuaries, lakes, rivers, or wetlands. Schnoor (1981) and Schnoor and McAvoy (1981) have summarized important issues relating to surface-water transport. Fugacity models have been developed for lakes and rivers by Mackay et al. (1983a,b).

At low concentrations, contaminants in natural waters exist in both a dissolved and a sorbed phase. In slow-moving surface waters (*e.g.*, lakes), both advection and dispersion are important. In rapidly moving water systems (*e.g.*, rivers), advection controls mass transport, and dissolved substances move at essentially the same velocity as the bulk water in the system. A water balance is the first step in assessing surface-water transport. A water balance is established by equating gains and losses in a water system with storage. Water can be stored within estuaries, lakes, rivers, and wetlands by a change in elevation. Water gains include inflows (both runoff and stream input) and direct precipitation. Water losses include outflows and evaporation.

The accuracy of modeling fresh-water systems depends on the ability to simulate the movement of water and sediment to and from the system (Schnoor 1981). There are two primary categories for fresh water: rivers and lakes. This model is based on that described in Mackay et al. (1983a,b). Table 4-1 summarizes the chemical gains and losses for the surface water compartment that are addressed in the current TRIM.FaTE library. Losses or changes due to transformation or degradation reactions also are modeled in TRIM.FaTE. Losses from the sediment due to colloidal diffusion and bioturbation are not addressed in the current TRIM.FaTE library.

¹Because of data limitations, in the current TRIM.FaTE library, algae are modeled as a third phase of the surface water compartment, instead of as a stand-alone biotic compartment.

Summary of Surface Water and Sediment Transfer Factors in TRIM.FaTE

ADVECTIVE TRANSFERS

Dry deposition of particles to surface water (solid phase): TF 4-1b

$$T_{Air \rightarrow SW}^{dry_dep} = \frac{A_{SWA} \times v_{dry}}{V_{Air}} \times f_{MS}$$

Wet deposition of particles to surface water (solid phase): TF 4-2b

$$T_{Air \rightarrow SW}^{wet_dep} = \frac{A_{SWA} \times v_{wet}}{V_{Air}} \times f_{MS}$$

Wet deposition of vapor-phase from air to surface water during rain (fugacity approach): TF 4-3a

$$T_{Air \rightarrow SW}^{WVdep}(rain) = \frac{A_{SWA}}{V_{Air}} \times rain \times \frac{Z_{pure_water}}{Z_{Total_air}}$$

Wet deposition of vapor-phase from air to surface water during rain (partitioning approach): TF 4-3b

$$T_{Air \rightarrow SW}^{WVdep}(rain) = \frac{A_{SWA}}{V_{Air}} \times rain \times w_{rV} \times f_{MV}$$

Deposition of suspended sediment to sediment bed (solid phase): TF 4-4

$$T_{SW \rightarrow Sed}^{dep} = \frac{A_{SedSW}}{V_{SW}} \times v_{Sed}^{dep} \times f_{MS}$$

Resuspension of sediment to surface water (solid phase): TF 4-5

$$T_{Sed \rightarrow SW}^{res} = \frac{A_{SedSW}}{V_{Sed}} \times v_{Sed}^{res} \times f_{MS}$$

Algal deposition rates (algal phase): TF 4-6

$$T_{Al \rightarrow Sed}^{dep} = \frac{A_{SedSW}}{V_{SW}} \times v_{Sed}^{Al} \times f_{MAI}$$

Outflow from flowing river to surface water advection sink (total phase): TF 4-7a

$$T_{SW-SW_sink}^{river} = outflow / V_{SW}$$

Outflow from lake or pond to surface water advection sink (total phase): TF 4-7b

$$T_{SW \rightarrow SW_sink}^{lake} = \frac{(flushes / yr)}{365}$$

Summary of Surface Water and Sediment Transfer Factors in TRIM.FaTE (cont.)

ADVECTIVE TRANSFERS (cont.)

Sediment burial (solid phase):

TF 4-8

$$T_{Sed \rightarrow Sed_sink}^{Total} = \frac{A_{Sed}}{V_{Sed}} \times burial_rate \times f_{MS}$$

Advection from one river compartment to another river or lake compartment:

TF 4-9

$$T_{i \rightarrow j}^{adv}(total) = flow / V_i$$

DIFFUSIVE/DISPERSIVE TRANSFERS

Diffusion from sediment to surface water compartments:

TF 4-10a

$$T_{SW \rightarrow Sed}^{dif} = \frac{A_{SedSW}}{V_{SW}} \times \left(\frac{1}{U_{SedSW} \times \frac{Z_{Total_Sed}}{Z_{Total_SW}}} + \frac{1}{U_{SWSed}} \right)^{-1}$$

Diffusion from surface water to sediment compartments:

TF 4-11a

$$T_{Sed \rightarrow SW}^{dif} = \frac{A_{SedSW}}{V_{Sed}} \times \left(\frac{1}{U_{SWSed} \times \frac{Z_{Total_SW}}{Z_{Total_Sed}}} + \frac{1}{U_{SedSW}} \right)^{-1}$$

Dispersive exchange flux between two surface water compartments:

TF 4-12

$$T_{SWi \rightarrow j}^{disp} = \frac{E_{ij} \times A_{ij}}{L_{ij} \times V_i}$$

Diffusive exchange between sediment compartment *i* and sediment compartment *j* below:

TF 4-13

$$T_{Sedi \rightarrow Sedj}^{dif} = \frac{A_{Sedij}}{V_{Sedi}} \times \frac{DSP_{Sed} \times \phi_{avg}}{L_{Sedij}} \times f_{MLi}$$

Diffusive exchange between sediment compartment *j* and sediment compartment *i* above:

TF 4-14

$$T_{Sedj \rightarrow Sedi}^{dif} = \frac{A_{Sedij}}{V_{Sedj}} \times \frac{DSP_{Sed} \times \phi_{avg}}{L_{Sedij}} \times f_{MLj}$$

Summary of Surface Water and Sediment Transfer Factors in TRIM.FaTE (cont.)

