2. ALGORITHM OVERVIEW

As described in TRIM.FaTE TSD Volume I, Chapter 4, TRIM.FaTE includes algorithms to model several types of transport and fate processes, including bulk advection, diffusion, dispersion, biotic processes, and chemical reactions and transformations. Because some of these algorithms are dependent on what phase (*e.g.*, liquid, solid) a chemical is in, TRIM.FaTE also contains equations to estimate phase distribution in abiotic compartments.[1] This chapter provides an overview of the general types of algorithms used by TRIM.FaTE, including those used to model phase distribution.

The main focus of this chapter is the methods and assumptions used to develop the advection algorithms, *i.e.*, the T-factors used to describe advective transport of a chemical between adjacent compartments. Mathematically, all that is required to calculate an advective transfer is the velocity of the moving phase and the amount of the chemical that is in the moving phase. Thus, the fraction of the total chemical in a compartment that is in the moving phase (*e.g.*, water) must be estimated. To estimate the fraction in the moving phase, the fraction of the total chemical that will be found in each phase (*i.e.*, the partitioning of the chemical among all phases within a compartment) must be estimated. Both fugacity and non-fugacity related approaches are used in TRIM.FaTE to model the partitioning of a chemical among phases within a compartment.

The remainder of this chapter is organized into six main sections. Section 2.1 focuses on multiphase calculations and how TRIM.FaTE estimates the fraction of the total chemical in a compartment that occurs in each phase within the compartment. Section 2.2 describes the general phase-distribution equations of Section 2.1 as they apply to soil, surface water, and sediment compartment types and different moving phases as modeled in TRIM.FaTE. Section 2.3 describes the general phase-distribution equations for the air compartment type. Section 2.4 then indicates, in general terms, how the various T-factors are estimated in TRIM.FaTE for the different fate and transport processes. Section 2.5 describes how some algorithms related to equilibrium processes (*e.g.*, diffusion between biotic and abiotic media) were modified from a steady-state equilibrium form to a time-dependent form that is suitable for use in TRIM.FaTE. Section, 2.6 demonstrates the equivalence of certain fugacity-based expressions to non-fugacity-based expressions. The last Section, 2.7, provides descriptions of the code in the TRIM.FATE library used to estimate the distribution of chemical among phases for each type of abiotic compartment. Table 2-1 at the end of this chapter summarizes the advective algorithms included in TRIM.FaTE.

2.1 PHASE-DISTRIBUTION CALCULATIONS

This section describes how the distribution of a chemical among multiple phases within a compartment is currently modeled in TRIM.FaTE. The most common phases considered for the

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[1] Although termed “abiotic” compartments, chemical transformations that may be biologically mediated (*e.g.*, by bacteria) can be simulated in these compartments. Additionally, in the current TRIM.FaTE library, algae is represented as an explicit phase of surface water rather than as a separate compartment.

abiotic compartments are liquid, gas, and solid. In the current TRIM.FaTE library, the liquid phase of the abiotic compartments is aqueous (*i.e.*, water and chemicals dissolved in water). Other phases included in some TRIM.FaTE compartments may include biotic phases (*e.g.*, algae in surface water). Section 2.1.1 describes the equations that result from assuming chemical equilibrium among the phases within a compartment. Section 2.1.2 illustrates how concentrations of a chemical in other phases are normalized to its concentration in the liquid phase to allow calculation of its concentration in each phase. Section 2.1.3 describes two general forms of equilibrium partitioning calculations: general and fugacity-based forms.

2.1.1 ASSUMED CHEMICAL EQUILIBRIUM

A fundamental assumption of the TRIM.FaTE algorithms is that within a single compartment, all phases are at chemical equilibrium with each other at all times. Because chemical equilibrium is assumed, the ratios of the concentrations among the individual phases are constant over time, and mass balance need only be tracked for the total amount of the chemical in a compartment. The amount of chemical in the compartment in a particular phase can be determined from the total amount in the compartment (described in the following text), characteristics of the chemical, and the relative volume fraction of the compartment that consists of that phase. It is possible that, in future versions of TRIM.FaTE, chemical equilibrium among phases in the same compartment will not be assumed, in which case the amount of chemical in different phases will need to be tracked as separate compartments.

As pointed out in Section 4.2 of TSD Volume I, TRIM.FaTE tracks the amount of chemical in each compartment using moles (actually conserved units, which are related to moles). The resultant molar quantities in each compartment are then used to estimate the modeling results in terms of mass or concentration by using a chemical's molecular weight. For the sake of simplicity, however, most of the equations in this chapter refer to the amount of chemical in compartments in units of mass, not moles. Exceptions include discussion of the gas laws, in which moles are used.

In any given compartment, the total amount of chemical is the sum of the amounts in the different phases:

$$\begin{aligned} N_{Total} &= Amount\_in\_gas\_phase + \\ &\qquad Amount\_in\_aqueous\_liquid\_phase + Amount\_in\_solid\_phase \\ &= C_{gas} \times V_{gas} + C_{liquid} \times V_{liquid} + C_{solid} \times V_{solid} \end{aligned} \qquad \text{(Eq. 2-1)}$$

where:

N_{Total} = total mass of chemical in the compartment (g[chemical]);
C_{gas} = concentration of chemical vapor in gas phase of the compartment (g[chemical vapor]/m^3[gas]);
V_{gas} = volume of gas in the compartment (m^3[gas]);
C_{liquid} = concentration of chemical in aqueous liquid phase of the compartment (g[chemical]/m^3[water]);
V_{liquid} = volume of aqueous liquid phase in the compartment (m^3[water]);

C_{solid} = concentration of chemical in solid phase of the compartment (g[chemical]/m^3[solids]); and
V_{solid} = volume of solid in the compartment (m^3[solids]).

As noted earlier, because chemical equilibrium among phases within the same compartment is assumed, the ratios of the concentrations between phases are constant over time.[2] However, care must be used in specifying the units of the concentration. This is because, in general practice, it is more common to present concentration ratios on a mass-by-mass basis rather than on a mass-by-volume basis, as in TRIM.FaTE.

2.1.2 NORMALIZATION TO LIQUID PHASE

This section describes the relevant formulas when the concentrations of a chemical in other phases are normalized to the concentration in the liquid phase. Normalization to the liquid phase means that the concentrations in other phases are to be expressed in terms of concentration in the liquid phase. This normalization is used for all soil, surface water, and sediment compartments (including the cases where additional phases are considered). Using the equilibrium assumptions, the following equations describe the concentration of the chemical in the solid and gas phases, respectively:

$$C_{solid} = (\rho_{solid} \times K_d \times CF) \times C_{liquid} \qquad \text{(Eq. 2-2)}$$

$$C_{gas} = \frac{H}{R \times T} \times C_{liquid} \qquad \text{(Eq. 2-3)}$$

where:

ρ_{solid} = density of a solid phase in the compartment (kg[solid phase]/m^3[solid phase]);
K_d = equilibrium partition coefficient; ratio of concentration in solid phase (g[chemical] /kg[solid phase]) to that in liquid phase (g[chemical]/liters(L)[liquid phase]);
CF = 10^{-3} (m^3/L), unit conversion factor from m^3 to L[liquid phase];
H = Henry's law constant for chemical (Pascal (Pa)-m^3/mol) in liquid phase;
R = ideal gas constant (8.314 m^3-Pa/mol-°K); and
T = temperature (°K).

UNIT CONVERSIONS

1 Pascal (Pa) = 9.869E-06 atmospheres or 7.5E-03 mm Hg
1 atmosphere = 760 mm Hg
1 m^3 = 1000 liters (L)
0 °K = -273.15 °C

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[2] Assuming a constant temperature.

Equation 2-2 expresses the equilibrium partitioning for a solid in contact with water. The density of the solid is included in the equation, because the concentrations C_{solid} and C_{liquid} are expressed on a mass-by-volume basis rather than on a mass-by-mass basis (see Equation 2-1).

Equation 2-3 is derived from the ideal gas law and Henry's law. The ideal gas law states:

$$P_{gas} \times V = n \times R \times T \qquad \text{(Eq. 2-4)}$$

where:

P_{gas} = gas pressure (Pa);
V = volume (m^3); and
n = number of moles.

Henry's law states:

$$P_{air} = H \times C_{liquid} \qquad \text{(Eq. 2-5)}$$

where:

P_{air} = partial pressure in air (Pa); and
C_{liquid} = concentration of the chemical in a liquid phase (moles[chemical]/ m^3[liquid]).

