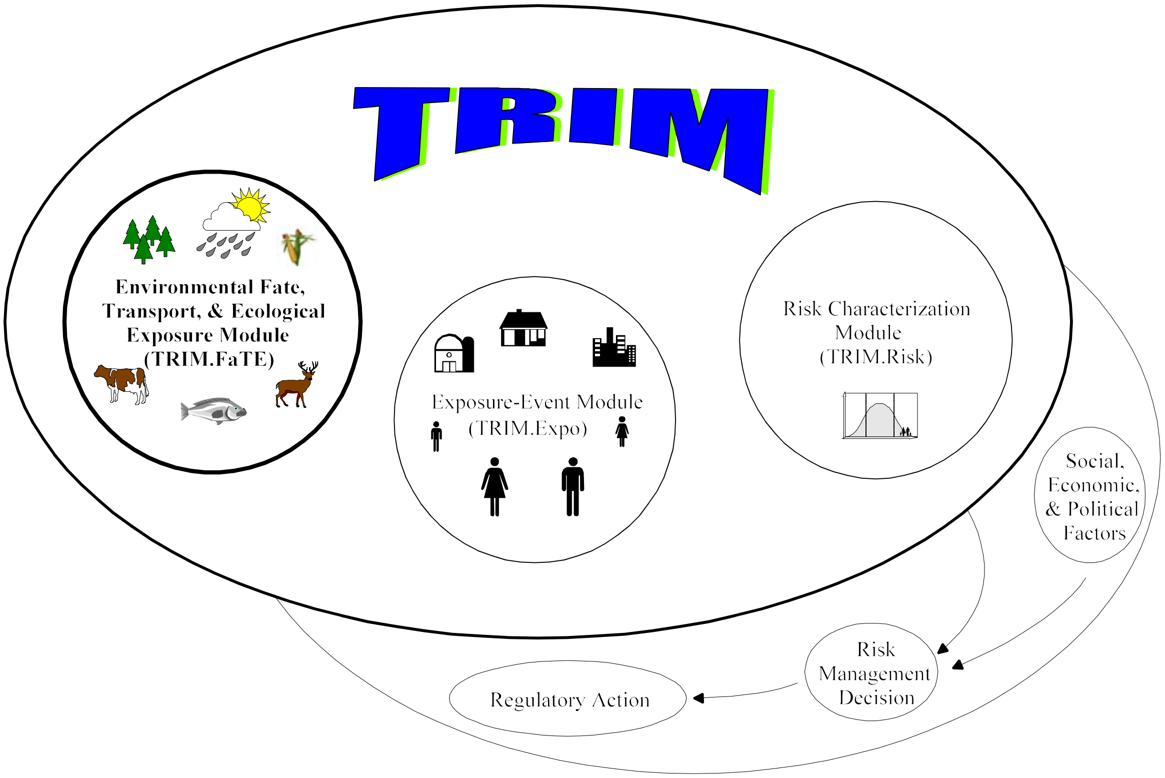
Total Risk Integrated Methodology

TRIM.FaTE Technical Support Document

Volume II: Description of Chemical Transport and Transformation Algorithms



EPA-453/R-02-011b
September 2002

TRIM
Total Risk Integrated Methodology

TRIM.FaTE
Technical Support Document
Volume II: Description of Chemical Transport and Transformation Algorithms

U.S. Environmental Protection Agency
Office of Air Quality Planning and Standards
Emissions Standards & Air Quality Strategies and Standards Divisions
Research Triangle Park, North Carolina

[This page intentionally left blank.]

DISCLAIMER

[This page intentionally left blank.]

ACKNOWLEDGMENTS

As described in this report, the Office of Air Quality Planning and Standards (OAQPS) of the U.S. Environmental Protection Agency (EPA) is developing the Total Risk Integrated Methodology. Individuals and organizations who have been involved in the TRIM.FaTE development effort and in the preparation of this report are listed below.

Steve Fine, EPA, Office of Research and Development
Robert G. Hetes, EPA, Office of Air Quality Planning and Standards
John Langstaff, EPA, Office of Air Quality Planning and Standards
Thomas McCurdy, EPA, Office of Research and Development
Deirdre L. Murphy, EPA, Office of Air Quality Planning and Standards
Ted Palma, EPA, Office of Air Quality Planning and Standards
Harvey M. Richmond, EPA, Office of Air Quality Planning and Standards
Amy B. Vasu, EPA, Office of Air Quality Planning and Standards

Deborah Hall Bennett, Lawrence Berkeley National Laboratory
David Burch, ICF Consulting
Rebecca A. Efroymson, Oak Ridge National Laboratory
Alison Eyth, MCNC-Environmental Modeling Center
Baxter Jones, ICF Consulting
Daniel S. Jones, Oak Ridge National Laboratory
Mark Lee, MCNC - Environmental Modeling Center
Bradford F. Lyon, University of Tennessee
Thomas E. McKone, Lawrence Berkeley National Laboratory & University of California, Berkeley
Margaret E. McVey, ICF Consulting
Randy Maddalena, Lawrence Berkeley National Laboratory

The following external experts reviewed a previous draft of this document.

Science Advisory Board Reviewers

Chair
Mitchell Small, Professor, Department of Civil Engineering & Public Policy,
Carnegie Mellon University, Pittsburgh, PA

Members

Steven M. Bartell, Senior Associate,
Cadmus Group, Inc., Oak Ridge, TN

Calvin Chien, Senior Environmental Fellow,
E.I. DuPont Company,
Wilmington, DE

Kai-Shen Liu, Epidemiologist, California
Department of Health Services,
Environmental Health Laboratory Branch,
Berkeley, CA

Paulette Middleton, Associate Director,
Environmental Science and Policy Center,
RAND Corporation, Boulder, CO

Ishwar Murarka, Chief Scientist and
President, ISH Inc., Cupertino, CA

Consultants

M. Bruce Beck, Professor & Eminent
Scholar, Warnell School of Forest
Resources,
University of Georgia, Athens GA

Linfield Brown, Professor, Department of
Civil and Environmental Engineering,
Tufts University, Medford, MA

Arthur J. Gold, Professor, Department of
Natural Resources Science,
University of Rhode Island, Kingston, RI

Helen Grogan, Research Scientist, Cascade
Scientific, Inc., Bend, OR

Wu-Seng Lung, Professor, Department of
Civil Engineering,
University of Virginia, Charlottesville, VA

Jana Milford, Associate Professor,
Department of Mechanical Engineering,
University of Colorado, Boulder, CO

Thomas Theis, Professor & Chair,
Department of Civil and Environmental
Engineering, Clarkson University,
Potsdam, NY

The following EPA individuals reviewed a previous draft of this document.

EPA Models 2000 TRIM Review Team

Robert F. Carousel
National Exposure Research Laboratory
Office of Research and Development

[*]S. Steven Chang
Office of Emergency and Remedial Response
Office of Solid Waste and Emergency Response

Ellen Cooter
National Exposure Research Laboratory
Office of Research and Development

Stan Durkee
Office of Science Policy
Office of Research and Development

Harvey Holm
National Exposure Research Laboratory
Office of Research and Development

John S. Irwin
Office of Air Quality Planning and Standards
Office of Air and Radiation

Linda Kirkland
National Center for Environmental Research and Quality Assurance
Office of Research and Development

Matthew Lorber
National Center for Environmental Assessment
Office of Research and Development

Haluk Özkaynak
National Exposure Research Laboratory
Office of Research and Development

William Petersen
National Exposure Research Laboratory
Office of Research and Development

Ted W. Simon
Region 4

Amina Wilkins
National Center for Environmental Assessment
Office of Research and Development

[*] Team Leader

Review by Other Program Offices

Pam Brodowicz, Office of Air and Radiation, Office of Mobile Sources
William R. Effland, Office of Pesticide Programs
John Girman, Office of Air and Radiation, Office of Radiation and Indoor Air
Steven M. Hassur, Office of Pollution Prevention and Toxics
Terry J. Keating, Office of Air and Radiation, Office of Policy Analysis and Review
Russell Kinerson, Office of Water
Stephen Kroner, Office of Solid Waste
David J. Miller, Office of Pesticide Programs

[This page intentionally left blank.]

PREFACE

This document, the *TRIM.FaTE Technical Support Document*, is part of a series of documentation for the overall Total Risk Integrated Methodology (TRIM) modeling system. The detailed documentation of TRIM's logic, assumptions, algorithms, equations, and input parameters is provided in comprehensive Technical Support Documents (TSDs) and/or user's guidance for each of the TRIM modules. This report, which supersedes earlier versions (U.S. EPA 1998a, U.S. EPA 1999a,b), documents the Environmental Fate, Transport, and Ecological Exposure module of TRIM (TRIM.FaTE) and is divided into two volumes. The first volume provides a description of terminology, model framework, and functionality of TRIM.FaTE, and the second volume presents a detailed description of the algorithms used in the module.

Comments and suggestions are welcomed. The OAQPS leads on the various modules are provided below with their individual roles and addresses.

TRIM coordination and TRIM.FaTE

Deirdre L. Murphy
REAG/ESD/OAQPS
C404-01
RTP, NC 27711
[murphy.deirdre@epa.gov]

TRIM.Expo [Inhalation]

Ted Palma
REAG/ESD/OAQPS
C404-01
RTP, NC 27711
[palma.ted@epa.gov]

Harvey M. Richmond
HEEG/AQSSD/OAQPS
C404-01
RTP, NC 27711
[richmond.harvey@epa.gov]

TRIM.Expo [Ingestion]

Amy B. Vasu
REAG/ESD/OAQPS
C404-01
RTP, NC 27711
[vasu.amy@epa.gov]

TRIM.Risk

Terri Hollingsworth
REAG/ESD/OAQPS
C404-01
RTP, NC 27711
[hollingsworth.terri@epa.gov]

[This page intentionally left blank.]

ACRONYMS, ABBREVIATIONS, AND SYMBOLS

ACRONYMS

BAF	Bioaccumulation Factor
B(a)P	Benzo(a)pyrene
BASS	Bioaccumulation and Aquatic System Simulator
BCF	Bioconcentration Factor
BMR	Basal Metabolic Rate
BW	Body Weight
D	Dust
DOC	Dissolved Organic Carbon
EPA	United States Environmental Protection Agency
FIR	Free-living Inhalation Rate
GI	Gastrointestinal
GIS	Geographic Information Systems
GW	Ground Water
HAP	Hazardous Air Pollutant
IEM	Indirect Exposure Methodology
K_{AW}	Air/Water Parition Coefficient
K_{OA}	Octanol/Air Partition Coefficient
K_{OW}	Octanol/Water Partition Coefficient
LSODE	Livermore Solver for Ordinary Differential Equations
NERL	National Exposure Research Laboratory
OAQPS	EPA Office of Air Quality Planning and Standards
OPPT	Office of Pollution Prevention and Toxics
ORD	Office of Research and Development
OW	Office of Water
PAH	Polycyclic Aromatic Hydrocarbon
R-MCM	Regional Mercury Cycling Model
SAB	Science Advisory Board
SCF	Stem Concentration Factor
SW	Surface Water
TF	Transfer Factor
TOC	Total Organic Carbon
TRIM	Total Risk Integrated Methodology
TRIM.Expo	TRIM Exposure-Event module
TRIM.FaTE	TRIM Environmental Fate, Transport, and Ecological Exposure module
TRIM.Risk	TRIM Risk Characterization module
TSCF	Transpiration Stream Concentration Factor
TSD	Technical Support Document
WASP	Water Quality Analysis Simulation Program

UNIT ABBREVIATIONS

		µg	microgram
°C	degrees Centigrade	ng	nanogram
°K	degrees Kelvin	mm	millimeter
g	gram	mol	mole
hr	hour	nmol	nanomole
kg	kilogram	nM	nanomolar
L	liters	Pascals	Pa
m	meter	yr	year

SYMBOLS USED FOR VARIABLES

Greek

α (alpha)	proportion of equilibrium value
κ (kappa)	von Karmen's constant
κ_j	the equilibrium ratio between the concentration in phase j and the phase to which one is normalizing
ϵ (epsilon)	volume fraction gas/vapor/pure air
θ (theta)	volume fraction liquid
ϕ (phi)	porosity (volume fraction not solid)
ψ(psi)	volume fraction of compartment
ρ (rho)	density
φ (alternate phi)	fraction sorbed to solids
γ(gamma)	gradient of soil concentration change
δ (delta)	boundary layer thickness
Θ (Theta)	temperature correction factor
λ (lamda)	dimensionless viscous sublayer thickness
λ_i	removal rate constant for soil compartment I
μ (mu)	viscosity
ν (nu)	velocity
υ (upsilon)	volumetric flow rate
ω (omega)	volume fraction occupied by a fluid (where fluid = air or water)

Roman

A	area
AE	assimilation efficiency
BW	body weight
C	concentration
d	depth
D	diffusion coefficient
DSP	dispersion coefficient (between surface water compartments)
E	elimination (wildlife)
f	fraction
FIR	free-living inhalation rate (not normalized to body weight)
g	conductance
H	Henry's law constant
I	interception fraction

IN	ingestion, inhalation, or intake (normalized to body weight)
IR	inhalation rate (not normalized to body weight)
k	rate constant
k	transfer coefficient (Chapter 3)
K	partition coefficient
L	characteristic mixing length
m	mass of an organism
M	mass of chemical
M_W	molecular weight
n	number
na_S	number of stomata in leaf multiplied by the area of a single stomata divided by the area of the leaf
N	chemical inventory (mass)
p	proportion
P	permeance
P	pressure (P_{vapor})
Q	flux
R	universal gas constant
$R_{[sub]}$	resistance [subscript]
rh	relative humidity
f_{ML}	fraction mass disolved/volume fraction liquid
f_{MS}	fraction mass solid particle-phase/volume fraction solid particles
f_{MV}	fraction mass vapor-phase/volume fraction gas
S	rate of sediment deposition (or resuspension)
T	transfer factor or
T	temperature
U	mass transfer coefficient
V	volume
v	velocity
ve	effective velocity
WI	water ingestion (not normalized to body weight)
Z	fugacity capacity

ABBREVIATIONS USED IN VARIABLE SUBSCRIPTS

acc	accumulation
adv	advection
Al	Algae
Arth	Arthropod
ASF	Allometric Scaling Factor
avail	available
B	Boundary layer
BI	Benthic Invertebrates
C	Conductance
d	drag
D	Diet
dep	depuration (fish)
dep	deposition (abiotic media)
dif	diffusion
e	effective
ef	excretion via urine/feces
eg	excretion from gills
ET	total elimination
f	unspecified fish
ff	fur, feathers (or hair)
Fbo	Fish, benthic omnivore
Fh	Fish, herbivore
Fwch	Fish, water column herbivore
Fwco	Fish, water column omnivore
G	Growth (fish algorithms)
G	Gas (air algorithms)
L	load (e.g., D_L = Dust load)
L	liquid (e.g., R_L = liquid phase resistance)
lact	lactation
m	melting; or
m	mesophyl
met	metabolism
Mp	Macrophyte
N	normalized
oc	organic carbon
ow	octanol water
P	Particle
Ph	Phloem
r	ratio
rV	ratio for Vapor
R	Root
Rcv	Receiving
res	resuspension/resuspend
S	Soil (*e.g.*, A_S = soil area); or
S	Stomatal (*e.g.*, g_S = total stomatal conductance)
Sed	Sediment
SSed	Suspended sediments
Send	Sending
Snk	Sink
Sr	root-zone Soil
Ss	surface Soil
Sv	vadose-zone Soil
St	Stem
SWD	dissolved in surface water
t	time
T	Temperature
Tprey	Terrestrial prey
Twl	Terrestrial wildlife
uf	urine/feces
U	Uptake
fuSs	eliminated to surface soil
fuSW	eliminated to surface water
W	Water
WD	dissolved in water
v	volatilization
VAF	vegetation attenuation factor
Worm	Earthworm
WV	Wet Vapor
Xy	Xylem

TABLE OF CONTENTS

APPENDICES

[This page intentionally left blank.]

1. INTRODUCTION

This volume of the TRIM.FaTE Technical Support Document (TSD) presents the equations available in the current TRIM.FaTE library that can be used to describe the transport and transformation of chemicals in TRIM.FaTE simulations. These equations are used to simulate the physical, chemical, and biological processes that drive chemical transport and transformation in the environment. As explained in Volume I of this report, the TRIM.FaTE modeling framework can incorporate first-order and higher order equations. At the present time, however, only first-order equations have been included in the TRIM.FaTE library and applied using the model.

First-order transfer between compartments in TRIM.FaTE is described mathematically by ***transfer factors***, referred to as T-factors or TFs. This volume documents all of the TF algorithms currently included in the TRIM.FaTE library. A T-factor is the instantaneous flux of the chemical into the receiving compartment normalized by the amount of chemical in the sending compartment (see Section 4.2 in TRIM.FaTE TSD Volume I (U.S. EPA 2002a) for more discussion about T-factors and related issues). That is, $T \times N(t)$ is the instantaneous flux at time t in units of chemical amount/time, where $N(t)$ is the chemical amount in the sending compartment at time t. Thus, the unit for a T-factor is inverse time (in TRIM.FaTE, per day).

Because it is a normalized flux, a large T-factor in itself does not imply that the flux is large; the actual flux also depends on the amount of chemical in the sending compartment. The T-factor is not the same as the fraction of mass transported from the sending to receiving compartment (or transformed or degraded from one chemical form to another) in a given time interval, although the two quantities are related. When the fraction of mass lost is small, these two quantities are approximately the same, but they differ significantly when the fraction of mass lost is larger. In particular, $T = -\ln(1-p)$, where p is the proportion (fraction) of mass lost in one simulation time step, and the units of time are the same as those for T.

The remainder of this volume is organized in seven chapters. Chapter 2 describes the general methods and assumptions used to model fate and transport in TRIM.FaTE, focusing on advection algorithms and the equations to estimate the fraction of the total chemical in a compartment that occurs in each phase *(i.e.*, solid, liquid, vapor) within the compartment. Chapters 3 through 5 present the abiotic transfer factor algorithms for air (Chapter 3), surface water and sediment (Chapter 4), and soil and ground water (Chapter 5). For simplicity, the T-factor algorithms used to describe intermedia transport are presented in only one of the relevant chapters and referenced in the other. Chapters 6 and 7 present the algorithms for transfers between biotic compartment types and between biotic and abiotic compartment types. Chapter 6 describes the algorithms associated with aquatic biota, while Chapter 7 describes those associated with terrestrial biota. Chapters 3 through 7 begin with (or begin each major subsection with) a brief summary of the T-factor algorithms described in the chapter and then explain each algorithm in greater detail. Each chapter also describes supporting equations that are located in the compartment sections of the TRIM.FaTE code library instead of in the T-factor algorithm sections. Chapter 8 provides the references cited in this volume.

This volume includes four appendices. Appendix A presents chemical-specific algorithms for mercury, and Appendix B presents chemical-specific algorithms for polycyclic aromatic hydrocarbons (PAHs). Appendix C describes key aspects of running TRIM.FaTE using the steady-state solution feature. Appendix D lists and describes the input parameters in the current library.

The derivation of T-factors begins in different ways in some chapters, reflecting differences in typical presentations of transfer or partitioning models in the literature among the related disciplines. An effort has been made, however, to use a standard set of variable names throughout this volume (see Acronyms, Abbreviations, and Symbols on pages ix to xii.)

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

---

[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

---

[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:

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

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:

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

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

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

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:

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

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.

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

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:

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

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

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

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:

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

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

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

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:

$$K_d = K_{oc} \times f_{oc} \quad \text{(Eq. 2-44)}$$

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:

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

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

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

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

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

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

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

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

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:

$$Z_{solid} = Z_{air} \times \frac{C_{solid}}{C_{gas}} \qquad \text{(Eq. 2-51a)}$$

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

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:

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

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:

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

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:

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

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

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:

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

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:

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

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:

$$\begin{aligned} T_{i \to j}^{adv}(phase) &= \frac{Q(phase) \times Z_i(phase)}{V_i(Total) \times Z_i(Total)} \\ &= \frac{\upsilon_{ij}(phase) \times A_{ij} \times Z_i(phase)}{V_i(Total) \times Z_i(Total)} \end{aligned} \qquad \text{(Eq. 2-63)}$$

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:

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

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:

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

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:

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

Solving for k_1 yields:

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

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:

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

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

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

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:

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

an equation for Z_{air} can be derived:

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

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:

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

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

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

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	$= 1 - \left(\dfrac{1}{1 + \left(K_P \times D_L \times 1\mathrm{E}^9 \; (\mu\mathrm{g/kg}) \right)} \right)$	$= \dfrac{V_{SW} \times (1 - \theta) \times Kd \times \rho_{Sed} \times 0.001 \; (\mathrm{m}^3/\mathrm{L})}{GenDenom_{SW}}$
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	$= \dfrac{V_{SW} \times fV_{Algae} \times RatioConc_{Algae} \left(\mathrm{g/m}^3 \right) \times 0.001 \; (\mathrm{m}^3/\mathrm{L})}{GenDenom_{SW}}$
GenericDenominatorfor PhaseCalculations, or *GenDenom*	NA, not used	$= V_{SW} \times (fV_{Algae} \times RatioConc_{Algae} \times AC(\mathrm{g/m}^3) \times 0.001 \; (\mathrm{m}^3/\mathrm{L})$ $+ (1 - \theta) \times Kd \times \rho_{Sed} \times 0.001 \; (\mathrm{m}^3/\mathrm{L}) + \theta)$

[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	$= \dfrac{V_{Sed} \times (1 - \phi) \times Kd \times \rho_{Sed} \times 0.001\,(\mathrm{m^3/L})}{GenDenom_{Sed}}$	$= \dfrac{V_S \times \left(Kd \times \rho_S\right) \times (1 - \theta - \varepsilon)}{GenDenom_S}$
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*	$= V_{Sed} \times (1 - \phi) \times Kd \times \rho_{Sed} \times 0.001\,(\mathrm{m^3/L}) + V_{Sed} \times \theta$	$= V_S \times ((Kd \times \rho_S) \times (1 - \theta - \varepsilon) + (\theta \times 1000) + (\varepsilon \times \dfrac{Z_{pure\_air}}{Z_{pure\_water}} \times 1000))$

---

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

3. AIR ALGORITHMS

In this chapter, the algorithms for the horizontal transport of chemical species between air compartments and those for diffusion/volatilization between air compartments and surface water are presented. A description of deposition from air compartments to surface water can be found in Chapter 4, and a description of the transport processes between air compartments and soil can be found in Chapter 5. The text box on the next page provides a summary of the T-factor algorithms developed in this chapter and definitions of the parameters used in those algorithms.

3.1 AIR-TO-AIR ALGORITHMS

For a given wind speed and direction, there are two types of transfer processes that account for the majority of chemical mass that moves from one air compartment to another:

- Advective transfer (bulk) due to the component of the wind vector normal to the boundary between the compartments; and
- Dispersive transfer (bulk) calculated from the component of the wind vector parallel to the boundary between the compartments.

The total transfer factor from one air compartment to an adjacent air compartment is the sum of these two transfers.

The current TRIM.FaTE library incorporates only the advective transfer due to the wind vector normal to the boundary between compartments. This is because of the complexity and technical challenges related to the representation of dispersive transfers in a compartment-based modeling system such as TRIM.FaTE. Note that diffusion between air compartments is considered negligible and thus is not included in TRIM.FaTE.

Let *Air_Rcv* and *Air_Send* denote the adjacent receiving and sending air compartments. If the boundary between the two air compartments is composed of *n* distinct line segments, then the transfer factor from the sending to the receiving air compartment is calculated as:

$$T^{adv}_{Air\_Send \rightarrow Air\_Rcv} = \frac{1}{V_{Send}} \times \sum_{t=1}^{n} A_i \times (u_i^{(D)} + u_i^{(L)}) \qquad \text{(Eq. 3-1)}$$

where:

V_{Send} = volume of the sending air compartment (m^3);
A_i = interfacial area across i^{th} boundary (m^2);
$u_i^{(D)}$ = direct (D) advective wind velocity across the i^{th} boundary (m/day); and
$u_i^{(L)}$ = lateral (L)/dispersive wind velocity across the i^{th} boundary (m/day).

The direct wind flow across an air compartment boundary (notation $u_i^{(D)}$ is used above) is calculated by finding the projection of the wind vector onto the normal vector to the boundary between the air compartments.

Summary of Transfer Factors for Air in TRIM.FaTE

AIR ADVECTION

Air compartment to air compartment: (TF 3-1)

$$T^{adv}_{Air\_Send \to Air\_Rcv} = \frac{1}{V_{Air\_Send}} \times \sum_{i=1}^{n} A_i \times \left(u_i^{(D)}\right)$$

AIR DIFFUSION/VOLATILIZATION

Diffusion from air compartment to surface water compartment: (TF 3-2)

$$T^{dif}_{Air \to SW} = \frac{A_{SWA}}{V_{Air}} \times \frac{k_v}{H/(R \times T)} \times f_{MV}$$

Volatilization from surface water compartment to air compartment: (TF 3-3)

$$T^{vol}_{SW \to Air} = \frac{A_{SWA}}{V_{SW}} \times k_v \times f_{ML}$$

LIST OF SYMBOLS USED IN AIR TRANSFER FACTOR ALGORITHMS

V_{Air_Send} = volume of the sending air compartment (m^3).
A_i = interfacial area across *i*th boundary (m^2).
$u_i^{(D)}$ = direct advective wind velocity across the *i*th boundary (m/day).
A_{SWA} = interfacial area between the surface water and air compartments (m^2).
V_{Air} = volume of air compartment (m^3).
k_v = volatilization transfer rate (m/day).
H = Henry's law coefficient for the air-water partitioning of the chemical (atm-m^3/mole).
R = universal gas constant (8.206×10^{-5} atm-m^3/mole °K).
T = water temperature (°K).
f_{MV} = fraction of chemical mass in the air compartment that is in the vapor phase divided by the volume fraction of the compartment that is air (*i.e.*, excluding particles) (unitless).
V_{SW} = volume of the surface water compartment (m^3).
f_{ML} = fraction of chemical mass in the surface water compartment that is dissolved in water divided by volume fraction of the surface water compartment that is water (*i.e.*, excluding suspended sediments and algae) (unitless).

Let $P_1 = (x_1, y_1)$ and $P_2 = (x_2, y_2)$ be the points defining the line that is the projection of the boundary onto the *xy*-plane (*i.e.*, the view from above the vertical plane defining the boundary). It is assumed that the points P_1 and P_2 are ordered so that the receiving compartment is on the right side of the directed line segment starting at P_1 and ending at P_2. The unit vector $\vec{v}$ perpendicular to this line segment that is in the direction of the receiving compartment is given by:

$$\vec{v} = \frac{1}{\sqrt{(y_2 - y_1)^2 + (x_2 - x_1)^2}} \times \left\langle y_2 - y_1, \; -(x_2 - x_1) \right\rangle = \left\langle \sin\varphi, \cos\varphi \right\rangle \qquad \text{(Eq. 3-2)}$$

where:

φ = the angle measured clockwise from due north.

If the wind is blowing with speed u toward the direction ϑ (measured clockwise from due north), then the wind vector, denoted by $\vec{w}$, can be written:

$$\begin{aligned} \vec{w} &= \left\langle u \times \cos(\pi/2 - \vartheta), u \times \sin(\pi/2 - \vartheta) \right\rangle \\ &= u\left\langle \sin\vartheta, \cos\vartheta \right\rangle \end{aligned} \qquad \text{(Eq. 3-3)}$$

The projection of the wind vector $\vec{w}$ onto $\vec{v}$ is just the dot product ($\vec{w} \cdot \vec{v}$) of the two vectors, which is given by:

$$\begin{aligned} \vec{w} \cdot \vec{v} &= \frac{u}{\sqrt{(y_2 - y_1)^2 + (x_2 - x_1)^2}} \times \left[(y_2 - y_1)\sin\vartheta - (x_2 - x_1)\cos\vartheta \right] \\ &= u\left[\sin\vartheta \sin\varphi + \cos\vartheta \cos\varphi \right] \\ &= u\cos(\vartheta - \varphi) \end{aligned} \qquad \text{(Eq. 3-4)}$$

Since $\vec{v}$ is a unit vector, the dot product in this case is the component of the vector $\vec{w}$ in the direction of $\vec{v}$. The wind flow rate from the sending compartment to the receiving compartment is defined to be the dot product if it is positive; otherwise, it is zero. In other words:

$$\textit{Wind speed perpendicular to compartment boundary} = u_{\perp} = \max\left\{ 0, u\cos(\vartheta - \varphi) \right\} \qquad \text{(Eq. 3-5)}$$

If the wind is blowing perpendicular to the boundary (*i.e.,* $\varphi = \vartheta$), then the wind flow rate across the boundary is just the wind speed; otherwise, it is flowing across the boundary with a velocity less than the wind speed, the magnitude of which depends on the angular difference between the wind vector and the unit vector normal to the boundary.

Although Equation 3-1 includes lateral/dispersive wind velocity, the equation implemented in TRIM.FaTE for the horizontal air-to-air compartment transfer factor includes only the direct advective wind velocity:

$$T^{adv}_{Air\_Send \rightarrow Air\_Rcv} = \frac{1}{V_{Air\_Send}} \times \sum_{i=1}^{n} A_i \times \left(u_i^{(D)} \right) \qquad \text{(TF 3-1)}$$

where:

$T^{adv}_{Air\_Send \rightarrow Air\_Rcv}$ = advective transfer factor for wind in air from sending (*Send*) to receiving (*Rcv*) air compartments (/day);
V_{Send} = volume of sending air compartment (m^3);
A_i = interfacial area across the i^{th} boundary (m^2); and
$u_i^{(D)}$ = direct (*D*) advective wind velocity across the i^{th} boundary (m/day).

The advective transport can occur both horizontally, based on the horizontal component of the wind speed, and vertically, based on the vertical component of the wind speed and the stability class assigned to the air layers. The advective transport Equations 3-1 through 3-5 are hard coded in the main TRIM.FaTE program. The transfer factor in the TRIM.FaTE library passes the information on wind speed and direction to the main TRIM.FaTE program to solve the equations. In initial applications of TRIM.FaTE involving only one layer of air compartments, any chemical transported vertically out of the compartments goes to an air sink.[1] If there is to be no vertical loss of chemical due to vertical advection to the air sink, the user can set the vertical wind speed to zero.

Advective transport in air also can carry the chemical horizontally beyond the boundary of the modeling domain to an air sink for the chemical mass. The transfer factor would be the same as TF 3-1, except that the receiving compartment would be the air sink.

3.2 AIR-TO-SOIL ALGORITHMS

The algorithms describing the transfer of chemical mass between air and soil are presented in Section 5.3.3.

3.3 AIR-TO-SURFACE-WATER ALGORITHMS

Several processes can move chemical mass between the air and surface water compartments, including deposition (Section 3.3.1) and diffusion and volatilization (Section 3.3.2).

3.3.1 DEPOSITION

The algorithms describing the deposition of chemical mass from air to surface water are presented in Section 4.2.1.

3.3.2 DIFFUSION AND VOLATILIZATION

Transfer of chemical between an air compartment and a surface water compartment can occur by advection (*i.e.*, wet and dry deposition of particle-bound chemical and wet deposition of vapor-phase chemical). The advective transfers between air and surface water are described in the surface water chapter (Chapter 4). The diffusion (and volatilization) transfer factors are

---

[1] The single air layer can vary in height (*i.e.*, mixing height) depending on environmental conditions.

described in Section 3.3.2.1. Section 3.3.2.2 includes several methods available to calculate the gas-phase transfer coefficient and the liquid-phase transfer coefficient.

3.3.2.1 Diffusion and Volatilization Transfer Between Air and Surface Water

The following describes the method used for estimating volatilization transfer between air and surface water for any chemical that has a non-zero Henry's law constant. The method is a two-layer resistance model first presented by Whitman (1923) and incorporated into the EPA Water Quality Analysis Simulation Program (WASP) (Ambrose et al. 1995). The following discussion is based primarily on the WASP model documentation.

Volatilization is the movement of a chemical across the air/water interface as the concentration of the dissolved chemical tends toward equilibrium with its vapor-phase concentration. Equilibrium occurs when the partial pressure exerted by the chemical in solution equals the partial pressure of the chemical in the overlying atmosphere. The rate of exchange is proportional to the gradient between the dissolved concentration and the concentration in air.

With the approach described in Whitman (1923), the dissolved concentration in the surface water is assumed to attempt to equilibrate with the gas-phase concentration in the atmosphere via the general equation:

$$\left(\frac{dC_{dissolved}}{dt}\right) = \frac{k_v}{d_W} \times \left(C_{dissolved} - \frac{C_{Air}}{\left(H/\left(R \times T\right)\right)}\right) \qquad \text{(Eq. 3-6)}$$

where:

$C_{dissolved}$ = concentration of dissolved chemical (g[chemical]/m^3[water]);
k_v = volatilization transfer rate (m/day);
d_W = water depth (m), assumed to be generally the same throughout the water body;
C_{Air} = vapor-phase concentration of chemical in air (g[chemical]/m^3[air]);
H = Henry's law constant for the air-water partitioning of the chemical (Pa-m^3/mole);
R = universal gas constant (8.314 m^3-Pa/mol-^{o}K); and
T = water temperature (^{o}K).

The volatilization transfer rate can range from near 0 to 25 m/day, depending on conditions (Ambrose et al. 1995). Multiplying the above equation by the volume of the surface water compartment, denoted here by V_{SW}, yields:

$$\begin{gathered} Net\ Flux\ air\ to\ water\ (g[chemical]/day) = \\ V_{SW} \times \frac{k_v}{d_W} \times \left(C_{dissolved} - C_{Air}\,\frac{1}{(H/(R \times T))}\right) \end{gathered} \qquad \text{(Eq. 3-7)}$$

The term V_{SW}/d_W will be equal to the surface area of the water compartment, if the depth of the water compartment is approximately constant. This area is also the interfacial area between the air and water compartments, so that:

$$\textit{Net Flux air to water} = A_{SWA} \times k_v \times \left(\begin{array}{l} \dfrac{Fraction\_Mass\_Dissolved}{Volume\_Fraction\_Liquid} \times \dfrac{N_{SW}}{V_{SW}} \\ - \dfrac{Fraction\_Mass\_Vapor}{Volume\_Fraction\_Vapor} \times \dfrac{N_{Air}}{V_{Air}} \times \dfrac{1}{(H/(R \times T))} \end{array} \right) \tag{Eq. 3-8}$$

or, using the notation of transfer factors and Equations 2-81 and 2-80:

$$T^{dif}_{Air \rightarrow SW} = \frac{A_{SWA}}{V_{Air}} \times \frac{k_v}{\left(H/(R \times T)\right)} \times f_{MV} \tag{TF 3-2}$$

$$T^{vol}_{SW \rightarrow Air} = \frac{A_{SWA}}{V_{SW}} \times k_v \times f_{ML} \tag{TF 3-3}$$

where:

$T^{dif}_{Air \rightarrow SW}$ = transfer of chemical from air to surface water via diffusion (/day);
A_{SWA} = interfacial area between the surface water and air compartments (m^2);
V_{Air} = volume of air compartment (m^3);
k_v = volatilization transfer rate (m/day) [see below for details];
H = Henry's law coefficient for the air/water partitioning of the chemical (Pa-m^3/mole).
R = universal gas constant (8.314 m^3-Pa/mole-^{o}K);
T = water temperature (^{o}K);
f_{MV} = fraction of chemical mass in the air compartment that is in the vapor phase divided by the volume fraction of the compartment that is gas (*i.e.*, excluding particles);
$T^{vol}_{SW \rightarrow Air}$ = transfer of chemical from surface water to air via volatilization (/day);
V_{SW} = volume of surface water compartment (m^3); and
f_{ML} = fraction of the chemical mass in the water compartment that is dissolved in water divided by the volume fraction of the compartment that is water (*i.e.*, excluding suspended sediments or algae) (unitless).

The two-layer resistance method assumes that two "stagnant films" are bounded on either side by well mixed compartments. Concentration differences serve as the driving force for volatilization from the water. Pressure differences drive the diffusion from the air layer. From mass balance considerations, it is obvious that the same mass must pass through both films; thus, the two resistances combine in series, so that the conductivity is the reciprocal of the total resistance. Thus, the volatilization transfer rate is estimated in the current TRIM.FaTE library as:

$$k_v = \left(R_L + R_G\right)^{-1} = \left[k_L^{-1} + \left(k_G \times \frac{H}{R \times T}\right)^{-1}\right]^{-1} \qquad \text{(Eq. 3-9)}$$

where:

R_L = liquid-phase resistance (day/m);
k_L = liquid-phase transfer coefficient (m/day);
R_G = gas-phase resistance (day/m); and
k_G = gas-phase transfer coefficient (m/day).

There is actually yet another resistance involved, the transport resistance between the two interfaces, but it is assumed to be negligible (although this may not be true in very turbulent conditions or in the presence of surface-active contaminants).

The value of k_v, the volatilization transfer rate, or conductivity, depends on the intensity of turbulence in a water body and in the overlying atmosphere. Mackay and Leinonen (1975) have discussed conditions under which the value of k_v is primarily determined by the intensity of turbulence in the water. As Henry's law coefficient increases, the conductivity tends to be increasingly influenced by the intensity of turbulence in water. As Henry's law coefficient decreases, the value of the conductivity tends to be increasingly influenced by the intensity of atmospheric turbulence.

Henry's law coefficient generally increases with increasing vapor pressure of a chemical and generally decreases with increasing solubility of a chemical. Thus, highly volatile low-solubility chemicals are more likely to exhibit mass-transfer limitations in water, and relatively nonvolatile high-solubility chemicals are more likely to exhibit-mass transfer limitations in the air. Volatilization is usually of relatively lower magnitude in lakes and reservoirs than in rivers and streams.

In cases where it is likely that the volatilization rate is regulated by the turbulence level in the water phase, estimates of volatilization can be obtained from results of laboratory experiments. As discussed by Mill et al. (1982), small flasks containing a solution of a pesticide dissolved in water that have been stripped of oxygen can be shaken for specified periods of time. The amount of pollutant lost and oxygen gained through volatilization can be measured and the ratio of conductivities (K_{VOG}) for pollutants and oxygen can be calculated. As shown by Tsivoglou and Wallace (1972), this ratio should be constant irrespective of the turbulence in a water body. Thus, if the reaeration coefficient for a receiving water body is known or can be estimated and the ratio of the conductivity for the pollutant to reaeration coefficient has been measured, the pollutant conductivity can be estimated.

The volatilization rate constant is for a temperature of 20°C. It is adjusted for segment temperature using the equation:

$$k_{v,T} = k_{v,20} \times \Theta_v^{T-20} \qquad \text{(Eq. 3-10)}$$

where:

$k_{v,20}$ = calculated volatilization transfer rate (m/day) at 20°C;
Θ_v^{T-20} = temperature correction factor for volatilization (unitless); and
T = water temperature (°C).

3.3.2.2 Calculation of Volatilization Transfer Rates for the Whitman Two-layer Resistance Model

There are a variety of methods for estimating the transfer rates k_G and k_L for stagnant and flowing water bodies, many of which are available in the current TRIM.FaTE library. These methods are summarized in Tables 3-1 and 3-2 at the end of this chapter.

3.4 AIR-TO-PLANT ALGORITHMS

The algorithms describing the transfer of chemical mass between air and plants are presented in Sections 7.2.1 (advection processes) and 7.2.2 (diffusion processes).

3.5 TRANSFORMATIONS AND DEGRADATION

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 air due to all mechanisms that might apply (*e.g.,* oxidation, photolysis) is reflected by the user input for the half-life of the chemical in air. The algorithm relating the degradation rate constant to the chemical half-life in the air compartment is presented in Chapter 2 (Equation 2-64), and the corresponding transfer factor is TF 2-1. The degradation transfer factor moves the chemical mass to a degradation sink.

TRIM.FaTE has the capability to track the newly formed compounds, when they are of particular interest to the user. Transformations of a chemical into another form(s) that is tracked in TRIM.FaTE are named for the processes (*e.g.*, oxidation, methylation, reduction of mercury species). In the TRIM.FaTE air 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.

3.6 AIR BOUNDARY CONTRIBUTIONS

The TRIM.FaTE library includes algorithms to allow transport of chemical into the modeling region from the ambient air located outside the modeling area. For many of the chemicals that will be modeled using TRIM.FaTE, so-called "background" concentrations in the absence of the modeled source(s) are not zero. Trace or higher concentrations of a chemical of interest might be found in ambient air due to natural causes or due to releases from other facilities outside the modeling region.

To model chemical inputs to the modeling region via advection of ambient levels of chemical in air from beyond the boundary of the modeling region in TRIM.FaTE, the user can set a boundary concentration for any outside interface of an air compartment located just inside the boundary of the modeled region. In the TRIM.FaTE definition of properties for each of the outside air volume elements, there is a property called the BoundaryConcentration_g_per_m3 for which the user may specify an ambient air concentration of the chemical in the absence of the source(s) being modeled.