LIST OF SYMBOLS USED IN TRANSFER FACTOR ALGORITHMS		
w_{rV}	=	vapor washout ratio ($m^3[\text{air}]/m^3[\text{rain}]$).
f_{MV}	=	fraction chemical mass in air compartment that is vapor-phase divided by volume fraction of the air compartment that is gas-phase (unitless).
A_{SWA}	=	area of surface water/air interface ($m^2[\text{interface}]$).
V_{Air}	=	volume of the air compartment ($m^3[\text{air}]$).
f_{MS}	=	fraction mass of chemical sorbed to sediment particles divided by the volume fraction of the compartment (surface water or sediment) that is solid particles (unitless).
<i>rain</i>	=	rainfall rate (m/day).
$Z_{\text{pure_water}}$	=	fugacity capacity of chemical in the aqueous phase ($\text{mol}/m^3\text{-Pa}$).
$Z_{\text{Total_Air}}$	=	total fugacity capacity of chemical in the air compartment ($\text{mol}/m^3\text{-Pa}$).
A_{SedSW}	=	area of surface water/sediment interface ($m^2[\text{interface}]$).
V_{SW}	=	volume of surface water compartment ($m^3[\text{water}]$).
$v_{\text{sed}}^{\text{dep}}$	=	volumetric deposition rate of suspended sediment to sediment bed ($m^3[\text{suspended sediment particles}]/m^2$ (area)-day).
V_{Sed}	=	volume of sediment compartment (m^3).
$v_{\text{Sed}}^{\text{res}}$	=	volumetric resuspension rate of benthic sediment to water column ($m^3[\text{benthic sediment particles}]/m^2$ [benthic sediment]-day).
$v_{\text{Sed}}^{\text{Al}}$	=	volumetric algal deposition rate to benthic sediments ($m^3[\text{algae}]/m^2[\text{sediment/water interface}]\text{-day}$).
f_{MAI}	=	fraction mass of chemical in algae divided by the volume fraction of the surface water compartment that consists of algal cells (unitless).
<i>outflow</i>	=	volumetric outflow of water from surface water compartment to advection sink (m^3/day).
<i>flushes/yr</i>	=	outflow measured as number of complete changes (flushes) of water per year.
<i>burial_rate</i>	=	sediment burial rate ($m^3[\text{sediment particles}]/m^2[\text{sediment}]\text{-day}$).
<i>flow</i>	=	volumetric flow of water from one river compartment to another river or lake compartment (m^3/day).
A_{Sed}	=	area of the sending sediment compartment (m^2).
$U_{\text{SW}^{\text{Sed}}}$	=	mass transfer coefficient between surface water and sediment (m/day).
$U_{\text{Sed}^{\text{SW}}}$	=	mass transfer coefficient between sediment and surface water (m/day).
E_{ij}	=	dispersion coefficient for exchange between water compartments <i>i</i> and <i>j</i> (m^2/day).
A_{ij}	=	interfacial area between water compartments <i>i</i> and <i>j</i> (m^2).
L_{ij}	=	characteristic mixing length between water compartments <i>i</i> and <i>j</i> (m).
V_i	=	volume of water compartment <i>i</i> (m^3).
$A_{\text{Sed}ij}$	=	interfacial area between sediment compartments <i>i</i> and <i>j</i> (m^2);
V_{Sedi}	=	volume of the sending sediment compartment <i>i</i> (m^3);
V_{Sedj}	=	volume of the sending sediment compartment <i>j</i> (m^3);
DSP_{Sed}	=	diffusive exchange coefficient between sediment compartments (m^2/day);
ϕ_{avg}	=	average porosity at the interface between sediment compartments <i>i</i> and <i>j</i> (unitless);
$L_{\text{Sed}ij}$	=	characteristic mixing length between sediment compartments <i>i</i> and <i>j</i> (m);
f_{MLi}	=	fraction of the chemical mass in sediment compartment <i>i</i> that is dissolved in water divided by volume fraction sending sediment compartment <i>i</i> that is liquid (unitless).
f_{MLj}	=	fraction of the chemical mass in sediment compartment <i>j</i> that is dissolved in water divided by volume fraction sending sediment compartment <i>j</i> that is liquid (unitless).

Table 4-1
Summary of the Chemical Gains and Losses for Surface Water Compartments
Addressed in TRIM.FaTE

Gains	Type of Process	Relevant Phase	Losses	Type of Process	Relevant Phase
From Surface Soil					
Erosion	Advection (TF 5-11)	Solid			
Runoff	Advection (TF 5-10)	Aqueous			
From Air			To Air		
Diffusion from air	Diffusion (TF 3-2)	Vapor	Diffusion to air	Diffusion (TF 3-3)	Aqueous
Dry deposition of particles/ aerosols from air	Advection (TF 4-1)	Solid			
Wet deposition of particles/ aerosols from air	Advection (TF 4-2)	Solid			
Wet deposition of vapor from air	Advection (TF 4-3)	Vapor			
From Sediment			To Sediment		
Diffusion from sediment	Diffusion (TF 4-10a,b)	Aqueous	Diffusion to sediment	Diffusion (TF 4-11a,b)	Aqueous
Resuspension of sediment	Advection (TF 4-5)	Solid	Deposition to sediment	Advection (TF 4-4)	Solid
From Rivers			To Lake		
Compartment to compartment flow	Advection (TF 4-9)	Total	River to lake advective flow	Advection (TF 4-9)	Total
From Aquatic Biota			To Aquatic Biota		
Elimination from fish	Advection (TF 6-8)	Total	Uptake by fish via gills	Advection (TF 6-5)	Total
Elimination from macrophytes	Diffusion (TF 6-1)	Aqueous	Uptake by macrophytes	Diffusive (TF 6-2)	Aqueous
			Ingestion of algae by fish	Advection (TF 6-6)	Algae
From Terrestrial Birds and Mammals			To Terrestrial Birds and Mammals		
Elimination from semi-aquatic wildlife	Advection (TF 7-32)	Total	Ingestion by wildlife	Advection (TF 7-21)	Total
From Surface Water Transformations			To Sink(s)		
			Decay to reaction sinks	Degradation (TF 2-1)	Total
			Outflow to advection sink	Advection (TF 4-7)	Total

The general manner in which the algorithms are presented below is intended to provide model flexibility and to facilitate implementing different algorithms to describe specific processes.

4.2 ADVECTIVE PROCESSES

This section describes the advective processes between different compartment types as follows:

- Between air and surface water (Section 4.2.1);
- Between sediment and surface water (Section 4.2.2);
- From sediment/surface water to advection sinks (Section 4.2.3); and
- From surface soil to surface water (Section 4.2.4).

4.2.1 ADVECTIVE PROCESSES BETWEEN AIR AND SURFACE WATER

The advective processes considered between air and surface water are wet and dry deposition of solid-phase particles and wet deposition of vapor that is dissolved into the water phase.² For all of these processes, the air compartment is the sending compartment and the surface water compartment is the receiving compartment.

The following subsections describe the transfer algorithms for advective processes between air and surface soil and surface water:

- dry deposition of particles to surface water (Section 4.2.1.1);
- wet deposition of particles to surface water (Section 4.2.1.2); and
- wet deposition of vapor-phase to surface water (Section 4.2.1.3).

4.2.1.1 Dry Deposition of Particles to Surface Water

A unidirectional flux equation that expresses dry deposition of particles from air to surface water, from van de Water (1995), follows. Note that the boundaries of the surface water and air parcels may not be congruent; that is, the area of the surface water and the area associated with a contiguous air compartment may be different. The change in the chemical mass in the surface water from dry deposition of chemical sorbed to atmospheric dust particles can be estimated as:

$$\frac{dN_{SW}}{dt} = \frac{N_{Air}}{V_{Air}} \times v_{dry} \times \frac{D_L}{\rho_P} \times \frac{Z_{pure_solid}}{Z_{Total_Air}} \times A_{SWA} \quad (\text{Eq. 4-1})$$

where:

$$\begin{aligned} N_{SW} &= \text{mass of chemical in the surface water compartment (g[chemical]);} \\ N_{Air} &= \text{mass of chemical in the air compartment (g[chemical]);} \end{aligned}$$

²See Appendix A for a description of a net dry vapor deposition algorithm for divalent mercury.