Combining Equations 2-1, 2-4, and 2-5, with $P_{air} = P_{gas}$, yields Equation 2-6, from which Equation 2-3 can be derived because $C_{gas} = n/V$:

$$\frac{n \times R \times T}{V} = H \times C_{liquid} \qquad \text{(Eq. 2-6)}$$

Applying Equations 2-2 and 2-3 to Equation 2-1 yields:

$$N_{Total} = C_{liquid} \times \left(\frac{H}{R \times T} \times V_{gas} + V_{liquid} + \rho_{solid} \times K_d \times CF \times V_{solid} \right) \qquad \text{(Eq. 2-7)}$$

The volumes of the various phases in the compartment can be expressed as fractions of the total volume of the compartment, in which case the previous equation yields:

$$N_{Total} = C_{liquid} \times V_{Total} \times \left(\frac{H \times V_{gas}}{R \times T \times V_{Total}} + \frac{V_{liquid}}{V_{Total}} + \rho_{solid} \times K_d \times CF \times \frac{V_{solid}}{V_{Total}} \right) \qquad \text{(Eq. 2-8)}$$

where:

$$V_{Total} = V_{gas} + V_{liquid} + V_{solid} \qquad \text{(Eq. 2-9)}$$

The term $C_{Total} = N_{Total}/V_{Total}$ is the total concentration of the chemical in the compartment. Using the assumed equilibrium relationships, the concentrations in the individual phases can be recovered from the total amount of mass in the compartment, as follows:

$$C_{liquid} = \frac{\dfrac{N_{Total}}{V_{Total}}}{\left(\dfrac{H}{R \times T} \times \dfrac{V_{gas}}{V_{Total}} + \dfrac{V_{liquid}}{V_{Total}} + \rho_{solid} \times K_d \times CF \times \dfrac{V_{solid}}{V_{Total}}\right)} \qquad \text{(Eq. 2-10)}$$

$$C_{gas} = \frac{H}{R \times T} \times C_{liquid} = \frac{\dfrac{H}{R \times T} \times \dfrac{N_{Total}}{V_{Total}}}{\left(\dfrac{H}{R \times T} \times \dfrac{V_{gas}}{V_{Total}} + \dfrac{V_{liquid}}{V_{Total}} + \rho_{solid} \times K_d \times CF \times \dfrac{V_{solid}}{V_{Total}}\right)} \qquad \text{(Eq. 2-11)}$$

$$C_{solid} = \rho_{solid} \times K_d \times CF \times C_{liquid} = \frac{(\rho_{solid} \times K_d \times CF) \times \dfrac{N_{Total}}{V_{Total}}}{\left(\dfrac{H \times V_{gas}}{R \times T \times V_{Total}} + \dfrac{V_{liquid}}{V_{Total}} + \rho_{solid} \times K_d \times CF \times \dfrac{V_{solid}}{V_{Total}}\right)} \qquad \text{(Eq. 2-12)}$$

For cases in which the concentration in the water phase is negligible (*e.g.*, when the compartment is air, or the chemical has a very low solubility), the concentrations must be normalized to another phase.

2.1.3 CONCENTRATIONS OF CHEMICAL IN EACH PHASE

TRIM.FaTE includes two types of equations for estimating concentrations in multiple phases: the general form of the equilibrium approach (Section 2.1.3.1) and the fugacity form (Section 2.1.3.2). As discussed earlier, all of the equations assume that the phases are in equilibrium with each other.

2.1.3.1 General Form

If a chemical is in equilibrium among several phases within a compartment, it is straightforward to calculate the concentration of the chemical that is in each phase. If there are *n* phases in equilibrium, the concentration of the chemical in each phase can be calculated using the following equations:

$$\begin{aligned} C_{j=1} &= \kappa_{j=1} \times C_{norm} \\ &\vdots \\ C_{j=n} &= \kappa_{j=n} \times C_{norm} \end{aligned} \qquad \text{(Eq. 2-13)}$$

where:

C_j = the concentration of the chemical in phase j (g[chemical]/m^3[phase j]);
C_{norm} = the concentration in the phase to which one is normalizing; and
κ_j = the equilibrium ratio between the concentration in phase j and the phase to which one is normalizing, with units of (g[chemical]/m^3[phase j])/(g[chemical]/m^3[phase to which one is normalizing]).

The κ_j ratios are generally expressed in terms of other environmental and/or chemical parameters. The total mass of chemical in the compartment, denoted by N_{Total}, is:

$$\begin{aligned} N_{Total} &= \sum_{j=1}^{n} V_j \times C_j \\ &= \sum_{j=1}^{n} V_j \times \kappa_j \times C_{norm} \\ &= C_{norm} \times \sum_{j=1}^{n} V_j \times \kappa_j \end{aligned} \qquad \text{(Eq. 2-14)}$$

Where V_j is the volume of phase j in the compartment and the sum of the Vj values for all n compartments equals V_{Total}. The fraction of mass of chemical in phase j is then given by:

$$\begin{aligned} \frac{Mass\ of\ chemical\ in\ phase\ j\ in\ compartment}{Total\ mass\ of\ chemical\ in\ compartment} &= V_j \times C_j \big/ N_{Total} \\ &= \frac{V_j \times \kappa_j \times C_{norm}}{C_{norm} \times \sum_{j'=1}^{n} V_{j'} \times \kappa_{j'}} \\ &= \frac{V_j \times \kappa_j}{\sum_{j'=1}^{n} V_{j'} \times \kappa_{j'}} \end{aligned} \qquad \text{(Eq. 2-15)}$$

When applied to the previous section (and using the notation introduced there), we have that $C_{norm} = C_{water}$, and the κ terms are given by:

$$\kappa_{water} = 1 \qquad \text{(Eq. 2-16)}$$

$$\kappa_{gas} = \frac{H}{R \times T} \qquad \text{(Eq. 2-17)}$$

$$\kappa_{solid} = \rho_{solid} \times \rho_d \times CF \qquad \text{(Eq. 2-18)}$$

2.1.3.2 Fugacity-based Notation

The concept of fugacity often is used to simplify the algorithms needed to describe the partitioning of a chemical among phases within a compartment. Fugacity is defined as a substitute for pressure in the real gas system so that the ideal gas equation (*i.e.*, $P \times V = n \times R \times T$) can be applied to the real gas system (Mackay 1991).

The fugacity of a chemical in a phase other than the gas phase is defined as the fugacity of the chemical in the gas phase that is in equilibrium with the phase of interest. Fugacity represents the escaping tendency of a chemical from a phase or compartment. ***When chemical equilibrium is reached within a compartment, the fugacities of the chemical in each phase are equal.***

The concentration of a chemical in a phase can be linearly related to fugacity using the following equation:

$$C_j = f_j \times Z_j \qquad \text{(Eq. 2-19)}$$

where:

C_j = concentration of a chemical in phase *j* (mol/m^3);
f_j = fugacity of the chemical in phase *j* (Pa); and
Z_j = fugacity capacity of the chemical in phase *j* (mol/m^3-Pa).

At equilibrium within a compartment, $f_1 = f_2 = \ldots f_j$. Thus, when two phases achieve chemical equilibrium, the chemical fugacities are equal and partitioning can be described in terms of their Z values, which are essentially "half" partition coefficients as shown below.

$$\frac{C_1}{C_2} = \frac{f_1 \times Z_1}{f_2 \times Z_2} = \frac{Z_1}{Z_2} = K_{12} \qquad \text{(Eq. 2-20)}$$

where:

C_1, C_2 = concentration of a chemical in phases 1 and 2, respectively (mol/m^3);
Z_1, Z_2 = the fugacity capacity of the chemical in phases 1 and 2 (mol/m^3-Pa);
f_1, f_2 = the fugacity of the chemical in phases 1 and 2, where $f_1 = f_2$ (Pa); and
K_{12} = partition coefficient (ratio of concentrations in phase 1 to phase 2) (g[chemical]/m^3[phase 1] per g[chemical]/m^3[phase 2] or m^3[phase 2]/m^3[phase 1]).