Chemical mass enters the air compartments located just inside the boundary of the modeling region via an air advection algorithm that incorporates wind speed, wind direction, and the boundary concentration of the chemical (see above). The use of wind speed and wind direction in this algorithm is identical to the approach that is used for the air-to-air advection algorithm.

Note that TRIM.FaTE does not model changes in chemical concentrations in the air external to the modeling region that might occur as a consequence of emissions from the modeled source. Losses of chemical via air advection from the modeling region to areas external to that region are modeled as transfers of the chemical to an air sink.

Table 3-1
Methods for Determining Gas-Phase Transfer Coefficient $k_G{}^a$ for the Whitman Two-Layer Resistance Volatilization Model Between Air and Surface Water

Water Body Type	Method	k_G, Gas phase transfer coefficient (m/day)	Reference
Stagnant Pond or Lake	1*	$k_G = u^* \times \left(\frac{\kappa^{0.33}}{\lambda_2} \right) \times Sc_{air}{}^{-0.67}$ where: u^* = the shear velocity (m/day) computed from $u^* = C_d{}^{0.5} \; W_{10} \times 86{,}400$ where: C_d = drag coefficient (= 0.0011), W_{10} = wind velocity 10 m above water surface (m/sec), and 86,400 = unit conversion factor (sec/day); κ = von Karmen's constant (= 0.74) (unitless); λ_2 = dimensionless viscous sublayer thickness = (4) (unitless); and Sc_{air} = air Schmidt Number, computed from $\mathrm{Sc_{air}} = \frac{\mu_{\mathrm{air}}}{10000 \times \mathrm{D_{air}}}$, where: μ_{air} = viscosity of air, internally calculated from air temperature (cm^2/sec), $= \frac{\left(1.32 \; + \; 0.009 \; \mathrm{T_{airC}}\right)}{10}$, where: T_{airC} = air temperature (°C), and D_{air} = diffusivity of chemical in air (m^2/sec) $= \frac{1.9 \times 10^{-4}}{M_W{}^{2/3}}$ where: M_W = molecular weight of compound (g/mole).	O'Connor (1983), Ambrose et al. (1995)
Stagnant Pond or Lake	2	See Method (1) for definition of terms. $k_G = 10^{-3} + 0.0462 \times \; u^* \times \; Sc_{air}{}^{-0.67}$	Mackay and Yeun (1983), Ambrose et al. (1995)
Flowing Water or Estuary	1*	Same as Method (1) for stagnant water body.	
Flowing Water or Estuary	2	Same as Method (2) for stagnant water body.	
Flowing Water or Estuary	3*	Input value of 100 m/day.	Ambrose et al. (1995)

[a] Used in the calculation of the volatilization transfer rate k_v: $k_v = \left(R_L + R_G\right)^{-1} = \left[k_L^{-1} + \left(k_G \times \frac{H}{R \times T_K} \right)^{-1} \right]^{-1}$. *Available in current TRIM.FaTE Library.

Table 3-2
Methods for Determining Liquid-Phase Transfer Coefficient k_L ^{a} for the Whitman Two-Layer Resistance Volatilization Model Between Air and Surface Water

Water Body Type	Method	k_L, Liquid phase transfer coefficient (m/day)	Reference
Stagnant Pond or Lake	1*	$k_L = k_a \times K_{vo}$ where: k_a (user input) = reaeration velocity (m/day); and K_{vo} (user input) = ratio of volatilization rate to reaeration rate (unitless).	Ambrose et al. (1995)
Stagnant Pond or Lake	2*	$k_L = k_a \times (32/M_W)^{0.5}$ where: M_W = molecular weight	Ambrose et al. (1995)
Stagnant Pond or Lake	3*	$k_L = u^* \times \left(\frac{\rho_a}{\rho_w}\right)^{0.5} \times \left(\frac{\kappa^{0.33}}{\lambda_2}\right) \times Sc_w^{-0.67}$ where: u^* = the shear velocity (m/day) computed from $u^* = C_d^{0.5} \times W_{10} \times 86{,}400$ where: C_d = drag coefficient (= 0.0011), W_{10} = wind velocity 10 m above water surface (m/sec), and 86,400 = unit conversion factor (sec/day); ρ_a = density of air, internally calculated from air temperature (kg/m^3); ρ_w = density of water, internally calculated from water temperature (kg/m^3); κ = von Karmen's constant (= 0.74) (unitless); and λ_2 = dimensionless viscous sublayer thickness (= 4) (unitless). Sc_w = water Schmidt Number, computed from $Sc_w = \frac{\mu_w}{\rho_w \times D_w}$ where: μ_w = viscosity of water, internally calculated from water temperature (kg/m-sec) = 10^(-3.30233 + 1301/(998.333+8.1855(T_w-20) + 0.00585 (T_w-20)^2), where: T_W = water temperature (°C) D_w = diffusivity of chemical in water (m^2/sec) $= \frac{22 \times 10^{-9}}{M_W^{2/3}}$ where: M_W = molecular weight of compound (g/mole).	O'Connor (1983), Ambrose et al. (1995)

Table 3-2 (continued)
Methods for Determining Liquid Phase Transfer Coefficient k_L for the Whitman Two-Resistance Volatilization Model Between Air and Surface Water

Water Body Type	Method	k_L, Liquid phase transfer coefficient (m/day)	Reference
Stagnant Pond or Lake	4*	$k_L = 10^{-6} + 0.00341 \times u^* \times Sc_w^{-0.5}$ if $u^* > 0.3$ m/s $k_L = 10^{-6} + 0.0144 \times u^{*0.22} \times Sc_w^{-0.5}$ if $u^* < 0.3$ m/s See Method (3) for definition of terms.	Mackay and Yeun (1983), Ambrose et al. (1995)
Flowing Water or Estuary	1*	Same as Method (1) for stagnant water body.	
Flowing Water or Estuary	2	Same as Method (2) for stagnant water body.	
Flowing Water or Estuary	3*	Same as Method (3) for stagnant water body.	
Flowing Water (*e.g.*, stream, river) or Estuary	4*	$k_L = k_a \times K_{vo}$, where: $k_a = 5.349 \times \frac{u^{0.67}}{d_W^{\ 0.85}}$ if $d_W < 0.61$ m $k_a = 8.64 \times 10^4 \times \sqrt{\frac{D_w \times u}{d_W}}$ if $d_W \geq 0.61$ m and ($u < 0.518$ m/s or $d_W > 13.584 \times u^{0.29135}$) $k_a = 5.049 \times \frac{u^{0.969}}{d_W^{\ 0.673}}$ else K_{vo} = input or $= \sqrt{\frac{32}{M_W}}$ where: u = velocity of water (m/sec); d_W = water compartment depth (m); D_w = diffusivity of chemical in water (m^2/sec) (= 22E-9 / $M_W^{2/3}$); K_{vo} = input = ratio of volatilization rate to reaeration rate (unitless); and k_a = input = reaeration velocity (m/day).	Covar (1976), Ambrose et al. (1995)

[a] Used in the calculation of the volatilization transfer rate k_v: $k_v = \left(R_L + R_G\right)^{-1} = \left[k_L^{-1} + \left(k_G \times \frac{H}{R \times T_K}\right)^{-1}\right]^{-1}$.

* = Available in current TRIM.FaTE Library.

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.

---

[1] Because 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

$$T_{Air \to SW}^{dry\_dep} = \frac{A_{SWA} \times \upsilon_{dry}}{V_{Air}} \times f_{MS}$$

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

$$T_{Air \to SW}^{wet\_dep} = \frac{A_{SWA} \times \upsilon_{wet}}{V_{Air}} \times f_{MS}$$

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

$$T_{Air \to SW}^{WVdep}(rain) = \frac{A_{SWA}}{V_{Air}} \times rain \times \frac{Z_{pure\_water}}{Z_{Total\_air}}$$

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

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

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

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

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

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

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

$$T_{Al \to Sed}^{dep} = \frac{A_{SedSW}}{V_{SW}} \times \upsilon_{Sed}^{Al} \times f_{MAl}$$

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

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

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[air]/m^3[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[interface]).
V_{Air} = volume of the air compartment (m^3[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).
rain = rainfall rate (m/day).
Z_{pure_water} = fugacity capacity of chemical in the aqueous phase (mol/m^3-Pa).
Z_{Total_Air} = total fugacity capacity of chemical in the air compartment (mol/m^3-Pa).
A_{SedSW} = area of surface water/sediment interface (m^2[interface]).
V_{SW} = volume of surface water compartment (m^3[water]).
υ_{sed}^{dep} = volumetric deposition rate of suspended sediment to sediment bed (m^3[suspended sediment particles]/m^2 (area)-day).
V_{Sed} = volume of sediment compartment (m^3).
υ_{Sed}^{res} = volumetric resuspension rate of benthic sediment to water column (m^3[benthic sediment particles]/m^2 [benthic sediment]-day).
υ_{Sed}^{Al} = volumetric algal deposition rate to benthic sediments (m^3[algae]/m^2[sediment/ water interface]-day).
f_{MAl} = fraction mass of chemical in algae divided by the volume fraction of the surface water compartment that consists of algal cells (unitless).
outflow = volumetric outflow of water from surface water compartment to advection sink (m^3/day).
flushes/yr = outflow measured as number of complete changes (flushes) of water per year.
burial_rate = sediment burial rate (m^3[sediment particles]/m^2[sediment]-day).
flow = 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_{SWSed} = mass transfer coefficient between surface water and sediment (m/day).
U_{SedSW} = mass transfer coefficient between sediment and surface water (m/day).
E_{ij} = dispersion coefficient for exchange between water compartments *i* and *j* (m^2/day).
A_{ij} = interfacial area between water compartments *i* and *j* (m^2).
L_{ij} = characteristic mixing length between water compartments *i* and *j* (m).
V_i = volume of water compartment *i* (m^3).
A_{Sedij} = interfacial area between sediment compartments *i* and *j* (m^2);
V_{Sedi} = volume of the sending sediment compartment *i* (m^3);
V_{Sedj} = volume of the sending sediment compartment *j* (m^3);
DSP_{Sed} = diffusive exchange coefficient between sediment compartments (m^2/day);
ϕ_{avg} = average porosity at the interface between sediment compartments *i* and *j* (unitless);
L_{Sedij} = characteristic mixing length between sediment compartments *i* and *j* (m);
f_{MLi} = fraction of the chemical mass in sediment compartment *i* that is dissolved in water divided by volume fraction sending sediment compartment *i* that is liquid (unitless).
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).

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:

$$\frac{dN_{SW}}{dt} = \frac{N_{Air}}{V_{Air}} \times v_{dry} \times \frac{D_L}{\rho_P} \times \frac{Z_{pure\_solid}}{Z_{Total\_Air}} \times A_{SWA} \qquad \text{(Eq. 4-1)}$$

where:

N_{SW} = mass of chemical in the surface water compartment (g[chemical]);
N_{Air} = mass of chemical in the air compartment (g[chemical]);

---

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

V_{Air} = volume of air compartment (m^3);
v_{dry} = dry deposition velocity of particles (m/day);
D_L = atmospheric dust load in air compartment (kg[particles]/m^3[air]);
ρ_P = density of dust particles (kg[particles]/m^3[particles]);
Z_{pure_solid} = fugacity capacity of the chemical in or sorbed to solid particles (mol/m^3-Pa);
Z_{Total_Air} = total fugacity capacity of chemical in bulk air, including atmospheric dust particles (mol/m^3-Pa); and
A_{SWA} = area of the interface between surface water and air (m^2).

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

$$T_{Air \to SW}^{dry\_dep} = \frac{A_{SWA}}{V_{Air}} \times v_{dry} \times \frac{D_L \times Z_{pure\_solid}}{\rho_P \times Z_{Total\_Air}} \qquad \text{(TF 4-1a)}$$

where:

$T_{Air \to SW}^{dry\_dep}$ = 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/m^3-Pa); and
Z_{Total_Air} = total fugacity capacity of chemical in the air compartment (mol/m^3-Pa).

It is also true that:

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

where:

υ_{dry} = volumetric dry deposition rate (m^3[dust]/m^2[surface water/air interface]-day);

and:

$$\frac{Z_{pure\_solid}}{Z_{Total\_Air}} = \frac{Mass\_Fraction\_Sorbed}{Volume\_Fraction\_Solid} = f_{MS} \qquad \text{(Eq. 4-3)}$$

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:

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

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:

$$\frac{dN_{SW}}{dt} = \frac{N_{Air}}{V_{Air}} \times w_r \times rain \times \frac{D_L}{\rho_P} \times \frac{Z_{pure\_solid}}{Z_{Total\_Air}} \times A_{SWA} \qquad \text{(Eq. 4-4)}$$

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 (m^3);
w_r = scavenging or washout ratio for particles in air (ranges from 50,000 to 200,000) (m^3[air]/m^3[rain]);
$rain$ = rate of rainfall (m/day);
D_L = dust load, *i.e.*, density of dust particles in air (kg[particles]/m^3[air]);
ρ_P = density of dust particles (kg[particles]/m^3[particles]);
Z_{pure_solid} = fugacity capacity of the chemical in or sorbed to solid particles (mol/m^3-Pa);
Z_{Total_Air} = total fugacity capacity of chemical in bulk air, including atmospheric dust particles (mol/m^3-Pa); and
A_{SWA} = area of surface water/air interface (m^2).

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

$$T_{Air \rightarrow SW}^{wet\_dep} = \frac{A_{SWA}}{V_{Air}} \times w_r \times rain \times \frac{D_L \times Z_{pure\_solid}}{\rho_P \times Z_{Total\_Air}} \qquad \text{(TF 4-2a)}$$

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:

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

where:

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

and:

f_{MS} = $Z_{pure\_solid}/Z_{Total\_Air}$ as described for Equation 4-3 above (unitless); and
υ_{wet} = volumetric wet deposition rate (m^3[dust particles]/m^2[surface water/air interface]-day).

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.

$$\frac{dN_{SW}}{dt} = \frac{N_{Air}}{V_{Air}} \times rain \times \frac{Z_{pure\_water}}{Z_{Total\_Air}} \times A_{SWA} \Rightarrow \qquad \text{(Eq. 4-6)}$$

$$T_{Air \rightarrow SW}^{WVdep}(rain) = \frac{A_{SWA}}{V_{Air}} \times rain \times \frac{Z_{pure\_water}}{Z_{Total\_Air}} \qquad \text{(TF 4-3a)}$$

where:

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

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:

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

where:

w_{rV} = vapor washout ratio (g[chemical dissolved]/m^3[rain] per g[chemical vapor-phase]/m^3[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]/m^3[air] per g[chemical]/ m^3[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:

$$Z_{Total\_SW} = Z_{pure\_water} + Z_{pure\_solid} + Z_{Algae} \qquad \text{(Eq. 4-7)}$$

where:

Z_{Total_SW} = total fugacity capacity of chemical in surface water compartment (mol/m^3-Pa);
Z_{pure_water} = fugacity capacity of chemical in liquid phase, *i.e.*, water (mol/m^3-Pa);
Z_{pure_solid} = fugacity capacity of chemical in the solid phase (mol/m^3-Pa); and

Z_{Algae} = fugacity capacity of chemical in algae (mol/m^3-Pa).

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

$$\begin{aligned} Z_{Total\_SW} = & \left(Z_{pure\_water} \times Volume\_Fraction\_Liquid\right) + \\ & \left(Z_{pure\_solid} \times Volume\_Fraction\_Solid\right) + \\ & \left(Z_{Algae} \times Volume\_Fraction\_Algae\right) \end{aligned} \qquad \text{(Eq. 4-8)}$$

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

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

where:

C_{Algae} = chemical concentration in algae (g[chemical]/m^3[algae]);
C_{SW} = concentration of chemical dissolved in the liquid phase of surface water (g[chemical]/m^3[water]);
CA = concentration (density) of algae in surface water (g[algae wet wt]/ m^3[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:

$$\begin{aligned} Z_{Total\_Sed} = & \left(Z_{pure\_water} \times Volume\_Fraction\_Liquid\right) + \\ & \left(Z_{pure\_solid} \times Volume\_Fraction\_Solid\right) \end{aligned} \qquad \text{(Eq. 4-10)}$$

Z_{Total_Sed} = total fugacity capacity of chemical in the sediment compartment (mol/m^3-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):

$$T_{SW \to Sed}^{dep} = \frac{A_{SedSW}}{V_{SW}} \times \frac{S_{dep}}{\rho_{Sed}} \times \frac{Z_{pure\_solid}}{Z_{Total\_SW}} \qquad \text{(TF 4-4a)}$$

where:

$T_{SW \to Sed}^{dep}$ = advective transfer factor for deposition of suspended sediment in surface water to sediment bed (/day);
A_{SedSW} = area of surface water/sediment interface (m^2);
V_{SW} = volume of surface water compartment (m^3);
S_{dep} = deposition rate of suspended sediment to sediment bed (kg[suspended sediment]/m^2[surface water/sediment interface]-day)
ρ_{Sed} = density of solid sediment particles (kg[sediment particles]/m^3[sediment particles]);
Z_{pure_solid} = fugacity capacity of the solid phase (mol/m^3-Pa); and
Z_{Total_SW} = total fugacity capacity of the surface water compartment (mol/m^3-Pa).

In the TRIM.FaTE library:

υ_{Sed}^{dep} = volumetric sediment deposition rate (m^3[sediment]/m^2[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:

$$T_{SW \to Sed}^{dep} = \frac{A_{SedSW}}{V_{SW}} \times \upsilon_{Sed}^{dep} \times f_{MS} \tag{TF 4-4b}$$

Resuspension of sediment to surface water (solid phase):

$$T_{Sed \to SW}^{res} = \frac{A_{SedSW}}{V_{Sed}} \times \frac{S_{res}}{\rho_{Sed}} \times \frac{Z_{pure\_solid}}{Z_{Total\_Sed}} \tag{TF 4-5a}$$

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:

$$T_{Sed \to SW}^{res} = \frac{A_{SedSW}}{V_{Sed}} \times \upsilon_{Sed}^{res} \times f_{MS} \tag{TF 4-5b}$$

where:

$T_{Sed \to SW}^{res}$ = advective transfer factor for resuspension of sediment to surface water (/day);
A_{SedSW} = area of sediment/surface water interface (m^2);
V_{Sed} = volume of sediment compartment (m^3);
S_{res} = resuspension rate of benthic sediment to water column (kg[benthic sediment particles]/m^2[sediment/surface water interface]-day);
ρ_{Sed} = density of solid sediment particles (kg[particles]/m^3[particles]);
Z_{pure_solid} = fugacity capacity of the chemical in solid phase (mol/m^3-Pa);
Z_{Total_Sed} = total fugacity capacity of the chemical in the sediment compartment (mol/m^3-Pa);
υ_{Sed}^{res} = volumetric sediment resuspension rate (m^3[sediment]/m^2[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:

$$\upsilon_{Sed}^{dep} = \frac{S_{dep}}{\rho_{Sed}} \tag{Eq. 4-9}$$

where:

υ_{Sed}^{dep} = volumetric sediment deposition rate (m^3[sediment particles]/m^2[surface water/sediment interface]-day);

S_{dep} = deposition rate of suspended sediment to sediment bed (kg[suspended sediment particles]/m^2[surface water/sediment interface]-day); and
ρ_{Sed} = density of suspended sediment particles (kg[particles]/m^3[particles]).

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

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

where:

v_{dep} = sediment deposition velocity (m/day); and
TSS = total suspended sediment concentration (kg[suspended sediment particles]/m^3[surface water compartment]);

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

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

where:

υ_{Sed}^{res} = volumetric sediment resuspension rate (m^3[sediment particles]/m^2[surface water/sediment interface]-day);
S_{res} = resuspension rate of benthic sediment to surface water (kg[benthic sediment]/m^2[sediment/surface water interface]-day); and
ρ_{Sed} = density of solid sediment particles (kg[sediment particles]/m^3[sediment particles]).

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

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

where:

v_{res} = sediment resuspension velocity (m/day); and
BSC = benthic solids concentration (kg[sediment particles]/m^3[sediment compartment]).

In the TRIM.FaTE library:

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

where:

ϕ = porosity, which for the sediment compartment is equal to the volume fraction liquid , *i.e.*, water (m^3[pore water]/m^3[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:

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

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);
υ_{Algae}^{dep} = algal deposition rate (m^3[algae]/m^2[sediment/surface water interface]-day); and
f_{MAl} = 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:

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

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:

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

where:

CS_{dep} = carbon sedimentation rate (g[carbon]/m2[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:

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

where:

CC	=	chlorophyll concentration in water (mg[chlorophyll]/m^3[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:

$$T^{river}_{SW\rightarrow SW\_sink} = outflow/V_{SW} \qquad \text{(TF 4-7a)}$$

where:

$T^{river}_{SW\rightarrow SW\_sink}$	=	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 (m^3[bulk water]/day); and
V_{SW}	=	volume of surface water compartment (m^3[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:

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

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 (m^3[bulk water]/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:

$$T_{Sed\rightarrow Sed\_sink}^{Total} = \frac{A_{Sed}}{V_{Sed}} \times burial\_rate \times f_{MS} \qquad \text{(TF 4-8)}$$

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 (m^3[sediment particles] /m^2[sediment]-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:

$$burial\_rate = \max(0,\ \upsilon_{sed}^{dep} - \upsilon_{sed}^{res}) \qquad \text{(Eq. 4-17)}$$

where:

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

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

where:

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

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

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

where:

U_{SWSed} = mass transfer coefficient from surface water to sediment (m/day);
U_{SedSW} = 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):

$$De_{SW} = D_{pure\_water} \qquad \text{(Eq. 4-19)}$$

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

where:

D_{pure_water} = diffusivity of chemical in liquid phase, *i.e.*, water (m^2/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:

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

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

$$T^{dif}_{Sed \to SW} = \frac{A_{SedSW}}{V_{Sed}} \times \left(\frac{1}{U_{SWSed} \times \frac{Z_{Total\_SW}}{Z_{Total\_Sed}}} + \frac{1}{U_{SedSW}} \right)^{-1} \qquad \text{(TF 4-10a)}$$

where:

$T^{dif}_{Sed \to SW}$ = diffusive transfer factor from sediment to surface water (/day);
A_{SedSW} = interfacial area between the sediment and surface water compartments (m^2);
Z_{Total_SW} = total fugacity capacity of chemical in the surface water compartment (mol/m^3-Pa); and
Z_{Total_Sed} = total fugacity capacity of chemical in the sediment compartment (mol/m^3-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:

$$T^{dif}_{SW \to Sed} = \frac{A_{SedSW}}{V_{SW}} \times \left(\frac{1}{U_{SedSW} \times \frac{Z_{Total\_Sed}}{Z_{Total\_SW}}} + \frac{1}{U_{SWSed}} \right)^{-1} \qquad \text{(TF 4-11a)}$$

where:

$T^{dif}_{SW \to Sed}$ = 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_{SWSed} = 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:

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

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

where:

N_{Sed} = chemical mass in the underlying sediment compartment (g[chemical]/day);

DSP_{SWSed} = diffusive exchange coefficient between surface water and sediment compartments (m^2[surface water/sediment interface]/day);

A_{SWSed} = interfacial area between surface water and sediment compartments (m^2);

L_{SWSed} = 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:

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

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

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):

$$\frac{C_{Algae}}{C_{pure\_water}} = BCF = \frac{Z_{Algae}}{Z_{pure\_water}} \tag{Eq. 4-24}$$

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:

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

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

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* (m^2/day);
A_{ij} = interfacial area between surface water compartments *i* and *j* (m^2);
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/m^3);
N_i, N_j = mass of chemical in surface water compartments *i* and *j*, respectively (g[chemical]/m^3[water]); and
V_i, V_j = volume of surface water compartments *i* and *j*, respectively (m^3).

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

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

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} m^2/sec (8.64×10^{-6} m^2/day) for molecular diffusion to 5×10^{2} m^2/sec (4.32×10^{7} m^2/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:

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

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* (m^2);
V_{Sedi} = volume of the sending sediment compartment *i* (m^3);
DSP_{Sed} = diffusive exchange coefficient (m^2/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:

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

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* (m^3); 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.

[This page intentionally left blank.]

5. SOIL ALGORITHMS

In this chapter, the T-factors for the transport and transformation of chemical species within and among soil compartments, including the ground-water stratum, are described. In addition, algorithms for the transport of a chemical between soil compartments and the lower atmosphere and between soil compartments and surface water are presented. The text box on the next page and continued on the following pages provides a summary of the T-factor algorithms developed in this chapter and defines all parameters used in those algorithms.

The remainder of this chapter is divided into five subsections. The first outlines the four soil compartment types and the general transport processes that apply to each (Section 5.1). The next (Section 5.2) describes the transformation and degradation processes that apply to the soil compartments. The third subsection develops the T-factor algorithms for vertical-transport between compartments (Section 5.3), while the fourth subsection describes the horizontal-transport algorithms that apply to the surface soil compartments (Section 5.4). Finally, the algorithms related to the ground-water compartment are described (Section 5.5).

5.1 SOIL COMPARTMENTS AND TRANSPORT PROCESSES

In TRIM.FaTE, soil is modeled as four distinct compartment types: surface soil, plant root-zone soil, vadose-zone soil above the saturated zone, and the saturated zone or ground water. In TRIM.FaTE, the root-zone and vadose-zone soils can be sub-divided into one or more vertically stacked compartments for the purpose of assessing mass transfer. Tables 5-1 and 5-2 summarize the gains and losses for surface and subsurface soil compartments, respectively, that are addressed in the current TRIM.FaTE library.

As indicated in Table 5-1, the uppermost surface soil compartment exchanges mass with the lowest compartment of the atmosphere by a combination of diffusion and advection processes. There are two advective processes addressed in TRIM.FaTE that can potentially transport a chemical from a surface soil compartment to down-gradient surface soil compartments or to surface water: erosion of surface soil particles and runoff of water from surface soil. Erosion applies to the solid phase, while runoff and recharge apply to the dissolved phase.

As indicated in Table 5-2, two of the primary transport processes in subsurface soils are exchanges by diffusion and advection. Transport can occur both in the gas and liquid phases. The predominant transport mechanism in the aqueous phase is advection, and that in the gas phase is diffusion. The advective transport of contaminants in the liquid or gas phase depends on the velocity of that phase. There currently is only one advective process included in the TRIM.FaTE library that can potentially transport a chemical from the vadose-zone soil compartment to ground water, that is percolation. Recharge of ground water to surface water also is included. Important physicochemical properties include solubility, molecular weight, vapor pressure, and diffusion coefficients in air and water. The important landscape properties include temperatures of air, rainfall rates, soil properties (*i.e.*, bulk density, porosity), and the depth of each soil compartment.

Summary of Transfer Factors for Soil in TRIM.FaTE

VERTICAL EXCHANGES BETWEEN SURFACE SOIL AND ATMOSPHERE

Diffusion of vapor-phase from air to surface soil: (TF 5-1)

$$T^{dif}_{Ss \rightarrow Air} = \frac{f_A \times A_{Ss}}{Z_{Total\_Ss} \times V_{Ss}} \times \left(\frac{1}{Z_{pure\_air} \times U_{Air}} + \frac{1}{Z_{Total\_Ss} \times U_{Ss}} \right)^{-1}$$

Diffusion of vapor-phase from surface soil to air: (TF 5-2)

$$T^{dif}_{Air \rightarrow Ss} = \frac{f_A \times A_{Ss}}{Z_{Total\_Air} \times V_{Air}} \times \left(\frac{1}{Z_{pure\_air} \times U_{Air}} + \frac{1}{Z_{Total\_Ss} \times U_{Ss}} \right)^{-1}$$

Dry deposition of particle-phase from air to surface soil: (TF 5-3b) [a]

$$T^{dry\_dep}_{AirP \rightarrow Ss} = \frac{\upsilon_{dry} \times (1 - I_{dry}) \times A_{Ss}}{V_{Air}} \times f_{MS}$$

Wet deposition of particle-phase from air to surface soil during rain:

(TF 5-4)

$$T^{wet\_dep}_{AirP \rightarrow Ss} = \frac{\upsilon_{wet} \times (1 - I_{wet}) \times A_{Ss}}{V_{Air}} \times f_{MS}$$

Wet deposition of vapor-phase from air to surface soil during rain (fugacity approach): (TF 5-5a)

$$T^{Vwet\_dep}_{Air \rightarrow Ss} = \frac{A_{Ss}}{V_{Air}} \times rain \times (1 - I_{wet}) \times \frac{Z_{pure\_water}}{Z_{Total\_Air}}$$

Wet deposition of vapor-phase from air to surface soil during rain (partitioning approach): (TF 5-5b)

$$T^{Vwet\_dep}_{Air \rightarrow Leaf} = \frac{A_{Ss}}{V_{Air}} \times w_{rV} \times rain \times \left(1 - I_{wet}\right) \times f_{MV}$$

Dry resuspension of particle-phase to air from surface soil compartment: (TF 5-6)

$$T^{res}_{Ss \rightarrow AirP} = \frac{A_{Ss}}{V_{Ss}} \times \frac{res}{\rho_P} \times \frac{Z_{pure\_solid}}{Z_{Total\_Ss}}$$

---

[a] TF 5-5a represents the same basic equation, but uses the fugacity notation. TF 5-5b is the expression of the equation in the current TRIM.FaTE library.

Summary of Transfer Factors for Soil in TRIM.FaTE (cont.)

VERTICAL EXCHANGES BETWEEN SOIL COMPARTMENTS

Diffusion downward from soil compartment *i* to the soil compartment *j* directly below it: (TF 5-7)

$$T^{dif}_{Si \to Sj} = \frac{Y_{Sij}}{d_{Si} \times Z_{Total\_Si}}$$

Diffusion upward from soil compartment *j* to the soil compartment *i* immediately above it: (TF 5-8)

$$T^{dif}_{Sj \to Si} = \frac{Y_{Sij}}{d_{Sj} \times Z_{Total\_Sj}}$$

Percolation downward from soil compartment *i* to soil compartment *j*: (TF 5-9)

$$T^{perc}_{Si \to Sj} = \frac{ve_{Si} \times \gamma_{Si}}{\left(e^{+\gamma_{Si} \times d_{Si}} - 1\right)}$$

HORIZONTAL EXCHANGES ACROSS SURFACE SOIL COMPARTMENTS

Runoff during rain from surface soil compartment *i* to surface soil compartment *j*: (TF 5-10a)

$$T^{runoff}_{Ssi \to Ssj} = runoff \times f_{runoff}(Ssi \to Ssj) \times \frac{A_{Ssi}}{V_{Ssi}} \times f_{ML}$$

Erosion during rain from surface soil compartment *i* to surface soil compartment *j*: (TF 5-11a)

$$T^{erosion}_{Ssi \to Ssj} = erosion \times f_{erosion}(Ssi \to Ssj) \times \frac{A_{Ssi}}{V_{Ssi}} \times \frac{f_{MS}}{\rho_P}$$

Runoff during rain from surface soil compartment *i* to surface soil sink, same as TF 5-10a but with *Ss_sink* replacing *Ssj*: (TF 5-10c)

Erosion during rain from surface soil compartment *i* to surface soil sink, same as TF 5-11a but with *Ss_sink* replacing *Ssj*: (TF 5-11c)

HORIZONTAL TRANSFER FROM SURFACE SOIL TO SURFACE WATER

Runoff during rain from surface soil compartment *i* to surface water compartment: (TF 5-10b)

$$T^{runoff}_{Ssi \to SW} = runoff \times f_{runoff}(Ssi \to SW) \times f_{avail\_runoff} \times \frac{A_{Ssi}}{V_{Ssi}} \times f_{ML}$$

Erosion during rain from surface soil compartment *i* to surface water compartment: (TF 5-11b)

$$T^{erosion}_{Ssi \to SW} = erosion \times f_{erosion}(Ssi \to SW) \times f_{avail\_erosion} \times \frac{A_{Ssi}}{V_{Ssi}} \times \frac{f_{MS}}{\rho_P}$$

Summary of Transfer Factors for Soil in TRIM.FaTE (cont.)

VERTICAL EXCHANGES WITH GROUND WATER

Percolation from vadose-zone soil to ground water: (TF 5-12)

$$T_{Sv \rightarrow GW} = \frac{ve_{Sv} \times \gamma_{Sv}}{\left(e^{+\gamma_{Sv} \times d_{Sv}} - 1\right)}$$

Recharge from ground water to surface water: (TF 5-13)

$$T_{GW \rightarrow SW} = \frac{A_{SWGW}}{V_{GW}} \times \frac{Z_{pure\_water}}{Z_{Total\_GW}} \times recharge$$

LIST OF SYMBOLS USED IN TRANSFER FACTOR ALGORITHMS

f_A = fraction of area available for vertical diffusion (from 0 to 1.0);
A_{Ss} = horizontal area of the surface soil compartment (m^2). (This is the area assumed to be shared between the top soil compartment and the atmosphere.)
Z_{Total_Ss} = total fugacity capacity of surface soil compartment (mol/m^3-Pa).
V_{Ss} = volume of surface soil compartment (m^3).
Z_{pure_air} = fugacity capacity of chemical in pure air, = 1/RT (mol/m^3-Pa).
U_{Air} = mass transfer coefficient on the air side of the air/soil boundary (m/day). (It is typical to represent the mass transfer coefficient in air as the ratio of the diffusion coefficient in air, D_{air}, divided by the turbulent boundary compartment thickness, δ_{air}. For many compounds, D_{air} is on the order of 0.4 m/day and δ_{air} is on the order of 0.0005 m, so that U_{air} is on the order of 800 m/day.)
V_{Air} = volume of the air compartment (m^3).
Z_{Total_Air} = total fugacity capacity of chemical in the air compartment (includes gas and particle phase of the atmosphere) (mol/m^3-Pa).
υ_{dry} = volumetric dry particle deposition rate (m^3[dust particles]/m^2[surface water]-day).
I_{dry} = fraction of dry particle deposition that is intercepted by plants (unitless).
f_{MS} = fraction of total chemical mass in compartment that is sorbed to solid particles divided by volume fraction of the compartment that consists of particles (unitless).
υ_{wet} = volumetric wet particle deposition rate (m^3[dust particles]/m^2[surface water]-day).
I_{wet} = fraction of wet particle deposition that is intercepted by plants (unitless).
$rain$ = rate of rainfall (m^3[rain]/m^2[surface soil]-day).
Z_{pure_water} = fugacity capacity of chemical in the moving phase, water (mol/m^3-Pa).
w_{rV} = vapor washout ratio (g[chemical dissolved]/m^3[rain] per g[chemical vapor-phase]/m^3[air]).
f_{MV} = fraction chemical mass in air compartment that is in vapor-phase divided by the volume fraction of air compartment that is gas (unitless).
res = rate of resuspension of dust particles from soil to air (kg[dust particles]/m^2[surface soil]-day).
ρ_p = density of dust or soil particles in air (kg[particles]/m^3[particles]).
Z_{pure_solid} = fugacity capacity of chemical in the moving phase, dust particles (mol/m^3-Pa).
γ_{Si} = gradient of soil concentration change in soil compartment *i* (/m).
d_{Si} = thickness of surface soil compartment *i* (m).
Y_{Sij} = fugacity-capacity adjusted mass transfer coefficient between soil compartments *i* and *j* (mol/m^2-Pa-day), and is given by:

Summary of Transfer Factors for Soil in TRIM.FaTE (cont.)

LIST OF SYMBOLS USED IN TRANSFER FACTOR ALGORITHMS (cont.)

$$Y_{Sij} = \frac{(Z_{Total\_Si} \times De_{Si} \times \gamma_{Si}) + (Z_{Total\_Sj} \times De_{Sj} \times \gamma_{Sj})}{2 \times \left[\frac{(e^{+\gamma_{Si} \times d_{Si}} - 1)}{\gamma_{Si} \times d_{Si}} - \frac{(1 - e^{-\gamma_{Si} \times d_{Si}})}{\gamma_{Sj} \times d_{Sj}} \right]}$$

d_{Si}, d_{Sj} = thickness of soil compartments *i* and *j,* respectively (m).
Z_{Total_Si} = total fugacity capacity of chemical in soil compartment *i* (mol/m^3-Pa).
Z_{Total_Sj} = total fugacity capacity of chemical in soil compartment *j* (mol/m^3-Pa).
γ_{Si}, γ_{Sj} = gradient of soil concentration change in soil compartments *i* and *j,* respectively (/m).
De_{Si} = effective diffusion coefficient in soil compartment *i* (m^2[soil]/day].
ve_i = effective advection velocity of a chemical in the soil compartment *i* (m/day), and equal to the rate of soil-solution movement, v_i (see below), multiplied by the fugacity capacity of the moving phase (water) divided by the total fugacity capacity of the soil compartment *i*; $ve_i = (v_i \times Z_{pure\_water})/Z_{Total\_Si}$.
v_i = average velocity of the moving phase (assumed to be water) in soil compartment *i* (/m).
runoff = flux of water transported away from surface soil compartment *i* (m^3[water]/m^2[soil]-day).
$f_{runoff}(Ssi \rightarrow Ssj)$ = fraction of water that runs off of surface soil compartment *i* that is transported to surface soil compartment *j* (unitless).
f_{avail_runoff} = fraction of surface soil available for runoff (between 0 and 1.0).
f_{ML} = fraction of chemical in compartment that is dissolved in water divided by the volume fraction of the compartment that is liquid (water).
erosion = flux of soil particles transported away from surface soil compartment *i* (kg[soil particles]/m^2[soil]-day).
$f_{erosion}(Ssi \rightarrow Ssj)$ = fraction of soil that erodes from surface soil compartment *i* that is transported to surface soil compartment *j* (unitless).
$f_{avail\_erosion}$ = fraction of surface soil available for erosion (between 0 and 1.0).
ve_{Sv} = effective advection velocity of a chemical in the vadose-zone soil compartment (m/day).
γ_{Sv} = gradient of soil concentration change in vadose-zone soil compartment (/m).
A_{SWGW} = interfacial area between ground-water and surface-water compartments (m^2).
V_{GW} = volume of ground-water compartment (m^3).
Z_{Total_GW} = total fugacity of chemical in the ground-water compartment (mol/m^3-Pa).
recharge = average daily recharge from ground water into surface water (m/day).

A future version of the TRIM.FaTE library could include algorithms for diffusive transfers between the vadose-zone soil compartment and the ground-water compartment.

5.2 TRANSFORMATIONS AND DEGRADATION

The transformation of chemicals in soil layers can have a profound effect on their potential for persistence. Chemical transformations, which may occur as a result of biotic or abiotic processes, can significantly reduce the concentration of a substance in soil.

Table 5-1
Summary of the Chemical Gains and Losses for Surface Soil Compartments Addressed in TRIM.FaTE

Gains	Type of Process	Relevant Phase	Losses	Type of Process	Relevant Phase
From Air			**To Air**		
Diffusion from air	Diffusion (TF 5-1)	Vapor	Diffusion to air	Diffusion (TF5-2)	Vapor
Dry deposition of particles/ aerosols from air	Advection (TF 5-3)	Solid	Dry resuspension of particle phase	Advection (TF 5-6)	Solid
Wet deposition of particles/ aerosols from air	Advection (TF 5-4)	Solid			
Wet deposition of vapor from air	Advection (TF 5-5)	Vapor			
From Surface Soils			**To Surface Soils**		
Erosion from upgradient soils	Advection (TF 5-10a)	Solid	Erosion to downgradient soils	Advection (TF 5-10a)	Solid
Runoff from upgradient soils	Advection (TF 5-11a)	Aqueous	Runoff to downgradient soils	Advection (TF 5-11a)	Aqueous
From Plants			**To Plants**		
Deposition of leaves during litter fall	Advection (TF 7-15)	Solid			
Deposition of particles on leaves during litter fall	Advection (TF 7-16)	Solid			
From Surface Water			**To Surface Water**		
			Erosion	Advection (TF 5-11b)	Solid
			Runoff	Advection (TF 5-10b)	Aqueous
From Terrestrial Birds and Mammals			**To Terrestrial Birds and Mammals**		
Elimination from terrestrial and semi-aquatic wildlife	Advection (TF 7-31)	Total	Ingestion by wildlife	Advection (TF 7-22)	Total
From Root-Zone Soil			**To Root-Zone Soil**		
Upward diffusion	Diffusion (TF 5-8)	Aqueous & Vapor	Percolation	Advection (TF 5-9)	Aqueous
			Diffusion	Diffusion (TF 5-7)	Aqueous & Vapor
From Surface Soil Transformations			**To Sink(s)**		
			Runoff off-site to sink	Advection (TF 5-10c)	Aqueous
			Erosion off-site to sink	Advection (TF 5-11c)	Solid
			Decay to reaction sinks	Degradation (TF 2-1)	Total

Table 5-2
Summary of the Chemical Gains and Losses for Sub-surface Soil Compartment *j* Addressed in TRIM.FaTE[a]

Gains	Type of Process	Relevant Phase	Losses	Type of Process	Relevant Phase
From Vertically Adjacent Soil Compartment			**To Vertically Adjacent SoilCompartment**		
Downward diffusion from soil compartment *i*	Diffusion (TF 5-7)	Aqueous	Downward diffusion from soil compartment *j*	Diffusion (TF 5-7)	Aqueous
Upward diffusion from soil compartment *l*	Diffusion (TF 5-8)	Aqueous	Upward diffusion from soil compartment *j*	Diffusion (TF 5-8)	Aqueous
Percolation downward from soil compartment *i*	Advection (TF 5-9)	Aqueous	Percolation downward from soil compartment *j*	Advection (TF 5-9)	Aqueous
			To Plants		
Release from plant roots	Diffusion (TF 7-11)		Uptake from root-zone soil by plant roots	Diffusion (TF7-10)	Aqueous
			Uptake by plant stems from root-zone soil via flow of transpired water	Advection (TF 7-12a)	Aqueous
From Ground Water			**To Ground Water**		
			Percolation from vadose-zone soil	Advection (TF 5-12)	Aqueous
From Surface Water			**To Surface Water**		
			Recharge from ground water	Advection (TF 5-13)	Aqueous
From Soil Transformations			**To Sink(s)**		
			Decay to reaction sinks	Degradation (TF 2-1)	Total

[a] Sub-surface soil compartment *i* is higher than *j* is higher than *l*.