- V_{Air} = volume of air compartment (m³);
 v_{dry} = dry deposition velocity of particles (m/day);
 D_L = atmospheric dust load in air compartment (kg[particles]/m³[air]);
 ρ_P = density of dust particles (kg[particles]/m³[particles]);
 Z_{pure_solid} = fugacity capacity of the chemical in or sorbed to solid particles (mol/m³-Pa);
 Z_{Total_Air} = total fugacity capacity of chemical in bulk air, including atmospheric dust particles (mol/m³-Pa); and
 A_{SWA} = area of the interface between surface water and air (m²).

Thus, the transfer factor for dry deposition of chemical associated with air particles can be estimated using the fugacity approach:

$$T_{Air \rightarrow SW}^{dry_dep} = \frac{A_{SWA}}{V_{Air}} \times v_{dry} \times \frac{D_L \times Z_{pure_solid}}{\rho_P \times Z_{Total_Air}} \quad (\text{TF 4-1a})$$

where:

- $T_{Air \rightarrow SW}^{dry_dep}$ = advective transfer (dry deposition) of chemical sorbed to particles from air to surface water (/day);
 Z_{pure_solid} = fugacity capacity of chemical in the solid phase (mol/m³-Pa); and
 Z_{Total_Air} = total fugacity capacity of chemical in the air compartment (mol/m³-Pa).

It is also true that:

$$v_{dry} = v_{dry} \times \frac{D_L}{\rho_P} \quad (\text{Eq. 4-2})$$

where:

- v_{dry} = volumetric dry deposition rate (m³[dust]/m²[surface water/air interface]-day);

and:

$$\frac{Z_{pure_solid}}{Z_{Total_Air}} = \frac{Mass_Fraction_Sorbed}{Volume_Fraction_Solid} = f_{MS} \quad (\text{Eq. 4-3})$$

where:

- f_{MS} = mass fraction of the chemical sorbed to atmospheric dust particles divided by the volume fraction of the air compartment that consists of particles (see Equations 2-71 and 2-79) (unitless).

Therefore, the transfer factor for dry deposition of particles in air to surface water can also be expressed as the following equation, which is coded in the current TRIM.FaTE library:

$$T_{Air \rightarrow SW}^{dry_dep} = \frac{A_{SWA}}{V_{Air}} \times v_{dry} \times f_{MS} \quad (\text{TF 4-1b})$$

4.2.1.2 Wet Deposition of Particles to Surface Water

Nonionic organic chemicals in the atmosphere can be either in the vapor phase, attached to particles or aerosols, or as fine aerosols. TF 4-3a (see Section 4.2.1.3) is used for wet deposition of vapor. TF 4-2a is used for the wet deposition of aerosols, regardless of whether the chemical is attached to the aerosol or particle or is present as a fine aerosol of the chemical itself.

The change in the chemical mass in the surface water from wet deposition of chemical sorbed to atmospheric dust particles during a rain event can be estimated as:

$$\frac{dN_{SW}}{dt} = \frac{N_{Air}}{V_{Air}} \times w_r \times rain \times \frac{D_L}{\rho_P} \times \frac{Z_{pure_solid}}{Z_{Total_Air}} \times A_{SWA} \quad (\text{Eq. 4-4})$$

where:

- N_{SW} = mass of chemical in the surface water compartment (g[chemical]);
- N_{Air} = mass of chemical in the air compartment (g[chemical]);
- V_{Air} = volume of air compartment (m³);
- w_r = scavenging or washout ratio for particles in air (ranges from 50,000 to 200,000) (m³[air]/m³[rain]);
- $rain$ = rate of rainfall (m/day);
- D_L = dust load, *i.e.*, density of dust particles in air (kg[particles]/m³[air]);
- ρ_P = density of dust particles (kg[particles]/m³[particles]);
- Z_{pure_solid} = fugacity capacity of the chemical in or sorbed to solid particles (mol/m³-Pa);
- Z_{Total_Air} = total fugacity capacity of chemical in bulk air, including atmospheric dust particles (mol/m³-Pa); and
- A_{SWA} = area of surface water/air interface (m²).

Thus, the transfer factor for wet deposition of chemical associated with air particles can be estimated as follows:

$$T_{Air \rightarrow SW}^{wet_dep} = \frac{A_{SWA}}{V_{Air}} \times w_r \times rain \times \frac{D_L \times Z_{pure_solid}}{\rho_P \times Z_{Total_Air}} \quad (\text{TF 4-2a})$$

where:

- $T_{Air \rightarrow SW}^{wet_dep}$ = advective transfer (wet deposition) of chemical sorbed to particles from air to surface water (/day).

Using the same relationships described in Section 4.2.1.1, algorithm TF 4-2a can be rearranged to TF 4-2b, which reflects the code in the TRIM.FaTE library:

$$T_{Air \rightarrow SW}^{wet_dep} = \frac{A_{SWA}}{V_{Air}} \times v_{wet} \times f_{MS} \quad (\text{TF 4-2b})$$

where:

$$v_{wet} = w_r \times rain \times \frac{D_L}{\rho_P} \quad (\text{Eq. 4-5})$$

and:

$$\begin{aligned} f_{MS} &= Z_{pure_solid}/Z_{Total_Air} \text{ as described for Equation 4-3 above (unitless); and} \\ v_{wet} &= \text{volumetric wet deposition rate (m}^3\text{[dust particles]/m}^2\text{[surface water/air interface]-day).} \end{aligned}$$

4.2.1.3 Wet Deposition of Vapor-phase Chemical to Surface Water

There also is advective flux of vapor-phase chemical from rainfall. As the rain falls, it gathers chemical from the air, coming into equilibrium with the fugacity of the air compartment.

$$\frac{dN_{SW}}{dt} = \frac{N_{Air}}{V_{Air}} \times rain \times \frac{Z_{pure_water}}{Z_{Total_Air}} \times A_{SWA} \Rightarrow \quad (\text{Eq. 4-6})$$

$$T_{Air \rightarrow SW}^{WVdep}(rain) = \frac{A_{SWA}}{V_{Air}} \times rain \times \frac{Z_{pure_water}}{Z_{Total_Air}} \quad (\text{TF 4-3a})$$

where:

$$\begin{aligned} N_{SW} &= \text{total mass of chemical in the surface water compartment (g[chemical]);} \\ N_{Air} &= \text{total mass of chemical in the air compartment (g[chemical]);} \\ V_{Air} &= \text{volume of air compartment (m}^3\text{);} \\ rain &= \text{rainfall rate (m/day);} \\ Z_{pure_water} &= \text{fugacity capacity of the chemical in aqueous phase of surface water (i.e., excluding suspended sediments) (mol/m}^3\text{-Pa);} \\ Z_{Total_Air} &= \text{total fugacity capacity of the chemical in the air compartment (mol/m}^3\text{-Pa);} \\ A_{SWA} &= \text{area of surface water/air interface (m}^2\text{); and} \\ T_{Air \rightarrow SW}^{WVdep}(rain) &= \text{advective transfer factor for wet deposition of vapor from air to surface water (/day).} \end{aligned}$$

The fugacity approach and TF 4-3a are well suited for nonionic organic chemicals. For inorganic chemicals for which vapor washout ratios have been determined empirically, the transfer factor is calculated in the current TRIM.FaTE library as:

$$T_{Air \rightarrow SW}^{WVdep}(rain) = \frac{A_{SWA}}{V_{Air}} \times rain \times w_{rV} \times f_{MV} \quad (\text{TF 4-3b})$$

where:

- w_{rV} = vapor washout ratio (g[chemical dissolved]/m³[rain] per g[chemical vapor-phase]/m³[air]); and
- f_{MV} = the fraction of the chemical mass in the air compartment that is in the vapor phase divided by the volume fraction of the air compartment that is gas/vapor (*i.e.*, the fraction that is not particulate (see Equation 2-73 in Chapter 2)).