When concentrations are relatively low, as for most environmental contaminants, the fugacity of a chemical in air (f_{air}) is equal to the partial pressure of the chemical in air (P_{air}). Thus, at equilibrium:

$$f_{air} = P_{air} \tag{Eq. 2-21}$$

which equals the fugacity in the other phases (*e.g.*, phase *j*), so that $f_j = f_{air} = P_{air}$. Thus:

$$Z_j = C_j / P_{air} \tag{Eq. 2-22}$$

According to Henry's law, $C_{liquid} / P_{air} = 1/H$. Thus, letting phase *j* = water:

$$Z_{water} = 1/H \tag{Eq. 2-23}$$

Substituting Henry's law $C_{water} = P_{air}/H$ into equations (2-2) and (2-3), respectively, and solving for C_j / P_{air} leads to the definition of fugacity capacities for the chemical in water, air, and solid phases:

$$Z_{water} = 1/H \tag{Eq. 2-24}$$

$$Z_{air} = 1/(R \times T) \tag{Eq. 2-25}$$

$$Z_{solid} = \rho_{solid} \times K_d \times CF \times Z_{water} \tag{Eq. 2-26}$$

where:

Z_{water} = fugacity capacity of chemical in the liquid phase, *i.e.*, water (mol/m^3-Pa);
Z_{air} = fugacity capacity of chemical in the gas phase, *i.e.*, air (mol/m^3-Pa);
Z_{solid} = fugacity capacity of chemical in the solid phase (mol/m^3-Pa);
ρ_{solid} = density of solid phase in compartment (kg[solid phase]/m^3[solid phase]);
K_d = equilibrium partition coefficient; ratio of concentration in solid phase (g [chemical]/kg[solid phase]) to that in liquid phase (g[chemical]/L[liquid phase]); and
CF = 10^{-3} (m^3/L), conversion factor to convert m^3 to L[liquid phase].

Substituting Henry's law, $C_{water} = P_{air}/H$, into equation (2-9), solving for C_{Total}/P_{gas}, and inserting Z_{air}, Z_{water}, Z_{solid}, and Z_{Total} yields:

$$Z_{Total} = Z_{air} \times \frac{V_{air}}{V_{Total}} + Z_{water} \times \frac{V_{water}}{V_{Total}} + Z_{solid} \times \frac{V_{solid}}{V_{Total}} \tag{Eq. 2-27}$$

Since the fugacity of a chemical in phase 1 and phase 2 within a compartment at equilibrium is equal:

$$\frac{C_{phase_1}}{C_{phase_2}} = \frac{Z_{phase_1}}{Z_{phase_2}} \qquad \text{(Eq. 2-28)}$$

Applying these relationships shows that:

$$C_{water} = \frac{Z_{water}}{Z_{Total}} \times \frac{N_{Total}}{V_{Total}} = \frac{Z_{water}}{Z_{Total}} \times C_{Total} \qquad \text{(Eq. 2-29)}$$

$$C_{air} = \frac{Z_{air}}{Z_{Total}} \times \frac{N_{Total}}{V_{Total}} = \frac{Z_{air}}{Z_{Total}} \times C_{Total} \qquad \text{(Eq. 2-30)}$$

$$C_{solid} = \frac{Z_{solid}}{Z_{Total}} \times \frac{N_{Total}}{V_{Total}} = \frac{Z_{solid}}{Z_{Total}} \times C_{Total} \qquad \text{(Eq. 2-31)}$$

where:

C_{Total} = total concentration of the chemical in the compartment (g[chemical]/ m^3[total compartment]).

From these relationships, in general, the amount of mass in the different phases is given by:

$$N_{water} = V_{water} \times C_{water} = V_{water} \times \frac{Z_{water}}{Z_{Total}} \times \frac{N_{Total}}{V_{Total}} = V_{water} \times \frac{Z_{water}}{Z_{Total}} \times C_{Total} \qquad \text{(Eq. 2-32)}$$

$$N_{air} = V_{air} \times C_{air} = V_{air} \times \frac{Z_{air}}{Z_{Total}} \times \frac{N_{Total}}{V_{Total}} = V_{air} \times \frac{Z_{air}}{Z_{Total}} \times C_{Total} \qquad \text{(Eq. 2-33)}$$

$$N_{solid} = V_{solid} \times C_{solid} = V_{solid} \times \frac{Z_{solid}}{Z_{Total}} \times \frac{N_{Total}}{V_{Total}} = V_{solid} \times \frac{Z_{solid}}{Z_{Total}} \times C_{Total} \qquad \text{(Eq. 2-34)}$$

where:

N_{water} = chemical mass in the liquid phase (*i.e.*, water, excluding suspended particles) (g[chemical]);
N_{air} = chemical mass in the gas phase (*i.e.*, air, excluding suspended particles) (g[chemical]); and
N_{solid} = chemical mass in the solid phase (g[chemical]).

If there are other phases in equilibrium with the chemical dissolved in the water phase, then the fugacity capacities of that phase can be defined in a manner consistent with that above. For example, if $C_{other} = \kappa_{other} \times C_{water}$, where C_{other} has units of g[chemical]/m^3[*other* phase], then the fugacity capacity of the other phase is defined by:

$$Z_{other} = \kappa_{other} \times Z_{water} \qquad \text{(Eq. 2-35)}$$

and the total fugacity capacity of the chemical in the compartment is given by:

$$Z_{Total} = Z_{air} \times \frac{V_{air}}{V_{Total}} + Z_{water} \times \frac{V_{water}}{V_{Total}} + Z_{solid} \times \frac{V_{solid}}{V_{Total}} + Z_{other} \times \frac{V_{other}}{V_{Total}} \qquad \text{(Eq. 2-36)}$$

where V_{other} is the volume of the other phase, in units of m^3 [other phase].

In the following sections, the general equations presented in this section for multiple phase calculations are applied to specific compartment types. The use of these equations in the following sections generally adheres to notations commonly used in the literature for the different media.

2.2 APPLICATION TO SOIL, SURFACE WATER, AND SEDIMENT COMPARTMENT TYPES

For soil, surface water, and sediment compartment types, the concentrations are normalized to the concentration in the liquid phase, and the same notation is used to represent the relevant parameters. In a soil compartment, the solid phase consists of the soil particles. In a surface water compartment, the solid phase consists of the sediment suspended in the water column. In a sediment compartment, the solid phase consists of clay, silt, or sand particles as opposed to the water phase that fills the interstitial space between the sediment solid particles. Table 2-1 shows all of the phases modeled in TRIM.FaTE. Both the general form (Section 2.2.1) and the fugacity-based form (Section 2.2.2) are described below.

2.2.1 GENERAL FORM

Following common practice, the volume fractions of each phase are denoted as follows:

$$\frac{V_{liquid}}{V_{Total}} = \theta \qquad \text{(Eq. 2-37)}$$

$$\frac{V_{gas}}{V_{Total}} = \varepsilon \qquad \text{(Eq. 2-38)}$$

$$\frac{V_{solid}}{V_{Total}} = 1 - \theta - \varepsilon = 1 - \phi \qquad \text{(Eq. 2-39)}$$

where:

θ = (theta) volume fraction liquid (*i.e.*, water) (unitless);
ϵ = (epsilon) volume fraction gas (*i.e.*, air) (unitless);
$1\text{-}\theta\text{-}\epsilon$ = volume fraction solid (*i.e.*, $1 - \phi$) (unitless); and
ϕ = (phi) total porosity of the compartment (*i.e.*, $\theta + \epsilon$).

Table 2-1
Phases Explicitly Modeled in TRIM.FaTE by Abiotic Compartment Type

Type of Abiotic Compartment	Phases Modeled in TRIM.FaTE	Description
Air	Solid	Airborne particles, where particles can be solids, aerosols, or water droplets
	Gas	Vapors/gases in air
Soil (surface, root-zone, and vadose zone soils)	Solid	Soil particles
	Liquid	Soil pore water
	Gas	Vapors/gases in soil air spaces
Ground water	Solid	Soil particles
	Liquid	Soil pore water
Surface water	Solid-algae	Suspended algal cells/particles
	Solid-other	Suspended sediments (particles other than algae)
	Liquid	Water (excluding suspended sediments and algae)
Sediment	Solid	Sediment particles
	Liquid	Sediment pore water

Using Equation 2-8, the equation for the total mass of chemical in the compartment and in the different phases is then given by:

$$N_{Total} = C_{liquid} \times V_{Total} \times \left(\frac{H}{R \times T} \times \varepsilon + \theta + \rho_{solid} \times K_d \times CF \times (1 - \phi) \right) \qquad \text{(Eq. 2-40)}$$

If there are other phases in equilibrium with the chemical in the liquid (aqueous) phase, then the previous equation is augmented as follows:

$$N_{Total} = C_{liquid} \times V_{Total} \times$$
$$\left(\left(\frac{H}{R \times T} \times \varepsilon \right) + \theta + \left(\rho_{solid} \times K_d \times C_f \times \left(1 - \phi - \sum_{j=1}^{m} \psi_j \right) \right) + \sum_{j=1}^{m} K_j \times \psi_j \right) \qquad \text{(Eq. 2-41)}$$

where:

K_j = equilibrium ratio of concentration of chemical in phase *j* and concentration dissolved in the aqueous phase (g[chemical]/m^3[phase *j*])/(g[chemical]/m^3[water]); and

ψ_j = volume fraction of compartment composed of phase j (m^3[phase j]/ m^3[total]).