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 the model. In TRIM.FaTE, the degradation of chemicals in soil due to all mechanisms that might apply (*e.g.*, degradation by soil microfauna, photolysis at the soil surface, hydrolysis in the saturated zone) is reflected by the user input for the half-life of the chemical in the particular soil compartment. The algorithm relating the degradation rate constant to the chemical half-life in a soil compartment is presented in Chapter 2 (Equation 2-64).

Transformations of a chemical into another form of the chemical that is tracked in TRIM.FaTE are reflected in algorithms that are named for the process (*e.g.*, oxidation, methylation, reduction of mercury species). In the TRIM.FaTE soil layers, all transformation processes 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 and the transformation rate constant. The transformation rate constant is the inverse of the residence time with respect to that reaction.

5.3 VERTICAL TRANSPORT ALGORITHMS

The transfer factors in the subsurface are a function of the advective flux (gas phase plus liquid phase) and the diffusive flux (gas phase plus liquid phase). In the subsections below, upward and downward transfer factors are developed for the top three soil compartments (*i.e.*, excluding ground water). No provisions are made for preferential flow regions in the vadose zone that could lead to higher concentrations in the ground water, because in most cases, the proportion of exposure from ground water is minimal for air pollutants.

5.3.1 THEORETICAL BASIS FOR THE TRANSPORT ALGORITHMS

The algorithms below are developed by assuming that chemical concentration in each compartment decreases exponentially with depth in that compartment. This type of concentration gradient has been demonstrated as the correct analytical solution of the one-dimensional, convective-dispersive, solute-transport equation in a vertical layer with a steady-state concentration maintained at its upper surface (ARS 1982). With the assumption of exponentially decreasing vertical concentration for each soil compartment, *i*, the variation in concentration with depth in that compartment is given by:

$$C_i(x) = C_i(0) \times \exp(-\gamma_i x) \qquad \text{(Eq. 5-1)}$$

where:

x = distance into the soil compartment measured from the top of the soil column (m);

$C_i(0)$ = peak chemical concentration in soil compartment *i* (g[chemical]/m^3[soil]), which is related to the total inventory N_i (g[chemical]) in this soil compartment (this relationship is provided below); and

γ_i = the gradient of soil concentration change in soil compartment *i* (/m), which is obtained from the inverse of the normalized or characteristic depth X^*, which is $\gamma_i = 1/X^*$.

X^* can be input by the user. If the user does not provide a value, a value for X* is calculated as follows. Let:

λ_i = removal rate constant for a chemical in soil compartment *i*, based on chemical transformation (/day); then

If $\lambda_i > 0$ then $X^* = \text{Minimum}(DX_1, DX_2)$,
Otherwise (*i.e.*, $\lambda_i = 0$), then $X^* = DX_2$. (Eq. 5-2)

DX_1 is the Damkoehler distance (the distance at which the soil concentration falls by 1/e based on the aggregate results of diffusion, advection, and reaction) in units of meters and is given by:

$$DX_1 = \frac{ve_i + \sqrt{ve_i + 4De_{Si}}}{2\lambda_i} \tag{Eq. 5-3a}$$

Equation 5-3a can be rearranged as follows to arrive at Equation 5-3d, which is the form of the equation in the TRIM.FaTE library:

$$DX_1 = \frac{ve_i}{2\lambda_i} + \frac{\sqrt{(ve_i)^2 + (4De_{Si} \times \lambda_i)}}{2\lambda_i} \tag{Eq. 5-3b}$$

$$DX_1 = \frac{ve_i}{2\lambda_i} + \sqrt{\frac{(ve_i)^2}{4\lambda_i^{\,2}} + \left(\frac{4De_{Si} \times \lambda_i}{4\lambda_i^{\,2}}\right)} \tag{Eq. 5-3c}$$

$$DX_1 = \frac{ve_i}{2\lambda_i} + \sqrt{\left(\frac{ve_i}{2\lambda_i}\right)^2 + \left(\frac{De_{Si}}{\lambda_i}\right)} \tag{Eq. 5-3d}$$

If $ve_i = 0$, then:

$$DX_1 = \sqrt{\frac{De_{Si}}{\lambda_i}} \tag{Eq. 5-3e}$$

In Equations 5-3a through 5-3e, the following parameter definitions apply:

De_{Si} = effective diffusion coefficient in soil compartment *i* (m^2[soil]/day), which is derived below in Equation 5-7; and

ve_i = the effective advection velocity of a chemical in the soil compartment, *i* (m/day), and equal to the rate of soil-solution movement, v_i, multiplied by the fugacity capacity of the moving phase and divided by the fugacity capacity of soil compartment *i*:

$$ve_i = (v_i \times Z_{pure\_water}) / Z_{Total\_Si} \tag{Eq. 5-4}$$

where:

v_i = average velocity of the moving liquid phase (assumed to be water) in the soil column *i* (m/day);

Z_{pure_water} = fugacity capacity of chemical in the moving phase, water (mol/m^3-Pa); and

Z_{Total_Si} = total fugacity capacity of chemical in soil compartment *i* (mol/m^3-Pa).

DX_2 is the depth that establishes the concentration gradient in soil in the absence of any reaction or transformation processes, in units of meters. It is obtained as follows:

If $ve_i > 0$, then DX_2 = Minimum $[(4 \times De_i/ve_i), (2d_i \times \sqrt{\pi})]$
Otherwise (*i.e.*, $ve_i = 0$), $DX_2 = (2d_i \times \sqrt{\pi})$ (Eq. 5-5)

where:

d_i = the thickness of soil compartment *i* (m).

As an average, the property v_i (m/day), the average velocity of the moving liquid phase (assumed to be water) in the soil column *i*, is intended to be representative of the range of velocities occurring, and not be limited only to the velocity during rainfall events. The user should check that the value used for v_i in the TRIM.FaTE library is consistent with the precipitation data in the scenario (adjusted for infiltration) (see the TRIM.FaTE user guidance).

Compartments such as soils and sediments are neither homogeneous nor single phase. When air and water occupy the tortuous pathways between stationary particles in a porous medium such as a soil or sediment, Millington and Quirk (1961) have shown that the effective diffusivity is given by:

$$De = (\omega^{10/3} / \phi^2) \times D_{pure} \qquad \text{(Eq. 5-6)}$$

where:

De = effective diffusivity of a chemical in either the air or water phase of the mixture (m^2[fluid]/day);
ω = volume fraction occupied by that fluid (either air or water) (unitless);
ϕ = porosity or total void fraction in the medium (the volume occupied by all fluids) (unitless); and
D_{pure} = diffusion coefficient of the chemical in the pure fluid (m^2[fluid]/day).

Jury et al. (1983) have shown that the effective tortuous diffusivity in the water and air of a soil compartment *i*, such as the root-zone soil(s), is given by:

$$De_{Si} = \frac{Z_{pure\_air}}{Z_{Total\_Si}} \times (\varepsilon_i^{10/3} / \phi_i^2) \times D_{air} + \frac{Z_{pure\_water}}{Z_{Total\_Si}} \times (\theta_i^{10/3} / \phi_i^2) \times D_{water} \qquad \text{(Eq. 5-7)}$$

where:

De_{Si} = the effective tortuous, mixed-phase diffusion coefficient in the soil compartment *i* (m^2[soil]/day);
ϵ_i = volume fraction of soil compartment *i* that is air (unitless);
θ_i = volume fraction of soil compartment *i* that is water (unitless);
Z_{pure_air} = fugacity capacity of chemical in the gas-phase of air (mol/m^3-Pa);
Z_{pure_water} = fugacity capacity of chemical in the soil water (mol/m^3-Pa);
Z_{Total_Si} = total fugacity capacity of chemical in soil compartment *i* (mol/m^3-Pa);
D_{air} = the diffusion coefficient of the chemical in air (excluding atmospheric dust particulates) (m^2[air]/day); and

D_{water} = the diffusion coefficient of the chemical in water (excluding suspended sediments (m^2[water]/day).

5.3.2 RELATIONSHIP BETWEEN INVENTORY, N_{Si}, AND PEAK CONCENTRATION, $C_{Si}(0)$

The assumptions of a peak chemical concentration and an exponential gradient of chemical concentration within a soil compartment make it possible to define $C_{Si}(0)$ in terms of the inventory, N_{Si}:

$$N_{Si} = A_{Si} \times \int_0^{d_i} C_{Si}(0) \times \exp(-\gamma_{Si} x) dx \qquad \text{(Eq. 5-8)}$$

$$N_{Si} = A_{Si} \times [C_{Si}(0) / \gamma_{Si}] \times [1 - \exp(-\gamma_{Si} \times d_{Si})] \qquad \text{(Eq. 5-9)}$$

where:

N_{Si} = inventory of chemical in soil compartment *i* (g[chemical]);
A_{Si} = horizontal area of the soil compartment *i* (m^2);
C_{Si} = chemical concentration in soil compartment *i* (g[chemical]/m^3[soil]);
γ_{Si} = the gradient of soil concentration change in soil compartment *i* (/m) (see Equation 5-1); and
d_{Si} = thickness of soil compartment *i* (m).

Solving Equation 5-9 for $C_{Si}(0)$ yields:

$$C_{Si}(0) = \frac{N_{Si} \times \gamma_{Si}}{A_{Si} \times [1 - \exp(-\gamma_{Si} \times d_{Si})]} \qquad \text{(Eq. 5-10)}$$

5.3.3 VERTICAL MASS EXCHANGE BETWEEN AIR AND THE SURFACE SOIL COMPARTMENT

Both diffusive and advective processes can transfer a chemical between the air and the surface soil compartment. The diffusive process can result in a two-way exchange of vapor-phase chemical between the surface soil and air above it (Section 5.3.3.1). The advective processes are one-way, from air to surface soil. These include the wet and dry deposition of particle-bound chemical (*i.e.*, solid phase) (Section 5.3.3.2) and the wet deposition of vapor-phase chemical scavenged from the air during rain.

5.3.3.1 Diffusive Processes

The algorithm for representing diffusion exchange at the air/soil interface is based on defining the flux from air to soil in terms of the concentration gradient at the point of contact between air and soil (Eq. 5-11) and the flux from soil to air in terms of the bulk chemical concentration in the surface soil layer (Eq. 5-12):

$$Flux\ (air\ side) = U_{Air} \times \left[C_{Air} - C_{Ss}(0) \times \frac{Z_{pure\_air}}{Z_{Total\_Ss}} \right] \quad \text{(Eq. 5-11)}$$

$$Flux\ (soil\ side) = U_{Ss} \times \left[C_{Ss}(0) - C_{Ss} \right] \quad \text{(Eq. 5-12)}$$

where:

$Flux$ = transfer rate per unit area (g[chemical]/m^2[air/soil interface]-day);
U_{Air} = mass-transfer coefficient on the air side of the air/soil interface (m/day) (It is typical to represent the mass transfer coefficient in air as the ratio of the diffusion coefficient in air, D_{air}, divided by the turbulent boundary compartment thickness, δ_{air}. For many compounds, D_{air} is on the order of 0.4 m/day, and δ_{air} is on the order of 0.0005 m, so that U_{Air} is on the order of 800 m/day.);
C_{Air} = concentration of the chemical in the gas phase of the lowest compartment of the atmosphere (g[chemical]/m^3[gas-phase air]), derived in Equation 5-16 below;
$C_{Ss}(0)$ = chemical concentration at the top of the uppermost (*i.e.*, surface) soil compartment in a vertical set of soil compartments (g[chemical]/m^3[soil]), as given for $C_i(0)$ in Equation 5-10;
Z_{pure_air} = fugacity capacity of chemical in air, = 1/RT (mol/m^3-Pa);
Z_{Total_Ss} = total fugacity capacity of chemical in surface soil compartment (mol/m^3-Pa);
U_{Ss} = mass-transfer coefficient on the soil side of the air/soil interface (m/day); and
$C_{Ss}\ (bulk)$ = total chemical concentration in bulk surface soil (g[chemical]/ m^3[soil]).

Rearranging Equations 5-11 and 5-12 yields Equations 5-13 and 5-14, respectively:

$$\frac{Flux}{Z_{pure\_air} \times U_{Air}} = \left[\frac{C_{Air}}{Z_{pure\_air}} - \frac{C_{Ss}(0)}{Z_{Total\_Ss}} \right] \quad \text{(Eq. 5-13)}$$

$$\frac{Flux}{Z_{Total\_Ss} \times U_{Ss}} = \left[\frac{C_{Ss}(0)}{Z_{Total\_Ss}} - \frac{C_{Ss}(bulk)}{Z_{Total\_Ss}} \right] \quad \text{(Eq. 5-14)}$$

Adding Equations 5-13 and 5-14 together yields:

$$Flux \times \left[\frac{1}{Z_{pure\_air} \times U_{Air}} + \frac{1}{Z_{Total\_Ss} \times U_{Ss}} \right] = \left[\frac{C_{Air}}{Z_{pure\_air}} - \frac{C_{Ss}(bulk)}{Z_{Total\_Ss}} \right] \qquad \text{(Eq. 5-15)}$$

$$Flux = \left[\frac{C_{Air}}{Z_{pure\_air}} - \frac{C_{Ss}(bulk)}{Z_{Total\_Ss}} \right] \times \left[\frac{1}{Z_{pure\_air} \times U_{Air}} + \frac{1}{Z_{Total\_Ss} \times U_{Ss}} \right]^{-1} \qquad \text{(Eq. 5-16)}$$

The bulk concentration of the chemical in the lowest compartment of the atmosphere is given by:

$$C_{Air} = \frac{N_{Air} \times Z_{pure\_air}}{V_{Air} \times Z_{Total\_Air}} \qquad \text{(Eq. 5-17)}$$

where:

N_{Air} = inventory of chemical in the air compartment above the soil (g[chemical]);
Z_{pure_air} = fugacity capacity of chemical in gas-phase air (mol/m^3-Pa);
V_{Air} = volume of the air compartment (m^3[air]); and
Z_{Total_Air} = total fugacity capacity of chemical in air compartment (including gas and particle phases of the air) (mol/m^3-Pa).

The bulk concentration of the chemical in the surface soil layer is given by:

$$C_{Ss} = \frac{N_{Ss}}{V_{Ss}} \qquad \text{(Eq. 5-18)}$$

where:

N_{Ss} = inventory of chemical in the surface soil compartment (g[chemical]); and
V_{Ss} = volume of the surface soil compartment (m^3[soil]).

Finally, the chemical flow between the air and surface soil compartments is determined from the flux and the area of the air/soil interface (as well as the fraction of that area that is not covered by an impervious material):

$$Flow = Flux \times f_A \times A_{Ss} \qquad \text{(Eq. 5-19)}$$

where:

$Flow$ = diffusive flow (g[chemical]/day);
f_A = fraction of area available for vertical diffusion (unitless, ranges from 0 to 1); and
A_{Ss} = area of surface soil compartment (m^2).

Making the appropriate substitutions, the net flow of chemical mass between the air and surface soil compartments by diffusion is calculated as:

Net Diffusion Flow (Air↔Ss) (g[chemical]/day) = $(T_{Air \rightarrow Ss} \times N_{Air}) - (T_{Ss \rightarrow Air} \times N_{Ss})$ =

$$f_A \times A_{Ss} \times \left(\frac{N_{Air}}{Z_{Total\_air} \times V_{Air}} - \frac{N_{Ss}}{Z_{Total\_Ss} \times V_{Ss}} \right) \times \left(\frac{1}{Z_{pure\_air} \times U_{Air}} + \frac{1}{Z_{Total\_Ss} \times U_{Ss}} \right)^{-1} \quad \text{(Eq. 5-20)}$$

where:

Z_{pure_air} = fugacity capacity of chemical in pure air (mol/m^3-Pa);
V_{Air} = volume of the air compartment (m^3);
Z_{Total_Ss} = total fugacity capacity of chemical in surface soil compartment (mol/m^3-Pa);
V_{Ss} = volume of the surface soil compartment (m^3);
U_{Air} = mass transfer coefficient on the air side of the air/soil boundary (m/day); and
U_{Ss} = mass transfer coefficient on the soil side of the air/soil boundary (m/day).

This implies the following:

$$T^{dif}_{Ss \rightarrow Air} = \frac{f_A \times A_{Ss}}{Z_{Total\_Ss} \times V_{Ss}} \times \left(\frac{1}{Z_{pure\_air} \times U_{Air}} + \frac{1}{Z_{Total\_Ss} \times U_{Ss}} \right)^{-1} \quad \text{(TF 5-1)}$$

where:

$T^{dif}_{Ss \rightarrow Air}$ = transfer factor for diffusion of chemical from surface soil compartment to air (/day).

It also implies:

$$T^{dif}_{Air \rightarrow Ss} = \frac{f_A \times A_{Ss}}{Z_{Total\_air} \times V_{Air}} \times \left(\frac{1}{Z_{pure\_air} \times U_{Air}} + \frac{1}{Z_{Total\_Ss} \times U_{Ss}} \right)^{-1} \quad \text{(TF 5-2)}$$

where:

$T^{dif}_{Air \rightarrow Ss}$ = transfer factor for diffusion of chemical from air to surface soil compartment (/day).

The mass transfer coefficient for the soil side of the air/soil boundary, U_{Ss}, can be estimated as follows:

$$U_{Ss} = \frac{De_{Ss}}{d_{Ss}} \quad \text{(Eq. 5-21)}$$

where :

De_{Ss} = effective diffusion coefficient in surface soil compartment (m^2/d) (derived in Equation 5-7); and

d_{Ss} = the thickness of the surface soil compartment (m).

It is important to ensure that the area used to calculate the flux, A_{Ss}, is the area of the surface soil compartment that is shared with the lowest atmosphere compartment. This is not necessarily the surface area of the lowest atmosphere compartment.

Note: In the current TRIM.FaTE library, these transfer factor algorithms apply to all chemicals except divalent mercury, which is reactive in air. Therefore, a separate algorithm representing net diffusion from air to surface soil is used for divalent mercury (see vapor dry deposition algorithms for Hg(2) described in Appendix A, Section A.1.1).

5.3.3.2 Wet and Dry Deposition of Particles

For wet and dry deposition of particles from air to surface soil, the rate of mass flow is given by:

$$\frac{dN_{Ss}}{dt} = \frac{A_{Ss}}{V_{Air}} \times v \times (1-I) \times \frac{D_L}{\rho_P} \times \frac{Z_{pure\_solid}}{Z_{Total\_Air}} \times N_{Air} \qquad \text{(Eq. 5-22)}$$

where:

N_{Ss} = inventory of chemical in surface soil compartment (g[chemical]);
A_{Ss} = area of contact between the surface soil compartment and the lowest air compartment (m^2[soil]);
V_{Air} = volume of the air compartment (m^3[air]);
v = air-to-soil deposition velocity, where the velocity is different for wet and dry deposition of particles (m/day);
I = fraction of deposition that is intercepted by plants, where the interception fraction is different for wet and dry deposition of particles (unitless);
D_L = dust load (*i.e.*, particulate matter concentration) in air (kg[dust particles]/m^3[air]);
ρ_P = density of dust particles (kg[dust particles]/m^3[dust particles]);
Z_{pure_solid} = fugacity capacity of chemical in dust particles (mol/m^3-Pa);
Z_{Total_Air} = total fugacity capacity of chemical in air compartment (including dust particles) (mol/m^3-Pa); and
N_{Air} = total inventory of chemical in air compartment, vapor- and solid-phase (g[chemical]).

***Dry deposition of particle-phase chemical**:*

Thus, the transfer factor for *dry* deposition of chemical sorbed to air particles to the surface soil is as follows:

$$T_{AirP \to Ss}^{dry\_dep} = \frac{A_{Ss}}{V_{Air}} \times v_{dry} \times (1-I_{dry}) \times \frac{D_L}{\rho_P} \times \frac{Z_{pure\_solid}}{Z_{Total\_Air}} \qquad \text{(TF 5-3a)}$$

where:

ν_{dry} = air-to-soil dry deposition velocity (m/day); and
I_{dry} = fraction of dry deposition that is intercepted by plants (unitless) (see Equation 7-2).

It is also true that:

$$\upsilon_{dry} = \nu_{dry} \times \frac{D_L}{\rho_P} \qquad \text{(Same as Eq. 4-1)}$$

where:

υ_{dry} = volumetric dry deposition rate (m^3[dust]/m^2[air]-day);

and:

$$\frac{Z_{pure\_solid}}{Z_{Total\_Air}} = \frac{Mass\_Fraction\_Sorbed}{Volume\_Fraction\_Solid} = f_{MS} \qquad \text{(Eq. 5-23)}$$

where:

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

Therefore, the transfer factor can be calculated as:

$$T_{AirP \rightarrow Ss}^{dry\_dep} = \frac{\upsilon_{dry} \times (1 - I_{dry}) \times A_{Ss}}{V_{Air}} \times f_{MS} \qquad \text{(TF 5-3b)}$$

where:

$T_{AirP \rightarrow Ss}^{dry\_dep}$ transfer factor for dry deposition of particulate-bound chemical to surface soil compartment (/day);
υ_{dry} = volumetric dry deposition rate (m^3[dust]/m^2[surface soil]-day);
I_{dry} = fraction of dry deposition that is intercepted by plants (unitless);
A_{Ss} = area of contact between the surface soil compartment and the lowest air compartment (m^2); and
V_{Air} = volume of the air compartment (m^3[air]).

***Wet deposition of particle-phase chemical**:*

The transfer factor for wet deposition of particle-phase chemical to the surface soil can be calculated as:

$$T_{AirP \rightarrow Ss}^{wet\_dep} = \frac{\upsilon_{wet} \times (1 - I_{wet}) \times A_{Ss}}{V_{Air}} \times f_{MS} \qquad \text{(TF 5-4)}$$

where:

$T^{wet\_dep}_{AirP \rightarrow Ss}$ transfer factor for wet deposition of particulate-bound chemical to surface soil compartment (/day);
υ_{wet} = volumetric wet deposition rate (m^3[dust]/m^2[surface soil]-day);
I_{wet} = fraction of wet deposition that is intercepted by plants (unitless) (see Equation 7-4);
A_{Ss} = area of contact between the surface soil compartment and the lowest air compartment (m^2);
V_{Air} = volume of the air compartment (m^3[air]); and
f_{MS} = mass fraction of the chemical sorbed to air particles divided by the volume fraction of the air compartment that consists of particles (unitless).

The wet deposition rate is calculated as:

$$\upsilon_{wet} = w_r \times rain \times \frac{D_L}{\rho_P} \qquad \text{(Same as Eq. 4-5)}$$

where:

w_r = washout ratio for particles in air (m^3[air]/m^3[rain]);
$rain$ = rate of rainfall (m/day);
D_L = dust load (*i.e.*, particulate matter concentration) in air (kg[dust particles]/m^3[air]); and
ρ_P = density of dust particles (kg[dust particles]/m^3[dust particles]).

5.3.3.3 Wet Deposition of Vapor-phase Chemical

Chemical vapors can be scavenged (absorbed) by the rain water and deposited to the surface soil with the rain. During rain, the advection flow of chemical from air to the upper surface soil compartment is given by:

$$\frac{dN_{Ss}}{dt} = \frac{A_{Ss}}{V_{Air}} \times rain \times \left(1 - I_{wet}\right) \times \frac{Z_{pure\_water}}{Z_{Total\_Air}} \times N_{Air} \qquad \text{(Eq. 5-24)}$$

where:

N_{Ss} = inventory of chemical in the surface soil compartment (g[chemical]);
A_{Ss} = area of the surface soil compartment (m^2[soil]);
$rain$ = rate of rainfall (m/day);
V_{Air} = volume of the air compartment (m^3[air]);
Z_{pure_water} = fugacity capacity chemical in water (excluding suspended sediments) (mol/m^3-Pa);
Z_{Total_Air} = total fugacity capacity of chemical in the air compartment (including dust particles) (mol/m^3-Pa);

I_{wet} = fraction of wet deposition that is intercepted by plants (unitless) (see Equation 7-4); and

N_{Air} = total chemical inventory in the air compartment, both vapor- and solid-phase (g[chemical]).

Therefore, the transfer factor for wet deposition of vapor-phase chemical to surface soil can be calculated as:

$$T_{Air \rightarrow Ssi}^{Vwet\_dep} = \frac{A_{Ss}}{V_{Air}} \times rain \times (1 - I_{wet}) \times \frac{Z_{pure\_water}}{Z_{Total\_Air}} \qquad \text{(TF 5-5a)}$$

where:

$T_{Air \rightarrow Ssi}^{Vwet\_dep}$ = transfer factor for wet vapor deposition from air to surface soil compartment *i* during a rainfall event (/day).

In the current TRIM.FaTE library, TF 5-5a is used for organic chemicals. For the mercury species, a slightly different algorithm is used:

$$T_{Air \rightarrow Leaf}^{Vwet\_dep} = \frac{A_{Ss}}{V_{Air}} \times w_{rV} \times rain \times \left(1 - I_{wet}\right) \times f_{MV} \qquad \text{(TF 5-5b)}$$

where:

w_{rV} = vapor washout ratio (g[chemical dissolved]/m^3[rain] per g[chemical vapor-phase]/m^3[air]) = 1/K_{AW}, where:
K_{AW} = air/water partition coefficient (g[chemical/m^3[air] per g[chemical]/m^3[water]); 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.*, fraction that is not particulate) (see Equation 2-81 in Chapter 2).

The derivation of these algorithms is explained in more detail in Chapter 7, Section 7.2.1.6.

5.3.3.4 Dry Resuspension of Dust from Soil to Air

For resuspension of dust from the first surface soil compartment to the lower compartment of the atmosphere, the chemical transfer from soil to air is given by:

$$T_{Ss \rightarrow AirP}^{res} = \frac{A_{Ss}}{V_{Ss}} \times \frac{res}{\rho_P} \times \frac{Z_{pure\_solid}}{Z_{Total\_Ss}} \qquad \text{(TF 5-6)}$$

where:

res = rate at which dust particles are resuspended from the soil surface (kg[particles]/m^2[soil surface]-day);
ρ_P = density of the dust particles (kg[particles]/m^3[particles]);
Z_{pure_solid} = fugacity capacity of chemical in dust particles (mol/m^3-Pa); and
Z_{Total_Ss} = total fugacity capacity of chemical in surface soil compartment (including dust particles) (mol/m^3-Pa).

If a value cannot be determined for *res*, then it can be estimated using the equation:

$$res = \upsilon_{dry} \times \rho_P \tag{Eq. 5-25}$$

where:

υ_{dry} = volumetric dry deposition rate (m^3[particles]/m^2[surface soil]-day).

5.3.4 VERTICAL MASS EXCHANGE BETWEEN TWO VERTICALLY ADJACENT SOIL COMPARTMENTS

The vertical exchange of a chemical substance between two vertically adjacent soil compartments occurs through advection and diffusion. Only the net advection in the downward direction is considered due to long-term infiltration of rain water. This percolation occurs only in the downward direction, and not laterally. Diffusion in the current TRIM.FaTE library is represented in both an upward and downward direction, but not horizontally. The focus is on vertical diffusion because it is assumed that the vertical transport of chemicals in soils exceeds the horizontal transport when the major source of contamination is from the air.

5.3.4.1 Vertical Diffusive Transfers

According to Equation 5-1, the concentration in each soil compartment *i* is given by:

$$C_{Si}(x) = C_{Si}(0)\exp(-\gamma_{Si}x) \tag{same as Eq. 5-1}$$

where:

x = distance into the soil compartment measured from the top of the soil column (m);
$C_{Si}(0)$ = peak chemical concentration in soil compartment *i* (g[chemical]/m^3[soil]), which is related to the total inventory N_{Si} (g[chemical]) in this soil compartment (this relationship is provided below in Equation 5-30); and
γ_{Si} = the gradient of soil concentration change in soil compartment *i* (/m), which is obtained from the inverse of the normalized or characteristic depth X^*, which is $\gamma_{Si} = 1/X^*$.

Thus, the diffusive flow at the lower boundary of soil compartment *i* to compartment *j* is given by:

$$\mathit{Diffusion\ Flow} = -A_{Sij} \times De_{Si} \times \left.\frac{dC}{dx}\right|_{d_{Si}} = A_{Sij} \times De_{Si} \times C_{Si}(0) \times \gamma_{Si} \times e^{-\gamma_{Si} \times d_{Si}} \qquad \text{(Eq. 5-26)}$$

where:

Diffusion Flow = movement of chemical mass from soil compartment *i* to *j* (g[chemical]/day);
A_{Sij} = area of interface between soil compartments *i* and *j* (m^2[interface]);
De_{Si} = effective diffusion coefficient in soil compartment *i* (m^2/day);
γ_{Si} = the gradient of soil concentration change in soil compartment *i* (/m); and
d_{Si} = the thickness of soil compartment *i* (m).

Conservation of mass requires that the flow specified by Equation 5-26 out of soil compartment *i* must equal the flow into soil compartment *j* at the upper boundary of compartment *j*, that is:

$$\mathit{Diffusion\ Flow} = -A_{Sij} \times De_{Sj} \left.\frac{dC}{dx}\right|_{0} = A_{Sij} \times De_{Sj} \times C_{Sj}(0) \times \gamma_{Sj} \qquad \text{(Eq. 5-27)}$$

where:

De_{Sj} = effective diffusion coefficient in soil compartment *ji* (m^2/day);
γ_{Sj} = the gradient of soil concentration change in soil compartment *j* (/m); and
d_{Sj} = the thickness of soil compartment *j* (m).

Combining Equations 5-26 and 5-27 gives:

$$\mathit{Diffusion\ Flow} = A_{Sij} \times \frac{\left[De_{Si} \times C_{Si}(0) \times \gamma_i \times e^{-\gamma_{Si} \times d_{Si}} + De_{Sj} \times C_{Sj}(0) \times \gamma_{Sj}\right]}{2} \qquad \text{(Eq. 5-28)}$$

$C_{Si}(0)$ is found from the condition:

$$N_{Si} = A_{Sij} \times \int_0^{d_{Si}} C_{Si}(0) \times e^{-\gamma_{Si} x} dx = A_{Sij} \times \frac{C_{Si}(0)}{\gamma_{Si}} \times \left(1 - e^{-\gamma_{Si} \times d_{Si}}\right) \qquad \text{(Eq. 5-29)}$$

where:

N_{Si} = total chemical inventory in soil compartment *i* (g[chemical]).

Rearranging gives:

$$C_{Si}(0) = \frac{N_{Si} \times \gamma_{Si}}{A_{Sij} \times \left(1 - e^{-\gamma_{Si} \times d_{Si}}\right)} \qquad \text{(Eq. 5-30)}$$

In order to conserve concentration equilibrium at the boundary between two soil compartments, the following condition must hold:

$$C_{Sj}(0) = \frac{Z_{Total\_Sj}}{Z_{Total\_Si}} \times C_{Si}(0) \times e^{-\gamma_{Si} d_{Si}} = \frac{Z_{Total\_Sj}}{Z_{Total\_Si}} \times \frac{N_{Si} \times \gamma_{Si} \times e^{-\gamma_{Si} \times d_{Si}}}{A_{Sij} \times \left(1 - e^{-\gamma_{Si} \times d_{Si}}\right)} \qquad \text{(Eq. 5-31)}$$

where:

Z_{Total_Sj} = total fugacity capacity of the chemical in soil compartment *j* (mol/m^3-Pa); and
Z_{Total_Si} = total fugacity capacity of the chemical in soil compartment *i* (mol/m^3-Pa).

Substituting Equations 5-30 and 5-31 into Equation 5-28 gives:

$$Diffusion\ Flow = \frac{N_{Si} \times \gamma_{Si}}{Z_{Total\_Si} \times \left(e^{+\gamma_{Si} \times d_{Si}} - 1\right)} \times \left(\frac{De_{Si} \times \gamma_{Si} \times Z_{Total\_Si} + De_{Sj} \times \gamma_{Sj} \times Z_{Total\_Sj}}{2}\right) \qquad \text{(Eq. 5-32)}$$

Then in order to express mass transfer between two compartments, the diffusion flow is represented in the following form:

$$Diffusion\ Flow = A_{Sij} \times Y_{Sij} \times \left(\frac{N_{Si}}{Z_{Total\_Si} \times V_{Si}} - \frac{N_{Sj}}{Z_{Total\_Sj} \times V_{Sj}}\right) \qquad \text{(Eq. 5-33)}$$

where:

N_{Sj} = the total chemical inventory in soil compartment *j* (g[chemical]);
V_{Si} = volume of soil compartment *i* (m^3);
V_{Sj} = volume of soil compartment *j* (m^3); and
Y_{Sij} = fugacity-capacity adjusted mass transfer coefficient between soil compartments *i* and *j*, mol/(m^2-Pa-day).

The total chemical inventory, N_{Sj}, in soil compartment *j*, is given by:

$$N_{Sj} = A_{Sj} \times \int_0^{d_{Sj}} C_{Sj}(0) \times e^{-\gamma_{Sj} x} dx = A_{Sj} \times \frac{C_{Sj}(0)}{\gamma_{Sj}} \times \left(1 - e^{-\gamma_{Sj} \times d_{Sj}}\right) \qquad \text{(Eq. 5-34)}$$

Substituting Equation 5-31 in Equation 5-34 gives:

$$N_{Sj} = \frac{Z_{Total\_Sj} \times N_{Si} \times \gamma_{Si} \times \left(1 - e^{-\gamma_{Sj} \times d_{Sj}}\right)}{Z_{Total\_Si} \times \gamma_{Sj} \times \left(e^{+\gamma_{Si} \times d_{Si}} - 1\right)} \qquad \text{(Eq. 5-35)}$$

An expression for Y_{Sij} is obtained by substituting Equation 5-35 for N_{Sj} in Equation 5-33 and then setting Equation 5-33 equal to Equation 5-32:

$$\begin{aligned} &\frac{N_{Si} \times \gamma_{Si}}{Z_{Total\_Si} \times \left(e^{+\gamma_{Si} \times d_{Si}} - 1\right)} \times \left(\frac{De_{Si} \times \gamma_{Si} \times Z_{Total\_Si} + De_{Sj} \times \gamma_{Sj} \times Z_{Total\_Sj}}{2} \right) = \\ &Y_{Sij} \times \frac{N_{Si}}{Z_{Total\_Si}} \times \left(\frac{1}{d_{Si}} - \frac{\gamma_{Si} \times \left(1 - e^{-\gamma_{Sj} \times d_{Sj}}\right)}{d_{Sj} \times \gamma_{Sj} \times \left(e^{+\gamma_{Si} \times d_{Si}} - 1\right)} \right) \end{aligned} \tag{Eq. 5-36}$$

Rearranging gives:

$$Y_{Sij} = \frac{(Z_{Total\_Si} \times De_{Si} \times \gamma_{Si}) + (Z_{Total\_Sj} \times De_{Sj} \times \gamma_{Sj})}{2 \times \left[\frac{(e^{+\gamma_{Si} \times d_{Si}} - 1)}{\gamma_{Si} \times d_{Si}} - \frac{(1 - e^{-\gamma_{Si} \times d_{Si}})}{\gamma_{Sj} \times d_{Sj}} \right]} \tag{Eq. 5-37}$$

The definition of Y_{Sij} in Equation 5-37 completes the definition of all terms in Equation 5-33.

For the diffusive transfer of chemical from the higher soil compartment *i* (*e.g.*, root-zone soil) to the soil compartment *j* below (*e.g.*, vadose-zone soil), the transfer factor can be calculated as follows:

$$T^{dif}_{Si \rightarrow Sj} = \frac{Y_{Sij}}{d_{Si} \times Z_{Total\_Si}} \tag{TF 5-7}$$

For the diffusive transfer of chemical from the lower soil compartment *j* (*e.g.*, vadose-zone soil) to the soil compartment *i* above (*e.g.*, root-zone soil), the transfer factor can be calculated as follows:

$$T^{dif}_{Sj \rightarrow Si} = \frac{Y_{Sij}}{d_{Sj} \times Z_{Total\_Sj}} \tag{TF 5-8}$$

Note that both TF 5-7 and TF 5-8 assume that the normalized depth of the higher soil compartment i is thinner than the lower soil compartment *j* (*i.e.*, $d_{Si} \times \gamma_{Si} < d_{Sj} \times \gamma_{Sj}$). The variable γ_{Si}, the soil penetration gradient (/m), is used to normalize depth in each soil compartment as shown above.

5.3.4.2 Downward Advective Transfer (Percolation)

The advection flow (*i.e.*, percolation) from soil compartment *i* to *j* at the lower end, d_i, of compartment *i* is given by:

$$Advection\ Flow(Si \rightarrow Sj) = A_{Sij} \times ve_i \times C_{Si}(0)\exp(-\gamma_{Si} \times d_{Si}) \tag{Eq. 5-38}$$

where:

Advection Flow = movement of chemical mass from soil compartment *i* to *j* (g[chemical]/day);
ve_i = the effective advection velocity of a chemical in the soil compartment *i* (m/day), which is equal to the rate of soil-solution movement, v_i, multiplied by the fugacity capacity of the moving phase and divided by the total fugacity capacity of soil compartment *i*:

$$ve_i = \frac{v_i \times Z_{pure\_water}}{Z_{Total\_Si}} \tag{Eq. 5-39}$$

where:

v_i = the average downward velocity of the moving phase (assumed to be water) in the soil compartment *i* (m/day).

Substituting Equation 5-30 for $C_i(0)$ in Equation 5-38 gives:

$$\frac{dN_{Sj}}{dt} = \frac{N_{Si} \times \gamma_{Si} \times ve_i}{\left(e^{+\gamma_{Si} \times d_{Si}} - 1\right)} \tag{Eq. 5-40}$$

where:

N_{Sj} = chemical inventory in soil compartment *j* (g[chemical]); and
N_{Si} = chemical inventory in soil compartment *i* (g[chemical]).

From this equation, we can derive terms for the advective transfer of chemical downward from soil compartment *i* to soil compartment *j* below as:

$$T^{perc}_{Si \rightarrow Sj} = \frac{ve_i \times \gamma_{Si}}{\left(e^{+\gamma_{Si} \times d_{Si}} - 1\right)} \tag{TF 5-9}$$

5.4 STORM-WATER RUNOFF ALGORITHMS

Horizontal transport processes included in TRIM.FaTE include runoff (Section 5.4.1) and erosion (Section 5.4.2) due to rainfall.

5.4.1 AQUEOUS-PHASE TRANSPORT PROCESSES

During a rainfall event, some of the water travels laterally across the soil as runoff. As the water travels over the soil, the concentration of the water approaches that of the soil pore water beneath it. Although the water flowing over the soil does not necessarily reach equilibrium instantaneously, some researchers use an approximation that runoff is in equilibrium with the soil pore water (Wallach et al. 1989). Currently in TRIM.FaTE, an equilibrium relationship between the runoff water and the soil pore water is used. Runoff water is considered a phase of the surface soil compartment at each spatial location. A mass-balance approach is used to determine the concentration in runoff water that moves from one surface soil compartment to a horizontally adjacent compartment.

Runoff transport is assumed to carry chemical from the surface soil compartment of one land unit to the next. During a rain event the surface soil compartment is assumed to be saturated with rain water and this water is assumed to be in equilibrium with the soil solids on the surface. It should be recognized that at times (*e.g.*, short rain events, during very dry periods of the year) the soil will not necessarily be fully saturated with rain water. However, the assumption of saturation by rain is not expected to have a large impact on results for events when the soil is not saturated. Moreover, a lack of information on the extent to which soil is saturated during rain makes this a convenient starting point. The assumption of chemical equilibrium between the surface soil water and surface soil solids has more uncertainty and needs further research.