Note that $w_{rV} = 1/K_{AW}$, where:

- K_{AW} = air/water partition coefficient (g[chemical]/m³[air] per g[chemical]/m³[water]).

4.2.2 ADVECTIVE PROCESSES BETWEEN SEDIMENT AND SURFACE WATER

The two advective processes between sediment and surface water involve the transport of the chemical from the surface water to the sediment and from the sediment to the surface water via movement of sediment particles. “Sediment deposition” refers to the transport of the chemical sorbed to sediment particles from the surface water to the benthic sediment bed, and “sediment resuspension” refers to the reverse process. Both processes involve only the solid-phase chemical; thus, it is necessary to estimate the partitioning of a chemical among the phases in the surface water compartment and in the sediment compartment. Section 2.7 provides the equations in the current TRIM.FaTE library that implement the general equilibrium approach to calculating the chemical distribution among phases. The fugacity-based equations in the TRIM.FaTE library are described below.

As indicated above, there are three surface-water phases in the current TRIM.FaTE library: liquid-phase water, suspended particle solids, and algae. Thus, to calculate the total fugacity of a chemical in the surface water compartment, it is necessary to add the fugacity capacity of those three components:

$$Z_{Total_SW} = Z_{pure_water} + Z_{pure_solid} + Z_{Algae} \quad (\text{Eq. 4-7})$$

where:

- Z_{Total_SW} = total fugacity capacity of chemical in surface water compartment (mol/m³-Pa);
- Z_{pure_water} = fugacity capacity of chemical in liquid phase, *i.e.*, water (mol/m³-Pa);
- Z_{pure_solid} = fugacity capacity of chemical in the solid phase (mol/m³-Pa); and

Z_{Algae} = fugacity capacity of chemical in algae (mol/m³-Pa).

Thus, the total fugacity of the chemical in the surface water compartment is estimated in the current TRIM.FaTE library as:

$$Z_{Total_SW} = \left(Z_{pure_water} \times Volume_Fraction_Liquid \right) + \left(Z_{pure_solid} \times Volume_Fraction_Solid \right) + \left(Z_{Algae} \times Volume_Fraction_Algae \right) \quad (\text{Eq. 4-8})$$

The fugacity capacity in algae, Z_{Algae} , is calculated as:

$$Z_{Algae} = \frac{C_{Algae}}{C_{SW}} \times \frac{CA}{1000} \times Z_{pure_water} \quad (\text{Eq. 4-9})$$

where:

- C_{Algae} = chemical concentration in algae (g[chemical]/m³[algae]);
- C_{SW} = concentration of chemical dissolved in the liquid phase of surface water (g[chemical]/m³[water]);
- CA = concentration (density) of algae in surface water (g[algae wet wt]/m³[water]); and
- 1000 = units conversion factor (g/kg).

Note that C_{Algae}/C_{SW} is equivalent to a bioconcentration factor (BCF) of the chemical in algae and is represented in the TRIM.FaTE library as *RatioOfConcInAlgaeToConcDissolvedInWater*.

The sediment compartment in the current TRIM.FaTE library consists of two phases: liquid-phase water and solid sediment particles. Thus, to calculate the total fugacity of a chemical in the sediment compartment, it is only necessary to add the fugacity capacity of those two components:

where:

$$Z_{Total_Sed} = \left(Z_{pure_water} \times Volume_Fraction_Liquid \right) + \left(Z_{pure_solid} \times Volume_Fraction_Solid \right) \quad (\text{Eq. 4-10})$$

Z_{Total_Sed} = total fugacity capacity of chemical in the sediment compartment (mol/m³-Pa).

The following subsections describe the sediment deposition and resuspension transfer factors (Section 4.2.2.1), the equations used to calculate the phase flow velocities (Section 4.2.2.2), and algal deposition rates (Section 4.2.2.3), since living and dead algal cells can settle out of the water column onto the sediment bed.

4.2.2.1 Sediment Deposition and Resuspension

The algorithms for sediment deposition and resuspension are similar and are described below.

Deposition of suspended sediment to sediment bed (solid phase):

$$T_{SW \rightarrow Sed}^{dep} = \frac{A_{SedSW}}{V_{SW}} \times \frac{S_{dep}}{\rho_{Sed}} \times \frac{Z_{pure_solid}}{Z_{Total_SW}} \quad (\text{TF 4-4a})$$

where:

- $T_{SW \rightarrow Sed}^{dep}$ = advective transfer factor for deposition of suspended sediment in surface water to sediment bed (/day);
- A_{SedSW} = area of surface water/sediment interface (m²);
- V_{SW} = volume of surface water compartment (m³);
- S_{dep} = deposition rate of suspended sediment to sediment bed (kg[suspended sediment]/m²[surface water/sediment interface]-day)
- ρ_{Sed} = density of solid sediment particles (kg[sediment particles]/m³[sediment particles]);
- Z_{pure_solid} = fugacity capacity of the solid phase (mol/m³-Pa); and
- Z_{Total_SW} = total fugacity capacity of the surface water compartment (mol/m³-Pa).

In the TRIM.FaTE library:

- v_{Sed}^{dep} = volumetric sediment deposition rate (m³[sediment]/m²[surface water/sediment interface]-day) (see Section 4.2.2.2 below);

and:

- f_{MS} = mass fraction of chemical sorbed to suspended sediment particles divided by the volumetric fraction of the surface water compartment that is suspended sediments (unitless) (*i.e.*, $Mass_Fraction_Sorbed / Volume_Fraction_Solid$), which:
= $Z_{pure_solid} / Z_{Total_Air}$ (see Equations 2-71 and 2-79).