2.2.2 FUGACITY-BASED NOTATION

If fugacity-based notation is to be used, then the total fugacity of the chemical in the total compartment is given by:

$$Z_{Total} = Z_{air} \times \varepsilon + Z_{water} \times \theta + Z_{solid} \times (1 - \phi) \tag{Eq. 2-42}$$

In the general case when there are additional equilibrium phases (up to *m* phases) considered:

$$Z_{Total} = Z_{air} \times \varepsilon + Z_{water} \times \theta + Z_{solid} \times (1 - \phi - \sum_{l=1}^{m} \psi_l) + \sum_{l=1}^{m} Z_l \times \psi_l \tag{Eq. 2-43}$$

where:

Z_l = fugacity capacity of the chemical in phase l (mol/m^3-Pa).

NOTE: For the ground water, surface water, and sediment compartment types, the volume fractions in the gas phase (ϵ) are assumed to be zero.

The soil/water partition coefficients (K_d) in each compartment (the various soil, ground water, surface water, and sediment compartments) may be either input or calculated. At present, they are input for mercury species and calculated for nonionic organic chemicals (Karickhoff 1981) by:

$$K_d = K_{oc} \times f_{oc} \tag{Eq. 2-44}$$

where:

K_d = soil/water partition coefficient (g[chemical]/kg[soil wet wt] per g[chemical]/L[water] or L[water]/kg[soil wet wt]);
K_{oc} = organic carbon/water partition coefficient (g[chemical]/kg[organic carbon] per g[chemical]/L[water]); and
f_{oc} = fraction of organic carbon in the total compartment (kg[organic carbon]/kg[soil wet wt].

2.3 APPROACH FOR AIR

Because the volume of water in an air compartment is so small relative to the volumes of the solid and gas phases, there has not been a historical development of K_d's (*i.e.*, ratio of concentration in the solid phase to that in the dissolved phase) for the atmosphere, although the concept still applies. Instead, often the solid and gas phases only are addressed for the air compartment. In TRIM.FaTE, solid particles and water (or chemical) droplets in clouds or mists are all modeled as solid particles in the air (*i.e.*, dust).

Section 2.3.1 describes the equations for multiphase partitioning in the air compartment type, and Section 2.3.2 describes two different approaches to calculating the fraction of chemical that is bound to air particles.

2.3.1 MULTIPHASE PARTITIONING IN THE AIR COMPARTMENT TYPE

If chemical equilibrium is assumed between the solid and gas phases in air (liquid phase is considered absent), then a normalization other than to the liquid concentration is required. Section 2.3.1.1 describes the general approach, while Section 2.3.1.2 describes the fugacity-based approach.

2.3.1.1 General Approach

At present, the volume fractions in each phase in an air compartment are given by:

$$\frac{V_{liquid}}{V_{Total}} = 0 \qquad \text{(Eq. 2-45)}$$

$$\frac{V_{solid}}{V_{Total}} = \frac{D_L}{\rho_P} \qquad \text{(Eq. 2-46)}$$

$$\frac{V_{gas}}{V_{Total}} = 1 - \frac{D_L}{\rho_P} \qquad \text{(Eq. 2-47)}$$

where:

D_L = atmospheric dust particle load in the air compartment (kg[dust particles]/ m^3[air]), where dust could include any type of aerosol; and
ρ_P = density of dust particles (kg[particles]/m^3[particles]).

The dust load and density are specified properties of each air compartment. To normalize to either the gas or solid phase, the equilibrium ratio of the concentrations in the two phases must be estimated. The fraction of the chemical bound to particles is denoted by φ here and by *Fraction_Mass_Sorbed* in the air compartment of TRIM.FaTE. It is estimated using a method developed by Junge (1977) for organic chemicals, and a more recent method developed by Harner and Bidleman (1998) that is applied for mercury, both of which are discussed in Section 2.3.2. Use of this term in the current notation yields:

$$\frac{V_{solid} \times C_{solid}}{V_{gas} \times C_{gas}} = \frac{\varphi}{1-\varphi} \qquad \text{(Eq. 2-48)}$$

where:

φ = fraction of chemical in the air compartment that is sorbed to particles in air (unitless).

From this, the equilibrium ratio of the concentration in the solid phase to that in the gas phase in an air compartment is given by:

$$\frac{C_{solid}}{C_{gas}} = \frac{\varphi / V_{solid}}{(1-\varphi) / V_{gas}} \tag{Eq. 2-49a}$$

$$= \frac{\varphi / (D_L / \rho_P)}{(1-\varphi) / (1 - D_L / \rho_P)} \tag{Eq. 2-49b}$$

$$= \frac{\varphi \times (1 - D_L / \rho_P)}{(1-\varphi) \times (D_L / \rho_P)} \tag{Eq. 2-49c}$$

The total mass of chemical in the air compartment is then:

$$N_{Total} = C_{gas} \times V_{Total} \times \left((1 - D_L / \rho_P) + \frac{C^{solid}}{C^{gas}} \times (D_L / \rho_P) \right) \tag{Eq. 2-50a}$$

$$= C_{gas} \times V_{Total} \times \left((1 - D_L / \rho_P) + \frac{\varphi \times (1 - D_L / \rho_P)}{(1-\varphi) \times (1 - D_L / \rho_P)} \times (D_L / \rho_P) \right) \tag{Eq. 2-50b}$$

$$= C_{gas} \times V_{Total} \times \left((1 - D_L / \rho_P) + \frac{\varphi \times (1 - D_L / \rho_P)}{(1-\varphi)} \right) \tag{Eq. 2-50c}$$

$$= C_{gas} \times V_{Total} \times (1 - D_L / \rho_P) \times \left(1 + \frac{\varphi}{(1-\varphi)} \right) \tag{Eq. 2-50d}$$

2.3.1.2 Fugacity-based Notation

For the air compartment, the fugacity capacity in the solid phase can be determined by use of the relationship as follows:

$$Z_{solid} = Z_{air} \times \frac{C_{solid}}{C_{gas}} \tag{Eq. 2-51a}$$

$$= Z_{air} \times \frac{\varphi \times (1 - D_L / \rho_P)}{(1-\varphi) \times (D_L / \rho_P)} \tag{Eq. 2-51b}$$

where:

Z_{air} = $1/(RT)$;
R = ideal gas constant (8.314 m^3-Pa/mol-K); and
T = temperature (°K).

The total fugacity in the air compartment is then given by:

$$Z_{Total} = Z_{air} \times \frac{V_{gas}}{V_{Total}} + Z_{solid} \times \frac{V_{solid}}{V_{Total}} \qquad \text{(Eq. 2-52a)}$$

$$= Z_{air} \times (1 - D_L/\rho_P) + Z_{solid} \times (D_L/\rho_P) \qquad \text{(Eq. 2-52b)}$$

2.3.2 CALCULATION OF THE FRACTION OF CHEMICAL BOUND TO AIR PARTICLES

The fraction of chemical bound to particulate in the air compartment, denoted by φ, can be calculated using one of two methods. The first method is the K_{OA}-based method discussed in Harner and Bidleman (1998) (Section 2.3.2.1), while the second is from Junge (1977) (Section 2.3.2.2). The current TRIM.FaTE library includes the method of Harner and Bidleman (1998). Note that in each of these methods, a chemical with extremely low or essentially zero vapor pressure (*e.g.,* cadmium, lead) is assumed to be 100 percent bound to particulate matter in the air.

2.3.2.1 K_{OA}-based Method

In Harner and Bidleman (1998), a "K_{OA} adsorption model" is shown to fit to PCB data better than a Junge-Pankow model similar to the Junge (1977) model. Further, the parameters needed are considered to be more easily measurable than the parameters for the Junge-Pankow model. This K_{OA} model is in the current TRIM.FaTE library. Using the notation of Harner and Bidleman (1998), the K_{OA} model first estimates the particle/gas partition coefficient (K_P) in terms of the octanol/air partition coefficient and the fraction of organic matter attached to particles. It then calculates the fraction of chemical in the particle phase via the relationship:

$$\varphi = \frac{K_P \times TSP}{1 + K_P \times TSP} \qquad \text{(Eq. 2-53)}$$

where:

φ, = *Fraction_Mass_Sorbed*, *i.e.*, fraction of chemical bound to dust particles in the air compartment (unitless);
K_P = particle/gas partition coefficient for chemical (ng[chemical]/µg[particles])/(ng[chemical]/m^3[air]); and
TSP = total suspended particle concentration (µg[particles]/m^3[air]).