During periods of no rain, the total fugacity capacity of the i^{th} surface soil compartment, Z_{Total_Ssi}, is given by:

$$Z_{Total\_Ssi} = \varepsilon \times Z_{pure\_air} + \theta \times Z_{pure\_water} + (1 - \phi) \times Z_{pure\_solid} \qquad \text{(Eq. 5-41)}$$

During periods of rain, when the soil becomes saturated with water, we account for the different composition of the soil by writing the fugacity capacity of the chemical in the surface soil compartment as follows:

$$Z_{Total\_Ssi} = [(Rh + \phi \times d_{Ssi}) \times Z_{pure\_water} + (1 - \phi \times d_{Ssi}) \times Z_{pure\_solid}] \times d_{Ssi} \qquad \text{(Eq. 5-42)}$$

where:

Z_{Total_Ssi} = total fugacity capacity of the chemical in the i^{th} surface soil compartment (mol/m^3-Pa);
Z_{pure_air} = fugacity capacity of chemical in air (excluding suspended particles) (mol/m^3-Pa);
Z_{pure_water} = fugacity capacity of chemical in water (excluding suspended sediments) (mol/m^3-Pa);
Z_{pure_solid} = fugacity capacity of the chemical in solid phase in the surface soil compartment (mol/m^3-Pa);
ϵ = volume fraction of the surface soil compartment that is gas (unitless);
θ = volume fraction of the surface soil compartment that is water (unitless);
ϕ = total void fraction (or porosity) in surface soil, $\phi = \epsilon + \theta$ (unitless);
Rh = hydraulic radius of the water flowing over the surface soil during a rain event (m); and
d_{Ssi} = depth of the surface soil compartment (m).

The hydraulic radius, *Rh*, for flow of water on top of the soil surface is site specific and depends on the hydraulic gradient (slope of the flow), the rainfall rate, and the recharge rate. It is considered an uncertain variable. A hydraulic balance is needed to determine the flow of the water and the depth of the runoff stream. From the Geographic Information System (GIS) data, the runoff is estimated.

Although runoff occurs only during rain events, in the current TRIM.FaTE library, it is modeled as a continuous process based on an annual average runoff value divided by 365 days. The horizontal advective flow of chemical in water from surface soil compartment *i* to adjacent compartment *j* is given by:

$$Runoff\ \ Flow\,(Ssi \rightarrow\ Ssj) = \frac{runoff \times f_{runoff}(Ssi \rightarrow\ Ssj) \times f_{avail\_runoff} \times Z_{pure\_water}}{Z_{Total\_Ssi} \times d_{Ssi}} \times N_{Ssi} \tag{Eq. 5-43}$$

where:

$Runoff\ Flow\ (Ssi \rightarrow Ssj)$ = average daily horizontal transfer of chemical carried in surface soil pore water down-gradient from surface soil compartment *i* to surface soil compartment *j* (g[chemical]/day);
$runoff$ = aereal flux of water that is transported away from surface soil compartment *i* (m^3[water]/m^2[surface soil]-day);
$f_{runoff}(Ssi \rightarrow Ssj)$ = fraction of water that runs off of surface soil compartment *i* that is transported to compartment *j* (unitless);
f_{avail_runoff} = fraction of surface soil compartment *i* that is available for runoff (unitless);
Z_{Total_Ssi} = total fugacity capacity of the chemical in the *i*th surface soil compartment (mol/m^3-Pa) as determined in Equation 5-42;
Z_{pure_water} = fugacity capacity of chemical in water (excluding suspended sediments) (mol/m^3-Pa); and
N_{Ssi} = total chemical inventory in the surface soil compartment *i* (g[chemical]).

Using substitutions for $1/d_{Ssi}$ and $Z_{pure\_water}/Z_{Total\_Ssi}$ as indicated below, Equation 5-43 is equivalent to:

$$\frac{dN_{Ssj}}{dt} = runoff \times f_{runoff}(Ssi \rightarrow\ Ssj) \times f_{avail\_runoff} \times \frac{A_{Ssi}}{V_{Ssi}} \times f_{ML} \times N_{Ssi} \tag{Eq. 5-44}$$

where:

$1/d_{Ssi}$ = A_{Ssi}/V_{Ssi} (m)*, i.e.*, the area of surface soil compartment *i* (m^2) divided by the volume of the surface soil compartment *i* (m^3);

and:

$$\frac{Z_{pure\_water}}{Z_{Total\_Ssi}} = \frac{Mass\_Fraction\_Dissolved}{Volume\_Fraction\_Liquid} = f_{ML} \qquad \text{(Eq. 5-45)}$$

as described in Chapter 2, Equation 2-80 (*i.e.*, f_{ML} equals the fraction of the mass of total chemical in surface soil compartment *i* that is dissolved in water divided by the volume fraction of the surface soil compartment that is liquid (water)) (unitless).

From Equation 5-44, the expression for $T_{Ssi \to Ssj}(runoff)$ that is in the TRIM.FaTE library can be obtained:

$$T^{runoff}_{Ssi \to Ssj} = runoff \times f_{runoff}(Ssi \to Ssj) \times f_{avail\_runoff} \times \frac{A_{Ssi}}{V_{Ssi}} \times f_{ML} \qquad \text{(TF 5-10a)}$$

$$T^{runoff}_{Ssi \to SW} = runoff \times f_{runoff}(Ssi \to SW) \times f_{avail\_runoff} \times \frac{A_{Ssi}}{V_{Ssi}} \times f_{ML} \qquad \text{(TF 5-10b)}$$

Runoff from a surface soil compartment might flow into an adjacent to a surface water (*SW*) body. The equation for that transfer is the same as for runoff to an adjacent surface soil compartment, except that the receiving compartment is the surface water compartment instead:

Finally, for a surface soil compartment adjacent to the boundary of the modeling region, runoff from the compartment can move out of the modeling region, which is modeled as a transfer to the surface soil sink (*Ss_sink*). The equation for runoff to a surface soil sink is similar to the previous equation:

$$T^{runoff}_{Ssi \to Ss\_sink} = runoff \times f_{runoff}(Ssi \to Ss\_sink) \times f_{avail\_runoff} \times \frac{A_{Ssi}}{V_{Ssi}} \times f_{ML} \qquad \text{(TF 5-10c)}$$

It is possible for all three of these different runoff algorithms to apply to a given surface soil compartment *i*. The sum of the f_{runoff} values across all of the runoff algorithms applied to the same surface soil compartment cannot exceed 1.0.

5.4.2 SOLID-PHASE TRANSPORT PROCESSES

The algorithm for erosion runoff is based on knowledge of the erosion factor for the region being modeled. Similar to solution runoff, erosion is also applied only to the surface soil layer. Although erosion is most likely to occur during rain events, erosion can be modeled as a continuous event. The flow of chemical (mol/d) from one surface soil compartment to another by erosion is represented by the following expression:

$$Erosion\ Flow\ (Ssi \to Ssj) = \frac{erosion \times f_{erosion}(Ssi \to Ssj) \times f_{avail\_erosion} \times Z_{pure\_solid} \times N_{Ssi}}{Z_{Total\_Ssi} \times \rho_P \times d_{Ssi}} \qquad \text{(Eq. 5-46)}$$

where:

Erosion Flow (Ssi → Ssj) = average daily horizontal transfer of chemical carried in surface soil particles down-gradient from surface soil compartment *i* to surface soil compartment *j* (g[chemical]/day);
erosion = erosion factor (kg[soil solids]/m^2[surface soil]-day);
$f_{erosion}(Ssi \rightarrow Ssj)$ = fraction of soil eroded from surface soil compartment *i* that is transported to surface soil compartment *j* (unitless);
$f_{avail\_erosion}$ = fraction of surface soil compartment *i* that is available for erosion (*e.g.*, not paved or otherwise covered by non-soil surfaces);
Z_{pure_solid} = fugacity capacity of chemical in the solid phase in the *i*th surface soil compartment (mol/m^3-Pa);
Z_{Total_SSi}= total fugacity capacity of chemical in the *i*th surface soil compartment (mol/m^3-Pa);
ρ_P = density of the soil particles (kg[particles]/m^3[particles]);
d_{Ssi} = depth of the surface soil compartment (m); and
N_{Ssi} = the total chemical inventory in soil compartment *i* (g[chemical]).

Substituting for $1/d_{Ssi}$ and $Z_{pure\_solid}/Z_{Total\_Ssi}$ as indicated below, Equation 5-46 is equivalent to:

$$\frac{dN_{Ssj}}{dt} = erosion \times f_{erosion}(Ssi \rightarrow Ssj) \times f_{avail\_erosion} \times \frac{A_{Ssi}}{V_{Ssi}} \times \frac{f_{MS}}{\rho_P} \times N_{Ssi} \qquad \text{(Eq.5-47)}$$

where:

$1/d_{Ssi}$ = A_{Ssi}/V_{Ssi} (m);
A_{Ssi} = area of surface soil compartment *i* (m^2);
V_{Ssi} = volume of the surface soil compartment *i* (m^3);

and:

$$f_{MS} = \frac{Z_{pure\_solid}}{Z_{Total\_Air}} = \frac{Mass\_Fraction\_Sorbed}{Volume\_Fraction\_Solid} \qquad \text{(same as Eq. 5-23)}$$

as described in Chapter 2, Equation 2-79 (*i.e.*, fraction of the mass of total chemical in surface soil compartment *i* that is sorbed to solid particles divided by the volume fraction of the surface soil compartment that is solid particles) (unitless).

From Equation 5-47, the expression for $T_{Ssi \rightarrow Ssj}(erosion)$ can be obtained:

$$T^{erosion}_{Ssi \rightarrow Ssj} = erosion \times f_{erosion}(Ssi \rightarrow Ssj) \times f_{avail\_erosion} \times \frac{A_{Ssi}}{V_{Ssi}} \times \frac{f_{MS}}{\rho_P} \qquad \text{(TF 5-11a)}$$

Erosion from a surface soil compartment might flow into an adjacent to a surface water body. The equation for that transfer is the same as for erosion to an adjacent surface soil compartment, except that the receiving compartment is the surface water body instead:

$$T_{Ssi \rightarrow SW}^{erosion} = erosion \times f_{erosion}(Ssi \rightarrow SW) \times f_{avail\_erosion} \times \frac{A_{Ssi}}{V_{Ssi}} \times \frac{f_{MS}}{\rho_P} \qquad \text{(TF 5-11b)}$$

Finally, for a surface soil compartment adjacent to the boundary of the modeling region, erosion from the compartment can move out of the modeling region, which is modeled as a transfer to the surface soil sink (*Ss_sink*). The equation for erosion to a surface soil sink is similar to the previous equation:

$$T_{Ssi \rightarrow SW}^{erosion} = erosion \times f_{erosion}(Ssi \rightarrow SW) \times f_{avail\_erosion} \times \frac{A_{Ssi}}{V_{Ssi}} \times \frac{f_{MS}}{\rho_P} \qquad \text{(TF 5-11c)}$$

It is possible for all three of these different erosion algorithms to apply to a given surface soil compartment *i*. The sum of the $f_{erosion}$ values across all of the erosion algorithms applied to the same surface soil compartment cannot exceed 1.0.

5.5 GROUND-WATER ALGORITHMS

The horizontal flow of pollutants in the saturated zone (ground water) is not expected to be a significant pathway when considering air pollutants. Downward advective transport from the vadose zone to ground water has been simulated because it is a more significant process than diffusion/dispersion. However, the relative importance of diffusive/dispersive transfer compared with advective transport between the vadose zone and the ground-water zone needs to be investigated further.

In the current version of TRIM.FaTE, ground water is modeled as a receiving compartment for percolation from the vadose zone. The same equation used to estimate the transfer of chemical via percolation from one soil compartment to another soil compartment immediately below it (*i.e.*, TF 5-9) is used to estimate the transfer factor for percolation from the vadose-zone soil (*Sv*) compartment to ground water (*GW*):

$$T_{Sv \rightarrow GW} = \frac{ve_{Sv} \times \gamma_{Sv}}{\left(e^{+\gamma_{Sv} \times d_{Sv}} - 1\right)} \qquad \text{(TF 5-12)}$$

where:

$T_{Sv \rightarrow GW}$ = transfer factor from vadose-zone soil to ground water (/day);
ve_{Sv} = the effective advection velocity of a chemical in the vadose-zone soil compartment (m/day), which is equal to the rate of soil-solution movement, v_i, multiplied by the fugacity capacity of the moving phase

(water) and divided by the total fugacity capacity of the vadose-zone soil compartment;

γ_{Sv} = the gradient of soil concentration change in the vadose-zone soil compartment (/m); and

d_{Sv} = thickness of vadose-zone soil compartment (m).

The transfer factor from ground water to surface water is based on aqueous-phase advection only. It can be calculated as:
where:

$T_{GW \rightarrow SW}$ = transfer factor from ground-water to surface-water compartments (/day);

A_{SWGW} = interfacial area between the surface-water and ground-water compartments (m^2);

V_{GW} = volume of the ground-water compartment (m^3);

Z_{pure_water} = fugacity capacity of the chemical in pure water (mol/m^3-Pa);

Z_{Total_GW} = total fugacity capacity of the chemical in the ground-water compartment (mol/m^3-Pa);

recharge = annual average daily recharge from ground water into surface water (m/day); and

$$T_{GW \rightarrow SW} = \frac{A_{SWGW}}{V_{GW}} \times \frac{Z_{pure\_water}}{Z_{Total\_GW}} \times recharge \qquad \text{(TF 5-13a)}$$

$$= \frac{A_{SWGW}}{V_{GW}} \times f_{ML} \times recharge \qquad \text{(TF 5-13b)}$$

f_{ML} = $Z_{pure\_water}/Z_{Total\text{-}GW}$, which equals *Mass_Fraction_Dissolved / Volume_Fraction_Liquid* (*i.e.*, fraction of the mass of total chemical in the ground-water compartment that is dissolved in water divided by the volume fraction of the ground-water compartment that is liquid water, see Equations 2-72 and 2-80) (unitless).

[This page intentionally left blank.]

6. AQUATIC BIOTA ALGORITHMS

In this chapter, algorithms for transfers among aquatic biotic compartment types and other biotic or abiotic compartment types are presented. The aquatic biotic components include algae, macrophytes, benthic invertebrates, and several trophic groups of fish. The transfer factor algorithms are based on diffusive or advective transfer.

Most of the algorithms in this chapter apply to all air pollutants, although some are applicable only to mercury species and others that involve octanol-water partition coefficients are only applicable to nonionic organic chemicals. Some of the equations represent dynamic processes, while others are simple models for which a time-to-equilibrium is calculated. The text box on the next page and continued on the following pages provides a summary of the transfer-factor algorithms developed in this chapter and defines all parameters used in those algorithms. The derivation of chemical-specific algorithms and input parameters is presented in Appendix A for mercury and in Appendix B for polyaromatic hydrocarbons (PAHs).

The remainder of this chapter is organized in four sections. Section 6.1 briefly discusses the process of selecting aquatic compartments for use in a TRIM.FaTE scenario. Section 6.2 addresses algorithms associated with aquatic plants. Section 6.3 covers the algorithms for benthic infauna (animals living in sediment), which are represented in the current TRIM.FaTE library by a single compartment type. Section 6.4 develops and describes the transfer factor algorithms associated with the fish compartments.

6.1 AQUATIC BIOTA COMPARTMENT TYPES

The aquatic compartments in the current TRIM.FaTE library are listed in the text box to the right. Trophic level 1, the primary producers, are represented by algae[1] and macrophytes. The 2nd trophic level is represented by herbivorous fish and benthic infauna, while the 3rd and 4th levels are represented by two fish trophic levels (omnivores, that might feed on a combination of plant and animal material, and carnivores).

Use of aquatic biotic compartment types in a TRIM.FaTE scenario is described in Section 3.2.2 of TRIM.FaTE TSD Volume I. Additional guidance on how to select aquatic biota for compartments is provided in more detail in the TRIM.FaTE user guidance.

AQUATIC BIOTA COMPARTMENT TYPES

Algae (actually represented as a phase of the surface water)
Macrophyte
Water column herbivore (fish)
Water column omnivore (fish)
Water column carnivore (fish)
Benthic herbivore (invertebrate)
Benthic omnivore (fish)
Benthic carnivore (fish)

---

[1] Algae are represented as a phase of the surface water compartment than as a separate compartment.

Summary of Transfer Factors for Aquatic Biota in TRIM.FaTE

AQUATIC PLANT AND BENTHIC INVERTEBRATE TRANSFERS

Surface water to macrophytes (nonionic organic chemicals): F 6-1a

$$T_{SW \rightarrow Mp} = \frac{k_{Mp,acc-W} \times V_{Mp}}{V_{SW}} \times f_{ML} \quad \text{where} \quad k_{Mp,acc-W} = \text{Eq. 6-3}$$

Macrophytes to surface water (nonionic organic chemicals): TF 6-2a

$$T_{Mp \rightarrow SW} = k_{Mp,dep-W} \quad \text{where} \quad k_{Mp,dep-W} = \text{Eq. 6-4}$$

Surface water to macrophytes (other chemicals): TF 6-1b

$$T_{SW \rightarrow Mp} = \left[\frac{-\ln(1-\alpha)}{t_{\alpha}^{MpW}}\right] \times \frac{K_{Mp-W} \times V_{Mp} \times \rho_{Mp} \times 1}{V_{SW}} \times f_{ML}$$

Macrophytes to surface water (other chemicals): TF 6-2b

$$T_{Mp \rightarrow SW} = \frac{-\ln(1-\alpha)}{t_{\alpha}^{MpW}}$$

Sediment water (interstitial or overlying) to benthic invertebrates: TF 6-3a

$$T_{SedW \rightarrow BI} = \frac{n_{BI} \times m_{BI} \times k_{BI,\ acc-SedW}}{V_{Sed}} \times f_{ML}$$

Benthic invertebrates to sediment water (interstitial or overlying): TF 6-4a

$$T_{BI \rightarrow SedW} = k_{BI,\ dep-SedW}$$

Bulk sediment to benthic invertebrates: TF 6-3b

$$T_{Sed \rightarrow BI} = \frac{n_{BI} \times m_{BI} \times k_{BI,\ acc-Sed}}{V_{Sed} \times \rho_{Sed}}$$

Benthic invertebrates to bulk sediment: TF 6-4b

$$T_{BI \rightarrow Sed} = k_{BI,\ dep-Sed}$$

FISH TRANSFERS

Gill uptake by fish, bioenergetic-based kinetic model: TF 6-5

$$T_{SW \rightarrow fish}^{gill} = \frac{n_f \times m_f \times k_u}{V_{SW}} \times f_{ML} \times 1000$$

Summary of Transfer Factors for Aquatic Biota in TRIM.FaTE (cont.)

FISH TRANSFERS (cont.)

Ingestion with food by fish, bioenergetic-based kinetic model: TF 6-6

$$T_{diet \rightarrow fish} = \frac{n_f \times m_f}{n_{diet} \times m_{diet}} \times IN_D \times AE_D$$

Ingestion with algae by water column herbivorous fish, bioenergetic-based kinetic model: TF 6-7

$$T_{Algae \rightarrow Fwch} = \frac{n_{Fwch} \times m_{Fwch}}{\left(f_{MA} / m_{Algae}\right)} \times IN_D \times p_{Algae} \times AE_D$$

Fish excretion to surface water via gills, feces, and urine, bioenergetic-based kinetic model: TF 6-8

$$T_{fish \rightarrow SW}^{excretion} = k_E$$

Ingestion with food by fish, time-to-equilibrium-based kinetic model : TF 6-9

$$T_{diet \rightarrow fish} = \frac{n_f \times m_f}{n_{diet} \times m_{diet}} \times \left[\frac{-\ln(1-\alpha)}{t_{\alpha}^{fd}}\right] \times K_{fish-diet}$$

Ingestion with algae by herbivorous water column fish, time-to-equilibrium-based kinetic model: TF 6-10

$$T_{Algae \rightarrow Fwch} = \frac{n_{Fwch} \times m_{Fwch}}{(f_{MA} / m_{Algae})} \times \left[\frac{-\ln(1-\alpha)}{t_{\alpha}^{FwchAl}}\right] \times K_{Fwch-Algae}$$

Transfer from fish compartment to diet compartment, time-to-equilibrium-based kinetic model: TF 6-11

$$T_{fish \rightarrow diet} = \left[\frac{-\ln(1-\alpha)}{t_{\alpha}^{fd}}\right]$$

LIST OF SYMBOLS USED IN AQUATIC BIOTA TRANSFER FACTORS

V_{Mp} = volume of the macrophyte compartment (L).
$k_{Mp,\ acc\text{-}W}$ = bioaccumulation rate constant for macrophyte in water (/day).
V_{SW} = volume of the surface water compartment (L).
f_{ML} = fraction chemical mass dissolved divided by volume fraction of compartment that is liquid *i.e.,* water (unitless).
$k_{Mp,\ dep\text{-}W}$ = depuration rate constant for macrophyte in water (/day).
n_{BI} = number of organisms comprising the benthic invertebrate compartment (unitless).
m_{BI} = average mass per individual benthic invertebrate (kg[invertebrate wet wt]/individual).
$k_{BI,\ acc\text{-}SedW}$ = benthic invertebrate uptake rate constant from interstitial water in sediment compartment (/day).

Summary of Transfer Factors for Aquatic Biota in TRIM.FaTE (cont.)

LIST OF SYMBOLS USED IN AQUATIC BIOTA TRANSFER FACTORS (cont.)

$k_{BI,\ dep\text{-}SedW}$ = benthic invertebrate depuration rate constant to interstitial water in the sediment compartment (/day).
$k_{BI,\ acc\text{-}Sed}$ = benthic invertebrate uptake rate constant from bulk sediment (/day).
ρ_{Sed} = bulk density of sediment (kg[sediment wet wt]/m^3[sediment]).
$k_{BI,\ dep\text{-}Sed}$ = benthic invertebrate depuration rate constant to bulk sediment (/day).
n_f = number of fish in fish compartment (unitless).
m_f = mass per individual fish (kg[fish wet wt]/individual).
k_u = fish gill uptake rate constant for chemical dissolved in water (/day).
n_{diet} = number of individuals in diet compartment (unitless).
m_{diet} = mass per individual in diet compartment (kg[organism]/individual).
IN_D = food (diet) ingestion rate for fish (kg[food wet wt]/kg[fish wet wt]-day).
AE_D = assimilation efficiency of chemical from the diet (unitless).
f_{MA} = fraction of chemical mass in surface water compartment that is in the algal phase (unitless).
n_{Fwch} = number of water column herbivorous fish in that fish compartment (unitless).
m_{Fwch} = mass per individual water column herbivorous (kg[fish wet wt]/individual).
m_{Algae} = total mass of algae in the surface water compartment (kg[algae wet wt]).
p_{Algae} = proportion of total fish diet that consists of algae on a wet-weight basis (unitless).
k_E = total chemical excretion rate constant (/day).
α = proportion of equilibrium value reached (default = 0.95).
t_α = time to reach $100\times\alpha$ percent of equilibrium value (days).
$K_{fish\text{-}diet}$ = fish/diet partition coefficient (kg[diet wet wt]/kg[fish wet wt]).
$K_{Fwch\text{-}Algae}$ = fish(water column herbivore)/algae partition coefficient (kg[algae wet wt]/kg[fish (water column herbivore) wet wt]).

6.2 AQUATIC PLANTS

Aquatic vegetation is included as two separate components, algae (modeled as a phase of surface water in the current TRIM.FaTE library) and macrophytes (modeled as a separate compartment). Water is assumed to be the primary source of chemical to both vegetation types, and thus, uptake from water is the only pathway for which algorithms are currently included in the TRIM.FaTE library.

6.2.1 ALGAE

As mentioned previously, algae are modeled as a phase of the surface water compartment.[2] For modeling transfer of dissolved chemical from surface water to algae for nonionic organic chemicals or chemicals for which empirically based partition coefficients are available, Equation 4-24 can be used. A more detailed approach has been developed for mercury (see section A.1.2 of Appendix A), and is available in the current TRIM.FaTE library.

---

[2] The surface water compartment consists of three phases: liquid (dissolved), solid (particles), and algae.

6.2.2 MACROPHYTES

Although rooted macrophytes can derive some nutrients and chemicals from sediments, direct uptake from water is the primary pathway (Ribeyre and Boudou 1994). Transfers of chemical between macrophytes and surface water are described in Section 6.2.2.1. Limited chemical transformation by macrophytes is described in Section 6.2.2.2.

6.2.2.1 Transfers Between Macrophytes and Surface Water

Net uptake of chemicals dissolved in surface water by aquatic macrophytes (only the dissolved portion of the chemical is available for bioaccumulation by macrophytes) is given by the following concentration-based equation for the chemical flux rate:

$$Flow_{Mp} = \left(k_{Mp,acc-W} \times V_{Mp} \times \rho_{Mp} \times C_{SW} \times f_{ML}\right) - \left(k_{Mp,\,dep-W} \times V_{Mp} \times \rho_{Mp} \times C_{Mp}\right) \qquad \text{(Eq. 6-1)}$$

where:

$Flow_{Mp}$ = net flow of chemical into the macrophyte (g[chemical]/day);
$k_{Mp,\,acc\text{-}W}$ = macrophyte bioaccumulation rate constant from water (/day);
V_{Mp} = volume of the macrophyte compartment (L[macrophyte]);
ρ_{Mp} = density of macrophyte (kg[macrophyte wet wt]/L[macrophyte]);
C_{SW} = total chemical concentration in surface water (g[chemical]/L[bulk water]);
f_{ML} = mass fraction of chemical dissolved in surface water (unitless) divided by the volume fraction of the surface water compartment that is liquid, *i.e.*, water, (unitless, value close to 1.0), *i.e.*, *Fraction_Mass_Dissolved / Volume_Fraction_Liquid* (see Equations 2-72 and 2-80);
$k_{Mp,\,dep\text{-}W}$ = macrophyte depuration rate constant to water (/day); and
C_{Mp} = chemical concentration in macrophyte (g[chemical]/L[macrophyte wet wt]).

Note that:

$$Volume\_Fraction\_Liquid = 1 - \left(Vf_{SSed} + Vf_{Algae}\right) \qquad \text{(Eq. 6-2)}$$

where:

Vf_{SSed} = volume fraction of the surface water compartment that is suspended solid sediment particles (unitless); and
Vf_{Algae} = volume fraction of the surface water compartment that is algae (unitless).

The rate constants $k_{Mp,\,acc\text{-}SW}$ and $k_{Mp,\,dep\text{-}SW}$, for nonionic organic chemicals are estimated using the following equations (Gobas et al. 1991):

$$\frac{1}{k_{Mp,\,acc-W}} = 0.0020 + \frac{500}{K_{ow}} \qquad \text{(Eq. 6-3)}$$

$$1/k_{Mp,\,dep-W} = 1.58 + 0.000015\ K_{ow} \qquad \text{(Eq. 6-4)}$$

where:

K_{ow} = the octanol-water partitioning coefficient for the chemical (g[chemical]/kg[octanol] per g[chemical]/L[water] = L[water]/kg[octanol] or kg[water]/kg[octanol]).

The rate constants $k_{Mp,\,acc-W}$ and $k_{Mp,\,dep-W}$ for chemicals other than nonionic organic pollutants were derived from bioconcentration factors using the time-to-equilibrium conversion (see Section 2.5) as follows:

$$k_{Mp,\ acc-W} = \left[\frac{-\ln(1-\alpha)}{t_{\alpha}^{MpW}}\right] \times K_{Mp-W} \qquad \text{(Eq. 6-5)}$$

$$k_{Mp,\,dep-W} = \frac{-\ln(1-\alpha)}{t_{\alpha}^{MpW}} \qquad \text{(Eq. 6-6)}$$

where:

t_{α}^{MpW} = time (days) required to reach 100×α percent of the macrophyte/water interaction equilibrium when the concentration in water is approximately constant with time;
α = fraction of equilibrium value attained (default = 0.95) (unitless); and
K_{Mp-W} = macrophyte/water partition coefficient (g[chemical]/kg[macrophyte] per g[chemical]/L[water] = L[water]/kg[macrophyte] or L[water]/L[macrophyte] assuming that the density of macrophytes equals that of water).

The transfer of chemical mass from water to the macrophyte is given by:

$$\frac{dN_{Mp}}{dt} = \left(k_{Mp,\,acc-W} \times f_{ML} \times V_{Mp} \times \rho_{Mp} \times \frac{N_{SW}}{V_{SW}}\right) - \left(k_{Mp,\,dep-W} \times N_{Mp}\right) \qquad \text{(Eq. 6-7)}$$

where:

N_{Mp} = mass of chemical in the macrophyte (g[chemical]);
V_{Mp} = volume of the macrophyte (L);
N_{SW} = mass of chemical in the surface water compartment (g[chemical]); and
V_{SW} = volume of the surface water compartment (L[water]).

In the current TRIM.FaTE library, the chemical transfer factors for nonionic organic chemicals from water to macrophytes and for macrophytes to water are given by:

$$T_{SW \rightarrow Mp} = \frac{k_{Mp,\, acc-W} \times V_{Mp} \times \rho_{Mp}}{V_{SW}} \times 1 \times f_{ML}$$

$$= \frac{k_{Mp,\, acc-W} \times V_{Mp}}{V_{SW}} \times f_{ML} \qquad \text{(TF 6-1a)}$$

and:

$$T_{Mp \rightarrow SW} = k_{Mp,\, dep-W} \qquad \text{(TF 6-2a)}$$

where:

$T_{SW \rightarrow Mp}$ = transfer factor from surface water to macrophyte (/day);
ρ_{Mp} = wet density of macrophyte (kg[macrophyte wet wt]/L[macrophyte] equals same density as water, *i.e.*, 1 kg/L);
1 = unit conversion factor (L[water]/kg[water]); and
$T_{Mp \rightarrow SW}$ = transfer factor from macrophyte to surface water (/day).

The macrophyte/surface water transfer factors for other chemicals, including mercury, use Equations 6-5 and 6-6 to replace the rate constants $k_{Mp,\, acc-W}$ and $k_{Mp,\, dep-W}$ in TFs 6-1a and 6-2a. Thus, the transfer factors for other chemicals, including mercury, are:

$$T_{SW \rightarrow Mp} = \left[\frac{-\ln(1-\alpha)}{t_{\alpha}^{MpW}} \right] \times \frac{K_{Mp-W} \times V_{Mp} \times \rho_{Mp} \times 1}{V_{SW}} \times f_{ML} \qquad \text{(TF 6-1b)}$$

$$T_{Mp \rightarrow SW} = \frac{-\ln(1-\alpha)}{t_{\alpha}^{MpW}} \qquad \text{(TF 6-2b)}$$

6.2.2.2 Transformation and Degradation

Although the TRIM.FaTE library supports macrophyte transformation of mercury species (see below), it does not currently accommodate biodegradation of any chemicals (*i.e.*, transformation into chemicals that are not tracked in TRIM.FaTE) in macrophytes.

Biotransformation of elemental to divalent mercury in macrophytes is included in the TRIM.FaTE library and is described as a rapid (almost instantaneous) first-order rate constant (*i.e.*, 10^6 to 10^9). This is assumed because elemental mercury can be taken up by macrophytes but is not accumulated in macrophytes in the elemental form (*i.e.*, data showing Hg(0) in macrophytes were not found). Because data demonstrating methylation of divalent mercury or demethylation of methylmercury in macrophytes were not found, those transformations are not included for macrophytes in the current TRIM.FaTE library.

6.3 BENTHIC INFAUNA

The benthic community is typically comprised of many different classes and species of organisms, including those from the phyla Mollusca (*e.g.*, clams and snails), Annelida (*e.g.,* oligochaete worms), and Arthropoda (*e.g.*, crustaceans and larval insects). Several trophic levels are represented within this community. That is true even within some families of insects, such as the mayflies and chironomids. In the current TRIM.FaTE library, benthic infauna are considered to represent the lowest heterotrophic level of the benthic food chain, which includes those species that feed on algae and/or detritus, which is assumed to be derived largely from plant material.

An explicit dietary uptake component is not practical, given the highly variable diet among benthic infauna. Rather, uptake is modeled based on the extraction of chemical from water (interstitial or overlying) or bulk sediment. It should be noted that at this time only one chemical source (water or bulk sediment) is considered for a given chemical. Selection of the primary source of contamination is chemical dependent. Neutral organic chemicals (*e.g.*, PAHs) are typically evaluated based on uptake from water. If interstitial water is used, the results often are considered representative of total sediment exposures. Uptake of metals (*e.g.*, mercury) is based on uptake data from bulk sediments. Sediment chemical concentrations are not apportioned to separate inorganic and organic (living and detrital matter) compartments in TRIM.FaTE. Thus, uptake from sediment implicitly includes transfers from algal and detrital matter to the benthic invertebrate herbivores.

Algorithms describing the general case for uptake of chemicals by benthic invertebrates from sediment interstitial (*i.e*., pore) water are presented in Section 6.3.1. The chemicals to which these algorithms apply are those for which the measured partition coefficient between sediments and benthic invertebrates is based on the chemical concentration in sediment water only, not bulk sediment. An algorithm specific to PAHs that is available in the TRIM.FaTE library is described in Appendix B. Algorithms for chemicals for which the measured partition coefficient is based on bulk sediment rather than sediment pore water (*e.g.*, mercury) are presented in Section 6.3.2.

6.3.1 TRANSFERS BETWEEN SEDIMENT INTERSTITAL WATER AND BENTHIC INVERTEBRATES

Uptake of chemical by benthic invertebrates from sediment pore water is given by the following equation:

$$\frac{dC_{BI}}{dt} = \left(k_{BI,\,acc-W} \times C_{WD}\right) - \left(k_{BI,\,dep-W} \times C_{BI}\right) \qquad \text{(Eq. 6-8)}$$

where:

C_{BI} = chemical concentration in benthic invertebrates (g[chemical]/kg[invertebrates wet wt]);
C_{WD} = chemical concentration in liquid phase of sediment (*i.e.*, sediment pore water) (g[chemical dissolved]/L[water]);
$k_{BI,\,acc\text{-}W}$ = uptake rate constant for chemical from water (/day); and
$k_{BI,\,dep\text{-}W}$ = depuration rate constant for chemical to water (/day).

The rate constants $k_{BI,acc\text{-}W}$ and $k_{BI,dep\text{-}W}$ are derived from the bioconcentration factors using the time-to-equilibrium conversion described in Section 2.5:

$$k_{BI,\,acc-W} = \left[\frac{-\ln(1-\alpha)}{t_{\alpha}^{BIW}}\right] \times K_{BI-W} \qquad \text{(Eq. 6-9)}$$

$$k_{BI,\,dep-W} = \frac{-\ln(1-\alpha)}{t_{\alpha}^{BIW}} \qquad \text{(Eq. 6-10)}$$

where:

t_{α}^{BIW} = time (days) required to reach 100×α percent of the benthic invertebrate/water interaction equilibrium when the concentration in water is approximately constant with time;
α = fraction of equilibrium attained (default = 0.95) (unitless); and
$K_{BI\text{-}W}$ = benthic invertebrate/sediment pore water partition coefficient (L[water]/ kg[invertebrates wet wt]).

Converting to mass units (N) yields the following equation:

$$\frac{dN_{BI}}{dt} = \left(n_{BI} \times m_{BI} \times k_{BI,\,acc-W} \times \frac{N_{WD}}{V_W}\right) - \left(k_{BI,\,dep-W} \times N_{BI}\right) \qquad \text{(Eq. 6-11)}$$

where:

N_{BI} = mass of chemical in organisms comprising the benthic invertebrate compartment (g[chemical]);
n_{BI} = number of organisms comprising the benthic invertebrate compartment (unitless);
m_{BI} = average mass per individual benthic invertebrate (kg[invertebrates wet wt]/individual);
N_{WD} = mass of dissolved chemical in sediment compartment (g[chemical dissolved]);
V_W = volume of water in the sediment compartment (L) = $V_{Sed} \times \theta$, where:
  V_{Sed} = volume of sediment compartment (L); and
  θ = *Volume_Fraction_Liquid* (water) (unitless); *i.e.*:

= ϕ, the total porosity of the sediment compartment (unitless) (see Eq. 2-39; volume fraction gas assumed to be zero for sediments).

It is also true that:

$$N_{WD} = N_{Sed} \times Fraction\_Mass\_Dissolved \tag{Eq. 6-12}$$

where:

N_{Sed} = total mass of chemical in sediment compartment (g[chemical]); and
Fraction_Mass_Dissolved = fraction of chemical mass in sediment compartment that is dissolved in the water phase (unitless).

Thus, the transfer factors for water (interstitial or immediately overlying) to benthic invertebrates and for benthic invertebrates to water are given by:

$$\begin{aligned} T_{SedW \rightarrow BI} &= \frac{n_{BI} \times m_{BI} \times k_{BI,\,acc-SedW}}{V_{Sed}} \times \frac{Fraction\_Mass\_Dissolved}{\theta} \\ &= \frac{n_{BI} \times m_{BI} \times k_{BI,\,acc-SedW}}{V_{Sed}} \times f_{ML} \end{aligned} \tag{TF 6-3a}$$

$$T_{BI \rightarrow SedW} = k_{BI,dep-W} \tag{TF 6-4a}$$

where:

$T_{SedW \rightarrow BI}$ = transfer factor for chemical dissolved in sediment pore water to benthic invertebrate (/day);
$T_{BI \rightarrow SedW}$ = transfer factor for chemical from benthic invertebrate to the water phase of the sediment compartment (/day); and
f_{ML} = mass fraction of chemical dissolved in sediment pore water (unitless) divided by the volume fraction of the surface water compartment that is liquid, *i.e.*, water (unitless); which
= *Fraction_Mass_Dissolved/*θ*,* which
= *Fraction_Mass_Dissolved/Volume_Fraction_Liquid* (see Equation 2-80).

The designation of these two transfer factors as “a” indicates that they are to be used together for chemicals for which the partitioning coefficient applies to the water phase only of the sediment compartment (*e.g.*, nonionic organic chemicals). The alternative pair of transfer factor algorithms designated as TF 6-3b and TF 6-4b are for use with partitioning coefficients derived from bulk sediments (*e.g.*, for metals), as described in Section 6.3.2.

Note that for organic chemicals categorized as PAHs, specific algorithms for transfers between benthic invertebrates and sediments have been developed as described in Appendix B.

6.3.2 TRANSFERS BETWEEN BULK SEDIMENT AND BENTHIC INVERTEBRATES

Uptake of chemicals by benthic invertebrates from bulk sediment (*e.g.*, mercury) is given by the following equation:

$$\frac{dC_{BI}}{dt} = \left(k_{BI,\,acc-Sed} \times C_{Sed}\right) - \left(k_{BI,\,dep-Sed} \times C_{BI}\right) \qquad \text{(Eq. 6-13)}$$

where:

C_{BI} = chemical concentration in benthic invertebrates (g[chemical]/kg[invertebrates wet wt]);
C_{Sed} = chemical concentration in bulk sediments (g[chemical]/kg[sediment wet wt]);
$k_{BI,\ acc-Sed}$ = benthic invertebrate uptake rate constant from sediment (/day); and
$k_{BI,\ dep-Sed}$ = benthic invertebrate depuration rate constant to sediment (/day).

The rate constants $k_{BI,\ acc-Sed}$ and $k_{BI,\ dep-Sed}$ are derived from bioconcentration factors using the time-to-equilibrium conversion (see Section 2.5):

$$k_{BI,\,acc-Sed} = \left[\frac{-\ln(1-\alpha)}{t_{\alpha}^{BISed}}\right] \times K_{BI-Sed} \qquad \text{(Eq. 6-14)}$$

$$k_{BI,\,dep-Sed} = \frac{-\ln(1-\alpha)}{t_{\alpha}^{BISed}} \qquad \text{(Eq. 6-15)}$$

where:

$K_{BI\text{-}Sed}$ = benthic invertebrate/bulk sediment partition coefficient (kg[sediment wet wt]/kg[invertebrates wet wt]);
t_{α}^{BISed} = time (days) required to reach 100×α percent of the benthic invertebrate/bulk sediment interaction equilibrium value when the concentration in water is approximately constant with time; and
α = fraction of equilibrium attained (default = 0.95) (unitless).

Converting to mass units (N) yields the following equation:

$$\frac{dN_{BI}}{dt} = \left(n_{BI} \times m_{BI} \times k_{BI,\,acc-Sed} \times \frac{N_{Sed}}{V_{Sed} \times \rho_{Sed}}\right) - \left(k_{BI,\,dep-Sed} \times N_{BI}\right) \qquad \text{(Eq. 6-16)}$$

where:

N_{BI} = mass of chemical in organisms comprising the benthic invertebrate compartment (g[chemical]);

n_{BI} = number of organisms comprising the benthic invertebrate compartment (unitless);
m_{BI} = average mass per individual benthic invertebrate (kg[invertebrate wet wt]/individual);
N_{Sed} = total mass of chemical in sediment compartment (g[chemical]);
V_{Sed} = volume of sediment compartment (L[sediment]); and
ρ_{Sed} = bulk density of sediment (kg[sediment wet wt]/L[sediment]).