Thus, the transfer factor for deposition of suspended sediments to the sediment bed is represented in the TRIM.FaTE library as:

$$T_{SW \rightarrow Sed}^{dep} = \frac{A_{SedSW}}{V_{SW}} \times v_{Sed}^{dep} \times f_{MS} \quad (TF\ 4-4b)$$

Resuspension of sediment to surface water (solid phase):

$$T_{Sed \rightarrow SW}^{res} = \frac{A_{SedSW}}{V_{Sed}} \times \frac{S_{res}}{\rho_{Sed}} \times \frac{Z_{pure_solid}}{Z_{Total_Sed}} \quad (TF\ 4-5a)$$

As for Equations TF 4-4a and 4-4b above, TF 4-5a is coded in the TRIM.FaTE library as the equivalent expression shown in TF 4-5b:

$$T_{Sed \rightarrow SW}^{res} = \frac{A_{SedSW}}{V_{Sed}} \times v_{Sed}^{res} \times f_{MS} \quad (TF\ 4-5b)$$

where:

- $T_{Sed \rightarrow SW}^{res}$ = advective transfer factor for resuspension of sediment to surface water (/day);
- A_{SedSW} = area of sediment/surface water interface (m²);
- V_{Sed} = volume of sediment compartment (m³);
- S_{res} = resuspension rate of benthic sediment to water column (kg[benthic sediment particles]/m²[sediment/surface water interface]-day);
- ρ_{Sed} = density of solid sediment particles (kg[particles]/m³[particles]);
- Z_{pure_solid} = fugacity capacity of the chemical in solid phase (mol/m³-Pa);
- Z_{Total_Sed} = total fugacity capacity of the chemical in the sediment compartment (mol/m³-Pa);
- v_{Sed}^{res} = volumetric sediment resuspension rate (m³[sediment]/m²[sediment/surface water interface]-day) (see Section 4.2.2.2 below); and
- f_{MS} = mass fraction of chemical sorbed to sediment bed particles divided by the volume fraction of the sediment bed that is solid particles (unitless).

4.2.2.2 Sediment Deposition and Resuspension Rates

The volumetric sediment deposition and resuspension rates are estimated using similar equations in TRIM.FaTE. The equation for volumetric sediment deposition is:

$$v_{Sed}^{dep} = \frac{S_{dep}}{\rho_{Sed}} \quad (Eq.\ 4-9)$$

where:

- v_{Sed}^{dep} = volumetric sediment deposition rate (m³[sediment particles]/m²[surface water/sediment interface]-day);

S_{dep} = deposition rate of suspended sediment to sediment bed (kg[suspended sediment particles]/m²[surface water/sediment interface]-day); and
 ρ_{Sed} = density of suspended sediment particles (kg[particles]/m³[particles]).

The sediment deposition rate, S_{dep} , is calculated as:

$$S_{dep} = v_{dep} \times TSS \quad (\text{Eq. 4-10})$$

where:

v_{dep} = sediment deposition velocity (m/day); and
 TSS = total suspended sediment concentration (kg[suspended sediment particles]/m³[surface water compartment]);

The equation for volumetric sediment resuspension is similar to Equation 4-7:

$$v_{Sed}^{res} = \frac{S_{res}}{\rho_{Sed}} \quad (\text{Eq. 4-11})$$

where:

v_{Sed}^{res} = volumetric sediment resuspension rate (m³[sediment particles]/m²[surface water/sediment interface]-day);
 S_{res} = resuspension rate of benthic sediment to surface water (kg[benthic sediment]/m²[sediment/surface water interface]-day); and
 ρ_{Sed} = density of solid sediment particles (kg[sediment particles]/m³[sediment particles]).

In this case, the sediment resuspension rate, S_{res} , is calculated as:

$$S_{res} = v_{res} \times BSC \quad (\text{Eq. 4-12})$$

where:

v_{res} = sediment resuspension velocity (m/day); and
 BSC = benthic solids concentration (kg[sediment particles]/m³[sediment compartment]).

In the TRIM.FaTE library:

$$BSC = \rho_{Sed} \times (1 - \phi) \quad (\text{Eq. 4-13})$$

where:

ϕ = porosity, which for the sediment compartment is equal to the volume fraction liquid, *i.e.*, water (m³[pore water]/m³[sediment compartment]).

4.2.2.3 Algal Deposition Rates

Algal cells, both living and dead, can settle out of the water column onto the sediment bed. The transfer factor for that deposition process in TRIM.FaTE is similar in form to TF 4-4b:

$$T_{Algae \rightarrow Sed}^{dep} = \frac{A_{SedSW}}{V_{SW}} \times v_{Algae}^{dep} \times f_{MAI} \quad (\text{TF 4-6})$$

where:

$T_{Algae \rightarrow Sed}^{dep}$	=	deposition transfer factor for algae settling to the sediments (/day);
A_{SedSW}	=	interfacial area between the surface water and sediment compartments (m ²);
V_{SW}	=	volume of the surface water compartment (m ³);
v_{Algae}^{dep}	=	algal deposition rate (m ³ [algae]/m ² [sediment/surface water interface]-day); and
f_{MAI}	=	mass fraction of chemical in algal cells divided by the volume fraction of the surface water compartment comprised of algal cells (unitless).

The volumetric algal deposition rate can be estimated as:

$$v_{Algae}^{dep} = \frac{AS_{dep}}{CA \times 1000} \quad (\text{Eq. 4-14})$$

where:

AS_{dep}	=	algal deposition rate (g[algae]/m ² [sediment/surface water interface]-day);
CA	=	algae concentration (density) in water column (g[algae]/L[water]); and
1000	=	units conversion factor (L/m ³).

The mass-based algal deposition (sedimentation) rate can be estimated from:

$$AS_{dep} = \frac{CS_{dep}}{Al_{TOC} \times (1 - fW_{Algae})} \quad (\text{Eq. 4-15})$$

where:

CS_{dep}	=	carbon sedimentation rate (g[carbon]/m ² [sediment/surface water interface]-day);
Al_{TOC}	=	dry weight total carbon content of algae (g[carbon]/g[algae dry wt]); and
fW_{Algae}	=	mass fraction of the algae that consists of water (unitless).

Based on Baines and Pace (1994), the carbon sedimentation rate is estimated from the following formula:

$$CS_{dep} = 10^{1.82 + \frac{0.62 \times \ln(CC)}{\ln(10)}} \times \frac{1}{1000} \quad (\text{Eq. 4-16})$$

where:

CC = chlorophyll concentration in water (mg[chlorophyll]/m³[surface water]);
and
1000 = units conversion factor (mg/g).

Values for CC , Al_{TOC} , and fW_{Algae} can be obtained from the literature.

4.2.3 ADVECTIVE PROCESSES BETWEEN SEDIMENT/SURFACE WATER AND ADVECTIVE SINKS

The surface water advection sink represents outflow of the chemical from the study area. For sediment, the advection sink represents the burial of the chemical beneath the sediment layer. Following is a summary of the following advective processes between sediment/surface water and advective sinks:

- outflow from flowing river to surface water advection sink(s) (Section 4.2.3.1);
- outflow from a lake or pond to a surface water advection sink (Section 4.2.3.2);
and
- transfer of bulk sediment from the sediment bed to a sediment burial sink (Section 4.2.3.3).

4.2.3.1 Outflow from Flowing Water to Surface Water Advection Sink (Total Phase)

For flowing waters (*e.g.*, rivers and streams), chemical sorbed to suspended sediments and dissolved in the water can be carried downstream with the bulk water flow beyond the boundary of the modeling area, modeled as a transfer to a surface water advection sink. The transfer factor is based on the volumetric flow of the water body:

$$T_{SW \rightarrow SW_sink}^{river} = outflow / V_{SW} \quad (\text{TF 4-7a})$$

where:

$T_{SW \rightarrow SW_sink}^{river}$ = advective transfer factor from surface water compartment to surface water advection sink (downstream direction only) (/day);
 $outflow$ = volumetric outflow of bulk water (water and suspended sediments) from surface water compartment to advection sink (m³[bulk water]/day); and
 V_{SW} = volume of surface water compartment (m³[water]).