Using the notation of this section, the following relationship exists:

$$TSP = 10^9 \times D_L \qquad \text{(Eq. 2-54)}$$

where:

D_L = the dust load for the air compartment (kg[particles]/m^3[air]).

The particle/gas partition coefficient, K_P, is calculated via the regression-based equation:

$$\log(K_P) = \log(K_{OA}) + \log(f_{om}) - 11.91 \qquad \text{(Eq. 2-55)}$$

where:

K_P = particle/gas partition coefficient (g[chemical]/kg[particles] per g[chemical]/m^3[air] or m^3[air]/kg[particles]);
K_{OA} = octanol/air partition coefficient (g[chemical]/m^3[octanol] per g[chemical]/m^3[air] or m^3[air]/m^3[octanol]); and
f_{om} = fraction of dust comprised of organic material (on a weight basis; unitless).

In the current TRIM.FaTE library representation of the formula for K_P, log(f_{om}) is replaced by log(f_{om} + 1E-10) to prevent a log(zero) computer error if the user inputs zero as the value for the fraction of organic matter in the particles.

If the octanol/air partition coefficient is not available, it can be calculated from the octanol/water partition coefficient K_{OW} (g[chemical]/kg[octanol] per g[chemical]/L[water] or L[water]/kg[octanol]) via the relationship:

$$K_{OA} = K_{OW} \times \frac{R \times T}{H} \qquad \text{(Eq. 2-56)}$$

where the of R, T, and H are such that the quantity $R \times T/H$ is unitless.

2.3.2.2 Junge's Method

This method has been used in multimedia models, including prototype versions of TRIM.FaTE. It is not included in the TRIM.FaTE library for the reasons listed at the beginning of Section 2.3.2.1. The following discussion is based on that presented in CalTOX (McKone 1993a,b,c). With this method, the fraction of chemical bound to dust particles (or aerosol) is calculated via the formula:

$$\varphi = \frac{c \times SA}{P_{vapor} + (c \times SA)} \qquad \text{(Eq. 2-57)}$$

where:

P_{vapor} = vapor pressure or subcooled vapor pressure of the chemical (Pa);
c = empirical constant set to 0.173 (m-Pa) as in Junge (1977); and

SA = total surface of aerosols per volume of dust or aerosol particles (m^2[surface]/m^3[particles]) (denoted by θ in CalTOX).

There is a range of values for *SA*. Whitby (1978) reported a range of 4.2×10^{-5} m^2/m^3 for a "clean" continental site to 1.1×10^{-5} m^2/m^3 for urban sites.

Following CalTOX (McKone 1993a,b,c), the subcooled vapor pressure (*i.e.*, vapor pressure of subcooled liquid) is used if the temperature is below the melting point (T_m) of the chemical. In particular:

$$P_{vapor} = \begin{cases} P_{vapor} & if\ T > T_m \\ \exp[6.79(T_m/T - 1)] & if\ T \le T_m \end{cases} \tag{Eq. 2-58}$$

where:

P_{vapor} = vapor pressure or subcooled vapor pressure of the chemical (Pa);
T = temperature (°K); and
T_m = melting point (°K).

2.4 GENERAL FATE AND TRANSPORT PROCESSES

This section provides a brief overview of the forms of the algorithms used to calculate the T-factors in TRIM.FaTE for advective processes (Section 2.4.1), diffusive and dispersive processes (Section 2.4.2), reaction and transformation processes (Section 2.4.3), and biotic processes (Section 2.4.4).

2.4.1 ADVECTIVE PROCESSES

In general, the advective flux for a given phase (*e.g.*, attached to particles, or dissolved in water) from compartment *i* to compartment *j* is given by:

Advective flux from compartment i to compartment j =
(Volume of phase that moves from compartment i to compartment j per unit time) ×
(Amount of chemical in phase per volume of phase in compartment i) (Eq. 2-59)

or:

$$Advective\ Flux\ Compartment\ i \rightarrow Compartment\ j = Q(phase) \times \frac{N_i(t) \times f_i(phase)}{V_i(phase)} \tag{Eq. 2-60a}$$

$$= T^{adv}_{i \rightarrow j}(phase) \times N_i(t) \tag{Eq. 2-60b}$$

where:

$Q(phase)$ = volumetric flow of phase from compartment *i* to compartment *j* (m^3[phase]/day);
$N_i(t)$ = amount of chemical in compartment *i* at time (g[chemical]);

$f_i(phase)$ = fraction of chemical in compartment i that is in the moving phase (g [chemical in phase]/g[chemical in compartment i]);
$V_i(phase)$ = volume of phase that is in compartment i (m^3[phase]); and
$T_{i \to j}^{adv}(phase)$ = phase transfer factor for advective flux from compartment i to receiving compartment j (/day), given by:

$$T_{i \to j}^{adv}(phase) = \frac{Q(phase) \times f_i(phase)}{V_i(phase)} \tag{Eq. 2-61}$$

This formula for the transfer factor is valid for all advective processes from one compartment to another, and it does not rely on the fugacity concept.

Application of the concept of fugacity (as presented in Section 2.1.3.2) shows that:

$$f_i(phase) = \frac{Z_i(phase)}{Z_i(Total)} \times \frac{V_i(phase)}{V_i(Total)} \tag{Eq. 2-62}$$

where:

$Z_i(phase)$ = fugacity capacity for moving phase (mol/m^3[phase]-Pa);
$Z_i(Total)$ = total fugacity capacity for compartment i (mol/m^3[sending compartment i]-Pa); and
$V_i(Total)$ = total volume of compartment i (sum of volumes of each phase in compartment) (m^3[compartment i]).

Applying this shows that the fugacity-based form for the transfer factor for advective flux is:

$$T_{i \to j}^{adv}(phase) = \frac{Q(phase) \times Z_i(phase)}{V_i(Total) \times Z_i(Total)}$$

$$= \frac{\upsilon_{ij}(phase) \times A_{ij} \times Z_i(phase)}{V_i(Total) \times Z_i(Total)} \tag{Eq. 2-63}$$

where:

v_{ij} = volumetric flow rate per unit area or flow velocity (m^3[phase]/m^2[relevant area]-day or m/day); and
A_{ij} = area of interface between compartments i and j (m^2).

In most advective transfers between compartments, the volumetric flow rate *Q(phase)* of the phase is calculated as the product of a relevant area (A_{ij}) and the volumetric flow rate per unit area, or a flow velocity (v_{ij}). Usually the relevant area is the interfacial area between the sending and receiving compartments, but this is not always the case; *e.g.*, erosion from surface soil to surface water is usually reported in units of mass[soil]/area[soil layer]-time, in which case the relevant area is the surface area of the surface soil layer. Table 2-2 at the end of this chapter summarizes the advective volumetric flows included for compartment types in TRIM.FaTE. These flows are discussed in more detail in the chapters describing the specific compartment types.

2.4.2 DIFFUSIVE AND DISPERSIVE PROCESSES

In TRIM.FaTE, dispersion is explicitly addressed as a first-order process in transfers between surface water compartments and applies to the chemical in both liquid and solid phases. Modeling of dispersion has not been implemented for transfers between air compartments or for movement of a chemical through soils, either vertically or horizontally.

Diffusive processes are modeled in TRIM.FaTE for transfers between many different compartment types (see TSD Volume I). T-factors developed for diffusive processes between compartments often apply to the chemical found in only one of the phases in a compartment (*e.g.*, diffusion from air to surface water applies only to the vapor phase of the chemical in air). T-factors developed for diffusion between abiotic and biotic compartments also depend on characteristics, including the conductance, of the boundary layers between the two compartments.

2.4.3 REACTION AND TRANSFORMATION PROCESSES

At present, all reaction and transformation processes are modeled using a first-order rate constant *k* (units of 1/day). The reaction/transformation flux within a compartment is then given by $k\,N(t)$, where $N(t)$ is the mass of chemical in the compartment. There are a variety of ways in which the rate constant is determined, with the details depending on the compartment types and chemicals involved. The simplest is the case where the rate constant is an input (*e.g.*, for the current mercury species transformation algorithms).