Thus, the transfer factors for bulk sediment to benthic invertebrates and for benthic invertebrates to bulk sediment are given by:

$$T_{Sed \rightarrow BI} = \frac{n_{BI} \times m_{BI} \times k_{BI,\,acc-Sed}}{V_{Sed} \times \rho_{Sed}} \qquad \text{(TF 6-3b)}$$

$$T_{BI \rightarrow Sed} = k_{BI,\,dep-Sed} \qquad \text{(TF 6-4b)}$$

where:

$T_{Sed \rightarrow BI}$ = transfer factor for chemical in bulk sediment to benthic invertebrates (/day); and
$T_{BI \rightarrow Sed}$ = transfer factor for chemical in benthic invertebrates to the bulk sediment (/day).

For a given chemical, the user would specify either algorithms TF 6-3a and TF 6-4a (or, for PAHs, algorithms TF B-1 and TF B-2 from Appendix B) or algorithms TF 6-3b and TF 6-4b, but not both. The most appropriate algorithm depends on whether the available data on the partition coefficients were measured with respect to water only (*e.g.*, sediment pore water) or with respect to bulk sediments.

6.3.3 TRANSFORMATIONS AND DEGRADATION

Metabolic transformations of chemicals into different compounds that are tracked in TRIM.FaTE (*e.g.*, mercury species) can be included for biotic compartments. However, biotransformation from one chemical to another that is tracked in TRIM.FaTE is not included for benthic invertebrates in the current TRIM.FaTE library. Appropriate transformation rate data were not identified during initial applications of the model.

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 metabolic degradation of chemicals is determined from the user-input value for the half-life of the chemical in the benthic invertebrate compartment. The algorithm relating the general degradation rate constant to the chemical half-life in a compartment is presented in Chapter 2 (Equation 2-64), and the transfer factor is TF 2-1. The metabolic half-life reflects metabolic degradation only, and not excretion or elimination of the parent chemical to the sediment compartment.

6.4 FISH

The current TRIM.FaTE library includes two alternate approaches to estimate chemical uptake by fish: a bioenergetic-based kinetic model or a time-to-equilibrium-based kinetic model. Each model has strengths and weaknesses, which may weigh differently for different chemicals. The bioenergetic-based model is ideal for explicitly incorporating multiple exposure pathways, but finding data to assign values to some of the fish parameters may be difficult (*e.g.*, gill and fecal elimination rates). Data to set parameter values for the time-to-equilibrium-based kinetic model are generally available, but multiple pathways cannot be incorporated explicitly at the same time and the time required to reach equilibrium may be uncertain for strongly bioaccumulated chemicals. In applications to date, the bioenergetic model has been parameterized for PAHs and mercury, whereas the time-to-equilibrium model is parameterized for mercury only.

In comparison to the time-to-equilibrium model, the bioenergetic model provides the user greater flexibility in the specification of the fish compartments and associated diets for a given scenario. For example, the user may employ the five fish compartments currently available in the TRIM.FaTE library, assigning their diets as deemed appropriate to the modeling scenario, or the user may develop a different "set" of trophic compartments and diets to represent the fish community in a particular water body. For each fish compartment, the user can assign more than one diet item (*e.g.*, 20 percent of the diet consists of benthic invertebrates, 70 percent is benthic omnivorous fish, and 10 percent consists of omnivorous fish in the water column), creating a web-like set of trophic relationships, with some fish feeding from more than one trophic level or microenvironment. This approach is essentially the same as that used to model exposure via food ingestion for terrestrial wildlife (see Section 7.4). This approach is described in Subsection 6.4.1 below.

Another approach which has been used in initial TRIM.FaTE applications with both of the two bioaccumulation models, but which is particularly suited to the time-to-equilibrium model (which was developed to use input derived from measured chemical concentrations in fish at different trophic levels in the same water body) involves the adherence to a strict stepwise trophic structure with separate benthic and water column derived food chains. In this design, the existing five fish compartment types are presented as two separate food chains, one for water-column organisms and one for benthic organisms (see the conceptual model in Figure 4-1 of TSD Volume I), with each fish compartment feeding on only the compartment below it in the food chain. That is, water-column carnivores would consume only water-column omnivores, water-column omnivores consume only water-column herbivores (planktivores), water-column herbivores consume only algae (phytoplankton), benthic carnivores consume only benthic omnivores, and benthic omnivores consume only benthic invertebrates. In this type of design, both the benthic invertebrate (*i.e.*, feeding on algae and detritus, which is derived largely from plant material) and the herbivore compartments might be considered equivalent to trophic-level-2 organisms of other models (*e.g.*, Gobas 1993, Ambrose *et. al.* 1995). The "omnivore"compartments might be considered equivalent to the trophic-level-3 fish, and the carnivore compartments equivalent to the trophic-level-4 fish of the other models.

In initial TRIM.FaTE applications, a littoral food web (*i.e.*, including linkages between water-column and benthic food chains) was created from the linear benthic and pelagic food chain design described above by representing individual species as a combination of multiple compartments. For example, a given carnivore (*e.g.*, largemouth bass) may consume omnivores from both the water column and the benthos (*e.g.*, consume 50 percent water-column omnivores and 50 percent benthic omnivores). This diet can be accounted for in the simulation by assigning 50 percent of the bass biomass to each food chain (*i.e.,* 50 percent to the water-column carnivore and 50 percent to benthic carnivore compartments). The mass of fish to be assigned to each trophic level within each food chain may thus be derived from studies of the biomass of individual species in various aquatic ecosystems and studies of feeding strategies of those species. This method is described in detail in Subsection 6.4.2 below. When this approach is employed, interpretation of the model results with regard to individual species requires revisiting these data and calculations.

Regardless of the bioaccumulation model or food chain design employed, the entire fish biomass in the surface water body being modeled should be distributed among the modeled compartments. This will facilitate "realistic" partitioning of the modeled chemical within the biotic and abiotic compartments of the aquatic ecosystem. In addition, the relative distribution of biomass among the different fish compartment types should be as realistic as possible.

6.4.1 BIOENERGETIC-BASED KINETIC MODEL

This section describes the bioenergetic-based kinetic model for fish developed for use in TRIM.FaTE. First, the development of the full model is described (Section 6.4.1.1). Next, specific adaptations of the general model for nonionic organic chemicals (Section 6.4.1.2) and mercury (Section 6.4.1.3) are described. Then the equations for the transfer factor algorithms in the TRIM.FaTE library are presented (Section 6.4.1.4). Section 6.4.1.5 describes the TRIM.FaTE algorithms for chemical transformation and degradation by fish.

6.4.1.1 General Model

The following model for estimating chemical concentrations in fish is based on the model developed by Thomann (1989) and used in the derivation of the transfer factors associated with the fish compartment type in the bioenergetic model:

$$\frac{dC_f}{dt} = \left(U_{gill} \times C_{SWD}\right) + \left(AE_D \times \sum p_i \times C_{D,i}\right) - (E_{met} + E_{eg} + E_{ef} + E_G) \times C_f \qquad \text{(Eq. 6-17)}$$

where:

C_f = chemical concentration in fish (g[chemical]/kg[fish wet wt]);
U_{gill} = uptake from water via the gills (L[water]/kg[fish wet wt]-day);
C_{SWD} = dissolved chemical concentration in surface water (g[chemical dissolved]/L[water]);
AE_D = chemical assimilation (absorption) efficiency from diet (unitless);
p_i = proportion of the diet consisting of diet item *i* (unitless);
$C_{D,i}$ = chemical concentration in diet item *i* (g[chemical]/kg[food *i*]);
E_{met} = metabolic degradation or transformation of the chemical (/day);

E_{eg} = excretion of chemical in the fish (*i.e.*, absorbed chemical) via the gills (/day);
E_{ef} = excretion of chemical in the fish via feces and urine (/day); and
E_G = dilution of chemical concentration from growth (/day).

Assuming first-order rate constants to express both uptake and elimination, the following relationships hold:

U_{gill} = k_U = rate constant for uptake from water via the gills (L[water]/kg[fish wet wt]-day);
E_{met} = k_{met} = rate constant for metabolic transformation of chemical (/day);
E_{eg} = k_{eg} = rate constant for excretion of chemical via the gills (/day);
E_{ef} = k_{ef} = rate constant for excretion of chemical via feces and urine (/day); and
E_G = k_G = rate constant for dilution of chemical concentration from growth (/day).

This comprehensive model can be simplified consistent with the approach used in Thomann (1989) to:

$$\frac{dC_f}{dt} = \left(k_U \times C_{SWD}\right) + \left(AE_D \times \sum p_i \times C_{D,i}\right) - \left(k_{ET} + k_G\right) \times C_f \qquad \text{(Eq. 6-18)}$$

where:

k_{ET} = rate constant for total elimination via all excretory systems and via metabolic degradation to chemicals no longer tracked (/day);
= $k_{eg} + k_{ef} + k_{met}$ (in Thomann 1989).

This simplification is appropriate in TRIM.FaTE for chemicals that are not lost via metabolic degradation, only transformed among different species or compounds with a conserved element (*e.g.*, mercury) that is tracked individually in TRIM.FaTE. For those chemicals, $k_{met} = 0$; all metabolic reactions are tracked via transformations between species (*e.g.*, between elemental and divalent mercury and methylmercury).

For organic chemicals, that are metabolized to chemicals that are currently not tracked in TRIM.FaTE, such as PAHs, loss of chemical from the modeling system via metabolic degradation should be tracked separately from elimination of the parent chemical from fish back into the surface water compartment. Loss of chemical from the modeling system is simulated in TRIM.FaTE by transfers to a compartment sink, in this case, the fish degradation sink, that accumulates the mass of chemical lost from the system via this pathway. Thus, for use in TRIM.FaTE with organic chemicals that can be degraded, the "elimination" rate constant k_{ET} in Equation 6-18 would need to be separated into k_E, for the excretory pathways for transfer of the chemical back to surface water (*i.e.*, $k_{eg} + k_{ef}$), and k_{met}, for loss (transfer) of chemical to the fish degradation sink.

It is important to note that the equations in their present form exclude dermal uptake as a significant exposure route. Also, growth dilution (k_G) is not included in TRIM.FaTE, because a constant biomass for the entire fish population is assumed and growth of individual fish is not included in the current TRIM.FaTE library.

The bioenergetic-based kinetic model generally is used to estimate concentrations in individual fish of a species. Following is the derivation of the fish model for the entire fish population. Initially the model is derived for a population of two fish and then generalized for the case of *n* fish, where *n* is the fish population size. Thus, for two fish with concentrations C_{f1}, and C_{f2}, Equation 6-18 can be rewritten as:

$$\frac{dC_{f1}}{dt} = \left(k_{U1} \times C_{SWD}\right) + \left(AE_D \times \sum p_i \times C_{Di}\right) - \left(k_{ET1} \times C_{f1}\right) \qquad \text{(Eq. 6-19)}$$

$$\frac{dC_{f2}}{dt} = \left(k_{U2} \times C_{SWD}\right) + \left(AE_D \times \sum p_i \times C_{Di}\right) - \left(k_{ET2} \times C_{f2}\right) \qquad \text{(Eq. 6-20)}$$

To convert the concentrations to masses, it is assumed that:

$$C_{SWD} = \frac{N_{WD}}{V_{SW} \times \theta} \qquad \text{(Eq. 6-21)}$$

$$C_{f1} = \frac{N_1}{m_1} \qquad \text{(Eq. 6-22)}$$

$$C_{f2} = \frac{N_2}{m_2} \qquad \text{(Eq. 6-23)}$$

where:

C_{SWD} = concentration of dissolved chemical in surface water (g[chemical dissolved]/L[water]);
N_{WD} = mass of chemical dissolved in water (g[chemical dissolved]);
V_{SW} = volume of surface water compartment (L);
θ = volume fraction of surface water compartment that is water (unitless, ≈ 1.0);
m_1 = mass of fish 1 (kg[fish wet wt]);
m_2 = mass of fish 2 (kg[fish wet wt]);
N_1 = mass of chemical in fish 1 (g[chemical]); and
N_2 = mass of chemical in fish 2 (g[chemical]).

Note that:

$$\theta = 1 - \left(Vf_{SSed} + Vf_{Algae}\right) \qquad \text{(Same as Eq. 6-2)}$$

where:

Vf_{SSed} = volume fraction of the surface water compartment that is suspended sediment particles (unitless); and

Vf_{Algae} = volume fraction of the surface water compartment that is algae (unitless).

Substituting yields:

$$\frac{d(N_1/m_1)}{dt} = k_{U1} \times \frac{N_{WD}}{V_{SW} \times \theta} + (AE_D \times \sum p_i \times C_{Di}) - k_{ET1} \times \frac{N_1}{m_1} \qquad \text{(Eq. 6-24)}$$

$$\frac{d(N_2/m_2)}{dt} = k_{U2} \times \frac{N_{WD}}{V_{SW} \times \theta} + \left(AE_D \times \sum p_i \times C_{Di}\right) - k_{ET2} \times \frac{N_2}{m_2} \qquad \text{(Eq. 6-25)}$$

Adding Equations 6-24 and 6-25 yields the mass transfer equations for the total fish compartment type, as follows:

$$\begin{aligned}\frac{d(N_1/m_1 + N_2/m_2)}{dt} = {} & (k_{U1} + k_{U2}) \times \frac{N_{WD}}{V_{SW} \times \theta} + 2 \times \left(AE_D \times \sum p_i \times C_{Di}\right) \\ & - \left(k_{ET1} \times \frac{N_1}{m_1} + k_{ET2} \times \frac{N_2}{m_2}\right)\end{aligned} \qquad \text{(Eq. 6-26)}$$

Making the simplifying assumptions that individual fish mass is represented by a population average m_f ($m_1 = m_2 = m_f$), and that $k_{U1} = k_{U2} = k_U$, and $k_{ET1} = k_{ET2} = k_{ET}$, yields:

$$\frac{d\left(\dfrac{N_1 + N_2}{m_f}\right)}{dt} = 2 \times \left(k_U \times \frac{N_{WD}}{V_{SW} \times \theta} + \left(AE_D \times \sum p_i \times C_{Di}\right)\right) - k_{ET} \times \left(\frac{N_1 + N_2}{m_f}\right) \qquad \text{(Eq. 6-27)}$$

This equation can be generalized from 2 to n_f fish, with N_f ($= N_1 + N_2$) being the total chemical mass in the fish compartment type, to yield the following generalized chemical mass-transfer equation for a fish compartment type:

$$\frac{dN_f}{dt} = \left(n_f \times m_f \times k_U \times \frac{N_{WD}}{V_{SW}} \times f_{ML}\right) + \left(n_f \times m_f \times IN_D \times AE_D \times \frac{N_{diet}}{V_{diet}}\right) - \left(k_{ET} \times N_f\right) \qquad \text{(Eq. 6-28)}$$

where:

$$N_{WD} = N_{SW} \times Fraction\_Mass\_Dissolved \qquad \text{(Eq. 6-29)}$$

$$f_{ML} = \frac{Fraction\_Mass\_Dissolved}{Volume\_Fraction\_Liquid} \qquad \text{(Eq. 6-30)}$$

and:

n_f = total number of fish in surface water compartment;
IN_D = food (diet) ingestion rate constant (kg[food wet wt]/kg[fish wet wt]-day);
AE_D = assimilation (absorption) efficiency of chemical from the diet (unitless);
N_{SW} = total chemical inventory in the surface water compartment (both dissolved and sorbed to suspended sediment particles) (g[chemical]);
f_{ML} = fraction of chemical mass in surface water compartment that is dissolved in water divided by the volume fraction of the surface water compartment that is liquid, *i.e.*, water (unitless); and
θ = *Volume_Fraction_Liquid* (unitless).

Note that an AE_D of less than 1.0 implies that the fraction of chemical not absorbed was effectively left in the diet compartment(s). A future enhancement of TRIM.FaTE might be to transfer the unassimilated chemical to the suspended sediment phase of the surface water compartment or directly to the sediment bed to simulate the fecal elimination of unabsorbed chemical implied by the AE_D.

The food ingestion rate (IN_D) of an individual fish is given by the following bioenergetic model presented in Gobas (1993):

$$IN_D = 0.022 \times m_f^{0.85} \times e^{(0.06 \times T)} \qquad \text{(Eq. 6-31)}$$

where:

m_f = mass of the fish (kg); and
T = temperature (°C).

To illustrate how the dietary transfer calculation would differ between the different fish trophic groups, an equation for a benthic omnivore (*Fbo* = fish, benthic omnivore) is illustrated below.

$$\begin{aligned}\frac{dN_{Fbo}}{dt} = &\left(n_{Fbo} \times m_{Fbo} \times k_{Fbo} \times \frac{N_W}{V_W} \times f_{ML} \right) \\ &+ \left(n_{Fbo} \times m_{Fbo} \times IN_D \times AE_D \times \left(p_{Mp} \times \frac{N_{Mp}}{m_{Mp}} + p_{Fh} \times \frac{N_{Fh}}{m_{Fh}} + p_{BI} \times \frac{N_{BI}}{m_{BI}} \right) \right) \qquad \text{(Eq. 6-32)} \\ &- \left(k_{ET} \times N_{Fbo} \right)\end{aligned}$$

where:

n_{Fbo} = number of benthic fish omnivores in the surface water compartment (unitless);
m_{Fbo} = mass per individual benthic omnivore fish (kg[fish wet wt]/individual);

N_{Fbo} = chemical inventory in the benthic omnivore fish compartment (g[chemical]);
p_{Mp}, p_{Fh}, p_{BI} = proportion of the benthic omnivore fish's diet that is comprised of macrophytes, herbivorous fish, and benthic invertebrates, respectively (unitless);
N_{Mp}, N_{Fh}, N_{BI} = chemical inventory in the macrophyte, herbivorous fish, and benthic invertebrate compartments, respectively (g[chemical]); and
m_{Mp}, m_{Fh}, m_{BI} = total biomass of the macrophyte, herbivorous fish, and benthic invertebrate compartments, respectively (kg[biomass wet wt]).

Implicit in the previous equation is the assumption that the mass of an individual fish is constant over the time of the simulation. The dilution-due-to-growth factor (k_G) is not included in the equation because k_G is based on concentrations, while the mass transfer equations are in mass units.

6.4.1.2 Nonionic Organic Chemicals

For nonionic organic chemicals (*e.g.*, PAHs), the chemical uptake rate constant k_U for fish gills is estimated using the following formula in TRIM.FaTE if measured values are not available:

$$k_U = 10^3 \times \left(\frac{m_f^{-\gamma_{ASF}}}{f_{lipid}} \right) \times AE_g \qquad \text{(Eq. 6-33)}$$

where:

k_U = chemical uptake rate constant (L[water]/kg[fish wet wt]-day);
m_f = fish body mass (kg[fish wet wt]);
γ_{ASF} = allometric scaling factor (*e.g.*, 0.2 (Thomann 1989)) (unitless);
f_{lipid} = fraction lipid (kg[lipid]/kg[fish wet wt]); and
AE_g = chemical assimilation (absorption) efficiency of the gills (unitless).

There is an apparent increase in assimilation efficiency for smaller organisms; therefore, organisms have been divided into two weight groups: 10 to 100 g (wet) and more than 100 g (wet) weight (Thomann 1989). The chemical assimilation efficiency of the gills (AE_g) can be approximated for these two size classes of organisms as follows. For smaller organisms, the following equations should be used to estimate AE_g, where K_{ow} is the octanol/water partition coefficient (g[chemical]/kg[octanol] per g[chemical]/L[water] = L[water]/kg[octanol]):

For chemicals with $\log(K_{ow})$ = 2.00-4.99, $\log(AE_g) = -2.6 + 0.5 \log(K_{ow})$;
For chemicals with $\log(K_{ow})$ = 5.00-5.99, $AE_g = 0.8$; and
For chemicals with $\log(K_{ow})$ = 6.00-10, $\log(AE_g) = 2.9 - 0.5 \log(K_{ow})$.

For larger organisms, the following equations should be used to estimate AE_g:

For chemicals with $\log(K_{ow})$ = 2.00-2.99, $\log(AE_g) = -1.5 + 0.4 \log(K_{ow})$;
For chemicals with $\log(K_{ow})$ = 3.00-5.99, $AE_g = 0.5$; and
For chemicals with $\log(K_{ow})$ = 6.00-10, $\log(AE_g) = 1.2 - 0.25 \log(K_{ow})$.

There is a similar relationship between chemical assimilation efficiency from dietary items (AE_D) and K_{ow} (Thomann 1989). However, there does not appear to be an increase in the dietary assimilation efficiency for smaller organisms; therefore, the AE_D can be approximated for all size classes of organisms as follows:

For chemicals with $\log(K_{ow})$ = 2.00-4.99, $\log(AE_D) = -2.6 + 0.5 \log(K_{ow})$;
For chemicals with $\log(K_{ow})$ = 5.00-5.99, $AE_D = 0.8$; and
For chemicals with $\log(K_{ow})$ = 6.00-10, $\log(AE_D) = 2.9 - 0.5 \log(K_{ow})$.

Note that this is the same set of equations used to estimate AE_g for smaller organisms.

Thomann (1989) gives the total excretion rate constant (k_{ET}) for nonionic organic chemicals using the following equation:

$$k_{ET} = \frac{k_U}{K_{ow}} \tag{Eq. 6-34}$$

Note that in a subsequent publication, Thomann *et. al.* (1992a,b) state that k_{ET} accounts for elimination via the gills and "other losses...for example, fecal loss and metabolism". However, those publications (1) indicate that the simplified equation that includes a term for elimination via the gills only is approximately representative of observed excretion data for fish and (2) provide no data or formulas for estimating the values of the other types of losses (which we interpret as meaning fecal loss of biliary secretions and excretion in urine). We interpret the rate constant k_{ET} in Equation 6-34 as not including losses due to metabolism, because k_{ET} is set directly proportional to the gill uptake rate divided by K_{ow}. Therefore, the simplified Equation 6-35 from Thomann (1989) is used here to represent the total excretion rate constant for the absorbed chemical, k_E, *excluding* losses due to metabolism.

6.4.1.3 Mercury

For mercury (all forms), uptake from water is excluded from the transfer equations because accumulation in fish is primarily as methylmercury, for which uptake from water is negligible (Trudel and Rasmussen 1997).

The mercury excretion rate constant (k_E) (*i.e.*, transfer of absorbed mercury back to surface water) is given by a bioenergetic model from Trudel and Rasmussen (1997), as described in Appendix A, Section A.1.3. Trudel and Rasmussen (1997) based the excretion rate on the clearance of methylmercury only, because greater than 95 percent of mercury in fish is methylmercury, and the elimination of methylmercury is much slower than that of inorganic mercury (*i.e.*, the overall rate is dominated by the elimination of methylmercury).

6.4.1.4 Bioenergetic Model Transfer Factors

Using the bioenergetic model, the transfer factor for uptake of dissolved nonionic organic chemicals from a surface water compartment via gill uptake for a fish compartment (/day) can be expressed as:

$$T^{gill}_{SW\rightarrow fish} = \frac{n_f \times m_f \times k_U}{V_{SW}} \times f_{ML} \times 1000 \qquad \text{(TF 6-5)}$$

where:

n_f = total number of fish in surface water compartment;
m_f = mass per individual fish (kg[fish wet wt]);
k_U = fish gill uptake rate constant for chemical dissolved in water (/day);
V_{SW} = volume of the surface water compartment (L[water]);
f_{ML} = fraction of chemical mass in surface water compartment that is dissolved in water divided by the volume fraction of the surface water compartment that is liquid, *i.e.*, water (unitless); and
1000 = unit conversion factor (L/m^3) to match the units for all TRIM.FaTE compartment volumes.

For mercury, the transfer from surface water to the fish via the gills is set to zero (0) (see Appendix A, Section A.1.3).

The generalized transfer factors for chemical uptake from dietary items to a specific fish compartment are given by:

$$T_{diet\rightarrow fish} = \frac{n_f \times m_f}{n_{diet} \times m_{diet}} \times IN_D \times AE_D \qquad \text{(TF 6-6a)}$$

$$= \frac{biomass_{fish}}{biomass_{diet}} \times IN_D \times AE_D \qquad \text{(TF 6-6b)}$$

where:

n_{diet} = number of individuals in the diet compartment (unitless);
m_{diet} = mass per individual in the diet compartment (kg[organism]/individual);
IN_D = total diet (food) ingestion rate (kg[diet wet wt]/kg[fish wet wt]);
AE_D = assimilation efficiency of chemical from diet (unitless);
$biomass_{fish}$ = total biomass of the fish compartment (= $n_f \times m_f$); and
$biomass_{diet}$ = total biomass of the diet compartment (= $n_{diet} \times m_{diet}$).

Because algae is modeled as a phase of the surface water compartment in the current TRIM.FaTE library, consumption of algae by herbivorous fish is represented by a slightly different transfer factor algorithm:

$$T_{Algae \rightarrow Fwch} = \frac{n_{Fwch} \times m_{Fwch}}{\left(f_{MA} / m_{Algae}\right)} \times IN_D \times p_{Algae} \times AE_D \qquad \text{(TF 6-7)}$$

where:

$T_{Algae \rightarrow Fwch}$ = transfer factor from algae to water column herbivore (/day);
n_{Fwch} = number of water column herbivores in surface water compartment (unitless);
m_{Fwch} = mass per individual water column herbivore (g[fish wet wt]);
f_{MA} = fraction of chemical mass that is in the algal-phase of the surface water (kg[chemical]/kg[bulk surface water, including suspended sediments and algae]);
m_{Algae} = total mass of algae in surface water compartment (kg[algae wet wt]); and
p_{Algae} = proportion of the total diet that consists of algae on a wet-weight basis (unitless).

Using the same bioenergetic model, the transfer of chemicals from the fish population compartment to the surface water compartment can be expressed as:

$$\begin{aligned} T_{fish \rightarrow SW}^{excretion} &= k_{eg} + k_{ef} \\ &= k_E \end{aligned} \qquad \text{(TF 6-8)}$$

where:

k_E = rate constant for elimination of chemical from the fish to surface water via the gills and in urine and feces (/day).

Note that k_E applies only to the absorbed chemical in the fish compartment. Fecal loss of unabsorbed chemical was accounted for by the AE_D parameter. As described in Section 6.4.1.4, k_E does not include losses due to metabolic transformation or degradation.

6.4.1.5 Transformations and Degradation

Transformations of organic chemicals into biodegradation by-products that are no longer tracked in TRIM.FaTE are modeled as transfers to the fish degradation sinks. See the TRIM.FaTE user guidance for recommendations on how to identify rate constants for biodegradation separately from rate constants associated with chemical excretion from fish to surface water. Equation 2-64 (Chapter 2) is used to estimate the metabolic degradation (in TRIM.FaTE, called "general degradation") rate constant for an organic chemical from its metabolic half-life.

Metabolic transformations of inorganic chemicals into different compounds containing the same core chemical (*e.g.*, mercury) can be included in the TRIM.FaTE fish models. For example, biotransformation of Hg(0) to Hg(2) in fish is included as a rapid (almost instantaneous) first-order rate constant in the fish compartments. Thus, it is assumed that elemental mercury can be taken up by fish but is not accumulated in the fish (*i.e.*, data showing Hg(0) in fish were not found). It is also assumed that inorganic mercury is not methylated by fish. Demethylation in fish may occur as part of the excretory process, but it is not explicitly modeled here. Rather, it is assumed to be insignificantly small compared to the relative masses of the mercury species in the fish (*i.e.*, receiving compartments).

6.4.2 TIME-TO-EQUILIBRIUM-BASED KINETIC MODEL

The time-to-equilibrium model is based on the assumption that one pathway accounts for the vast majority of the chemical uptake. Thus, only one chemical "source" (*e.g.*, food) is explicitly considered for a given "receptor", (*e.g.*, fish). The general form of the model is:

$$\frac{dC_{receptor}}{dt} = \left[\frac{-\ln(1-\alpha)}{t_{\alpha}^{rs}}\right] \times K_{receptor-source} \times C_{source} - \left[\frac{-\ln(1-\alpha)}{t_{\alpha}^{rs}}\right] \times C_{receptor} \qquad \text{(Eq. 6-35)}$$

where:

$K_{receptor\text{-}source}$ = receptor/source partition coefficient (*e.g.*, fish/diet partition coefficient) (g[chemical]/kg[receptor wet wt] per g[chemical]/kg[source wet wt]);
$C_{receptor}$ = concentration in receptor (*e.g.*, fish) (g[chemical]/kg[receptor wet wt]);
C_{source} = concentration in source (*e.g.*, diet) (g[chemical]/kg[source wet wt]);
t_{α}^{rs} = time (days) required to reach 100×α percent of the receptor/source equilibrium value when the concentration in the source is approximately constant with time; and
α = fraction of the equilibrium value attained (default = 0.95; unitless).

If the sole chemical source is surface water, then $K_{receptor\text{-}source}$ is a bioconcentration factor (BCF). Bioaccumulation factors (BAFs) implicitly include uptake from food and water, though water is the identified source. This presumes that the concentration in the food item is essentially constant relative to the concentration in the water. An alternative approach is the use of diet as the primary source. Thus, empirically derived accumulation data are used to derive factors for each trophic transfer, and uptake from water is implicitly, rather than explicitly, included. This latter alternative is used here.

Following this approach requires that the dietary sources for a given fish compartment be restricted to one other trophic group. Thus, intratrophic group transfers and multitrophic group transfers are not explicitly included. These transfers are implicitly included to the extent that the empirical data used to derive the transfer factors are from systems possessing those transfers. Thus, the "fit" of the model results for any given case study will depend partly on how well the food chains at the sites used to derive the transfer factors match the food chains at the case study site (*e.g.*, length of the food chains, number of interconnections, degree of intratrophic group transfer, etc.).

Restriction of the dietary pathway can be achieved within TRIM.FaTE by defining the generic trophic compartment types to represent a straight food chain (*e.g.*, of three or four segments). As noted in Section 6.3, the benthic herbivore compartment type in initial TRIM.FaTE applications has been represented by all benthic invertebrates and in the use of this time-to-equilibrium approach, the bulk sediment (or interstitial water) is the chemical source. The benthic omnivore fish compartment type is the next trophic level up from the benthic invertebrates.

Like the benthic food chain, the chemical transfers in the water column food chain can be set to be unidirectional from lower to higher trophic levels. In initial applications following this design, it is important to note that zooplankton have been implicitly included in the transfers from algae to water column herbivores. That is, the biomass and chemical mass associated with zooplankton have not been explicitly tracked in TRIM.FaTE, but the dietary transfers were based on concentration ratios for planktivorous fish and algae. Some studies provide the intermediate transfer factors for algae to zooplankton, which might be used to include the zooplankton compartment type within future TRIM.FaTE simulations.

For each trophic level transfer, the general concentration-based equation is converted to the following mass-transfer equation:

$$\frac{dN_f}{dt} = n_f \times m_f \times \left[\frac{-\ln(1-\alpha)}{t_\alpha^{fd}}\right] \times K_{fish-diet} \times \frac{N_{diet}}{n_{diet} \times m_{diet}} - \left[\frac{-\ln(1-\alpha)}{t_\alpha^{fd}}\right] \times N_f \qquad \text{(Eq. 6-36)}$$

where:

n_f = number of fish in the compartment (unitless);
m_f = mass of individual fish (kg[fish wet wt]/individual);
t_α^{fd} = time (days) required to reach 100×α percent of the fish/diet interaction equilibrium value when the concentration in the source is approximately constant with time;
$K_{fish\text{-}diet}$ = fish/diet partition coefficient (kg[diet wet wt]/kg[receptor wet wt]);
N_{diet} = mass of chemical in items comprising the potential diet (g[chemical]);
n_{diet} = number of contaminated items comprising the potential diet (unitless);
m_{diet} = mass of individual items comprising the potential diet (kg[diet wet wt]/individual); and
N_f = mass of chemical in the fish (receptor) compartment (g[chemical]).

As an example, the mass transfer equation for water-column omnivores eating water-column herbivores is given as:

$$\frac{dN_{Fwco}}{dt} = n_{Fwco} \times m_{Fwco} \times \left[\frac{-\ln(1-\alpha)}{t_\alpha^{fd}}\right] \times K_{Fwco-Fwch} \times \frac{N_{Fwch}}{n_{Fwch} \times m_{Fwch}} - \left[\frac{-\ln(1-\alpha)}{t_\alpha^{fd}}\right] \times N_{Fwco} \qquad \text{(Eq. 6-37)}$$

where:

N_{Fwco} = mass of chemical in the fish water-column omnivore compartment (g[chemical]);
n_{Fwco} = number of fish comprising the water-column omnivore compartment (unitless);
m_{Fwco} = mass per individual fish in the water-column omnivore compartment (kg[fish wet wt]/individual);
$K_{Fwco\text{-}Fwch}$ = fish (water-column omnivore)/fish (water-column herbivore) partition coefficient (kg[*Fwch* wet wt]/kg[*Fwco* wet wt]);
N_{Fwch} = mass of chemical in fish water-column herbivore compartment (g[chemical]);
n_{Fwch} = number of fish comprising the water-column herbivore compartment (unitless); and
m_{Fwch} = mass per individual fish in the water-column herbivore compartment (kg[fish wet wt]/individual).

For each trophic level transfer, the generalized transfer factors for dietary items to a specific fish compartment type (*i.e.*, benthic omnivore, benthic carnivore, water-column herbivore, water-column omnivore, or water column carnivore) is given by:

$$T_{diet \rightarrow fish} = \frac{n_f \times m_f}{n_{diet} \times m_{diet}} \times \left[\frac{-\ln(1-\alpha)}{t_{\alpha}^{fd}} \right] \times K_{fish-diet} \qquad \text{(TF 6-9)}$$

Because algae is treated as a phase of the surface water compartment, the time-to-equilibrium transfer factor from algae to the water-column herbivore fish compartment is slightly different:

$$T_{Algae \rightarrow Fwch} = \frac{n_{Fwch} \times m_{Fwch}}{(f_{MA} / m_{Algae})} \times \left[\frac{-\ln(1-\alpha)}{t_{\alpha}^{FwchAlg}} \right] \times K_{Fwch-Algae} \qquad \text{(TF 6-10)}$$

where:

$T_{Algae \rightarrow Fwch}$ = transfer factor from algae to fish (water-column herbivore) (/day);
f_{MA} = fraction of chemical mass that is in the algal phase of the surface water compartment (unitless);
m_{Algae} = total mass of algae in surface water compartment (kg[algae wet wt]);
$t_{\alpha}^{FwchAlg}$ = time (days) required to reach 100×α percent of the fish/diet interaction equilibrium value when the concentration in the source is approximately constant with time; and
$K_{Fwch\text{-}Algae}$ = fish (water-column herbivore)/algae partition coefficient (kg[algae wet wt]/kg[fish wet wt]).

The generalized transfer factor in the other direction (to allow equilibirum) from a specific fish compartment to its diet compartment is given by:

$$T_{fish \rightarrow diet} = \left[\frac{-\ln(1-\alpha)}{t_{\alpha}^{fd}} \right] \qquad \text{(TF 6-11)}$$

Transformations and degradation are modeled using the same approach as described for the bioenergetic model (see Section 6.4.1.5).

6.4.3 OTHER EPA MODELS FOR BIOACCUMULATION BY FISH

Aquatox is a general ecological risk model that estimates the fate and effects of chemical and physical stressors in aquatic ecosystems (U.S. EPA 1998b). The model has been developed by the Office of Pollution Prevention and Toxics (OPPT) and the Office of Water (OW). The Bioaccumulation and Aquatic System Simulator (BASS), developed by the National Exposure Research Laboratory (NERL) of the Office of Research and Development (ORD), also simulates exposure and effects on fish (U.S. EPA 1999c).

Aquatox and BASS are designed to predict effects of chemical contaminants and environmental factors on fish populations, whereas TRIM.FaTE is designed to estimate the fate and transport of chemicals throughout aquatic and terrestrial environments, with an emphasis on a collection of identical, individual fish. This difference in purpose results in several differences in structure: (1) Aquatox and BASS include chemical toxicity data; TRIM.FaTE does not (although TRIM.Risk is designed to include such a database); (2) the toxicological data in Aquatox and BASS are used to predict mortality, which is used to modify the structures of the models (*e.g.*, age-class structure and predator-prey interactions); the biomass in the TRIM.FaTE fish compartments remains constant; (3) in Aquatox, decomposition of dead fish and contaminants are linked to the dissolved oxygen levels in water, which affect populations; in TRIM.FaTE dissolved oxygen levels in surface water are not modeled; and (4) growth estimation of fish is fundamental to the population dynamics component of BASS, whereas growth is not included in the current version of TRIM.FaTE.

BASS (U.S. EPA 1999c) and Aquatox (U.S. EPA 1998b) are bioenergetic models of a multiple-trophic-level aquatic ecosystem. Aquatox, like TRIM.FaTE, provides an explicit time-to-equilibrium model option, whereas BASS does not. Like TRIM.FaTE, Aquatox has a Monte Carlo component to permit probabilistic estimates of exposure or risk. The developers of BASS plan to include metabolism of organic compounds in future versions of the model, but, unlike TRIM.FaTE, these transformations are not a feature of the current version (U.S. EPA 1999c). Components of Aquatox or BASS could be integrated with TRIM.FaTE. The challenge would be to preserve mass balance and to provide adequate links to all TRIM.FaTE compartment types that are connected to surface water and/or fish.

7. TERRESTRIAL BIOTA ALGORITHMS

In this chapter, algorithms for transfers between terrestrial biotic compartment types and other biotic or abiotic compartment types are presented. The terrestrial biotic compartments include terrestrial plants, soil detritivores, and wildlife (*i.e.*, birds and mammals).

The algorithms in this chapter are based on diffusive or advective transfer, and the most common instances of the latter are transfers via wildlife ingestion of chemicals in their diet. Most algorithms apply to all air pollutants, although some apply only to mercury species, and others (*e.g.*, those that involve octanol/water partition coefficients) apply only to nonionic organic chemicals. Some of the equations represent dynamic processes, while others are simple models for which a time-to-equilibrium is calculated and used to estimate relevant transfer factors.

After a brief introduction to the selection of terrestrial biotic compartments for a TRIM.FaTE scenario (Section 7.1), the algorithms used to calculate the transfer factors for chemical transfers in and out of terrestrial biota are developed and presented. General algorithms for terrestrial plants, soil detritivores, and birds and mammals are presented in Sections 7.2, 7.3, and 7.4, respectively. The derivations of chemical-specific algorithms for mercury and polycyclic aromatic hydrocarbons (PAHs) are presented in Appendices A and B, respectively.

7.1 TERRESTRIAL BIOTA COMPONENTS

The general approach for selecting biotic compartment types to include in a TRIM.FaTE scenario is noted in Section 3.3 of TSD Volume I and described in more detail in the user guidance document. All major trophic levels in terrestrial systems are represented in the current TRIM.FaTE library. The user can select default, representative species, based on their prevalence at the test location and/or the availability of data to estimate parameter values for them. The user can also create compartments for additional species based on policy considerations, such as the Endangered Species Act. There are some aspects of selecting biotic compartments for the terrestrial environment that we emphasize here. For additional information on these issues and more detailed guidance, see the TRIM.FaTE user guidance.

For terrestrial surface volume elements or parcels, the user can select one of a number of land-use characteristics that influence the type of land cover and/or vegetation. There are four types of plant communities that have already been incorporated into the TRIM.FaTE libraries: deciduous forest, coniferous forest, grasses/herbs, and agricultural (*e.g.*, crop) lands. Each plant community type is represented in TRIM.FaTE by a plant composite compartment, which includes particles on the leaf surface, leaf, stem, and root compartments and associated parameter values for that type of plant community.

For biotic compartments in soil, the current TRIM.FaTE library includes two types of soil organisms: earthworms and soil arthropods. Both types are detritivores (*i.e.*, they feed on the decaying organic materials found in soils). Chemical transformation and degradation processes that might be mediated by soil bacteria are accounted for in the soil compartment transformation and degradation rates for a chemical.

Finally, the user can populate the vegetated surface volume elements with wildlife species, depending on the goals and objectives of the project as well as considerations of chemical mass distribution across wildlife biomass and trophic levels. Major herbivores at a site should be included to facilitate appropriate partitioning of a chemical within the terrestrial ecosystems. Higher trophic level birds and mammals would affect environmental partitioning to a lesser extent. The current TRIM.FaTE library includes parameterized compartments for several species of birds and mammals as described in Section 7.4.4.

For detailed guidance on how to select and parameterize terrestrial biotic compartments and how to distribute them among surface soil and surface water parcels, see the TRIM.FaTE user guidance.