Note that inflow of chemical from outside the boundary of the study area is possible if there are background concentrations of the chemical in the water upstream of the study area. That transfer is estimated using an inflow rate that is equal to the outflow rate for the surface water compartment just inside the modeling boundary and a user-specified concentration of the chemical upstream of the study site.

4.2.3.2 Outflow from Lake or Pond to Surface Water Advection Sink (Total Phase)

For non-flowing waters (*e.g.*, lakes and ponds), chemical in water can be lost from the surface-water body to one or more outflows that are not modeled in TRIM.FaTE:

$$T_{SW \rightarrow SW_sink}^{lake} = \frac{(\text{flushes} / \text{yr})}{365} \quad (\text{TF 4-7b})$$

where:

- $T_{SW \rightarrow SW_sink}^{lake}$ = advective transfer factor from surface water compartment to surface water advection sink (/day);
- flushes/yr = outflow of water measured as number of complete flushes per year from surface water compartment to advection sink ($\text{m}^3[\text{bulk water}]/\text{day}$); and
- 365 = unit conversion factor (days/year).

4.2.3.3 Movement of Sediment from Sediment Bed to Sediment Burial Sink (Solid Phase)

The burial of chemical mass below the sediment compartment (*i.e.*, in the sediment burial sink) is a function of the sediment deposition rates and sediment resuspension rates. Conceptually, as sediment particles suspended in the surface water settle, with their associated chemical mass, to the top sediment layer, there is a simultaneous burial of sediment particles and associated chemical from the bottom sediment layer into a sediment burial sink. The chemical mass in TRIM.FaTE sinks does not move back into the modeled system. Transfer of chemical mass from sediment to a sediment sink is then modeled as follows:

$$T_{Sed \rightarrow Sed_sink}^{Total} = \frac{A_{Sed}}{V_{Sed}} \times \text{burial_rate} \times f_{MS} \quad (\text{TF 4-8})$$

where:

- $T_{Sed \rightarrow Sed_sink}^{Total}$ = transfer factor for chemical mass in lower-most modeled sediment layer to the sediment burial sink (/day);
- A_{Sed} = area of the sending sediment compartment (m^2);
- V_{Sed} = volume of the sending sediment compartment (m^3);
- burial_rate = sediment burial rate ($\text{m}^3[\text{sediment particles}] / \text{m}^2[\text{sediment}]\text{-day}$, or m/day); and

f_{MS} = fraction of chemical mass sorbed to sediment particles divided by volume fraction of the sediment compartment that is solid (unitless).

In the current library, burial rate is derived as a non-negative value as follows:

$$burial_rate = \max(0, v_{sed}^{dep} - v_{sed}^{res}) \quad (\text{Eq. 4-17})$$

where:

v_{sed}^{dep} = sediment deposition rate ($\text{m}^3[\text{sediment}]/\text{m}^2\text{-day}$) (see Eq. 4-9); and
 v_{sed}^{res} = sediment resuspension rate ($\text{m}^3[\text{sediment}]/\text{m}^2\text{-day}$) (see Eq. 4-11).

While the model could accommodate scouring (*i.e.*, net resuspension of sediment from the sediment layer up into the water column), the burial algorithm currently does not provide for the transfer of chemical mass back into a sediment compartment from a sediment burial sink. To accommodate a scouring situation in which chemical previously buried would become available for resuspension, the user might consider using a more complex scenario involving multiple sediment compartments positioned as layers above the burial sink, where the depth of the layers (*i.e.*, the upper most ones) could change depending on deposition and resuspension rates.

4.2.4 ADVECTIVE PROCESSES FROM SURFACE SOIL TO SURFACE WATER

The advective algorithms for runoff and erosion from surface soil compartments to a surface water compartment are described in Chapter 5 (TF 5-10b and TF 5-11b, respectively).

4.3 DERIVATION OF RIVER COMPARTMENT TRANSFER FACTORS

The transfer factor from one river compartment to another, or to a lake compartment, was derived based on advective flow rates of a total pollutant mass between two compartments, as developed in Section 2.4.1. By substituting river flow for the total volumetric flow, the following transfer factor is derived.

$$T_{i \rightarrow j}^{adv}(total) = \frac{flow}{V_i} \quad (\text{TF 4-9})$$

where:

$T_{i \rightarrow j}^{adv}(total)$ = advective transfer factor for bulk river flow between river compartments i and j (/day);
 $flow$ = bulk volumetric water flow rate ($\text{m}^3[\text{bulk water}]/\text{day}$); and
 V_i = volume of compartment i ($\text{m}^3[\text{surface water}]$).

Because advection is being simulated for the total phase (*i.e.*, both the water and the suspended sediments), no phase partitioning is applied in this equation. This transfer factor is specified for a particular link between surface water compartments.

4.4 DIFFUSIVE PROCESSES

TRIM.FaTE models the diffusive exchanges of chemicals between surface water and air (Section 4.4.1) and between surface water and sediments (Section 4.4.2). Diffusive exchanges between surface water and algae are noted in Section 4.4.3.

4.4.1 DIFFUSIVE EXCHANGE BETWEEN SURFACE WATER AND AIR

The algorithms describing the diffusive exchange of chemical mass between surface water and air are presented in Section 3.3.2.1 (see TF 3-2 and TF 3-3).

4.4.2 DIFFUSIVE EXCHANGE BETWEEN SURFACE WATER AND SEDIMENTS

The diffusive exchange of chemical between surface water and sediments is modeled based on mass transfer coefficients between the two compartments. Transfer factors based on the fugacity approach are developed in Section 4.4.2.1. The transfer factors for diffusion based on the method described in the Water Quality Analysis Simulation Program (WASP) (Ambrose et al. 1995) model are developed in Section 4.4.2.2.

4.4.2.1 Transfer Factors Based on Fugacity Approach

Diffusive transfers of dissolved chemical between sediment pore water and the overlying surface water are estimated from chemical mass transfer coefficients as described in the following set of equations. First:

$$U_{SW\text{Sed}} = \frac{De_{SW}}{\delta_{SW}} \quad (\text{Eq. 4-18a})$$

$$U_{\text{Sed}SW} = \frac{De_{\text{Sed}}}{\delta_{\text{Sed}}} \quad (\text{Eq. 4-18b})$$

where:

$U_{SW\text{Sed}}$	=	mass transfer coefficient from surface water to sediment (m/day);
$U_{\text{Sed}SW}$	=	mass transfer coefficient from sediment to surface water (m/day);
De_{SW}	=	effective diffusivity of chemical in surface water (m ² /day);
De_{Sed}	=	effective diffusivity of chemical in sediment (m ² /day);
δ_{SW}	=	boundary layer thickness below water (m); and
δ_{Sed}	=	boundary layer thickness above sediment (m).