In other cases, the rate constant for an organic chemical reaction can be calculated from other environmental and/or chemical parameters (*e.g.*, from a half-life input by the user). In the current TRIM.FaTE library, a "degradation" rate constant, $k_{degradation}$ (/day), for organic chemicals is calculated as:

$$k_{degradation} = \ln(2) \,/\, half\!-\!life \qquad \text{(Eq. 2-64)}$$

Whenever a chemical is transformed into reaction products that are no longer tracked in TRIM.FaTE, the mass of the chemical is transferred to a "reaction/degradation sink" for the compartment in which the transformation occurs. This is accomplished by setting a one-way transfer factor from the compartment to the compartment degradation sink as equal to the degradation rate constant, $k_{degradation}$:

$$T_{Comp \rightarrow Comp\_Sink} = k_{degradation} \qquad \text{(TF 2-1)}$$

where:

$T_{Comp \rightarrow Comp\_Sink}$ = transfer factor from compartment to compartment degradation sink (/day).

2.4.4 BIOTIC PROCESSES

The biotic processes in TRIM.FaTE are well characterized by the descriptions of abiotic processes and conversions. Diffusive processes and advective processes are both included. The primary instance of advection is dietary uptake. Another prominent example is litter fall. Fugacity is used as a descriptor in algorithms where it is convenient (*e.g.*, in the uptake of contaminants by foliage from air). Because mechanisms of uptake of contaminants by some organisms are not well understood or are difficult to parameterize, some partitioning processes are assumed to be equilibrium relationships according to the form described in Section 2.5 (next section). These processes may be combinations of diffusion, active transport, and/or advection (*e.g.*, transport of contaminants into the plant root), and it is not necessary for the user to specify the mechanistic process, only the empirical relationship (*e.g.*, partition coefficient and time to equilibrium).

As with abiotic reactions and transformations (Section 2.4.3), biotic transformation rates are also described as first-order processes with respect to the average chemical concentration in the particular compartment of concern.

2.5 CONVERTING EQUATIONS WITH EQUILIBRIUM RELATIONSHIPS TO DYNAMIC FORM

In the course of converting equations to a form suitable for use within the intended TRIM.FaTE framework, it is possible to convert some algorithms that represent steady-state equilibrium relationships into time-dependent ones. This can be accomplished if an estimate of the time required for the concentration to reach some fraction of the equilibrium value is available. In particular, if the concentration in one compartment C_1 is related to the concentration in another compartment C_2 by an equilibrium relationship of the form $C_1 = K \times C_2$, where K is known and it is known that it takes time t_α in order to reach 100α percent of the equilibrium value when C_2 is approximately constant, then:

$$\frac{dC_1(t)}{dt} = \left(k_2 \times C_2\right) - \left(k_1 \times C_1\right) \qquad \text{(Eq. 2-65)}$$

where:

$$k_1 = \frac{-\ln(1-\alpha)}{t_\alpha} \qquad \text{(Eq. 2-66)}$$

$$k_2 = K \times k_1 \qquad \text{(Eq. 2-67)}$$

and where:

α = proportion of the equilibrium concentration reached in time t_α (unitless);
t_α = time required to reach 100α percent of equilibrium value (days); and
K = ratio of the concentration of the chemical in compartment 1 to its concentration in compartment 2 (g[chemical]/m^3[compartment 1] per g[chemical]/m^3[compartment 2]).

The value for α used as a default in TRIM.FaTE is 0.95, meaning that t_α is the time to reach 95 percent of the equilibrium concentration value. The precision and accuracy of empirical data available to estimate t_α decreases with increasing values for α.

The solution of the previous differential equation with initial condition $C_1(0) = 0$ is given by:

$$C_1(t) = \frac{k_2}{k_1} C_2 (1 - e^{-k_1 t}) \qquad \text{(Eq. 2-68)}$$

The steady-state equilibrium solution is $C_1(t) = (k_2/k_1)\ C_2$, and so $K = k_2/k_1$. The assumption that $100 \times \alpha$ percent (*e.g.*, 95 percent) of the equilibrium value is reached at time t_α means that:

$$1 - e^{-k_1 t_\alpha} = \alpha \qquad \text{(Eq. 2-69)}$$

Solving for k_1 yields:

$$k_1 = -\ln(1 - \alpha)/t_\alpha \qquad \text{(Eq. 2-70)}$$

When k_1 is determined, given K, k_2 can be determined (*i.e.*, Equation 2-67, $k_2 = k_1 \times K$).

2.6 RELATING FUGACITY AND EQUILIBRIUM NOTATIONS

In developing code for TRIM.FaTE, there were some equations that were most easily developed using fugacity notation and others that were most easily developed using ratios of fractions related to phases in a compartment. This section demonstrates the equivalence of certain fugacity expressions to certain phase-related ratios that are commonly used in the TRIM.FaTE code. Specifically, this section demonstrates that:

$$\mathit{Mass\_Fraction\_Sorbed/Volume\_Fraction\_Solid} = Z_{solid}/Z_{Total} \qquad \text{(Eq. 2-71)}$$

$$\mathit{Mass\_Fraction\_Dissolved/Volume\_Fraction\_Liquid} = Z_{water}/Z_{Total} \qquad \text{(Eq. 2-72)}$$

$$\mathit{Mass\_Fraction\_Vapor/Volume\_Fraction\_Vapor} = Z_{air}/Z_{Total} \qquad \text{(Eq. 2-73)}$$

where:

Mass_Fraction_Sorbed = fraction of the chemical mass in the total compartment that is sorbed to the solid phase material in the compartment (unitless);
Volume_Fraction_Solid = volume fraction of the total compartment that is solid or particulate (unitless);
Mass_Fraction_Dissolved = fraction of the chemical mass in the total compartment that is dissolved in the liquid-phase material (*i.e.*, water) in the compartment (unitless);
Volume_Fraction_Liquid = volume fraction of the compartment that is liquid (*i.e.*, water) (unitless);
Mass_Fraction_Vapor = fraction of the chemical mass in the total compartment that is in vapor phase (unitless); and
Volume_Fraction_Vapor = volume fraction of the compartment that is vapor/gas phase (*i.e.*, air) (unitless).

Starting with:

$$Z_{solid} = Z_{air} \times \frac{\varphi \times \left(1 - \dfrac{D_L}{\rho_P}\right)}{\left(1 - \varphi\right) \times \dfrac{D_L}{\rho_P}} \tag{Same as Eq. 2-51}$$

an equation for Z_{air} can be derived:

$$Z_{air} = Z_{solid} \times \frac{\left(1 - \varphi\right) \times \dfrac{D_L}{\rho_P}}{\varphi \times \left(1 - \dfrac{D_L}{\rho_P}\right)} \tag{Eq. 2-74}$$

where:

Z_{air} = fugacity capacity of chemical in gas-phase air (mol/m^3-Pa);
Z_{solid} = fugacity capacity of chemical in solid-phase (mol/m^3-Pa);
D_L = atmospheric dust load in the air compartment (kg[dust]/m^3[air compartment]), where dust could include any type of aerosol;
ρ_p = density of dust particles (kg[dust]/m^3[dust]); and
φ = fraction of chemical in the air compartment that is sorbed to particles in air (unitless).

It is also true that:

$$Z_{Total} = \left(Z_{air} \times \left(1 - \frac{D_L}{\rho_P}\right)\right) + \left(Z_{solid} \times \frac{D_L}{\rho_P}\right) \tag{Eq. 2-75}$$

Using Equation 2-74 to replace Z_{air} in Equation 2-75 yields:

$$Z_{Total} = Z_{solid} \times \frac{(1-\varphi) \times \dfrac{D_L}{\rho_P}}{\varphi \times \left(1 - \dfrac{D_L}{\rho_P}\right)} \times \left(1 - \frac{D_L}{\rho_P}\right) + \left(Z_{solid} \times \frac{D_L}{\rho_P}\right) \qquad \text{(Eq. 2-76)}$$

The term (1-D_L/ρ_P) divided by (1-D_L/ρ_P) equals one; therefore, Equation 2-76 can be rewritten as:

$$Z_{Total} = Z_{solid} \times \left(\frac{(1-\varphi)}{\varphi} \times \frac{D_L}{\rho_P} + \frac{D_L}{\rho_P}\right) \qquad \text{(Eq. 2-77a)}$$

$$= Z_{solid} \times \frac{D_L}{\rho_P} \times \left(\frac{(1-\varphi)}{\varphi} + 1\right) = Z_{solid} \times \frac{D_L}{\rho_P} \times \left(\frac{1-\varphi+\varphi}{\varphi}\right) \qquad \text{(Eqs. 2-77b, 2-77c)}$$

$$= Z_{solid} \times \frac{D_L}{\rho_P} \times \frac{1}{\varphi} \qquad \text{(Eq. 2-77d)}$$

Therefore:

$$\frac{Z_{solid}}{Z_{Total}} = \frac{\varphi}{(D_L / \rho_P)} \qquad \text{(Eq. 2-78)}$$

where:

φ = *Mass_Fraction_Sorbed*; and
(D_L/ρ_P) = *Volume_Fraction_Solid.*

Thus:

Z_{solid}/Z_{Total} = *Mass_Fraction_Sorbed / Volume_Fraction_Solid.* (same as Eq. 2-71)

Similar derivations demonstrate that:

Z_{water}/Z_{Total} = *Mass_Fraction_Dissolved / Volume_Fraction_Liquid.* (same as Eq. 2-72)

and:

Z_{air}/Z_{Total} = *Mass_Fraction_Vapor/Volume_Fraction_Vapor* (same as Eq. 2-73)

where:

$Z_{air} = Z_{vapor}$.