7.2 ALGORITHMS FOR TERRESTRIAL PLANTS

The text box on the next page and continued on the following pages provides a summary of the plant transfer-factor algorithms developed in this section and defines the parameters used in those algorithms.

In TRIM.FaTE, terrestrial plants consist of four compartment types which, taken together, represent an entire plant: leaf, stem, root, and particles on the leaf surface. All four compartments, parameterized for a specific type of plant community (*e.g.*, deciduous forest) are linked together in a single plant composite compartment named for that community. Although the particles on the leaf surface are not in the plant, it is useful to track this compartment type separately from the leaf because: (1) it can provide a reservoir for chemical moving to leaves, (2) herbivorous animals can ingest particulate matter on leaves, (3) particles can wash off leaves during rain, (4) particles can be blown off leaves by wind, and (5) humans can wash most of these particles off of leaves, prior to any consumption (*e.g.*, agricultural plants).

Several attributes of the plant compartments vary with time of day and with season. A logical parameter named *IsDay* in TRIM.FaTE controls whether the plant stomata are open (1 for “yes, it is day”) or closed (0 for “no, it is night”) for a specific simulation run. Diffusion of a vapor-phase chemical between the air and plant leaves through the stomata occurs only during the day when they are open. A logical parameter named *AllowExchange* is used to control whether the plant is actively growing and has leaves (yes) or is dormant and without leaves for the non-growing season (no). Chemical exchanges between the grasses and herbaceous and deciduous plants occur only during the growing season (*AllowExchange* = 1). *AllowExchange* always equals one (yes) for the coniferous plants.

There are, however, several problems that arise in modeling uptake and emissions of chemicals by plants:

- Little information is available on the transformations of chemicals in plants.

Summary of Transfer Factors for Plants in TRIM.FaTE

ABOVE-GROUND EXCHANGES

Dry deposition of particulate phase of air to particles-on-leaf compartment: TF 7-1

$$T_{Air \rightarrow LeafP}^{dry\_dep} = \frac{\upsilon_{dry} \times I_{dry} \times A_S}{V_{Air}} \times f_{MS}$$

Dry particles on leaf blown off to air: TF 7-2

$$T_{LeafP \rightarrow Air}^{blow\_off} = \frac{\upsilon_{dry} \times I_{dry} \times A_S}{V_{LeafP}}$$

Wet deposition of particles in air to the particles-on-leaf compartment: TF 7-3

$$T_{Air \rightarrow LeafP}^{wet\_dep} = \frac{\upsilon_{wet} \times I_{wet} \times A_S}{V_{Air}} \times f_{MS}$$

Wash off of particles on leaf to surface soil: TF 7-4a

$$T_{LeafP \rightarrow Ss}^{wash\_off} = \frac{\upsilon_{wet} \times I_{wet} \times A_{Ss}}{V_{LeafP}}$$

Particles on leaf to leaf: TF 7-5

$$T_{LeafP \rightarrow Leaf} = k_{LeafP-Leaf}$$

Leaf to particles on leaf: TF 7-6

$$T_{Leaf \rightarrow LeafP} = 0.01 \times k_{LeafP-Leaf}$$

Wet deposition of vapor-phase chemical from air to the leaf (partitioning approach): TF 7-7a

$$T_{Air \rightarrow Leaf}^{Vwet\_dep} = \frac{A_S}{V_{Air}} \times w_{rV} \times rain \times I_{wet} \times f_{MV}$$

Wet deposition of vapor-phase chemical from air to the leaf (fugacity approach): TF 7-7b

$$T_{Air \rightarrow Leaf}^{Vwet\_dep} = \frac{A_S}{V_{Air}} \times rain \times I_{wet} \times \frac{Z_{pure\_water}}{Z_{Total\_Air}}$$

Summary of Transfer Factors for Plants in TRIM.FaTE (cont.)

ABOVE-GROUND EXCHANGES (cont.)

Leaf to air (diffusion): TF 7-8a

$$T^{diff}_{Leaf \rightarrow Air} = (2LAI \times A_S \times g_C + LAI \times A_S \times g_S) \times \frac{1}{V_{Leaf}} \times \frac{Z_{pure\_air}}{Z_{Total\_Leaf}}$$

Air to leaf (diffusion): TF 7-9a

$$T^{diff}_{Air \rightarrow Leaf} = (2LAI \times A_S \times g_C + LAI \times A_S \times g_S) \times \frac{1}{V_{Air}}$$

BELOW-GROUND EXCHANGES

Bulk root-zone soil to root: TF 7-10a

$$T_{Sr \rightarrow Root} = \left[\frac{-\ln(1-\alpha)}{t_\alpha^{RSr}}\right] \times \frac{V_{Root}}{V_{Sr}} \times K_{Root-Sr} \quad where\ K_{Root-Sr} = input\ value$$

Root to bulk root-zone soil: TF 7-11a

$$T_{Root \rightarrow Sr} = \frac{-\ln(1-\alpha)}{t_\alpha^{RSr}}$$

Root-zone-soil pore water to root: TF 7-10b

$$T_{SrW \rightarrow Root} = \left[\frac{-\ln(1-\alpha)}{t_\alpha^{RSrW}}\right] \times \frac{V_{Root}}{V_{Sr}} \times K_{Root-SrW} \times \frac{Z_{pure\_water}}{Z_{Total\_Sr}}\ where:$$

$$K_{Root-SrW} = (fW_{Root} + fL_{Root} \times K^b_{ow}) \times \rho_{Root} \times 0.001$$

Root to root-zone-soil pore water: TF 7-11b

$$T_{Root \rightarrow SrW} = \frac{-\ln(1-\alpha)}{t_\alpha^{RSrW}}$$

PLANT STEM EXCHANGES

Bulk root-zone soil to stem: TF 7-12a

$$T_{Sr \rightarrow Stem} = \frac{Q_{Xy}}{V_{Sr}} \times f_{ML} \times TSCF$$

Summary of Transfer Factors for Plants in TRIM.FaTE (cont.)

PLANT STEM EXCHANGES (cont.)

Root-zone soil pore water to stem (simplification for nonionic organic compounds): TF 7-12b1

$$T_{SrW \rightarrow Stem} = \left[\frac{-\ln(1-\alpha)}{t_{\alpha}^{StSrW}} \right] \times \rho area_{Stem} \times \frac{SCF}{\rho_{SrW} \times d_{Sr}}$$

Stem to root-zone soil (simplification for nonionic organic compounds): TF 7-12b2

$$T_{Stem \rightarrow SrW} = \frac{-\ln(1-\alpha)}{t_{\alpha}^{StSrW}}$$

Leaf to stem: TF 7-13

$$T_{Leaf \rightarrow Stem} = Q_{Ph} \times \frac{1}{V_{Leaf} \times K_{LeafPh}}$$

Stem to leaf: TF 7-14

$$T_{Stem \rightarrow Leaf} = Q_{Xy} \times \frac{1}{V_{Stem} \times K_{StemXy}}$$

LITTER FALL

Leaf to surface soil: TF 7-15

$$T_{Leaf \rightarrow Ss} = k_L$$

Particles on leaf to surface soil: TF 7-16

$$T_{LeafP \rightarrow Ss} = k_L$$

LIST OF SYMBOLS USED IN PLANT TRANSFER FACTOR ALGORITHMS

υ_{dry} = volumetric dry deposition for particle-phase chemical (m^3[particles]/m^2[soil]-day).
I_{dry} = fraction of dry-depositing chemical that is intercepted by plant canopy (unitless).
A_S = area of associated soil (m^2).
V_{Air} = volume of air compartment (m^3).
f_{MS} = mass fraction of chemical in the air compartment that is sorbed to solid particles divided by the volume fraction of the air compartment that consists of particles (unitless).
V_{LeafP} = volume of particles-on-leaf compartment (m^3).
υ_{wet} = volumetric wet deposition rate of particle-phase chemical (m^3[particle]/m^2[soil]-day = m/day),
I_{wet} = plant interception fraction for wet deposition (unitless).
A_{Ss} = area of surface soil compartment (m^2).
$k_{LeafP\text{-}Leaf}$ = 1st -order rate constant for transfer of chemical from particles on leaf to leaf (/day).
w_{rV} = vapor washout ratio (g[chemical]/m^3[rain] per g[chemical]/m^3[air]).
$rain$ = rain rate (m/day).
f_{MV} = mass fraction of chemical compartment that is in vapor phase divided by the volume fraction of compartment that is gas/vapor phase (unitless).
Z_{pure_water} = fugacity capacity of chemical in aqueous phase (mol/Pa-m^3).

Summary of Transfer Factors for Plants in TRIM.FaTE (cont.)

LIST OF SYMBOLS USED IN PLANT TRANSFER FACTOR ALGORITHMS (cont.)

Z_{Total_Air} = total fugacity capacity of chemical in air compartment (mol/Pa-m^3).
LAI = one-sided leaf-area index (m^2[total leaf area]/m^2[soil]).
g_C = total conductance of the cuticular path, including the air boundary layer (m/day).
g_S = total conductance of stomatal pathway, including mesophyll and air boundary layer (m/day).
V_{Leaf} = volume of leaf compartment (m^3).
Z_{pure_air} = fugacity capacity of chemical in gas phase of air (mol/Pa-m^3).
Z_{Total_Leaf} = total fugacity capacity of chemical in leaf compartment (mol/Pa-m^3).
α = proportion of equilibrium value achieved (default = 0.95) (unitless).
t_α = time required to reach 100×α percent of equilbrium value (days) (value depends on the compartments and phases for which time-to-equilibrium is modeled).
V_{Root} = volume of root compartment (m^3).
V_{Sr} = volume of root-zone soil compartment (m^3[soil]).
$K_{Root\text{-}Sr}$ = root/bulk-soil partition coefficient (m^3[soil]/m^3[root]).
$K_{Root\text{-}SrW}$ = root/soil-pore-water partition coefficient (m^3[water])/m^3[root]).
Z_{Total_Sr} = total fugacity capacity of root-zone soil compartment (mol/Pa-m^3).
fW_{Root} = fraction water content of root compartment (kg[water]/kg[root wet wt]).
fL_{Root} = fraction lipid content of root compartment (kg[lipid]/kg[root wet wt]).
K_{ow} = octanol-water partition coefficient (g[chemical]/kg[octanol] per g[chemical]/L[water]).
b = correction exponent for the differences between octanol and lipids (unitless).
ρ_{Root} = density of fresh root (kg[root wet wt]/m^3[root]).
Q_{Xy} = flow of transpired water (m^3[xylem]/day).
f_{ML} = mass fraction dissolved ÷ volume fraction of soil compartment that is liquid (water) (unitless).
$TSCF$ = transpiration stream concentration factor (g[chemical]/m^3[xylem] per g[chemical]/m^3[soil pore water]).
$\rho area_{Stem}$ = areal density of stem on associated soil (kg[stem wet wt]/m^2[soil]).
SCF = stem concentration factor (g[chemical]/kg[stem wet wt] per g[chemical]/kg[soil pore water]).
ρ_{SrW} = density of soil pore water (kg[water]/m^3[water] = 1 kg/m^3).
d_{Sr} = depth of root-zone soil compartment (m^3).
Q_{Ph} = phloem flux into leaves (m^3[phloem]/day) due to advection.
K_{LeafPh} = partition coefficient between leaves and phloem water (g[chemical]/m^3[leaf] per g[chemical]/m^3[phloem])).
V_{Stem} = volume of stem compartment (m^3[stem]).
K_{StemXy} = partition coefficient between stem and xylem water (m^3[xylem]/m^3[stem]).
k_L = litter-fall rate constant (/day).

- The volatilization of chemicals from soils and uptake by plant foliage occurs at a scale that is not easy to model in TRIM.FaTE.

- Little is known about the rate at which chemicals enter plant leaves from particulate matter or rain water on the leaf surface.

- The transport of many chemical species within plants is not well understood.

- The accumulation of chemicals by wood is not well understood; therefore, trees in TRIM.FaTE currently consist of leaves only and not stems or roots, except to the extent that stems are conduits of chemicals away from leaves.

Despite these limitations in understanding and available data, the potentially important transfer processes have been modeled in TRIM.FaTE to the extent possible given the state of the science and modeling efforts to date. The user can assess the importance of the limitations identified above using the sensitivity and uncertainty analysis tools for any given scenario.

7.2.1 TRANSFERS BETWEEN THE AIR, PARTICLES, AND PLANT LEAVES

The particles on the leaf surface are represented by the particles-on-leaf compartment type in the current TRIM.FaTE library. This compartment is comprised of particulate matter deposited to the leaf by either wet or dry deposition. Deposition is defined here as the mass transfer of suspended particulates from air to the plant surface. Elsewhere (*e.g.*, Lindberg et al. 1992), the deposition of chemicals to plants is defined to include the gaseous fraction of the pollutants that come into contact with plants. The uptake of gaseous pollutants in TRIM.FaTE is described in Section 7.2.2.

Dry or wet deposition of particles to the particles-on-leaf compartment is calculated by multiplying the particle-deposition velocity by the leaf-interception fraction. The leaf-interception fraction (I) is the fraction of the depositing chemical mass that is intercepted and initially retained on the leaf. Thus, the quantity ($1-I$) is the fraction of depositing chemical mass that is transferred to the surface soil. The chemical mass that is transferred to the leaf surface via particle deposition is assumed to join the particle-phase chemical in the particles-on-leaf compartment. From there, transfers of chemical between the leaf itself and the particles on the surface of the leaf occur via diffusion (see Section 7.2.1.5).

It is common for a concentration of a deposited particulate chemical to be estimated with respect to the leaf or above-ground plant mass. However, when that concentration is estimated, it is often forgotten that most of the chemical mass is still *on* the plant rather than *in* it. This situation is treated explicitly in the current TRIM.FaTE library through the inclusion of a separate compartment for particles on leaf.

In the TRIM.FaTE code, the transfer factors for exchanges between plant leaves and the air or air particles include the variable *AllowExchange*, which must equal one (yes) for the transfer to occur.

7.2.1.1 Dry Deposition of Particles to Surface of Plant Leaves

Dry deposition is estimated by multiplying the predicted air concentration of airborne particles at ground level by the dry-particle-deposition velocity (U.S. EPA 1997a). A unidirectional flux equation that expresses dry deposition to the leaf, from van de Water (1995), follows. Note that, as the boundaries of the surface soil and air parcels may not be congruent, that is the area of soil and the area associated with a contiguous air compartment may be different. This algorithm describes the accumulation of chemical mass in the particles on leaves due to deposition from any air compartment to the area of the associated surface soil compartment that it spatially overlaps.

$$\frac{dN_{LeafP}}{dt} = \frac{N_{Air}}{V_{Air}} \times \upsilon_{dry} \times I_{dry} \times \frac{Z_{pure\_solid}}{Z_{Total\_Air}} \times A_S \qquad \text{(Eq. 7-1)}$$

where:

N_{LeafP} = mass of chemical in particles-on-leaf compartment (g[chemical]);
N_{Air} = mass of chemical in the air compartment (g[chemical]);
V_{Air} = volume of air compartment (m^3);
υ_{dry} = volumetric dry deposition of particles (m^3[particles]/m^2[soil]-day);
I_{dry} = fraction of dry-depositing chemical that is intercepted and initially retained by the plant canopy (unitless, below);
Z_{pure_solid} = fugacity capacity of the chemical in or sorbed to solid particles (mol/m^3-Pa);
Z_{Total_Air} = total fugacity capacity in bulk air, including atmospheric dust particles (mol/m^3-Pa); and
A_S = area of associated soil (m^2).

The volumetric dry deposition of particles is calculated as:

$$\upsilon_{dry} = v_{dep} \times \frac{D_L}{\rho_P} \qquad \text{(Same as Eq. 4-2)}$$

where:

v_{dep} = dry deposition velocity of air particles (m/day);
D_L = dust load in air compartment (kg[particles]/m^3[air]); and
ρ_P = density of dust particles (kg[particles]/m^3[particles]).

The interception fraction for dry deposition (I_{dry}) of particles is calculated using the following equation (Baes et al. 1984):

$$I_{dry} = 1 - e^{(1 - fW_{Leaf})(-\alpha_{VAF} \times \rho area)} \qquad \text{(Eq. 7-2)}$$

where:

fW_{Leaf} = water content of leaf (kg[water]/kg[leaf wet wt]);
α_{VAF} = vegetation attenuation factor (m^2[leaf]/kg[plant dry wt]); and
$\rho area$ = wet above-ground non-woody vegetation biomass inventory per unit area of the surface soil (kg[plant wet wt]/m^2[soil]).

Chamberlain (1970) describes the relationship between I_{dry} and above-ground (dry) biomass, and Prohl and Hoffman (1996) provide an excellent review of interception and loss processes along with values (and ranges) for the constants used to estimate I_{dry}.

The water content adjusts $\rho area$ to represent dry biomass. The equation was originally derived for pasture grasses and hay and expanded to other crops. For this reason, the biomass estimate should not include wood biomass in its calculation. The vegetation attenuation factor (sometimes called the foliar interception constant) is sometimes equivalent to the surface area of leaves divided by plant biomass (van de Water 1995) or the leaf biomass if the plant is woody.

Thus, TRIM.FaTE estimates the dry deposition of chemical mass associated with airborne particles to the particles-on-leaf compartment as:

$$T_{Air \rightarrow LeafP}^{dry\_dep} = \frac{\upsilon_{dry} \times I_{dry} \times A_S}{V_{Air}} \times f_{MS} \qquad \text{(TF 7-1)}$$

where:

$T_{Air \rightarrow LeafP}^{dry\_dep}$ = transfer factor for dry deposition of particulate-phase chemical in air to the particles on the surface of plant leaves when it is not raining (/day); and

f_{MS} = $Z_{pure\_solid}/Z_{Total\_Air}$, also the fraction of chemical mass in air compartment that is sorbed to solid dust particles divided by the volume fraction of air that consists of dust particles (see Equations 2-71 and 2-79) (unitless).

The implicit assumption in this algorithm is that depositing particles reach thermodynamic (chemical) equilibrium with the surrounding air before contacting the leaf surface. Accepting this assumption, the transfer to vegetation by dry deposition is related to the total chemical mass in the air compartment (combined gas- and particle-phase) using the particle/gas partition coefficient (normalized on a volume basis), K'_p, which is the dimensionless particle/gas partition coefficient (g[chemical]/m^3[particles] per g[chemical]/m^3[air compartment]). The factor f_{MP} is equivalent to K'_p.

7.2.1.2 Blow Off of Particles on Leaf to Air

The intent in the conceptual design of the leaf-particle transfer algorithms is to maintain a constant (although unknown) mass of particles on the leaf. The algorithm below is based on three assumptions: (1) particles are blown off the plant by wind at a rate that equals the deposition rate to leaves; (2) the concentration in the particles blown off the leaf is equal to the concentration in particles remaining on the leaf; and (3) all particles are dispersed in air.

$$T_{LeafP \rightarrow Air}^{blow\_off} = \frac{\upsilon_{dry} \times I_{dry} \times A_S}{V_{LeafP}} \qquad \text{(TF 7-2)}$$

where:

$T_{LeafP \rightarrow Air}^{blow\_off}$ = transfer factor for particle-phase chemical on surface of leaf blown off to air (dry resuspension of particles) when it is not raining (/day)]; and

V_{LeafP} = volume of the particles-on-leaf compartment (m^3).

The factor f_{MP} is not needed in the algorithm TF 7-2 because all of the chemical mass inventory in the particles-on-leaf compartment is sorbed to particles, and the compartment consists only of the solid phase. The particles blown off leaves into the air are then available for redeposition to leaves and the surface soil. Note that the algorithm for blow off of particles from leaves includes a meteorological toggle that turns the process off during rain (the analogous process during rain is wash off; see Section 7.2.1.4).

7.2.1.3 Wet Deposition of Particles to Surface of Plant Leaves

Rain scavenges some of the particulate-phase chemical from the air, depositing it on the surface of leaves. The concentration in the rain drop is related to the fraction of the chemical in the air that is associated with the particle and the scavenging ratio for particles in rain drops. Thus, wet deposition resulting from this process can be modeled using equations similar to dry deposition of particles. The rate of mass transfer of particle-phase chemicals from air to rain water and to the particles-on-leaf compartment can be described as:

$$\frac{dN_{LeafP}}{dt} = \frac{N_{Air}}{V_{Air}} \times w_r \times rain \times \frac{D_L}{\rho_P} \times I_{wet} \times \frac{Z_{pure\_solid}}{Z_{Total\_Air}} \times A_S \qquad \text{(Eq. 7-3)}$$

where:

N_{LeafP} = mass of chemical in particles-on-leaf compartment (g[chemical]);
N_{Air} = mass of chemical in the air compartment (g[chemical]);
V_{Air} = volume of air compartment (m^3);
w_r = scavenging or washout ratio for particles in air (ranges from 50,000 to 200,000) (m^3[air]/m^3[rain]);
$rain$ = rate of rainfall (m/day);
D_L = dust load, *i.e.*, density of dust particles in air (kg[particles]/m^3[air]);
ρ_P = density of dust particles (kg[particles]/m^3[particles]);
I_{wet} = wet interception fraction (unitless);
Z_{pure_solid} = fugacity capacity of the chemical in or sorbed to solid particles (mol/m^3-Pa);
Z_{Total_Air} = total fugacity capacity in bulk air, including atmospheric dust particles (mol/m^3-Pa); and
A_S = area of associated soil (m^2).

The washout ratio for particle-bound chemicals typically is restricted to empirical data on particle scavenging ratios (Wania et al. 1998). The expression $w_r \times J_{rain} \times (D_L/\rho_{dust})$ equals the volumetric particle wet deposition velocity, υ_{wet}:

υ_{wet} = volumetric wet deposition rate of air particles (m^3[particle]/m^2[soil]-day = m/day),
= $w_r \times rain \times (D_L/\rho_p)$.

Thus, the transfer factor that describes chemical deposition to the particles-on-leaf compartment from wet deposition of air particles is calculated as:

$$T_{Air \rightarrow LeafP}^{wet\_dep} = \frac{\upsilon_{wet} \times I_{wet} \times A_S}{V_{Air}} \times f_{MS} \qquad \text{(TF 7-3)}$$

where:

$T_{Air \rightarrow LeafP}^{wet\_dep}$ = transfer factor for wet deposition of particulate-phase chemical in air to the particles on plant leaves when it is raining (/day); and

f_{MS} = the mass fraction of chemical in the particle-phase divided by the volume fraction of the air compartment that is particulate (unitless).

The wet particle interception fraction in the preceding equations can be calculated using the following equation from Muller and Prohl (1993). The value of the fraction depends on how much water the leaf can hold, the total amount of rainfall during a rainfall event, and the ability of the element or compound to stick to the leaf.

$$I_{wet} = \frac{LAI \times S}{rain} \times \left[1 - e^{\left(\frac{-\ln(2)}{3 \times S} \times rain \right)} \right] \qquad \text{(Eq. 7-4)}$$

where:

LAI = one-sided leaf-area index (m^2[total leaf area]/m^2[underlying soil area]);
S = vegetation-dependent leaf-wetting factor (retention coefficient) (m); and
$rain$ = amount of rainfall during a rainfall event (m).

With the current TRIM.FaTE library, however, the user must specify a value for the wet deposition interception fraction or accept the default value of 0.2, which is based on five years of meteorological data for a site in Maine. Because it is a fraction, the upper bound for I_{wet} is 1.

7.2.1.4 Wash-off of Chemical from Plant Surface

During rain, the chemical sorbed to particles on the surface of the leaf can be washed off and deposited to the surface soil. In TRIM.FaTE, this transfer is estimated by an equation that is basically the same as TF 7-3, *i.e.*:

$$T_{LeafP \rightarrow Ss}^{wash\_off} = \frac{\upsilon_{wet} \times I_{wet} \times A_{Ss}}{V_{LeafP}} \qquad \text{(TF 7-4a)}$$

where:

$T_{LeafP \rightarrow Ss}^{wash\_off}$ = transfer factor for wash off of particle-phase chemical from particles-on-leaf compartment to surface soil (/day);

υ_{wet} = volumetric wet deposition rate of air particles (m^3[particles]/m^2[soil]-day);

I_{wet} = fraction of wet-depositing particle-phase chemical that is intercepted by plant canopy (unitless);
A_S = area of the associated soil (m^2[soil]); and
V_{LeafP} = volume of particles-on-leaf compartment (m^3).

This equation has been implemented to ensure that the particle mass on the leaves does not change (*i.e.*, as much is wet-deposited as is washed off). The factor f_{MS} is not needed in algorithm TF 7-4a because all of the chemical mass inventory in the particles-on-leaf compartment is sorbed to particles, and the compartment consists only of the solid phase. Note that the algorithm for wash off of particles from leaves includes a meteorological toggle that turns the process on during rain (the analogous process when it is not raining is blow off; see Section 7.2.1.2).

There are some data available on wash off of particles from the surface of conifer leaves during rain that indicate first-order kinetics with a rate constant of approximately 0.04 per min (McCune and Lauver 1986). The rate of 0.04 per min is equivalent to 2.4 per hour or 57.6 per day. It may be assumed that the particles deposited in rain water and the chemical dissolved in rain water is washed off at the same rate. Thus, an alternative equation to estimate wash-off from conifer leaves could be:

$$\frac{dN_{LeafP}}{dt} = -57.6 \times N_{LeafP} \qquad \text{(Eq. 7-5)}$$

and the associated transfer factor for the chemical wash off to the surface soil compartment is:

$$T_{LeafP \rightarrow Ss}^{wash\_off} = 57.6 \qquad \text{(TF 7-4b)}$$

This algorithm is not included in the current TRIM.FaTE library, but is included here for users who may prefer this value for coniferous forests.

7.2.1.5 Transfer of Chemical to Leaf from Particles on Leaf

The fraction of chemical sorbed to particles on the leaves that enters the leaf cuticle per day is very uncertain. It depends on the relative concentrations in the plant and particles at equilibrium (which is unknown), as well as the time to equilibrium. It is sometimes assumed that chemicals attached to particles reach instantaneous solution equilibrium with plant tissues when they land on the plant. If that assumption is made for some chemicals (*e.g.*, mercury), TRIM.FaTE is likely to overestimate the contribution of the particles to uptake of the chemical by the plant (Lindberg 1999a). For a chemical that is tightly and chemically bound to particles in air (*e.g.*, mercury), an initial assumption of 0.2 per day may be appropriate (*i.e.*, assume a half-life of one week). Because particles cover only a small fraction of the surface of the plant, it is assumed that the rate of transfer from leaves to particles is 1 percent of the rate constant for transfer in the other direction (*i.e.*, 0.002 per day). The rate may be higher for the transfer of mercury from the plant to a dissolved state in rain water, but no information is available on this. Note that these default values will change if units of time change. Thus, the transfer factors for exchange between the leaf and particles-on-leaf compartments are:

$$T_{LeafP \rightarrow Leaf} = k_{LeafP-Leaf} \tag{TF 7-5}$$

$$T_{Leaf \rightarrow LeafP} = 0.01 \times k_{LeafP-Leaf} \tag{TF 7-6}$$

where:

$T_{LeafP \rightarrow Leaf}$ = transfer factor for transfer of chemical from particles-on-leaf compartment to leaf compartment (/day);
$k_{LeafP\text{-}Leaf}$ = first-order rate constant for transfer of chemical from particles on leaf to leaf (/day); and
$T_{Leaf \rightarrow LeafP}$ = transfer factor for transfer of chemical from leaf to particles-on-leaf compartment (/day).

In the current TRIM.FaTE library, these transfer factors are numeric constants set by the user. Thus, to implement the relationship described here, the value of $T_{Leaf\text{->}LeafP}$ should be set to 0.01 times that of $T_{LeafP\text{->}Leaf}$.

7.2.1.6 Transfer of Vapor-phase Chemical to Leaf from Air During Rain

The rate of mass transfer of the vapor-phase chemical from air to rain water and to the plant leaf is described by the following equation (modified from van de Water 1995):

$$\frac{dN_{Leaf}}{dt} = \frac{N_{Air}}{V_{Air}} \times w_{rV} \times rain \times A_S \times I_{wet} \times f_{MV} \tag{Eq. 7-6}$$

where:

N_{Leaf} = mass of chemical in the leaf (g[chemical]);
N_{Air} = mass of chemical in air (g[chemical]);
V_{Air} = volume of air compartment (m^3[air]);
w_{rV} = vapor washout ratio (g[chemical dissolved]/m^3[rain] per g[chemical vapor-phase]/m^3[air]);
$rain$ = rain rate (m/day);
A_S = area of associated soil (m^2);
I_{wet} = interception fraction for wet deposition (unitless); 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.*, fraction that is not particulate).

It is difficult to know whether vapor-phase chemicals dissolved in rain and deposited to leaves will partition into the particles on the surface of the leaf or into the leaf cuticle. The water droplets on a leaf are small and persist for only a short period of time. The surface area of the leaf that is actually in contact with the water also can be much larger or smaller than the macroscopic surface of the leaf (Riederer 1995). Given the relative surface area of the leaf versus the surface particles, we assume that all wet deposition of vapor that is intercepted and initially retained by the leaf will interact directly with the leaf compartment. Deposited chemical can subsequently partition between the leaf and particles on the leaf (see Section 7.2.1.5).

The vapor wet interception fraction can be calculated using the same equation from Muller and Prohl (1993) that was used to estimate the particle wet interception fraction (Equation 7-4 above). As before, the value of the fraction depends on how much water the leaf can hold, the total amount of rainfall during a rainfall event, and the ability of the element or compound to stick to the leaf.

$$I_{wet} = \frac{LAI \times S}{rain} \times \left[1 - e^{\left(\frac{-\ln(2)}{3 \times S} \times rain \right)} \right] \qquad \text{(Same as Eq. 7-4)}$$

The vapor washout ratio, w_{rV}, is the equilibrium partition coefficient for a chemical between rain water and the vapor phase in air; in other words, the chemical concentration in rain divided by the chemical concentration in the gaseous phase. It can also be expressed as a ratio of Z factors (see Chapter 2):

$$w_{rV} = \frac{C_{rain\_water}}{C_{air}} = \frac{Z_{pure\_water}}{Z_{pure\_vapor}} = \frac{1}{K_{AW}} \qquad \text{(Eq. 7-7)}$$

where:

C_{rain_water} = concentration of chemical in rain water (g[chemical]/m^3[rain]);
C_{air} = concentration of vapor-phase chemical in gas-phase air (g[chemical]/m^3[air]);
Z_{pure_water} = fugacity capacity of chemical in aqueous phase (mol/m^3-Pa);
Z_{pure_air} = fugacity capacity of vapor-phase chemical in air (excluding dust particles) (mol/m^3-Pa); and
K_{AW} = air/water partition coefficient (g[chemical]/m^3[air] per g[chemical]/m^3[water], unitless).

For some chemicals (*e.g.*, the mercury species), the user can specify the washout ratio, w_{rV}, using an empirically derived equilibrium partition coefficient between the water and vapor phases of the chemical, K_{WA}. Thus, the transfer of vapor-phase chemical from air to plant leaves during a rainfall event is calculated as:

$$T_{Air \rightarrow Leaf}^{Vwet\_dep} = \frac{A_S}{V_{Air}} \times w_{rV} \times rain \times I_{wet} \times f_{MV} \qquad \text{(TF 7-7a)}$$

where:

$T_{Air \rightarrow Leaf}^{Vwet\_dep}$ = transfer factor for wet deposition of vapor-phase chemical in air to the leaf when it is raining (/day); and
w_{rV} = $1/K_{AW}$ as described in Equation 7-7 above.

For other chemicals (*e.g.*, nonionic organic chemicals), the expression $w_{rV} \times f_{MV}$ can be estimated from the expression $Z_{pure\_water}/Z_{Total\_Air}$ as follows. From Equation 7-7 and the definition of f_{MV} above:

$$w_{rV} \times f_{MV} = \frac{Z_{pure\_water}}{Z_{pure\_vapor}} \times \frac{Mass\_Fraction\_Vapor}{Volume\_Fraction\_Vapor} \qquad \text{(Eq. 7-8)}$$

From Equation 2-73:

$$Z_{Total\_Air} = Z_{pure\_vapor} \times \left[\frac{Volume\_Fraction\_Vapor}{Mass\_Fraction\_Vapor} \right] \qquad \text{(Eq. 7-9)}$$

Therefore:

$$w_{rV} \times f_{MV} = \frac{Z_{pure\_water}}{Z_{Total\_Air}} \qquad \text{(Eq. 7-10)}$$

Thus, an alternative algorithm for wet deposition of vapor-phase chemical to plant leaves is calculated as:

$$T^{Vwet\_dep}_{Air \to Leaf} = \frac{A_S}{V_{Air}} \times rain \times I_{wet} \times \frac{Z_{pure\_water}}{Z_{Total\_Air}} \qquad \text{(TF 7-7b)}$$

where:

$T^{Vwet\_dep}_{Air \to Leaf}$ = transfer factor for wet deposition of vapor-phase chemical in air to the leaf (/day); and

Z_{Total_Air} = total fugacity capacity of chemical in air compartment (mol/m^3-Pa).

7.2.2 UPTAKE OF GASEOUS CHEMICAL INTO FOLIAGE

The diffusion pathway between air and leaves is relevant for all gaseous forms of chemicals, including organic compounds and mercury species. The diffusion from air to plants is based on two resistances in parallel: (a) the series resistance of air boundary (Section 7.2.2.1), stomata (Section 7.2.2.2), and mesophyll (Section 7.2.2.3), and (b) the series resistance of air boundary (7.2.2.1) and cuticle (Section 7.2.2.5). It is assumed that the chemical fraction that is in the plant cuticle or mesophyll is inside of the plant, but that the chemical inside of the stomata but outside of the mesophyll is outside of the plant. It should be noted that the resistance is the inverse of the conductance. Damage to the plant (*e.g.*, from insect herbivory) can also modify the transport of nutrients from plant leaves (Hargrove 1999). However, the contribution of insect or other sources of damage to the diffusion of mercury and other chemicals into and out of the plant is unknown and not currently addressed in TRIM.FaTE.

7.2.2.1 Air Boundary-layer Conductance

The air boundary-layer conductance is defined by the following equation:

$$g_B = \frac{D_{pure\_air}}{\delta_{AP}} \qquad \text{(Eq. 7-11)}$$

where:

g_B = conductance of the air boundary layer (m/day);
D_{pure_air} = diffusion coefficient of chemical through still, pure air (m^2[air]/day); and
δ_{AP} = thickness of air boundary layer (*i.e.*, still air) over leaf surfaces (m).

The boundary layer thickness (δ_{AP} in m) may be approximated by Equation 7-12 below (Nobel 1999), or the value may be assumed (*e.g.*, 0.001 m in Riederer 1995, 0.005 m in McKone 1993a,b,c). The constant of 0.00389 in the following equation is the square root of the viscosity of air at 20° Celsius, 1.51×10^{-5} m^2/sec (Wilmer and Fricker 1996).

$$\delta_{AP} = 0.00389\sqrt{l / v} \qquad \text{(Eq. 7-12)}$$

where:

l = length of flat leaf (m); and
v = wind velocity (m/sec).

7.2.2.2 Stomatal Conductance

The stomatal conductance of gaseous chemicals into the leaf is calculated in the TRIM.FaTE library using the following equation (Riederer 1995):

$$g_{stomata} = \frac{D_{pure\_air} \times na_S \times IsDay \times \alpha_S}{x_S + y_S} \qquad \text{(Eq. 7-13)}$$

where:

$g_{stomata}$ = conductance of the chemical through the stomata (m/day);
D_{pure_air} = diffusion coefficient of the chemical in pure, still air (m^2[air]/day);
na_S = number of stomata in leaf (n) times area of 1 stomata divided by area of leaf (a_S) (unitless);
α_S = mean degree of opening of stomatal pores, between 0 and 1 (default = 1) (unitless);
$IsDay$ = a time-varying parameter that equals 1 during the day and 0 at night, to open and close the stomatal pores (unitless);
x_S = depth of elliptical pore (m); and
y_S = mean pore radius (m).

In the field, the degree of opening of stomatal pores tends toward one during the day and zero at night, unless the temperature is high and the humidity low, in which case the value of α_S will be less than one during the day. The default value in the TRIM.FaTE library for α_S during the day is one. The stomatal conductance is "turned off" when *IsDay* equals zero.

Analysis of data reported by Wilmer and Fricker (1996, p. 18) indicates that the value for the expression $(na_S)/(x_S + y_S)$ is relatively similar among plant species (*i.e.*, coefficient of variation ~0.5). Thus, that expression in Equation 7-13 is replaced in the TRIM.FaTE library by a single parameter:

$$S_N = \frac{na_S}{x_S + y_S} \qquad \text{(Eq. 7-14)}$$

where:

S_N = stomatal area, normalized for effective diffusion path length (/m).

Thus, in the TRIM.FaTE library:

$$g_{stomata} = D_{pure\_air} \times S_N \times \alpha_S \qquad \text{(Eq. 7-15)}$$

If this algorithm for $g_{stomata}$ is used, it should be noted that a model limitation is that conductance varies with temperature. In the 20° to 40°C temperature range, the vapor flux from leaves has been observed to double with a 10° rise in temperature (Leonard et al. 1998), so variability in temperature could contribute significantly to the uncertainty in this type of transfer.

If data on the effective diffusivity of the subject chemical in air, D_{pure_air}, are lacking, the following alternate equation can be used to estimate diffusivity (conductance) of the chemical through stomata based on diffusivity of water through stomata (Trapp 1995). In other words, the stomatal conductance of gaseous chemicals into the leaf may be approximated from the stomatal conductance of water vapor. The only chemical-specific parameter that is required is the molecular weight of the chemical:

$$g_{stomata} = \sqrt{18 / M_W} \times g_{water} \qquad \text{(Eq. 7-16)}$$

where:

18 = molecular weight of water (g[water]/mol[water]);
M_W = molecular weight of chemical (g[chemical]/mol[chemical]); and
g_{water} = conductance of water through the stomata (m/day).

Conductance of water through the stomata may be calculated using the following algorithm from Bennett et al. (1998):

$$g_{water} = \frac{461 \times T}{(1 - rh) \times 611 \times 10^{\frac{7.5(T-273)}{(237+(T-273))}}} \times \left(1\ \mathrm{kg} \times \mathrm{d}^{-1} \times \mathrm{m}^{2}\right) \qquad \text{(Eq. 7-17)}$$

where:

rh = relative humidity (unitless); and
T = temperature (°K).

Note that Equation 7-16 for stomatal conductance, with Equation 7-17 substituted for g_{water}, includes the resistance of the air-side boundary in series with the stomatal resistance. If those equations were to be implemented in TRIM.FaTE instead of Equation 7-15, it would be necessary to remove the air boundary-layer resistance from Equations 7-18 and 7-19 for total conductance of the stomatal pathway (see Section 7.2.2.4 below).

7.2.2.3 Conductance of Mesophyll

It is suggested that for most organic chemical species and most plant species, the stomatal or cuticular conductance is the rate-limiting pathway (Riederer 1995). Therefore, for most chemicals, there is no need to consider the conductance of mesophyll (inner tissue). However, some work with elemental mercury cited in Lindberg et al. (1992) suggests that "resistance on or within mesophyll surfaces dominates the atmosphere-leaf diffusive path of Hg^0" (see Section A.1.5 of Appendix A). Thus, conductance of the mesophyll is included when estimating the total conductance of the stomatal pathway for Hg(0), as described in the next subsection.

7.2.2.4 Total Conductance of the Stomatal Pathway

The total conductance of the stomatal pathway is:

$$g_S = \left(\frac{1}{g_{stomata}} + \frac{1}{g_m} + \frac{1}{g_B} \right)^{-1} \qquad \text{(Eq. 7-18)}$$

where:

g_S = total conductance of stomatal pathway, including mesophyll (m/day);
$g_{stomata}$ = conductance of stomata (m/day);
g_m = conductance of mesophyll (m/day); and
g_B = conductance of the air boundary layer (m/day) (see Section 7.2.2.1).

However, of the chemicals evaluated for TRIM.FaTE to date, only elemental mercury encounters significant resistance from the mesophyll (see Section 7.2.2.3). Thus, Equation 7-18 would be used in full for elemental mercury, but the middle term for the resistance of the mesophyll would be dropped from the equation for the two other mercury species (*i.e.*, divalent and methyl). The total conductance of the stomatal pathway for chemicals other than elemental mercury thus far included in the TRIM.FaTE library is:

$$g_S = \left(\frac{1}{g_{Stomata}} + \frac{1}{g_B} \right)^{-1} \qquad \text{(Eq. 7-19)}$$

7.2.2.5 Cuticular Conductance

The cuticular conductance (mass transfer coefficient for chemical transfer across the cuticle side of the air/plant interface) is defined by the following equation (Riederer 1995):

$$g_{cuticle} = \frac{P_{cuticle}}{K_{AW}} \qquad \text{(Eq. 7-20)}$$

where:

$g_{cuticle}$ = conductance of the cuticle (m/sec);
$P_{cuticle}$ = permeance of the cuticle (m/sec); and
K_{AW} = air/water partition coefficient, *i.e.*, equilibrium ratio between the chemical in water and in the vapor phase (g[chemical]/m^3[air] per g[chemical]/m^3[water]).