The values of De_{SW} and De_{Sed} are calculated using equations (Millington and Quirk 1961):

$$De_{SW} = D_{\text{pure_water}} \quad (\text{Eq. 4-19})$$

$$De_{\text{Sed}} = \phi^{(4/3)} \times D_{\text{pure_water}} \quad (\text{Eq. 4-20})$$

where:

$D_{\text{pure_water}}$ = diffusivity of chemical in liquid phase, *i.e.*, water (m²/day); and
 ϕ = porosity, or the volume fraction of the sediment compartment that is water (*i.e.*, θ , which = *Volume_Fraction_Liquid* given that ϵ , or *Volume_Fraction_Vapor*, in the sediment compartment = 0; unitless).

The value for δ_{Sed} can be input by the user. The value for δ_{SW} is estimated using the method from CalTox (McKone 1993b, Equation 58, p. 44) as:

$$\delta_{\text{SW}} = 318 \times De_{\text{Sed}}^{0.683} \quad (\text{Eq. 4-21})$$

The mass transfer coefficients are then used to estimate the diffusive transfer from sediment to surface water:

$$T_{\text{Sed} \rightarrow \text{SW}}^{\text{dif}} = \frac{A_{\text{SedSW}}}{V_{\text{Sed}}} \times \left(\frac{1}{U_{\text{SW} \rightarrow \text{Sed}} \times \frac{Z_{\text{Total_SW}}}{Z_{\text{Total_Sed}}}} + \frac{1}{U_{\text{SedSW}}} \right)^{-1} \quad (\text{TF 4-10a})$$

where:

$T_{\text{Sed} \rightarrow \text{SW}}^{\text{dif}}$ = diffusive transfer factor from sediment to surface water (/day);
 A_{SedSW} = interfacial area between the sediment and surface water compartments (m²);
 $Z_{\text{Total_SW}}$ = total fugacity capacity of chemical in the surface water compartment (mol/m³-Pa); and
 $Z_{\text{Total_Sed}}$ = total fugacity capacity of chemical in the sediment compartment (mol/m³-Pa).

The diffusive transfer from surface water to sediment is estimated by the same equations, but with the identity of the sending and receiving compartments reversed:

$$T_{\text{SW} \rightarrow \text{Sed}}^{\text{dif}} = \frac{A_{\text{SedSW}}}{V_{\text{SW}}} \times \left(\frac{1}{U_{\text{SedSW}} \times \frac{Z_{\text{Total_Sed}}}{Z_{\text{Total_SW}}}} + \frac{1}{U_{\text{SW} \rightarrow \text{Sed}}} \right)^{-1} \quad (\text{TF 4-11a})$$

where:

$T_{\text{SW} \rightarrow \text{Sed}}^{\text{dif}}$ = diffusive transfer factor from surface water to sediment compartments (/day);

A_{SedSW}	=	interfacial area between the sediment and surface water compartments (m ²);
U_{SedSW}	=	mass transfer coefficient from sediment to surface water compartments (m/day);
U_{SWsSed}	=	mass transfer coefficient from surface water to sediment compartments (m/day);
Z_{Total_SW}	=	total fugacity capacity of the chemical in the surface water compartment (mol/m ³ -Pa); and
Z_{Total_Sed}	=	total fugacity capacity of the chemical in the sediment compartment (mol/m ³ -Pa).

4.4.2.2 Transfer Factors Based on the WASP model

An alternative to the fugacity approach described in Section 4.4.2.1 is the diffusive method described in WASP (Ambrose et al. 1995). Diffusive transport between surface water and sediment compartments can be approximated as a first-order process using the method described for WASP. Based on the WASP model, the net diffusive exchange flux between a surface water compartment and a sediment compartment is modeled by:

$$\frac{dN_{Sed}}{dt} = \frac{DSP_{SWsSed} \times A_{SWsSed} \times \phi_{SWsSed}}{L_{SWsSed} / \phi_{SWsSed}} \times \left(\frac{f_{D_{Sed}} \times C_{Sed}}{\phi_{Sed}} - \frac{f_{D_{SW}} \times C_{SW}}{\phi_{SW}} \right) \quad (\text{Eq. 4-22a})$$

$$= \frac{DSP_{SWsSed} \times A_{SWsSed} \times \phi_{SWsSed}}{L_{SWsSed} / \phi_{SWsSed}} \times \left(\frac{f_{D_{Sed}} \times N_{Sed}}{V_{Sed} \times \phi_{Sed}} - \frac{f_{D_{SW}} \times N_{SW}}{V_{SW} \times \phi_{SW}} \right) \quad (\text{Eq. 4-22b})$$

where:

N_{Sed}	=	chemical mass in the underlying sediment compartment (g[chemical]/day);
DSP_{SWsSed}	=	diffusive exchange coefficient between surface water and sediment compartments (m ² [surface water/sediment interface]/day);
A_{SWsSed}	=	interfacial area between surface water and sediment compartments (m ²);
L_{SWsSed}	=	characteristic mixing length between surface water and sediment compartments (m);
C_{SW}, C_{Sed}	=	bulk concentration of chemical in surface water compartment and sediment compartment, respectively (g[chemical]/m ³ [compartment]);
N_{SW}, N_{Sed}	=	mass of chemical in surface water compartment and sediment compartment, respectively (g[chemical]);
V_{SW}, V_{Sed}	=	volume of surface water and sediment compartments, respectively (m ³ [compartment]);
f_{DSW}, f_{DSed}	=	dissolved fraction of chemical in surface water and sediment compartments, respectively (calculated);

ϕ_{SW}, ϕ_{Sed} = porosity of surface water and sediment compartments, respectively
(= volume fraction water, θ , for these compartments, see Chapter 2); and
 ϕ_{SWSed} = average porosity at interface ($(\phi_i + \phi_j)/2$).

The resulting transfer factors (units of /day) between the surface water and sediment compartments are given by:

$$T_{Sed \rightarrow SW}^{dif} = \frac{DSP_{SWSed} \times A_{SWSed} \times \phi_{SWSed}}{L_{SWSed} / \phi_{SWSed}} \times \left(\frac{f_{D_{Sed}}}{V_{Sed} \times \phi_{Sed}} \right) \quad (TF\ 4-10b)$$

$$T_{SW \rightarrow Sed}^{dif} = \frac{DSP_{SWSed} \times A_{SWSed} \times \phi_{SWSed}}{L_{SWSed} / \phi_{SWSed}} \times \left(\frac{f_{D_{SW}}}{V_{SW} \times \phi_{SW}} \right) \quad (TF\ 4-11b)$$

Following the method used in WASP (Ambrose et al. 1995, p. 25), the sediment compartment height is used as the characteristic mixing length L_{SWSed} . The porosity of the sediment compartment (ϕ_{Sed}) is calculated from the volume fraction of the sediment compartment that consists of water (*i.e.*, θ_{Sed}). The porosity of the surface water compartment is set to the volume of water compartment that is water (*i.e.*, 1 - (volume fraction suspended sediment + volume fraction algae)). Values for dispersion coefficients are as discussed in Section 4.5.1 for exchanges between horizontally adjacent surface water compartments *i* and *j*.

These transfer factors (TF 4-10b and TF 4-11b) are not available in the current TRIM.FaTE library, but are included here for users who might prefer to use the method used in WASP.