To simplify equations in Chapters 3 through 7, the variables f_{MS}, f_{ML}, and f_{MV} are defined as follows:

$$f_{MS} = Mass\_Fraction\_Sorbed / Volume\_Fraction\_Solid \qquad \text{(Eq. 2-79)}$$

$$f_{ML} = Mass\_Fraction\_Dissolved / Volume\_Fraction\_Liquid \qquad \text{(Eq. 2-80)}$$

$$f_{MV} = Mass\_Fraction\_Vapor/Volume\_Fraction\_Vapor \qquad \text{(Eq. 2-81)}$$

To ensure clarity in the presentation of equations throughout the remainder of this TSD, the following naming conventions have been used:

Z_{pure_air} = Z_{air} for fugacity capacity of the chemical vapor in gas-phase air *excluding* atmospheric dust particles;
Z_{Total_Air} = total fugacity capacity of chemical in bulk air, *including* atmospheric dust particles;
Z_{pure_water} = Z_{water} for fugacity capacity of the chemical dissolved in liquid-phase water *excluding* suspended sediment particles;
Z_{Total_SW} = total fugacity capacity of chemical in bulk surface water, *including* suspended sediment particles;
Z_{pure_solid} = Z_{solid} for fugacity capacity of the chemical in or sorbed to solid particles; and
Z_{Total_Sx} = total fugacity of chemical in a bulk soil compartment, *including* the gas/vapor (air) and liquid (water) phases in the interstitial spaces, where the subscript *Sx* equals *Ss* for surface soil, *Sr* for root-zone soil, and *Sv* for vadose-zone soil.

2.7 TRIM.FaTE CODE FOR DISTRIBUTION OF CHEMICAL AMONG PHASES

Tables 2-3a and 2-3b at the end of this chapter provide the equations in the current TRIM.FaTE library for calculating the distribution of chemical mass among phases in each abiotic compartment type, *i.e.*:

Fraction_Mass_Dissolved, the fraction in the aqueous liquid phase;
Fraction_Mass_Sorbed, the fraction in the solid phase;
Fraction_Mass_Vapor, the fraction in the vapor phase; and
Fraction_Mass_Algae, the fraction in algae.

All abiotic compartment types include a solid phase and hence the property *Fraction_Mass_Sorbed*. The property *Fraction_Mass_Algae* is included only in the surface water compartment. The air compartment does not include a liquid phase or the property *Fraction_Mass_Dissolved*. The surface water, sediment, and ground water compartments do not include a vapor/gas phase or the property *Fraction_Mass_Vapor*.

Each of the equations in Tables 2-3a and 2-3b are simply compartment-specific versions of the general equations developed earlier in this chapter. The definitions of the parameters in both tables are listed below:

1000 = units conversion factor (L/m^3);
V_{SW} = volume of the surface water compartment (m^3);
V_{Sed} = volume of the sediment compartment (m^3);
V_S = volume of the soil (or ground water) compartment (m^3);
θ = volume fraction liquid (*i.e.*, water) (unitless);
ϕ = total porosity (*i.e.* $\theta + \epsilon$) (unitless);
ϵ = volume fraction gas (*i.e.*, air) (unitless);
K_P = particle/gas partition coefficient (m^3[air]/kg[particles]);
Kd = soil/water partition coefficient (L[water]/kg[soil wet wt]);
$RatioConc_{Algae}$ = ratio of the concentration of chemical in algae to the concentration of chemical in surface water (excluding suspended sediments) (unitless);
ρ_{Sed} = density of sediment particles (kg[particles]/m^3[particles]);
ρ_S = density of soil particles (kg[particles]/m^3[particles]);
D_L = atmospheric dust load in the air compartment (kg[dust particles]/ m^3[air]);
AC = algal concentration (density) in the water column (g[algae]/m^3[water]);
fV_{Algae} = volume fraction of the surface water compartment comprised of algae (unitless), *i.e.*, *Volume_Fraction_Algae*;
Z_{pure_air} = fugacity capacity of chemical in air (excluding atmospheric dust particles) (mol/m^3-Pa); and
Z_{pure_water} = fugacity capacity of chemical in water (excluding suspended sediment particles) (mol/m^3-Pa).

The volume fraction of the surface water compartment that consists of algae is estimated as:

$$fV_{Algae} = (CA \times 1000) / \rho_{Algae} \qquad \text{(Eq. 2-82)}$$

where:

Vf_{Algae} = volume fraction of surface water compartment that is algae (m^3[algae]/m^3[surface water], unitless);
CA = algae concentration (density) in water column (g[algae]/L[water]);
ρ_{Algae} = density of algae (g[algae]/m^3[algae]); and
1000 = conversion factor (L/m^3).

Table 2-2
Summary of Advective Volumetric Flows Included in TRIM.FaTE[a,b]

Source/ Sending Compartment	Receiving Compart-ment	Moving Phase	Description of Advective Process	Units of Moving Phase	Method for Calculation of Volumetric Flow (Q)
Soil	Soil or Soil Sink	Liquid	Runoff (surface soil only)	m^3[water]/day	$= A_{Ss} \times runoff$ where: A_{Ss} = Area of surface soil layer (m^2) $runoff$ = Amount of runoff that reaches adjacent downgradient surface soil parcel per unit area of sending soil parcel (m^3[water]/m^2[area]-day)
			Precipitation driven percolation	m^3[water]/day	$= A \times v_{liquid}$ where: A = Area of soil/soil interface (m^2) v_{liquid} = Velocity of water (vertical) in sending soil compartment (m^3[water]/m^2[area]-day)
		Solid	Erosion (surface soil only)	m^3[soil particles]/day	Calculated from mass-based areal erosion rate and soil density: $= A_{Ss} \times erosion \; / \; \rho_P$ where: A_{Ss} = Area of surface soil layer (m^2) $erosion$ = erosion rate to adjacent downgradient surface soil parcel (kg [soil]/m^2[area]-day) ρ_P = density of eroding soil particles (kg[particles]/m^3[soil])

Source/ Sending Compartment	Receiving Compart- ment	Moving Phase	Description of Advective Process	Units of Moving Phase	Method for Calculation of Volumetric Flow (Q)
Soil	Air	Solid	Resuspension	m^3[soil particles]/day	It is assumed that volumetric flow of particles from soil is the same as that to soil. Volumetric resuspension rate is then = volumetric flow to soil = $A \times v_{dry} \times (D_L / \rho_P)$ where: A = Area of soil/soil interface (m^2) v_{dry} = Dry deposition velocity of particles (m/day) D_L = Atmospheric dust load in air compartment type (concentration of dust in air) (kg[particles]/m^3[air]) ρ_P = Density of dust particles (kg[particles]/m^3[particles])
	Surface Water	Solid	Erosion	m^3[soil particles]/day	Calculated from mass-based areal erosion rate and soil density: = $A_{Ss} \times erosion \ / \rho_P$ where: A_{Ss} = Area of surface soil layer (m^2) *erosion* = Erosion rate to surface water (kg[soil]/m^2[area]-day) ρ_P = Density of eroding soil particles (kg[particles]/m^3[soil])
		Liquid	Runoff	m^3[water]/day	= $A_{Ss} \times runoff$ where: A = Area of soil layer (m^2) *runoff* = Amount of runoff that reaches water body per unit area of watershed (m^3[water]/m^2[area]-day)
	Ground Water	Liquid	Percolation	m^3[water]/day	= $A \times percolation$ where: A = Area of vadose-zone soil interface with the ground water compartment (m^2) *percolation* = Volume of water flow per unit area of interface (m^3[water]/m^2[area]-day)
Ground Water	Surface Water	Liquid	Recharge	m^3[water]/day	= $A \times recharge$ where: A = Area of ground water soil/surface water interface (m^2) *recharge* = Volume of water flow per unit area of interface (m^3[water]/m^2[area]-day)

Table 2-2 (continued)
Summary of Advective Volumetric Flows Included in TRIM.FaTE[a,b]