Cuticular permeance is an experimentally derived value that describes the mass transfer velocity from water into the leaf. The dimensionless air/water partition coefficient is used to transform the chemical in the sending compartment from water-phase to the vapor-phase in air. Cuticular permeance has been measured in *Citrus aurantium* leaves, and the following relationship in Equation 7-21 (below) was derived from those data (Riederer 1995). The variability of this relationship among plant species is unknown.

$$\log\left(P_{cuticle}\right) = 0.704 \times \log(K_{OW}) - 11.2 \quad (r = 0.91) \qquad \text{(Eq. 7-21)}$$

We extend Equation 7-21 to estimate the conductance from bulk air, using Z_{Total_Air} / Z_{pure_water}. Thus:

$$g_{cuticle} = \left(\frac{10^{0.704 \log K_{ow} - 11.2}}{Z_{Total\_Air} / Z_{pure\_water}} \right) \times 86{,}400 \qquad \text{(Eq. 7-22)}$$

where:

Z_{pure_water} = fugacity capacity of chemical in aqueous phase (mol/Pa-m^3);
Z_{Total_Air} = total fugacity capacity of chemical in bulk air (mol/Pa-m^3); and
86,400 = units conversion factor (sec/day).

The cuticular conductance must be put in series with resistance through the air boundary on the leaf surface to yield the total cuticular conductance (air-to-plant), adjusted for the fugacity capacity of the air and leaf. Thus:

$$g_C = \left(\frac{1}{g_B} + \frac{1}{g_{cuticle}} \right)^{-1} \qquad \text{(Eq. 7-23)}$$

where:

g_C = total conductance of the cuticular path, including the air boundary layer (m/day);
g_B = conductance of the boundary layer (m/day); and
$g_{cuticle}$ = conductance of the cuticle (m/day).

7.2.2.6 Transfer Factors for Diffusion

Riederer (1995) has derived a flux equation for diffusion in and out of plant leaves:

$$\frac{dN_{Leaf}}{dt} = \left[A_{LeafA} \times (g_C + g_S) \times \frac{N_{Air}}{V_{Air}} \right] - \left[A_{LeafA} \times (g_C + g_S) \times \frac{N_{Leaf}}{V_{Leaf}} \times \frac{K_{AW}}{K_{LeafW}} \right] \qquad \text{(Eq. 7-24)}$$

where:

N_{Leaf} = mass of chemical in leaves (g[chemical]);
A_{LeafA} = effective interfacial area between leaf and air (m^2);
N_{Air} = mass of chemical in air (g[chemical]);
V_{Air} = volume of air (m^3);
V_{Leaf} = volume of leaves (m^3);
K_{AW} = air/water partition coefficient (g[chemical]/m^3[air] per g[chemical]/m^3[water]); and
K_{LeafW} = leaf/water partition coefficient (g[chemical]/m^3[leaf] per g[chemical]/m^3[water]).

If the Riederer (1995) equation (which is calculated with respect to one-sided leaf area; *i.e.*, Eq. 7-4) is used in TRIM.FaTE to estimate stomatal conductance, the following equation is used to estimate diffusion of vapor-phase chemical from the plant leaf into the air:

$$T^{diff}_{Leaf \rightarrow Air} = (2LAI \times A_S \times g_C + LAI \times A_S \times g_S) \times \frac{1}{V_{Leaf}} \times \frac{Z_{pure\_air}}{Z_{Total\_Leaf}} \qquad \text{(TF 7-8a)}$$

where:

$T^{diff}_{Leaf \rightarrow Air}$ = transfer factor for diffusion of vapor-phase chemical from leaf to the air (/day);
LAI = one-sided leaf-area index (for the area of one side of a leaf) (unitless);
A_S = area of associated soil (m^2);
g_C = total conductance of the cuticular pathway, including the air boundary layer (m/day);
g_S = total conductance of the stomatal pathway, including the air boundary layer (m/day);
V_{Leaf} = volume of leaf compartment (m^3);
Z_{pure_air} = fugacity capacity of chemical in gas-phase air (mol/m^3-Pa); and
Z_{Total_Leaf} = total fugacity capacity of chemical in the leaf compartment (mol/m^3-Pa).

The Riederer (1995) equation is the default implemented in the current TRIM.FaTE library.

If the alternative equation for stomatal conductance from Bennett et al. (1998) is used to calculate stomatal conductance (*i.e.*, Equations 7-16 and 7-17), the transfer factor for diffusion from leaf to air would be calculated as:

$$T^{diff}_{Leaf \rightarrow Air} = (2LAI \times A_S \times g_C + A_S \times g_S) \times \frac{1}{V_{Leaf}} \times \frac{Z_{pure\_air}}{Z_{Total\_Leaf}} \qquad \text{(TF 7-8b)}$$

Note that the contact area associated with the cuticular pathway is double the LAI, because cuticles cover the top and bottom of a leaf.

The total fugacity capacity of the chemical in the leaf compartment, Z_{Total_Leaf}, can be calculated using Equation 7-25 (below), which represents plants as a mixture of air, water, and nonpolar organic matter analogous to octanol (Paterson and Mackay 1995). It is assumed that the fugacity capacity of the chemical in a plant leaf is equivalent to that in a generic plant that is 18 percent air, 80 percent water, and 2 percent nonpolar organic matter.

$$Z_{Total\_Leaf} = 0.18 \times Z_{pure\_air} + 0.80 \times Z_{pure\_water} + 0.02 \times K_{OW} \times Z_{pure\_water} \qquad \text{(Eq. 7-25)}$$

Since the Riederer (1995) equation (which is calculated with respect to one-sided leaf area, *i.e.*, Equation 7-11) is used for the stomatal conductance in the current TRIM.FaTE library, the transfer factor for diffusion of the chemical from the air into the leaf is calculated in the library as:

$$T^{diff}_{Air \rightarrow Leaf} = (2LAI \times A_S \times g_C + LAI \times A_S \times g_S) \times \frac{1}{V_{Air}} \qquad \text{(TF 7-9a)}$$

If the Bennett et al. (1998) equation is used for the stomatal conductance (*i.e.*, Equations 7-16 and 7-17), the transfer factor for diffusion from air to leaf would be calculated as:

$$T^{diff}_{Air \rightarrow Leaf} = (2LAI \times A_S \times g_C + A_S \times g_S) \times \frac{1}{V_{Air}} \qquad \text{(TF 7-9b)}$$

7.2.3 UPTAKE FROM SOIL BY ROOT

The uptake of chemicals by plant roots is treated as an equilibrium process in the current library. Two alternative algorithms may be used to calculate the accumulation of a chemical by plants from soil: uptake from bulk soil (Section 7.2.3.1) or uptake from soil pore water (Section 7.2.3.2). Both algorithms are derived from an equilibrium relationship, an estimated time to equilibrium, and the assumption of a first-order rate of uptake. The selection of algorithms for bulk soil or for soil pore water depends on the measured partition coefficient (*i.e.*, whether it was measured relative to bulk soil or estimated relative to soil pore water). Due to uncertainties associated with modeling these root types, initial TRIM.FaTE applications have not applied these algorithms to woody tree roots or tuber crops. Further consideration of compartment design, parameter values, etc. may lead to some use of these or other algorithms for those root types.

7.2.3.1 Uptake from Bulk Soil

The uptake of chemicals from bulk soil by roots is described in TRIM.FaTE by an equation in the form of time to equilibrium between the roots and soil. Because of the linear relationships in TRIM.FaTE, uptake is described as proportional to the concentration of the chemical in soil even though some studies suggest that a log-log regression between soil and root concentrations is a more precise model of uptake (Efroymson et al. 2001).

The change in concentration of the chemical in the root over time can be estimated using a time-to-equilibrium model (see Section 2.5):

$$\frac{dC_{Root}}{dt} = \left[\frac{-\ln(1-\alpha)}{t_{\alpha}^{RSr}}\right] \times K_{Root-Sr} \times C_{Sr} - \left[\frac{-\ln(1-\alpha)}{t_{\alpha}^{RSr}}\right] \times C_{Root} \qquad \text{(Eq. 7-26)}$$

where:

C_{Root} = concentration of chemical in the root compartment (g[chemical]/m^3[roots]);
α = proportion of equilibrium value achieved (default = 0.95);
t_{α}^{RSr} = time (days) required for the root/bulk-soil interaction to reach 100×α percent (default $\alpha = 0.95$) of equilibrium when C_{Sr} is approximately constant with time;
$K_{Root\text{-}Sr}$ = user-specified value for the partition coefficient of the chemical between the root and bulk wet soil (or uptake factor, g[chemical]/m^3[root] per g[chemical]/m^3[soil wet wt]); and
C_{Sr} = concentration of the chemical in the root-zone soil (g[chemical]/m^3[soil]).

If the areal density of roots is approximately constant with time, then:

$$\frac{dN_{Root}}{dt} = \left[\frac{-\ln(1-\alpha)}{t_{\alpha}^{RSr}}\right] \times V_{Root} \times K_{Root-Sr} \times \frac{N_{Sr}}{V_{Sr}} - \left[\frac{-\ln(1-\alpha)}{t_{\alpha}^{RSr}}\right] \times N_{Root} \qquad \text{(Eq. 7-27)}$$

where:

N_{Root} = mass of chemical in roots (g[chemical]);
V_{Root} = volume of roots (m^3[root]);
N_{Sr} = total mass of chemical in all phases of bulk root-zone soil (g[chemical]); and
V_{Sr} = total volume of root-zone soil, which contains roots (m^3[soil]).

Thus:

$$T_{Sr\rightarrow Root} = \left[\frac{-\ln(1-\alpha)}{t_{\alpha}^{RSr}}\right] \times \frac{V_{Root}}{V_{Sr}} \times K_{Root-Sr} \tag{TF 7-10a}$$

where:

$T_{Sr\rightarrow Root}$ = transfer factor for transfer of chemical from root-zone soil to root (/day).

The transfer in the other direction, from the root to the bulk root-zone soil is represented as:

$$T_{Root\rightarrow Sr} = \frac{-\ln(1-\alpha)}{t_{\alpha}^{RSr}} \tag{TF 7-11a}$$

where:

$T_{Root\rightarrow Sr}$ = transfer factor for transfer of chemical from root to root-zone soil (/day).

7.2.3.2 Uptake from Soil Pore Water

An alternative method by which to estimate the root concentration of a chemical is as an equilibrium between root-tissue and soil-pore-water concentrations. Selection of the appropriate method (*i.e.*, for bulk soil or for soil pore water) depends on the experimental method used to derive the partition coefficient, *i.e.*, whether the data are reported based on pore water, bulk soil, or dry soil and wet or dry roots. The equilibrium relationship is a generalization of the Briggs et al. (1982) equation developed in Trapp (1995):

$$C_{Root} = K_{Root-SrW} \times C_{SrW} \tag{Eq. 7-28}$$

where:

C_{Root} = concentration in roots (g[chemical]/m^3[root wet wt]);
$K_{Root\text{-}SrW}$ = root/root-zone-soil-water partition coefficient (g[chemical]/m^3[root] per g[chemical]/m^3[water] or m^3[water]/m^3[root]); and
C_{SrW} = concentration in root-zone soil pore water (g[chemical]/m^3[water]).

The root/root-zone-soil-water partition coefficient is determined as:

$$K_{Root-SrW} = (fW_{Root} + fL_{Root} \times K_{ow}^{b}) \times \rho_{Root} \times 0.001 \tag{Eq. 7-29}$$

where:

fW_{Root} = fraction water content of root (kg[water]/kg[root wet wt]);
fL_{Root} = fraction lipid content of root (kg[lipid]/kg[root wet wt]);
K_{ow} = octanol/water partition coefficient (g[chemical]/kg[octanol] per g[chemical]/L[water] or L[water]/kg[octanol]);
b = correction exponent for the differences between octanol and lipids (unitless);

ρ_{Root} = volumetric density of fresh root (kg[root wet wt]/m^3[root]); and
0.001 = unit conversion factor (m^3/L).

Thus:

$$\frac{dC_{Root}}{dt} = \left[\frac{-\ln(1-\alpha)}{t_\alpha^{RSrW}}\right] \times K_{Root-SrW} \times C_{SrW} - \left[\frac{-\ln(1-\alpha)}{t_\alpha^{RSrW}}\right] \times C_{Root} \qquad \text{(Eq. 7-30)}$$

where:

t_α^{RSrW} = time (days) required for the root/soil-pore-water interaction to reach 100×α percent (default α = 0.95) of equilibrium when C_{SrW} is approximately constant with time.

The value of t_α for the root/soil-pore-water interaction can be determined from empirical studies using roots exposed to the chemical in water. In the absence of any data, this t_α can be estimated from the following equation:

$$t_\alpha^{RSrW} = \frac{2 \times \left(1.62 + e^{\log(Kow)-1.8}\right)}{24} \qquad \text{(Eq. 7-31)}$$

That equation is based on the equation for the plant-root/soil-water interaction from Hsu et al. (1990), and 24 is the unit conversion factor (hr/day). However, it is a rough estimate, and the proportion of equilibrium that it might represent is not specified.

If the areal density of roots is approximately constant with time, then:

$$\frac{dN_{Root}}{dt} = \left[\frac{-\ln(1-\alpha)}{t_\alpha^{RSrW}}\right] \times V_{Root} \times K_{Root-SrW} \times \frac{N_{SrW}}{V_{SrW}} - \left[\frac{-\ln(1-\alpha)}{t_\alpha^{RSrW}}\right] \times N_{Root} \qquad \text{(Eq. 7-32)}$$

where:

N_{Root} = mass of chemical in roots (kg);
V_{Root} = total volume of roots (m^3[root]);
N_{SrW} = total mass of chemical in root-zone-soil water (kg), which
= N_{Sr} × *Fraction_Mass_Dissolved* (*i.e.*, the total chemical mass in the soil compartment multiplied by the fraction of it that is dissolved in water); and
V_{SrW} = volume of root-zone soil water (m^3[water]), which
= V_{Sr} × *Volume_Fraction_Liquid* (*i.e.*, volume of the soil compartment multiplied by θ, the fraction of the root-zone soil compartment that is liquid (see Equation 2-37)).

Making the substitutions for N_{SrW} and V_{SrW} and using Equation 2-72 (Chapter 2) to substitute Z factors for the ratio of fractions, the transfer factors are:

$$\begin{aligned} T_{SrW\rightarrow Root} &= \left[\frac{-\ln(1-\alpha)}{t_{\alpha}^{RSrW}}\right] \times \frac{V_{Root}}{V_{Sr}} \times K_{Root-SrW} \times \frac{Fraction\_Mass\_Dissolved}{Volume\_Fraction\_Liquid} \\ &= \left[\frac{-\ln(1-\alpha)}{t_{\alpha}^{RSrW}}\right] \times \frac{V_{Root}}{V_{Sr}} \times K_{Root-SrW} \times \frac{Z_{pure\_water}}{Z_{Total\_Sr}} \end{aligned} \qquad \text{(TF 7-10b)}$$

$$T_{Root\rightarrow SrW} = \frac{-\ln(1-\alpha)}{t_{\alpha}^{RSrW}} \qquad \text{(TF 7-11b)}$$

where:

$T_{SrW\rightarrow \mathrm{Root}}$ = transfer factor for transfer of chemical from root-zone soil water to root (/day);
$T_{Root\rightarrow SrW}$ = transfer factor for transfer of chemical from root to root-zone soil water (/day);
Z_{pure_water} = fugacity capacity of the chemical in aqueous phase (mol/Pa-m^3); and
Z_{Total_Sr} = total fugacity capacity of the chemical in the root-zone soil compartment (mol/Pa-m^3); and
V_{Sr} = volume of the root-zone soil compartment (m^3[soil]).

Note that the user specifies either equations TF 7-10a and TF 7-11a (for transfers related to bulk soil) or TF 7-10b and TF 7-11b (for transfers related to soil pore water only) for a given chemical.

7.2.4 TRANSFERS INVOLVING THE STEM

The algorithms for the uptake of chemicals by the stem are taken from Trapp (1995), who derived them for organic chemicals.

7.2.4.1 Contribution from Soil Pore Water via Transpiration Stream (Xylem)

Trapp (1995) derived an equation for the unidirectional flux of chemical from the soil pore water into the stem driven by the plant transpiration stream through its xylem:
where:

$$\frac{dN_{Stem}}{dt} = Q_{Xy} \times TSCF \times \frac{N_{SrW}}{V_{SrW}} \qquad \text{(Eq. 7-33)}$$

N_{Stem} = mass of chemical in stems (g[chemical]);
Q_{Xy} = total flow of transpired water (m^3[xylem]/day, derived below);
$TSCF$ = transpiration stream concentration factor (g[chemical]/m^3[xylem] per g[chemical]/m^3[soil pore water] or m^3[water]/m^3[xylem]);
N_{SrW} = mass of chemical in root-zone-soil pore water (g[chemical]); and

V_{SrW} = volume of water in root-zone soil (m^3[water]).

Using the equation of Hsu et al. (1990):

$$TSCF = \left[0.7 \times e^{\left(-\left((\log(Kow) - 3.07)^2 \right) / 2.78 \right)} \right] \qquad \text{(Eq. 7-34)}$$

According to Crank et al. (1981):

$$Q_{Xy} = 4.8 \times 10^{-3} \times LAI \times A_S \qquad \text{(Eq. 7-35)}$$

where:

4.8×10^{-3} = empirical factor (m^3[water]/m^2[leaf]-day);
LAI = leaf-area index (m^2[leaf]/m^2[soil]); and
A_S = area of associated soil (m^2[soil]).

The quantity (N_{SrW}/V_{SrW}) in Equation 7-33 equals the concentration of the chemical in the root-zone soil pore water in g[chemical]/m^3[water]. That quantity can also be expressed as the fraction of the mass of the chemical in the root-zone soil compartment that is dissolved in water divided by the volume of the root-zone soil compartment that is liquid, which equals $Z_{pure\_water}/Z_{Total\_Sr}$ (see Section 2.6):

$$\frac{N_{SrW}}{V_{SrW}} = \frac{N_{Sr}}{V_{Sr}} \times \frac{Mass\_Fraction\_Dissolved}{Volume\_Fraction\_Liquid} = \frac{N_{Sr}}{V_{Sr}} \times \frac{Z_{pure\_water}}{Z_{Total\_Sr}} \qquad \text{(Eq. 7-36)}$$

Thus:

$$T_{Sr \to Stem} = \frac{Q_{Xy} \times Z_{pure\_water}}{V_{Sr} \times Z_{Total\_Sr}} \times TSCF$$

$$= \frac{Q_{Xy}}{V_{Sr}} \times f_{ML} \times TSCF \qquad \text{(TF 7-12a)}$$

where:

$T_{Sr \to Stem}$ = transfer factor for transfer of chemical from root-zone soil to stem (/day);
Z_{pure_water} = fugacity capacity of chemical in pure water (mol/Pa-m^3);
V_{Sr} = volume of the root-zone soil compartment (m^3);
$Z_{\text{Total\_Sr}}$ = total fugacity capacity of chemical in bulk root-zone soil (mol/Pa-m^3); and
f_{ML} = fraction of chemical mass that is dissolved in water divided by fraction of the volume of the root-zone soil compartment that is water (unitless), which
= $Z_{pure\_water}/Z_{Total\_Sr}$ (see Equations 2-72 and 2-80).

7.2.4.2 Alternative Algorithm for Soil/Stem Transfers

An alternative algorithm for uptake of nonionic organic chemicals by the stem from root-zone soil is an equilibrium relationship between the soil pore water and stem taken from Briggs et al. (1983):

$$C_{Stem} = SCF \times C_{SrW} \times \frac{\rho_{Stem}}{\rho_{SrW}} \qquad \text{(Eq. 7-37)}$$

where:

C_{Stem} = concentration of chemical in stem (g[chemical]/m^3[stem]);
C_{SrW} = concentration in root-zone-soil pore water (g[chemical]/m^3[water]);
SCF = stem concentration factor (g[chemical]/kg[stem wet wt] per g[chemical]/kg[water] or kg[water]/kg[stem wet wt]) (see below);
ρ_{Stem} = density of stem (kg[stem wet wt]/m^3[stem]); and
ρ_{SrW} = density of root-zone-soil pore water (kg[water]/m^3[water]).

The *SCF* may be calculated using the following equation from Briggs et al. (1983):

$$SCF = (10^{0.95 \times \log(K_{ow}) - 2.05} + 0.82) \times 0.784 \times e^{-(\log(K_{ow}) - 1.78)^2 / 2.44} \qquad \text{(Eq. 7-38)}$$

Thus, the change in chemical concentration in the stem is estimated as:

$$\frac{dC_{Stem}}{dt} = \left[\frac{-\ln(1-\alpha)}{t_{\alpha}^{StSrW}}\right] \times SCF \times \frac{\rho_{Stem}}{\rho_{SrW}} \times C_{SrW} - \left[\frac{-\ln(1-\alpha)}{t_{\alpha}^{StSrW}}\right] \times C_{Stem} \qquad \text{(Eq. 7-39)}$$

where:

t_{α}^{StSrW} = time (days) required for the stem/root-zone-soil-pore-water interaction to reach 100×α percent of the equilibrium value when C_{SrW} is approximately constant with time.

If the areal density of stems is approximately constant with time, then:

$$\frac{dN_{Stem}}{dt} = \left[\frac{-\ln(1-\alpha)}{t_{\alpha}^{StSrW}}\right] \times V_{Stem} \times SCF \times \frac{\rho_{Stem}}{\rho_{SrW}} \times \frac{N_{SrW}}{V_{SrW}} - \left[\frac{-\ln(1-\alpha)}{t_{\alpha}^{StSrW}}\right] \times N_{Stem} \qquad \text{(Eq. 7-40)}$$

where:

N_{Stem} = mass of chemical in fresh stems (g[chemical]);
V_{Stem} = total volume of stem compartment (m^3[stem]);
N_{SrW} = total mass of chemical in root-zone soil water (g[chemical]); and
V_{SrW} = volume of root-zone soil water (m^3[water]).

The total volume of the stem compartment can be calculated as follows:

$$V_{Stem} = \frac{\rho area_{Stem} \times A_{Sr}}{\rho_{Stem}} \qquad \text{(Eq. 7-41)}$$

where:

$\rho area_{Stem}$ = areal density of stem on associated soil (kg[stem wet wt]/m^2[soil]);
A_{Sr} = area of associated root-zone-soil compartment (m^2[soil]); and
ρ_{Stem} = wet density of stem (kg[stem wet wt]/m^3[stem]).

Thus, the transfer factors describing the transfer from root-zone-soil pore water to the stem and from the stem to the root-zone-soil pore water are:

$$T_{SrW \rightarrow Stem} = \left[\frac{-\ln(1-\alpha)}{t_{\alpha}^{StSrW}}\right] \times \rho area_{Stem} \times \frac{SCF}{\rho_{SrW} \times d_{Sr}} \qquad \text{(TF 7-12b1)}$$

and:

$$T_{Stem \rightarrow SrW} = \frac{-\ln(1-\alpha)}{t_{\alpha}^{StSrW}} \qquad \text{(TF 7-12b2)}$$

where:

$T_{SrW \rightarrow Stem}$ = transfer factor for transfer of chemical from root-zone soil water to stem (/day);
$T_{Stem \rightarrow SrW}$ = transfer factor for transfer of chemical from stem to root-zone soil water (/day); and
d_{Sr} = depth of root-zone soil compartment (m), which
= V_{Sr} (m^3) / A_{Sr} (m^2).

Note that this alternative algorithm for nonionic organic chemicals includes transfers in two directions (TF 7-12b1 and TF 7-12b2), whereas the default algorithm in the TRIM.FaTE library (TF 7-12a) is a one-way transfer from root-zone-soil pore water to the stem. Note that TFs 7-12b1 and 7-12b2 are not in the current TRIM.FaTE library. They are provided here for those users who may have data available for the SCF parameter but not one or more of the parameters needed for TF 7-12a (*e.g.*, TSCF, Q_{xy}).

7.2.4.3 Contribution from Leaves via Phloem

During the growing season, the stem can gain dissolved chemical from the leaves via phloem. Assuming that the chemical concentration in phloem sap is in equilibrium with that in leaves:

$$\frac{dN_{Stem}}{dt} = Q_{Ph} \times \frac{N_{Leaf}}{V_{Leaf} \times K_{LeafPh}} \qquad \text{(Eq. 7-42)}$$

where:

N_{Stem} = mass of chemical in stems (g[chemical]);
Q_{Ph} = phloem flux into leaves (m^3[phloem]/day), due to advection (assume 5 percent of Q_{Xy} [defined in Section 7.2.4.4], Paterson et al. 1991);
N_{Leaf} = mass of chemical in leaves (g[chemical]);
V_{Leaf} = volume of leaves (m^3[leaf]); and
K_{LeafPh} = partition coefficient between leaves and phloem water (g[chemical]/m^3[leaf] per g[chemical]/m^3[phloem] or m^3[phloem]/m^3[leaf])).

The following equation, adapted from an equation for sorption of contaminants to plant roots (Trapp 1995), can be used to calculate K_{LeafPh}:

$$K_{LeafPh} = (fW_{Leaf} + fL_{Leaf} \times K_{ow}^{b}) \times \frac{\rho_{Leaf}}{\rho_{Ph}} \qquad \text{(Eq. 7-43)}$$

where:

fW_{Leaf} = fraction of leaves consisting of water (kg[water]/kg[leaf wet wt]);
fL_{Leaf} = fraction of leaves consisting of lipid (kg[lipid]/kg[leaf wet wt]);
K_{ow} = octanol/water partition coefficient (g[chemical]/kg[octanol] per g[chemical]/L[water]);
b = correction exponent for differences between foliage lipids and octanol (unitless);
ρ_{Leaf} = density of leaf (kg[leaf wet wt]/m^3[leaf]); and
ρ_{Ph} = density of phloem (kg[phloem]/m^3[phloem]).

If the chemical in question is ionic, it may be assumed that K_{ow} is close to zero and that the concentration of the ionic species in the phloem is the same as that in leaf water. Thus:

$$T_{Leaf \rightarrow Stem} = Q_{Ph} \times \frac{1}{V_{Leaf} \times K_{LeafPh}} \qquad \text{(TF 7-13)}$$

where:

$T_{Leaf \rightarrow Stem}$ = transfer factor for leaf to stem (/day).

7.2.4.4 Loss from Stem to Leaf via Xylem

During the growing season, the stem can lose dissolved chemical to the leaves via the xylem:

$$\frac{dN_{Leaf}}{dt} = Q_{Xy} \times \frac{N_{Stem}}{V_{Stem} \times K_{StemXy}} \qquad \text{(Eq. 7-44)}$$

where:

N_{Leaf} = mass of chemical in leaf compartment (g[chemical]);
Q_{Xy} = flow of transpired water (m^3[xylem]/day);
N_{Stem} = mass of chemical in stem compartment (g[chemical]);
V_{Stem} = volume of stem (m^3[stem]); and
K_{StemXy} = partition coefficient between stem and xylem water (m^3[xylem]/m^3[stem])).

The following equation, adapted from an equation for sorption of contaminants to plant roots (Trapp 1995), may be used to calculate K_{StemXy}:

$$K_{StemXy} = (fW_{Stem} + fL_{Stem} \times K_{ow}^{b}) \times \frac{\rho_{Stem}}{\rho_{Xy}} \qquad \text{(Eq. 7-45)}$$

where:

fW_{Stem} = fraction water content of stem (kg[water]/kg[stem wet wt]);
fL_{Stem} = fraction lipid content of stem (kg[lipid]/kg[stem wet wt]);
K_{ow} = octanol/water partition coefficient (g[chemical]/kg[octanol] per g[chemical]/L[water] or L[water]/kg[octanol]);
b = correction exponent for differences between foliage lipids and octanol (unitless);
ρ_{Stem} = density of stem (kg[stem wet wt]/m^3[stem]); and
ρ_{Xy} = density of xylem fluid (kg[xylem]/m^3[xylem]).

If the chemical in question is ionic, it may be assumed that K_{ow} is zero and that the concentration of the ionic species in the xylem is the same as that in leaf water. Thus:

$$T_{Stem \rightarrow Leaf} = Q_{Xy} \times \frac{1}{V_{Stem} \times K_{StemXy}} \qquad \text{(TF-7-14)}$$

where:

$T_{Stem \rightarrow Leaf}$ = transfer factor for stem to leaf.

7.2.4.5 Loss from Phloem to Fruit

Depending on the application, it may not be necessary to implement a fruit compartment or this loss term in a TRIM.FaTE simulation. Things to consider may be the concentrations expected in fruit and the portion of the diet (wildlife or human) expected to be comprised of fruit. This algorithm has not yet been implemented in any applications of TRIM.FaTE. The concentration of any chemical in the phloem running through the stem is at the same concentration as xylem sap leaving the stem; both are in equilibrium with the stem. Thus:

$$\frac{dN_{Fruit}}{dt} = Q_{PhF} \times \frac{N_{Stem}}{V_{Stem} \times K_{StemXy}} \qquad \text{(Eq. 7-46)}$$

where:

N_{Fruit} = mass of chemical in fruit (g[chemical]);
Q_{PhF} = phloem flux into fruit (m^3[phloem]/day), due to advection (assume 5 percent of Q_{Xy}, Paterson et al. 1991);
N_{Stem} = mass of chemical in stem (g[chemical]);
V_{Stem} = volume of stem (m^3[stem]); and
K_{StemXy} = partition coefficient between stem and xylem water (m^3[xylem]/m^3[stem])).

7.2.5 UPTAKE BY WOOD AND TREE BARK

Wood is of interest in a mass-balanced chemical transport and fate model because of its potential for serving as a large reservoir of chemical mass. The few studies that exist suggest that there is some accumulation of air pollutants in bark and wood. Turner (1998) has collected limited data on the accumulation of mercury in wood, but the mechanism of accumulation is not understood. Simonich and Hites (1995) provide data on the accumulation of organochlorine compounds in tree bark; PAHs would be expected to have similar properties. Algorithms for the transfer of chemicals to wood and tree bark are not currently available in the TRIM.FaTE library because of a general lack of information for persistent air pollutants.

7.2.6 TRANSFORMATIONS AND DEGRADATION

All transformations are assumed to be first-order processes in TRIM.FaTE. The derivations of these values for mercury and PAHs are described in Appendices A and B of this volume, respectively. Transformations of chemicals associated with particles on the surface of plant leaves are assumed to occur with the same rate constants as transformations of chemicals associated with particles in air.

Transformations of chemicals into other chemicals that are no longer be tracked in TRIM.FaTE are called general degradation processes. In TRIM.FaTE, the degradation of a chemical in particles on leaves and vegetation due to all mechanisms that might apply (*e.g.,* photolysis, and metabolic activity) is reflected by the user input for the half-life of the chemical in the plant leaf, stem, and root, and for the chemical associated with particles on the surface of the leaf.

Transformations of a chemical into another form of the chemical that is tracked in TRIM.FaTE are named for the processes associated with the transformation (*e.g.*, oxidation, methylation, reduction of mercury species). The transformation rate constant is the inverse of the residence time with respect to that reaction.

7.2.7 LITTER FALL

The flux of chemical from leaves, including particles on leaves, to surface soil during litter fall at the end of the growing season may be expressed by the equation:

$$\frac{dN_{Ss}}{dt} = N_{Leaf} + k_L \times N_{LeafP} \qquad \text{(Eq. 7-47)}$$

where:

N_{Ss} = mass of chemical in surface soil in compartment (g[chemical]);
k_L = litter-fall rate constant (/day);
N_{Leaf} = mass of chemical in foliage in leaf compartment (g[chemical]); and
N_{LeafP} = mass of chemical in particles-on-leaf compartment (g[chemical]).

If it is assumed that 99 percent of the leaves of deciduous trees are dropped to surface soil between the day of first frost and a date that is 30 days later, k_L would be calculated according to the equations:

$$\frac{C}{C_0} = e^{-k_L} \qquad \text{(Eq. 7-48a)}$$

$$\ln(0.01) = -30k_L \qquad \text{(Eq. 7-48b)}$$

where:

C/C_0 = ratio of concentration in the leaf compartment after 30 days of litter fall, C, to the concentration in the leaf compartment at the beginning of litter fall, C_0, which equals 0.01 if 99 percent of the mass is lost in 30 days (g[chemical]/m^3[leaf] per g[chemical]/m^3[leaf]).

Thus, k_L would equal -ln(0.01)/30 days which is 0.15 /day.

Litter fall for conifers, on the other hand, usually occurs more gradually, with a complete turnover of leaves taking 2 to 10 or 11 years (Post 1999). Thus, if it is assumed for the purpose of a TRIM.FaTE scenario that the leaf turnover is 6 years, k_L would equal -ln(0.01)/ 2190 days, which is 0.0021/day. Moreover, that litter-fall rate could be set to a constant value for the year.

If it is assumed that herbaceous plants and grasses become “litter” on the surface of the soil during the 30-day period beginning the day of first frost, again, k_L would equal 0.15 /day.

If all of the plant material were harvested, the litter-fall rate constant would be set to 0/day and the chemical in the harvested plant compartments would need to be transferred to a chemical sink or to another compartment (*e.g.*, silage) for purposes of balancing mass in TRIM.FaTE. If only a portion of the plant crop (half of the leaves for example) were harvested and the remainder of the plant were allowed to remain in the “field”, the user would need to determine the fraction of the biomass that would be harvested. That fraction of the chemical in the harvested plant biomass could be sent to a harvest sink while the remainder could be sent to the surface soil compartment.

Thus:

$$T_{Leaf \rightarrow Ss} = k_L \qquad \text{(TF 7-15)}$$

where:

$T_{Leaf \rightarrow Ss}$ = transfer factor for leaf to surface soil (/day).

Also:

$$T_{LeafP \rightarrow Ss} = k_L \qquad \text{(TF 7-16)}$$

where:

$T_{LeafP \rightarrow Ss}$ = transfer factor for the particles-on-leaf to surface-soil compartments (/day).

Note that the transfer of chemical from litter to surface water is not implemented in TRIM.FaTE at this time.

7.2.8 SENESCENCE

Senesence is not considered in the current version of the TRIM.FaTE library. Senescence is the aging of plants, a process which affects the uptake of chemicals, growth, and plant parameters such as water content. If a user of TRIM.FaTE wants to include the process of senescence, candidate algorithms for changes in plant biomass may be found in Whicker and Kirchner (1987). Senescence of plants is assumed to be negligible prior to the date of first frost.

7.2.9 OTHER SEASONAL ISSUES

Plants only take up chemicals during the growing season, *i.e.*, the dates in the spring, summer, and fall between last frost and first frost. Although there may be uptake by conifers outside of the growing season, it is probably negligible for much of the non-growing season in cold environments (*e.g.*, in the Maine case study) (Lindberg 1999b) and is not considered for TRIM.FaTE modeling purposes. To limit plant uptake only to the growing season, the user must specify the time period considered outside of the growing season.

During the 30-day period of litter fall for deciduous trees at the end of the growing season, chemical mass is steadily decreased in the leaf compartment. Because the loss is modeled using a rate constant, at the end of 30 days, a small amount of chemical remains in the leaf compartment, and that amount remains throughout the winter. Note that in the current TRIM.FaTE library, the volume of the leaf compartment goes to zero on the date at which *AllowExchange* goes to zero, which is at the beginning of the 30-day litter-fall period. On that date, the leaf compartment is no longer available as a food source for terrestrial herbivores and omnivores.

An additional seasonal issue is deposition to the particles-on-leaf compartment type. Tree foliage and grasses only intercept deposition when they are present. Like the leaf compartment, the volume of the particles-on-leaf compartment is a function of *AllowExchange*, and so the volume of particles-on-leaf drops abruptly to zero for the winter, starting on the first day of litter fall. TRIM.FaTE assumes that no plant foliage is present in the non-growing season, except for that associated with conifers or other user-created evergreen vegetation types. All deposition in deciduous forests, old fields, and agricultural systems in the non-growing season goes directly to soil. Deposition to conifer foliage may continue in the winter, though accumulation of chemicals from particles or wet deposition is assumed to be negligible.

Chemical transformation within the plant is also assumed to cease in the non-growing season. There is no evidence to support or refute this assumption for most chemicals.

During the non-growing season, for herbivorous or omnivorous animals that do not hibernate or engage in winter sleep, the user may want to consider the significance of accumulation from alternative, non-plant dietary sources.

7.3 SOIL DETRITIVORES

In this section, the transfer factor algorithms associated with soil detritivores (*i.e.*, earthworms, Section 7.3.1, and soil arthropods, Section 7.3.2) are developed. A list of these algorithms is provided in the table on the next and following page.

7.3.1 EARTHWORMS

The uptake of chemicals by earthworms in TRIM.FaTE is described by an equation in the form of time to equilibrium between the earthworms and soil (see Section 2.5). There are two forms of the uptake equation in TRIM.FaTE: one for uptake of chemicals from an interaction with bulk soil (Section 7.3.1.1) and one for uptake of chemicals dissolved in soil pore water (Section 7.3.1.2). The choice of algorithm depends on the data available to derive the partition coefficients. Empirical data on the uptake of chemicals from bulk soil by earthworms are commonly available for inorganic chemicals and some organic compounds. Such empirical ratios are not usually available for earthworm uptake from soil pore water; however, an established relationship exists between octanol-water partition coefficients and earthworm/soil-pore-water partition coefficients.

7.3.1.1 Uptake of Chemicals from Bulk Soil

For simplicity, uptake from bulk soil is described as being proportional to the concentration of the chemical in soil, even though some studies suggest that a log-log regression between soil and earthworm concentrations is a more precise model of uptake (Sample et al. 1999). The concentration of the chemical in the earthworm (dry-weight basis) is equal to the dry worm/soil partition coefficient multiplied by the concentration of the chemical in the soil (dry-weight basis):

$$C_{Worm\text{-}dry} = K_{Worm\text{-}Sr\text{-}dry} \times C_{Sr\text{-}dry} \qquad \text{(Eq. 7-49)}$$

where:

$C_{worm\text{-}dry}$ = dry-weight concentration of chemical in earthworm (g[chemical]/kg[worm dry wt]);
$K_{Worm\text{-}Sr\text{-}dry}$ = earthworm/dry-soil partition coefficient (kg[soil dry wt]/kg[worm dry wt]); and
$C_{Sr\text{-}dry}$ = dry-weight concentration of chemical in root-zone soil (g[chemical]/kg[soil dry wt]).

Summary of Transfer Factors for Soil Detritivores in TRIM.FaTE

DIFFUSIVE TRANSFERS

Bulk root-zone soil to earthworm:

TF 7-17a

$$T_{Sr \rightarrow Worm} = \left[\frac{-\ln(1-\alpha)}{t_{\alpha}^{WSr}} \right] \times \frac{M_{Worm}}{M_{Sr}} \times K_{Worm-Sr}$$

Earthworm to bulk root-zone soil:

TF 7-18a

$$T_{Worm \rightarrow Sr} = \frac{-\ln(1-\alpha)}{t_{\alpha}^{WSr}}$$

Root-zone-soil pore water to earthworm: TF 7-17b

$$T_{SrW \rightarrow Worm} = \left[\frac{-\ln(1-\alpha)}{t_{\alpha}^{WSrW}} \right] \times \frac{M_{Worm}}{V_{Sr} \times \theta \times 1000} \times K_{Worm-SrW}$$

Earthworm to root-zone-soil pore water: TF 7-18b

$$T_{Worm \rightarrow SrW} = \frac{-\ln(1-\alpha)}{t_{\alpha}^{WSrW}}$$

Bulk soil to soil arthropod: TF 7-19

$$T_{S \rightarrow Arth} = \left[\frac{-\ln(1-\alpha)}{t_{\alpha}^{AS}} \right] \times \frac{M_{Arth}}{M_{S}} \times K_{Arth-S}$$

Soil arthropod to bulk soil: TF 7-20

$$T_{Arth \rightarrow S} = \frac{-\ln(1-\alpha)}{t_{\alpha}^{AS}}$$

LIST OF SYMBOLS USED IN SOIL DETRITIVORE TRANSFER FACTOR ALGORITHMS

α = fraction of equilibrium value achieved by time t_{α} (default = 0.95 or 95%).
t_{α} = time required to reach the fraction α of equilibrium (days) (value depends on the compartments and phases for which time-to-equilibrium is modeled).
M_{Worm} = total biomass of worms in root-zone soil compartment (kg[worm wet wt]).
M_{Sr} = total mass of root-zone soil compartment (kg[soil wet wt]).
$K_{Worm\text{-}Sr}$ = earthworm/bulk-soil partition coefficient (kg[soil wet wt]/kg[worm wet wt]).

Summary of Transfer Factors for Soil Detritivores in TRIM.FaTE (cont.)