4.4.3 DIFFUSIVE EXCHANGE BETWEEN ALGAE AND SURFACE WATER

The diffusive exchange between algae and surface water traditionally has been called bioconcentration, with the bioconcentration factor (BCF) being equal to the chemical concentration in algae divided by the concentration of chemical dissolved in the surface water. From Equation 4-9, the BCF also is equal to the ratio of the *Z* factors for algae and water (excluding suspended sediments):

$$\frac{C_{Algae}}{C_{pure_water}} = BCF = \frac{Z_{Algae}}{Z_{pure_water}} \quad (Eq.\ 4-24)$$

An equation to estimate C_{Algae}/C_{pure_water} for mercury in particular is presented in Appendix A, Section A.1.2.

4.5 DISPERSIVE PROCESSES

Dispersive transport between horizontally adjacent surface water compartments can be approximated as a first-order process using the method described in WASP (Ambrose et al.

1995). Dispersive water column exchanges significantly influence the transport of dissolved and particulate pollutants in such water bodies as lakes, reservoirs, and estuaries.

Based on the WASP model, the net dispersive exchange flux between two surface water compartments i and j at a given time is modeled by:

$$\frac{dN_j}{dt} = \frac{DSP_{ij} \times A_{ij}}{L_{ij}} \times (C_j - C_i) \quad (\text{Eq. 4-25a})$$

$$= \frac{DSP_{ij} \times A_{ij}}{L_{ij}} \times \left(\frac{N_j}{V_j} - \frac{N_i}{V_i} \right) \quad (\text{Eq. 4-25b})$$

where:

- N_j = chemical mass in surface water j (g[chemical] /day);
- DSP_{ij} = dispersion coefficient for exchange between surface water compartments i and j (m²/day);
- A_{ij} = interfacial area between surface water compartments i and j (m²);
- L_{ij} = characteristic mixing length between surface water compartments i and j (m);
- C_i, C_j = concentration of chemical in surface water compartments i and j , respectively (g/m³);
- N_i, N_j = mass of chemical in surface water compartments i and j , respectively (g[chemical]/m³[water]); and
- V_i, V_j = volume of surface water compartments i and j , respectively (m³).

In TRIM.FaTE, the dispersive transfer factor between surface water compartments is:

$$T_{SWi \rightarrow j}^{disp} = \frac{DSP_{ij} \times A_{ij}}{L_{ij} \times V_i} \quad (\text{TF 4-12})$$

where:

- $T_{SWi \rightarrow j}^{disp}$ = dispersive transfer factor from the i^{th} to the j^{th} surface water compartment (/day).

The distance between the midpoints of the two water compartments is used for the characteristic mixing length, L_{ij} . Values for dispersion coefficients can range from 10⁻¹⁰ m²/sec (8.64 × 10⁻⁶ m²/day) for molecular diffusion to 5 × 10² m²/sec (4.32 × 10⁷ m²/day) for longitudinal mixing in estuaries (Ambrose et al. 1995, p. 35).

4.6 TRANSPORT BETWEEN SEDIMENT COMPARTMENTS

A chemical can be transported between vertically adjacent sediment compartments via the sediment pore water and bioturbation. Although applications of TRIM.FaTE to date have involved only one sediment bed layer (above the sediment sink), a user might specify more than one sediment layer with differing characteristics (*e.g.*, porosity) above the sediment sink. In this case, transport of a chemical between the layers can occur. In the current TRIM.FaTE library, the only process modeled for this transfer is diffusion of the liquid-phase chemical across compartments via the interstitial water. Bioturbation is not included in the TRIM.FaTE library at this time.

The transfer factor for pore-water diffusion of chemical from one sediment compartment to another located below it is:

$$T_{Sedi \rightarrow Sedj}^{dif} = \frac{A_{Sedij}}{V_{Sedi}} \times \frac{DSP_{Sed} \times \phi_{avg}}{L_{Sedij}} \times f_{MLi} \quad (\text{TF 4-13})$$

where:

- $T_{Sedi \rightarrow Sedj}^{dif}$ = transfer factor for diffusion between sediment compartment *i* and sediment compartment *j* below it (/day);
- A_{Sedij} = interfacial area between sediment compartments *i* and *j* (m²);
- V_{Sedi} = volume of the sending sediment compartment *i* (m³);
- DSP_{Sed} = diffusive exchange coefficient (m²/day);
- ϕ_{avg} = average porosity at the interface between sediment compartments *i* and *j* (unitless), which equals $(\phi_{Sedi} + \phi_{Sedj}) / 2$;
- L_{Sedij} = characteristic mixing length (m), which equals the distance between the vertical midpoints of sediment compartments *i* and *j*; and
- f_{MLi} = fraction of the chemical mass in sediment compartment *i* that is dissolved in water divided by the volume fraction of sending sediment compartment *i* that is water (see Equations 2-72 and 2-80) (unitless).

The algorithm for pore-water diffusion of chemical from sediment compartment *j* to the one above it, sediment compartment *i*, is:

$$T_{Sedj \rightarrow Sedi}^{dif} = \frac{A_{Sedij}}{V_{Sedj}} \times \frac{DSP_{Sed} \times \phi_{avg}}{L_{Sedij}} \times f_{MLj} \quad (\text{TF 4-14})$$

where:

- $T_{Sedj \rightarrow Sedi}^{dif}$ = transfer factor for diffusion between sediment compartment *j* and sediment compartment *i* above it (/day);
- V_{Sedj} = volume of the sending sediment compartment *j* (m³); and
- f_{MLj} = fraction of the chemical mass in sediment compartment *j* that is dissolved in water divided by volume fraction sending sediment compartment *j* that is liquid (unitless).

The current TRIM.FaTE does not include algorithms for horizontal diffusion between sediment compartments in the same sediment layer.

4.7 TRANSFORMATIONS AND DEGRADATION

The transformation of chemicals in surface water and sediments can affect their persistence and environmental partitioning. Transformations of chemicals into compounds that will no longer be tracked in TRIM.FaTE (*e.g.*, non-toxic degradation products) are called general degradation processes. In TRIM.FaTE, the degradation of a chemical in surface water due to all mechanisms that might apply (*e.g.*, hydrolysis, photolysis, and aerobic degradation by microfauna) is reflected by the user input for the half-life of the chemical in a surface water compartment. Similarly, the degradation of a chemical in sediments due to all mechanisms that might apply (*e.g.*, aerobic and anaerobic bacterial degradation) is reflected by the user input for the chemical half-life in the sediment compartment. The algorithm relating the degradation rate constant to the chemical half-life in the soil compartment is presented in Chapter 2 (Equation 2-64), and the corresponding transfer factor is TF 2-1.

Transformations of a chemical into another form of the chemical that is tracked in TRIM.FaTE are named for the processes (*e.g.*, oxidation, methylation, reduction of mercury species). In the TRIM.FaTE surface water and sediment compartments, all transformations are modeled as first-order processes, that is, linear with inventory (*i.e.*, the quantity of chemical contained in a compartment). The rate of mass removal in a first-order transformation is calculated as the product of the total inventory of chemical in the compartment and the transformation rate constant specified in the corresponding transfer factor. The transformation rate constant is the inverse of the residence time with respect to that reaction.

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