Source/ Sending Compartment	Receiving Compart-ment	Moving Phase	Description of Advective Process	Units of Moving Phase	Method for Calculation of Volumetric Flow (Q)
Air	Surface Soil or Surface Water	Solid	Dry and Wet deposition of particles	m^3[dust particles]/day	$= A \times v_{dry} \times D_L / \rho_P$ (dry dep.); $= A \times v_{wd} \times D_L / \rho_P$ (wet dep.); where: A_{Ss} = Area of surface soil layer (m^2) v_{dry} = Dry deposition velocity of particles (m/day) v_{wet} = Wet deposition velocity of particles (m/day) D_L = Atmospheric dust load in air compartment type (concentration of dust in air) (kg[particles]/m^3[atmosphere]) ρ_P = Density of dust particles (kg[particles]/m^3[particles])
	Air or Air Advection Sink	Gas and solid	Wind advection	m^3[air]/day	$= A \times v_{wind}$ where: A = Area of air/air interface (m^2) v_{wind} = Wind velocity from sending to receiving air compartment (m/day)
Air	Plant Leaf (no rain)	Solid	Dry deposition of particles	m^3[dust particles]/day	$= A_S \times I_{dry} \times v_{dry} \times (D_L / \rho_P)$ where: A_S = Area of soil layer containing plant (m^2) I_{dry} = Interception fraction for dry-depositing chemical (see Section 7.2 for description of algorithm) v_{dry} = Dry deposition velocity of particles (m/day) D_L = Atmospheric dust load in air compartment type (concentration of dust in air) (kg[particles]/ m^3[atmosphere]) ρ_P = Density of dust particles (kg[particles]/m^3[particles])

Source/ Sending Compartment	Receiving Compart-ment	Moving Phase	Description of Advective Process	Units of Moving Phase	Method for Calculation of Volumetric Flow (Q)
	Plant Leaf (during rain)	Solid	Wet deposition of particles	m^3[dust particles]/day	$= A_S \times I_{wet} \times v_{wet} \times (D_L / \rho_P)$ where: A_S = Area of soil layer containing plant (m^2) I_{wet} = Interception fraction for wet-depositing chemical (see Section 7.2 for description of algorithm) v_{wet} = Wet deposition velocity of particles (m/day) D_L = Atmospheric dust load in air compartment type (concentration of dust in air) (kg[particles]/ m^3[atmosphere]) ρ_P = Density of dust particles (kg[particles]/m^3[particles])
Surface Water	Sediment	Solid	Sediment deposition	m^3[suspended sediment particles]/day	$= A_{SW\text{-}sed} \times S_{dep} / \rho_{SSed}$ where: $A_{SW\text{-}sed}$ = Area of surface water-sediment interface (m^2) S_{dep} = Deposition rate of suspended sediment particles to sediment bed (kg[suspended sediment]/m^2[area]-day) ρ_{SSed} = Density of suspended sediment (kg[suspended sediment]/ m^3[suspended sediment])
Surface Water	Surface Water	Liquid and solid	Water flow	m^3[water]/day	$= A \times v_R$ where: A = Area of river parcel interface (m^2) v_R = River velocity from sending to receiving river compartment (of same interfacial areas) (m/day), OR = *Flow* , where *Flow* = volumetric bulk water flow rate (m^3[water]/day) for connecting water bodies of different interfacial areas
Sediment	Surface Water	Solid	Sediment resuspension	m^3[benthic sediment particles]/day	$= A_{sed\text{-}SW} \times S_{resusp} / \rho_{bs}$ where: $A_{sed\text{-}SW}$ = Area of sediment-surface water interface (m^2) S_{resusp} = Resuspension rate of benthic sediment particles to water column (kg[benthic sediment particles]/m^2[area]-day) ρ_{bs} = Density of benthic sediment (kg[benthic sediment particles]/m^3[benthic sediment particles])

Table 2-2 (continued)
Summary of Advective Volumetric Flows Included in TRIM.FaTE[a,b]

Source/ Sending Compartment	Receiving Compart-ment	Moving Phase	Description of Advective Process	Units of Moving Phase	Method for Calculation of Volumetric Flow (Q)
	Sediment Burial Sink	Solid	Sediment burial	m^3[(benthic sediment particles]/day	Calculated so that amount of sediment buried is equal to maximum of 0 and amount deposited minus amount resuspended: $= A_{sed\text{-}SW} \times \max\{ 0, S_{dep}/\rho_{ss} - S_{resusp}/\rho_{BSed}\}$ where: $A_{sed\text{-}SW}$ = Area of sediment-surface water interface (m^2) S_{dep} = Deposition rate of suspended sediment particles to sediment bed (kg[suspended sediment]/m^2[area]day) ρ_{ss} = Density of suspended sediment (kg[suspended sediment]/m^3[suspended sediment]) S_{resusp} = Resuspension rate of benthic sediment to water column (kg[benthic sediment]/m^2[area]-day) ρ_{BSed} = Density of benthic sediment (kg[benthic sediment]/m^3[benthic sediment])

[a] Advection of chemicals to and from plants in particles and rain water and advection of chemicals to and from wildlife in dietary and excretory materials are not included. See Chapter 7.

[b] Equations for estimating chemical partitioning among phases are not included in this table. See individual chapters related to each type of transfer.

Table 2-3a
Equations for Estimating Chemical Mass Distribution Among Phases: Air and Surface Water[a]

Compartment Property	**AIR**	**SURFACE WATER**
Fraction_Mass_Dissolved	NA, assume no liquid phase in air	$= \dfrac{V_{SW} \times \theta}{GenDenom_{SW}}$
Fraction_Mass_Sorbed	$= 1 - \left(\dfrac{1}{1 + \left(K_P \times D_L \times 1\mathrm{E}^9 \; (\mu\mathrm{g/kg}) \right)} \right)$	$= \dfrac{V_{SW} \times (1 - \theta) \times Kd \times \rho_{Sed} \times 0.001 \; (\mathrm{m^3/L})}{GenDenom_{SW}}$
Fraction_Mass_Vapor	=1 - *Fraction_Mass_Sorbed*	NA, assume no gas/vapor phase in surface water
F*raction_Mass_Algae*	NA, no algae in air	$= \dfrac{V_{SW} \times fV_{Algae} \times RatioConc_{Algae} (\mathrm{g/m^3}) \times 0.001 \; (\mathrm{m^3/L})}{GenDenom_{SW}}$
GenericDenominatorfor PhaseCalculations, or *GenDenom*	NA, not used	$= V_{SW} \times (fV_{Algae} \times RatioConc_{Algae} \times AC(\mathrm{g/m^3}) \times 0.001 \; (\mathrm{m^3/L}) + (1 - \theta) \times Kd \times \rho_{Sed} \times 0.001 \; (\mathrm{m^3/L}) + \theta)$

[a] For parameter symbol definitions, see text of Section 2.7.

Table 2-3b
Equations for Estimating Chemical Mass Distribution Among Phases: Sediments, Soil, and Ground Water[a]

Compartment Property	**SEDIMENT**	**SOIL and GROUND WATER**
Fraction_Mass_Dissolved	$= \dfrac{V_{Sed} \times \theta}{GenDenom_{Sed}}$	$= \dfrac{V_S \times \theta \times 1000}{GenDenom_S}$
Fraction_Mass_Sorbed	$= \dfrac{V_{Sed} \times (1 - \phi) \times Kd \times \rho_{Sed} \times 0.001\ (\mathrm{m}^3/\mathrm{L})}{GenDenom_{Sed}}$	$= \dfrac{V_S \times \left(Kd \times \rho_S\right) \times (1 - \theta - \varepsilon)}{GenDenom_S}$
Fraction_Mass_Vapor	NA, assume no gas/vapor phase in sediments	$= \dfrac{V_S \times \varepsilon \times 1000 \times \left(\dfrac{Z_{pure\_air}}{Z_{pure\_water}}\right)}{GenDenom_S}$
Fraction_Mass_Algae	NA, assume no algae in sediments	NA, no algae in soil or ground water
GenericDenominatorfor PhaseCalculations, or *GenDenom*	$= V_{Sed} \times (1 - \phi) \times Kd \times \rho_{Sed} \times 0.001\ (\mathrm{m}^3/\mathrm{L})$ $+ V_{Sed} \times \theta$	$= V_S \times ((Kd \times \rho_S) \times (1 - \theta - \varepsilon) +$ $(\theta \times 1000) + (\varepsilon \times \dfrac{Z_{pure\_air}}{Z_{pure\_water}} \times 1000))$

[a] For parameter symbol definitions, see text of Section 2.7.