LIST OF SYMBOLS USED IN SOIL DETRITIVORE TRANSFER FACTOR ALGORITHMS (cont.)

V_{Sr} = volume of root-zone soil compartment (m^3).
θ = fraction root-zone soil compartment volume that is liquid (unitless).
$K_{Worm\text{-}SrW}$ = earthworm/soil-pore-water partition coefficient (L[water]/kg[worm wet wt]).
M_{Arth} = total biomass of arthropods in soil compartment (kg[arthropod wet wt]).
M_s = total mass of soil compartment (kg[soil wet wt]).
$K_{Arth\text{-}S}$ = arthropod/bulk-soil partition coefficient (kg[soil wet wt]/kg[arthropod wet wt]).

If masses are converted to wet mass, then:

$$C_{Worm} = (1\text{-}fW_{Worm}) \times C_{Worm}\text{-}dry \qquad \text{(Eq. 7-50)}$$

where:

C_{Worm} = concentration of chemical in earthworm (g[chemical]/kg[worm wet wt]); and
fW_{Worm} = water content of earthworm (kg[water]/kg[worm wet wt]).

It is also true that:

$$C_{Sr} = (1\text{-}fW_{Sr}) \times C_{Sr\text{-}dry} \qquad \text{(Eq. 7-51)}$$

where:

C_{Sr} = concentration of the chemical in the bulk root-zone soil (g[chemical]/kg[soil]);
fW_{Sr} = fraction water content of root-zone soil (kg[water]/kg[root-zone soil wet wt]).

Thus:

$$\frac{C_{Worm}}{\left((1 - fW_{Worm}\right)} = K_{Worm\_Sr\_dry} \times \frac{C_{Sr}}{(1 - fW_{Sr})} \qquad \text{(Eq. 7-52a)}$$

Rearranging gives:

$$\frac{C_{Worm}}{C_{Sr}} = K_{Worm\_Sr\_dry} \times \frac{(1 - fW_{Worm})}{(1 - fW_{Sr})} \qquad \text{(Eq. 7-52b)}$$

Thus:

$$K_{Worm-Sr} = \frac{(1 - fW_{Worm})}{(1 - fW_{Sr})} \times K_{Worm\_Sr\_dry} \qquad \text{(Eq. 7-53)}$$

where:

$K_{Worm\text{-}Sr}$ = earthworm/bulk-soil partition coefficient (g[chemical]/kg[worm wet wt] per g[chemical]/kg[soil wet wt] or kg[soil wet wt]/kg[worm wet wt]).

Using the approach described in Section 2.5, the change in chemical concentration in the earthworm compartment over time can be described as:

$$\frac{dC_{Worm}}{dt} = \left[\frac{-\ln(1-\alpha)}{t_{\alpha}^{WSr}}\right] \times K_{Worm-Sr} \times C_{Sr} - \left[\frac{-\ln(1-\alpha)}{t_{\alpha}^{WSr}}\right] C_{Worm} \qquad \text{(Eq. 7-54)}$$

where:

t_{α}^{WSr} = time (days) required for the earthworm/bulk-soil interaction to reach 100×α percent (default $\alpha = 0.95$) of equilibrium when C_{Sr} is approximately constant with time. The value of t_{α} must be determined from empirical studies reported in the literature.

If the areal density of earthworms is approximately constant with time, then:

$$\frac{dN_{Worm}}{dt} = \left[\frac{-\ln(1-\alpha)}{t_{\alpha}^{WSr}}\right] \times \rho area_{Worm} \times A_{Sr} \times K_{Worm-Sr} \times \frac{N_{Sr}}{M_{Sr}} - \left[\frac{-\ln(1-\alpha)}{t_{\alpha}^{WSr}}\right] \qquad \text{(Eq. 7-55)}$$

where:

N_{Worm} = mass of chemical in earthworm compartment (g[chemical]);
$\rho area_{Worm}$ = areal wet-weight density of earthworms in root-zone soil (kg[worm wet wt]/m^2[soil]);
A_{Sr} = area of root-zone soil compartment (m^2[soil]);
N_{Sr} = total mass of chemical in all phases of bulk root-zone soil (g[chemical]); and
M_{Sr} = bulk mass of root-zone soil compartment, including arthropods (kg[soil wet wt]).

Note that the quantity $(\rho area_{Worm} \times A_{Sr})$ is equal to the total biomass of worms (wet wt), M_{Worm}, in the soil compartment.

Thus, the transfer factors between the bulk root-zone soil and earthworm compartments are estimated as:

$$T_{Sr\rightarrow Worm} = \left[\frac{-\ln(1-\alpha)}{t_{\alpha}^{WSr}}\right] \times \frac{M_{Worm}}{M_{Sr}} \times K_{Worm-Sr} \qquad \text{(TF 7-17a)}$$

$$T_{Worm\rightarrow Sr} = \frac{-\ln(1-\alpha)}{t_{\alpha}^{WSr}} \qquad \text{(TF 7-18a)}$$

where:

$T_{Sr\rightarrow Worm}$ = transfer factor for transfer of chemical from root-zone soil compartment to earthworm compartment (/day);
$T_{Worm\rightarrow Sr}$ = transfer factor for transfer of chemical from earthworm to root-zone soil compartments (/day); and
M_{Worm} = total biomass of worms (kg[worm wet wt]) in the root-zone soil compartment (= $\rho area_{Worm} \times A_{sr}$).

7.3.1.2 Uptake of Chemicals from Soil Pore Water

For simplicity, uptake of chemicals from soil pore water is described as being proportional to the concentration of the chemical in soil pore water. This algorithm is used as an alternative to uptake from bulk soil. All calculations can be done in original wet weights, simplifying the derivation of the transfer factors. These equations are appropriate for any chemicals for which partition coefficients have been reported on a pore-water basis:

$$C_{Worm} = K_{Worm-SrW} \times C_{SrW} \qquad \text{(Eq. 7-56)}$$

where:

C_{Worm} = wet-weight concentration of chemical in earthworm (g[chemical]/kg[worm wet wt]);
C_{SrW} = concentration of chemical in root-zone-soil pore water (g[chemical]/L[water]); and
$K_{Worm\text{-}SrW}$ = earthworm/root-zone-soil-pore-water (or earthworm/water) partition coefficient (L[water]/kg[worm wet wt]).

The partition coefficient for the lipophilic organic chemical between the earthworm and the pore water of the root-zone soil can be calculated as:

$$K_{Worm\text{-}SrW} = K_{OW}/3.98 \qquad \text{(Eq. 7-57)}$$

where:

K_{OW} = the chemical's octanol-water partition coefficient (g[chemical]/kg[octanol] per g[chemical]/L[water] or L[water]/kg[octanol]).

Equation 7-57 was derived from studies of 32 lipophilic chemicals with log(K_{OW}) values from 1.0 to 6.5 (Connell and Markwell 1990, Suter et al. 2000). As for uptake calculated with respect to bulk soil, the equilibrium model for uptake from soil pore water can be changed to the following equation to estimate the change in concentration of the chemical in the earthworm over time:

$$\frac{dC_{Worm}}{dt} = \left[\frac{-\ln(1-\alpha)}{t_{\alpha}^{WSrW}}\right] \times K_{Worm-SrW} \times C_{SrW} - \left[\frac{-\ln(1-\alpha)}{t_{\alpha}^{WSrW}}\right] \times C_{Worm} \qquad \text{(Eq. 7-58)}$$

where:

t_{α}^{WSrW} = time (days) required for the worm/root-zone soil-pore-water interaction to reach 100×α percent (default α = 0.95) of equilibrium when C_{SrW} is approximately constant with time.

The value of this t_α can be determined from empirical studies reported in the literature, but these are rare. In the absence of any data, "t_α" can be estimated from the following equation if the octanol/ water partition coefficient (K_{OW}) is available:

$$t_{\alpha}^{WSrW} = \frac{2 \times 1.62 + e^{\left(\log(K_{OW}) - 1.8\right)}}{24} \qquad \text{(Eq. 7-59)}$$

This equation is based on the equation for the interaction of plant roots and soil water in Hsu et al. (1990), which is a rough estimate of the time to equilibrium. An empirical relationship derived from plant roots is used for earthworms because a model derived from earthworms is not yet available and the diffusive processes are likely similar. The corresponding proportion of the equilibrium concentration actually reached, however, is uncertain. Thus, the appropriate value to use for α (*e.g.*, 0.95, 0.99) is uncertain.

If the areal density of worms is approximately constant with time, then:

$$\begin{aligned}\frac{dN_{Worm}}{dt} = &\left[\frac{-\ln(1-\alpha)}{t_{\alpha}^{WSrW}}\right] \times M_{Worm} \times K_{Worm-SrW} \times \frac{N_{SrW}}{M_{SrW}} \\ &- \left[\frac{-\ln(1-\alpha)}{t_{\alpha}^{WSrW}}\right] \times N_{Worm}\end{aligned} \qquad \text{(Eq. 7-60)}$$

where:

N_{Worm} = mass of chemical in earthworms (g[chemical]);
M_{Worm} = total biomass of worms (kg[worm wet wt]);
N_{SrW} = mass of chemical in root-zone-soil pore water (g[chemical]); and
M_{SrW} = mass of root-zone-soil pore water (kg[water]).

It is also true that:

N_{SrW} = N_{Sr} × *Fraction_Mass_Dissolved* (*i.e.*, the total chemical mass in the total soil compartment multiplied by the fraction of the total chemical mass that is dissolved in water); and

M_{SrW} = V_{SrW} (volume of root-zone soil water in m^3) × 1 kg[water]/L[water] × 1000 L[water]/m^3[water]; where:

  V_{SrW} = V_{Sr} (m^3) × *Volume_Fraction_Liquid* (*i.e.*, total volume of the root-zone soil compartment multiplied by the volume fraction of the root-zone soil compartment that is liquid).

Making the substitutions for N_{SrW}, M_{SrW}, and then V_{SrW}, and using Equation 2-72 (Chapter 2) to substitute Z factors for the ratio of fractions, the transfer factors are:

$$T_{SrW \to Worm} = \left[\frac{-\ln(1-\alpha)}{t_{\alpha}^{WSrW}}\right] \times K_{Worm-SrW} \times \frac{M_{Worm} \times Fraction\_Mass\_Dissolved}{V_{Sr} \times 1000 \times Volume\_Fraction\_Liquid}$$

$$= \left[\frac{-\ln(1-\alpha)}{t_{\alpha}^{WSrW}}\right] \times K_{Worm-SrW} \times \frac{M_{Worm}}{V_{Sr} \times 1000} \times \frac{Z_{pure\_water}}{Z_{Total}} \qquad \text{(TF 7-17b)}$$

and:

$$T_{Worm \to SrW} = \frac{-\ln(1-\alpha)}{t_{\alpha}^{WSrW}} \qquad \text{(TF 7-18b)}$$

where:

$T_{SrW \to Worm}$ = transfer factor for transfer of chemical from root-zone-soil pore water to worm (/day);
$T_{Worm \to SrW}$ = transfer factor for transfer of chemical from worm to root-zone-soil pore water (/day);
$K_{Worm\text{-}SrW}$ = worm/soil-pore water partition coefficient (L[water]/kg[worm wet wt]);
Z_{pure_water} = fugacity capacity of chemical in pure water (mol/m^3-Pa); and
Z_{Total_Sr} = total fugacity capacity of chemical in root-zone soil compartment (mol/m^3-Pa).

7.3.2 SOIL ARTHROPODS

An equation for the uptake of chemicals by soil arthropods may be derived similarly to that for earthworms. Much of the available data relates the concentration of a chemical in the fresh (wet weight) arthropod to that in its food. The food may be plant matter rather than soil, but for the purposes of TRIM.FaTE, the uptake factor is assumed to apply to bulk soil. Bulk soil includes all phases (*i.e.*, solid, liquid, gas) of the soil compartment.

The user may include the soil arthropods in the root-zone or surface soil compartments or both. In initial applications of TRIM.FaTE, soil arthropods were included in the surface soils.

The concentration of the chemical in the arthropods equals the concentration in the bulk soil multiplied by the arthropod/bulk-soil partition coefficient:

$$C_{Arth} = K_{Arth-S} \times C_S \qquad \text{(Eq. 7-61)}$$

where:

C_{Arth} = concentration in arthropods (g[chemical]/kg[arthropod wet wt]);
$K_{Arth\text{-}S}$ = arthropod/bulk-soil partition coefficient (kg[soil wet wt]/kg[arthropod wet wt]); and
C_{Sr} = concentration of the chemical in bulk soil (g[chemical]/kg[soil wet wt]).

Thus,

$$\frac{dC_{Arth}}{dt} = \left[\frac{-\ln(1-\alpha)}{t_{\alpha}^{AS}}\right] \times K_{Arth-S} \times C_S - \left[\frac{-\ln(1-\alpha)}{t_{\alpha}^{AS}}\right] \times C_{Arth} \qquad \text{(Eq. 7-62)}$$

where:

t_{α}^{AS} = time (days) required for the arthropod/bulk-soil interaction to reach the fraction α (default = 0.95) of the equilibrium value when C_S is approximately constant with time.

If the areal density of arthropods is approximately constant with time, then:

$$\frac{dN_{Arth}}{dt} = \left[\frac{-\ln(1-\alpha)}{t_{\alpha}^{AS}}\right] \times \rho area_{Arth} \times A_S \times K_{Arth-S} \times \frac{N_S}{M_S} - \left[\frac{-\ln(1-\alpha)}{t_{\alpha}^{AS}}\right] \times N_{Arth} \qquad \text{(Eq. 7-63)}$$

where:

N_{Arth} = mass of chemical in arthropods (g[chemical]);
$\rho area_{Arth}$ = areal density of arthropod community in soil (kg[arthropod wet wt]/m^2[soil]);
A_S = area of soil compartment (m^2);
N_S = total mass of chemical in all phases of the soil compartment (g[chemical]); and
M_S = bulk mass of soil, including arthropods (kg[soil wet wt]).

Thus:

$$T_{S \rightarrow Arth} = \left[\frac{-\ln(1-\alpha)}{t_{\alpha}^{AS}}\right] \times \frac{M_{Arth}}{M_S} \times K_{Arth-S} \qquad \text{(TF 7-19)}$$

The corresponding algorithm for the release of chemical from the arthropods back to the soil is estimated as:

$$T_{Arth \rightarrow Sr} = \frac{-\ln(1-\alpha)}{t_{\alpha}^{AS}} \qquad \text{(TF 7-20)}$$

where:

$T_{S \rightarrow Arth}$ = transfer factor for transfer of chemical from soil to arthropods (/day);
$T_{Arth \rightarrow S}$ = transfer factor for transfer of chemical from arthropods to soil (/day); and
M_{Arth} = total biomass of arthropods (kg[arthropods wet wt]) in the soil compartment; which
= $\rho area_{Arth}$ (kg[arthropods wet wt]/m^2)× A_S (m^2[soil]).

The transfer factors TF 7-19 and TF 7-20 apply to both organic and inorganic chemicals in TRIM.FaTE at this time. The user must supply empirical data on the time to reach 95 percent (or other selected proportion) of the equilibrium value between the bulk soil and arthropods.

7.3.3 FLYING INSECTS

Flying insects are the food of insectivores, particularly aerial feeding insectivores such as tree swallows. In initial applications of TRIM.FaTE, these insects have been assumed to have emerged from benthic aquatic larvae living in the surface water bodies. As a consequence, the concentration of a chemical in flying insects was assumed to be equal to the concentration of that chemical in the benthic invertebrate compartment in the surface water body to which the aerial insectivore is linked in a given scenario (see Section 6.3).

7.3.4 TRANSFORMATIONS AND DEGRADATION

Transformations of organic chemicals into metabolic by-products that are no longer tracked in TRIM.FaTE are not included in the current TRIM.FaTE library for soil detritivores. Nor are metabolic transformations among chemicals containing the same core chemical (*e.g.*, transformation among mercury species) included in the current TRIM.FaTE library for soil detritivores. These processes are not included because no information could be found concerning chemical transformations and degradation in soil detritivores.

7.4 TERRESTRIAL WILDLIFE

Terrestrial wildlife, including mammals and birds, can be exposed to chemicals through food, soil, and water ingestion, and through inhalation of chemicals in air. In addition, chemicals can be taken up dermally via contact with contaminants in surface water, soil, or air. The rate of contact with water and soil, however, generally is unknown. In addition, sorption to the skin surface is unknown, the rate of uptake into the organism is unknown, and the proportion absorbed through the dermis is relatively low compared with the proportion absorbed through the gastrointestinal tract or lungs. Thus, dermal uptake is not included in the current TRIM.FaTE library. Elimination of chemicals from body tissues may occur through metabolic transformation of the chemical or excretion of the parent compound through urine, feces, milk (female mammals only), eggs (female birds and reptiles only), and excretion to fur, hair, or feathers.

In this section, terrestrial wildlife refers only to mammals and birds; no reptiles or amphibians are included in the TRIM.FaTE library at this time. The phrase “terrestrial wildlife” also includes the semi-aquatic species noted in the introduction to this chapter (*e.g.*, mink, loon). The text box on the next page and continued on the following pages provides a summary of the transfer-factor algorithms developed in this section and defines the parameters used in those algorithms.

7.4.1 GENERALIZED MODEL FOR TERRESTRIAL MAMMALS AND BIRDS

A generalized model for terrestrial wildlife (*Twl*), including all of the possible routes of exposure and of elimination, is presented below. In addition, the equation below applies to semi-aquatic populations, such as loons and raccoons. If particular rate constants are determined to be insignificant relative to others for a particular implementation of TRIM.FaTE (*e.g.*, excretion via eggs compared to excretion in urine or feces), those may be set to zero. Similarly, if rate constants for excretion and chemical transformation are determined with respect to the mass of a contaminant that is taken up in the diet rather than the mass that is assimilated, the dietary assimilation efficiencies may be ignored.

$$\begin{aligned}
&\frac{dC_{Twl}}{dt} = [(IN_W \times C_{SW} \times AE_W) + (IN_{Ss} \times C_{Ss} \times AE_S) + p_{Plant}(IN_D \times C_{Leaf} \times AE_{Plant}) + \\
&p_{Plant}(IN_D \times C_{LeafP} \times AE_S) + p_{Worm}(IN_D \times C_{Worm} \times AE_{Worm}) \\
&+ p_{Arth}(IN_D \times C_{Arth} \times AE_{Arth}) + p_{Twl-prey}(IN_D \times C_{Twl-prey} \times AE_{Twl}) \\
&+ p_{fish}(IN_D \times C_{fish} \times AE_{fish}) + p_{BI}(IN_D \times C_{BI} \times AE_{BI}) + (IN_{Air} \times C_{Air} \times AE_{Air})] \\
&- [C_{Twl} \times (E_{met} + E_{uf} + E_{lact} + E_{egg} + E_{ff})]
\end{aligned} \qquad \text{(Eq. 7-64)}$$

where:

C_{Twl} = total, whole-body, internal concentration in the terrestrial wildlife population (g[chemical]/kg[body wet wt]);
IN_W = water ingestion rate (m^3[water]/kg[body wet wt]-day);
C_{SW} = concentration of chemical in surface water ingested by wildlife (g[chemical]/m^3[water]);
AE_W = assimilation efficiency of chemical from water (unitless);
IN_{Ss} = surface soil ingestion rate (kg[soil dry wtl]/kg[body wet wt]-day);
C_{Ss} = concentration of chemical in surface soil (g[chemical]/kg[soil wet wt]);
AE_S = assimilation efficiency of chemical from soil (unitless);
p_{Plant} = proportion of plant matter in diet (unitless);
IN_D = diet ingestion rate normalized to body weight (kg[diet wet wt]/kg[body wet wt]-day);
C_{Leaf} = concentration of chemical in leaf component of diet (g[chemical]/kg[leaf wet wt]);

Summary of Transfer Factors for Wildlife in TRIM.FaTE

ADVECTIVE TRANSFERS

Surface water to semi-aquatic terrestrial wildlife (*i.e.*, bird or mammal): TF 7-21

$$T_{SW \rightarrow Twl} = Biomass_{Twl} \times \frac{IN_W \times AE_W}{V_{SW}}$$

Surface soil to terrestrial wildlife: TF 7-22

$$T_{Ss \rightarrow Twl} = Biomass_{Twl} \times \frac{IN_{Ss} \times AE_S}{V_{Ss} \times \rho_{Ss\_wet}}$$

Plant leaf to terrestrial wildlife: TF 7-23

$$T_{Leaf \rightarrow Twl} = \frac{\rho area_{Twl}}{\rho area_{Leaf}} \times p_{Plant} \times IN_D \times AE_{Plant}$$

Surface particles on plant leaf to terrestrial wildlife: TF 7-24

$$T_{LeafP \rightarrow Twl} = \frac{p_{LeafP} \times IN_D \times AE_S}{V_{LeafP} \times \rho_{LeafP}}$$

Earthworm to terrestrial vertebrate: TF 7-25

$$T_{Worm \rightarrow Twl} = \frac{\rho area_{Twl}}{\rho area_{Worm}} \times p_{Worm} \times IN_D \times AE_{Worm}$$

Soil arthropod to terrestrial vertebrate: TF 7-26

$$T_{Arth \rightarrow Twl} = \frac{\rho area_{Twl}}{\rho area_{Arth}} \times p_{Arth} \times IN_D \times AE_{Arth}$$

Terrestrial vertebrate to terrestrial vertebrate: TF 7-27

$$T_{Twl-prey-i \rightarrow Twl} = \frac{\rho area_{Twl}}{\rho area_{Tprey-i}} \times p_{Tprey-i} \times IN_D \times AE_{Twl}$$

Summary of Transfer Factors for Wildlife in TRIM.FaTE (cont.)

ADVECTIVE TRANSFERS (cont.)

Fish to terrestrial wildlife (*i.e.*, bird or mammal): TF 7-28

$$T_{fish-i \rightarrow Twl} = \frac{Biomass_{Twl}}{A_{SW} \times \rho area_{fish-i}} \times p_{fish-i} \times IN_D \times AE_{fish}$$

Benthic invertebrate or flying insect to terrestrial wildlife: TF 7-29

$$T_{BI \rightarrow Twl} = \frac{Biomass_{Twl}}{A_{Sed} \times \rho area_{BI}} \times p_{BI} \times IN_D \times AE_{BI}$$

Air to terrestrial wildlife: TF 7-30

$$T_{Air \rightarrow Twl} = Biomass_{Twl} \times \frac{IN_{Air} \times AE_{Air}}{V_{Air}}$$

Terrestrial wildlife to surface soil: TF 7-31

$$T_{Twl \rightarrow Ss} = f_{fuSs} \times k_{ET}$$

Terrestrial wildlife to water: TF 7-32

$$T_{Twl \rightarrow SW} = f_{fuSW} \times k_{ET}$$

LIST OF SYMBOLS USED IN WILDLIFE TRANSFER FACTOR ALGORITHMS:

$Biomass_{Twl}$ = biomass of terrestrial wildlife species in a compartment (kg[wildlife wet wt]), which
= $\rho area_{Twl}$ (kg[wildlife wet wt]/m^2]) × A_S (m^2[soil]).
IN_W = water ingestion rate normalized to body weight (m^3[water]/kg[body wet wt]-day).
V_{SW} = volume of surface water compartment (m^3).
AE_W = assimilation efficiency of chemical from water (unitless).
IN_{Ss} = surface soil ingestion rate (kg[soil dry wt]/kg[body wet wt]-day).
V_{Ss} = volume of surface soil compartment (m^3).
ρ_{Ss} = density of soil particles (kg[soil dry wt]/m^3[soil]).
AE_S = assimilation efficiency of chemical from soil (unitless).
$\rho area_{Twl}$ = terrestrial wildlife biomass density per unit area (kg[wildlife wet wt]/m^2[surface parcel]), which
= N_{area} (number[individuals]/m^2[soil]) × BW (kg[body wet wt]).
p_{Plant} = proportion of plant matter in diet (unitless).
IN_D = diet ingestion rate (kg[diet wet wt]/kg[body wet wt]-day).
AE_{Plant} = assimilation efficiency of chemical from plant in diet (unitless).
$\rho area_{Leaf}$ = areal biomass density of foliage (kg[leaves wet wt]/m^2[surface soil]).
$\rho area_{LeafP}$ = areal biomass density of particles on leaf surface (kg[leaf particles]/m^2[surface parcel]).
p_{Worm} = proportion of earthworm in diet (unitless).
AE_{Worm} = assimilation efficiency of chemical from earthworm in diet (unitless).

Summary of Transfer Factors for Wildlife in TRIM.FaTE (cont.)

LIST OF SYMBOLS USED IN WILDLIFE TRANSFER FACTOR ALGORITHMS (cont.)

$\rho area_{Worm}$ = areal biomass density of earthworms (kg[worms wet wt]/m^2[soil]).
p_{Arth} = proportion of soil arthropods in diet (unitless).
AE_{Arth} = assimilation efficiency of chemical from soil arthropods in diet (unitless).
$p_{Twl\text{-}prey\text{-}i}$ = proportion of terrestrial wildlife prey species *i* in diet (unitless).
$AE_{Twl\text{-}prey}$ = assimilation efficiency of chemical from wildlife prey in diet (unitless).
$\rho area_{Twl\text{-}prey\text{-}i}$ = areal biomass density of terrestrial wildlife prey species *i* in diet (kg[prey wet wt]/m^2[surface parcel]).
$p_{fish\text{-}i}$ = proportion of fish species *i* in diet (unitless).
AE_{fish} = assimilation efficiency of chemical from fish in diet (unitless).
$\rho area_{fish\text{-}i}$ = areal biomass density of fish species *i* (kg[fish wet wt]/m^2[surface water], use correct size range for diet).
A_{SW} = area of surface water compartment (m^2).
p_{BI} = proportion of benthic invertebrates (or emergent flying insects) in diet (unitless).
AE_{BI} = assimilation efficiency of chemical from benthic invertebrates (or flying insects) in diet (unitless).
$\rho area_{BI}$ = areal biomass density of benthic invertebrates (kg[invertebrates wet wt]/m^2[sediment]).
A_{Sed} = area of sediment compartment (m^2).
IN_{Air} = inhalation rate normalized to body weight (m^3[air]/kg[body wet wt]-day).
V_{Air} = volume of air compartment (m^3[air]).
AE_{Air} = assimilation efficiency of chemical from air (unitless).
k_{ET} = chemical elimination rate constant (through feathers or fur and urine and feces) (/day).
f_{fuSW} = fraction of elimination directed to surface water (unitless).
f_{fuSs} = fraction of elimination directed to surface soil (unitless).

AE_{Plant} = assimilation (absorption) efficiency of chemical from plant in diet (unitless);
C_{LeafP} = concentration of chemical in particles on leaves (g[chemical]/kg[particles on leaf dry wt]);
p_{Worm} = proportion of earthworm in diet (unitless);
C_{Worm} = concentration of chemical in earthworms (g[chemical]/kg[worm wet wt]);
AE_{Worm} = assimilation (absorption) efficiency of chemical from earthworm in diet (unitless);
p_{Arth} = proportion of insect in diet (unitless);
C_{Arth} = concentration of chemical in soil arthropod component of the diet (g[chemical]/kg[arthropod wet wt]);
AE_{Arth} = assimilation (absorption) efficiency of chemical from soil arthropods in diet (unitless);
$p_{Twl\text{-}prey}$ = proportion of other wildlife in diet (unitless);
$C_{Twl\text{-}prey}$ = concentration of chemical in the prey of the terrestrial wildlife (g[chemical]/ kg[prey wet wt]);
$AE_{Twl\text{-}prey}$= assimilation (absoprtion) efficiency of chemical from other wildlife in diet (unitless);
p_{fish} = proportion of fish in diet (by fish compartment type) (unitless);

C_{fish} = concentration of chemical in fish (by fish type) (g[chemical]/kg[fish wet wt]; use correct size range);
AE_{fish} = assimilation (absorption) efficiency of chemical from fish in diet (unitless);
p_{BI} = proportion of benthic invertebrates (or emergent flying insects) in diet (unitless);
C_{BI} = concentration of chemical in benthic invertebrates (or flying insects) (g[chemical]/kg[invertebrates wet wt]);
AE_{BI} = assimilation (absorption) efficiency of chemical from benthic invertebrates or emergent flying insects in diet (unitless);
IN_{Air} = normalized inhalation rate (m^3[air]/kg[body wet wt]-day);
C_{Air} = concentration of chemical in the air, including vapor phase and particles (g[chemcial]/m^3[air]);
AE_{Air} = assimilation (absorption) efficiency of chemical from air (unitless);
E_{met} = rate of metabolic transformation to another chemical(s) that is tracked in a given scenario or "degradation" to another chemical(s) that is not tracked in a given scenario (/day);
E_{uf} = rate of chemical elimination through excretory processes (urine and feces) (/day);
E_{lact} = rate of chemical elimination through lactation (milk production, mammals only) (/day);
E_{egg} = rate of chemical elimination through egg production, birds only (/day); and
E_{ff} = rate of chemical elimination to fur (hair) or feathers (/day).

Because the source of drinking water is not usually known and may include puddles, the uptake of the chemical from water has been ignored in initial TRIM.FaTE applications for all species except the semi-aquatic, which are associated with a single water body.

Thus, for a population:

$$\begin{aligned}\frac{dN_{Twl}}{dt} = {} & \rho area_{Twl} \times A_S \times \Big[\frac{IN_W \times N_{SW} \times AE_W}{V_{SW}} + \frac{IN_{Ss} \times N_{Ss} \times AE_S}{V_{Ss} \times \rho_{Ss}} + \frac{p_{Plant} \times IN_D \times N_{Leaf} \times AE_{Plant}}{A_{Ss} \times \rho area_{Leaf}} \\ & \frac{p_{Plant} \times IN_D \times N_{LeafP} \times AE_S}{V_{LeafP} \times \rho_P} + \frac{p_{Worm} \times IN_D \times N_{Worm} \times AE_{Worm}}{A_S \times \rho area_{Worm}} + \frac{p_{Arth} \times IN_D \times N_{Arth} \times AE_{Arth}}{A_S \times \rho area_{Arth}} \\ & + \frac{p_{Twl-prey} \times IN_D \times N_{Twl-prey} \times AE_{Twl}}{A_S \times \rho area_{Twl-prey}} + \frac{p_{fish} \times IN_D \times N_{fish} \times AE_{fish}}{A_{SW} \times \rho area_{fish}} + \frac{p_{BI} \times IN_D \times N_{BI} \times AE_{BI}}{A_{Sed} \times \rho area_{BI}} \\ & + \frac{IN_{Air} \times N_{Air} \times AE_{Air}}{V_{Air}}\Big] - [N_{Twl} \times (E_{met} + E_{uf} + E_{lact} + E_{egg} + E_{ff})]\end{aligned} \tag{Eq. 7-65}$$

where:

N_{Twl} = mass of chemical in terrestrial wildlife species (g[chemical]);
$\rho area_{Twl}$ = wildlife biomass density per unit area (kg[biomass wet wt]/m^2[surface volume element]);

A_S = area of associated soil (m^2);
N_{SW} = mass of chemical in surface water source (g[chemical]);
V_{SW} = volume of surface water (m^3);
N_{Ss} = mass of chemical in surface soil (g[chemical]);
V_{Ss} = volume of surface soil (m^3);
ρ_{Ss_wet} = bulk density of soil (kg[soil wet wt]/m^3[soil]);
N_{Leaf} = mass of chemical in plant leaf (g[chemical]);
$\rho area_{Leaf}$ = areal biomass density of foliage (kg[leaf wet wt]/m^2[surface soil]);
N_{LeafP} = mass of chemical in particles on leaf (g[chemical]);
V_{LeafP} = volume of particles on leaf (m^3[particles]);
ρ_P = density of particles on surface of leaf (kg[particles]/m^3[particles]);
N_{Worm} = mass of chemical in earthworm (g[chemical]);
$\rho area_{Worm}$ = areal biomass density of earthworms (kg[worm wet wt]/m^2[soil]);
N_{Arth} = mass of chemical in soil arthropods (g[chemical]);
$\rho area_{Arth}$ = areal biomass density of soil arthropods (kg[arthropod wet wt]/m^2[soil]);
$N_{Twl\text{-}prey}$ = mass of chemical in the wildlife prey species (g[chemical]);
$\rho area_{Twl\text{-}prey}$ = areal biomass density of the wildlife prey species (kg[body wet wt]/m^2);
N_{fish} = mass of chemical in the fish species (g[chemical]);
A_{SW} = area of surface water (m^2);
$\rho area_{fish}$ = areal biomass density of the fish species (kg[fish wet wt]/m^2[surface water]);
N_{BI} = mass of chemical in benthic invertebrates (emergent flying insects) (g[chemical]);
A_{Sed} = area of sediment (m_2);
$\rho area_{BI}$ = areal biomass density of benthic invertebrates (kg[invertebrates wet wt]/m^2[sediment]);
N_{Air} = total mass of chemical in air (g[chemical]); and
V_{Air} = volume of air (m^3).

7.4.2 TRANSFER-FACTOR ALGORITHMS

In TRIM.FaTE, each route of exposure and elimination indicated in the previous section is handled as a separate transfer factor, as described in subsections 7.4.2.1 through 7.4.2.12. In the following subsections, the subscript *Twl* refers to terrestrial wildlife, including the semi-aquatic wildlife species, because they breathe air.

7.4.2.1 Surface Water to Terrestrial Vertebrate Wildlife

The general transfer factor for ingesting a chemical while drinking surface water for a specific semi-aquatic wildlife species, either a bird or a mammal, is given by:

$$T_{SW \rightarrow Twl} = Biomass_{Twl} \times \frac{IN_W \times AE_W}{V_{SW}} \tag{TF 7-21}$$

where:

$T_{SW \rightarrow Twl}$ = transfer factor for transfer of chemical from surface water to bird or mammal (/day);
$Biomass_{Twl}$ = total biomass of wildlife compartment (kg);
IN_W = water ingestion rate normalized to body weight (m^3[air]/kg[body wet wt]-day);
AE_W = assimilation efficiency of chemical from water (unitless);
V_{SW} = volume of surface water compartment from which the animal is drinking (m^3[water]);

and:

$$Biomass_{Twl} = \rho area_{Twl} \times A \quad \text{(Eq. 7-66)}$$

or:

$$Biomass_{Twl} = PN_{Twl} \times BW_{Twl} \quad \text{(Eq. 7-67)}$$

where:

$\rho area_{Twl}$ = terrestrial wildlife wet biomass density per unit area (kg[biomass wet wt]/m^2[surface parcel]);
A = area of associated surface water compartment (*e.g.*, for loons and ducks) or area of associated soil compartment that borders surface water compartment (m^2);
PN_{Twl} = population size, or number of individuals in compartment (unitless); and
BW_{Twl} = body weight of the bird or mammal (kg).

(Note: In the current TRIM.FaTE library, the property *PopulationSize* in the wildlife compartments is actually calculated as *NumberofIndividualsPerSquareMeter* × *A*.)

The water ingestion rates for birds and mammals can be estimated from allometric equations that relate water ingestion rates to body weight, as described in Section 3.2 of EPA's (1993) *Wildlife Exposure Factors Handbook*. The allometric equations for water ingestion by mammals and birds are from Calder and Braun (1983):

$$WI_{mammals} = 0.099 \times BW^{0.90} \quad \text{(Eq. 7-68)}$$

$$WI_{birds} = 0.059 \times BW^{0.67} \quad \text{(Eq. 7-69)}$$

where:

WI = water ingestion rate (L/day); and
BW = body weight (kg[body wet wt]).

Therefore, the water ingestion rate normalized to body weight in m^3[water]/kg[body wet wt]-day is estimated by:[1]

$$IN_W\left(\frac{\mathrm{m}^3}{\mathrm{kg-day}}\right) = \frac{WI\left(\frac{\mathrm{L}}{\mathrm{day}}\right)}{BW(\mathrm{kg})} \times 0.0001\left(\frac{\mathrm{m}^3}{\mathrm{L}}\right) \qquad \text{(Eq. 7-70)}$$

7.4.2.2 Surface Soil to Terrestrial Vertebrate Wildlife

The general transfer factor for incidental ingestion of chemical with surface soil by a specific bird or mammal is given by:

$$T_{Ss \rightarrow Twl} = Biomass_{Twl} \times \frac{IN_{Ss} \times AE_S}{V_{Ss} \times \rho_{Ss\_wet}} \qquad \text{(TF 7-22)}$$

where:

$T_{Ss \rightarrow Twl}$ = transfer factor for transfer of chemical from surface soil to bird or mammal (/day);
IN_{Ss} = surface soil ingestion rate (kg[soil dry wt]/kg[body wet wt]-day);
AE_S = assimilation efficiency of chemical from soil (unitless);
V_{Ss} = volume of surface soil compartment (m^3); and
ρ_{Ss_wet} = bulk density of surface soil (kg[soil wet wt]/m^3[soil]).

To estimate the soil ingestion rate from data on the estimated percent soil in the consumed diet on a dry-weight basis (e.g., the data in Beyer et al. 1994), the following equations can be used, where:

IN_D = diet (no soil) ingestion rate (kg[diet wet wt]/kg[body wet wt]-day);
IN_{Ss} = ingestion rate of surface soil (kg[soil dry wt]/kg[body wet wt]-day);
IN_{D_dry} = dry diet (no soil) ingestion rate (kg[diet dry wt]/kg[body wet wt]-day); and
IN_{Total_dry} = total intake of dry food plus dry soil (kg[food + soil, dry wt]/kg[body wet wt]-day]).

Assuming the natural diet is 75 percent water:

$$IN_{D\_dry} = IN_D \times 0.25 \qquad \text{(Eq. 7-71)}$$

$$IN_{Total\_dry} = IN_{Ss} + IN_{D\_dry} \qquad \text{(Eq. 7-72)}$$

The data available in Beyer et al. (1994) and similar studies are in the form of:

---

[1] The algorithm described in Equation 7-70 is associated with mammal and bird compartment types in the current TRIM.FaTE library.

f_{intake_soil} = fraction of total dry-weight intake that is soil (unitless).

Therefore:

$$IN_{Total\_dry} = IN_{D\_dry} / (1 - f_{intake\_soil}) \qquad \text{(Eq. 7-73)}$$

Substituting Equation 7-73 for IN_{Total_dry} in Equation 7-72, using $IN_D \times 0.25$ for IN_{D_dry}, and rearranging the equation yields:

$$IN_{Ss} = \frac{IN_D \times 0.25}{(1 - f_{intake\_soil})} - IN_D \times 0.25 \qquad \text{(Eq. 7-74)}$$

The transfer factor for surface soil to terrestrial vertebrates should only be used for birds and mammals that forage on the ground (Beyer et al. 1994). For example, black-capped chickadees are arboreal feeders and are rarely observed on the ground (Smith 1993), meaning that soil ingestion for this species would be negligible. Representative species that ingest soil as a consequence of their feeding habits include the mallard, mule deer, black-tailed deer, white-tailed deer, long-tailed vole, raccoon, white-footed mouse, woodcock, and bobwhite quail. Representative species that do not feed on the ground – and consequently ingest only negligible amounts of soil or none at all – include the tree swallow, red-tailed hawk, long-tailed weasel, mink, and black-capped chickadee.

7.4.2.3 Plant Leaf to Terrestrial Vertebrate Wildlife

The general transfer factor for bird or mammal ingestion of a chemical in plant leaves is given by:

$$T_{Leaf \rightarrow Twl} = \frac{\rho area_{Twl}}{\rho area_{Leaf}} \times p_{Plant} \times IN_D \times AE_{Plant} \qquad \text{(TF 7-23)}$$

where:

$T_{Leaf \rightarrow Twl}$ = transfer factor for transfer of chemical from plant leaf to bird or mammal(/day);
p_{Plant} = proportion of plant matter in diet (unitless);
IN_D = diet ingestion rate (kg[diet wet wt]/kg[body wet wt]-day);
AE_{Plant} = assimilation efficiency of chemical from plant in diet (unitless); and
$\rho area_{Leaf}$ = areal biomass density of foliage (kg[leaves wet wt]/m^2[surface soil]).

Note that:

$$\rho area_{Twl} = PN_{area} \times BW \qquad \text{(Eq. 7-74)}$$

and:

$$Biomass_{Twl} = PN_{area} \times A \times BW \qquad \text{(Eq. 7-75)}$$

where:

A = area of containing surface volume element (m^2); and
PN_{area} = population size or number of individuals per unit area (/m^2[soil]).

The transfer factor for plant leaf to terrestrial vertebrates is most relevant for herbivores, which feed entirely on plant matter. It also is relevant for omnivores, for which plant matter makes up a portion of their diet. This transfer factor is not relevant for carnivores or predators/scavengers. The proportion of plant matter in the diet (p_{Plant}) varies by species, by season, and by location of the population of interest. In initial applications of TRIM.FaTE, p_{Plant} has varied by species.

7.4.2.4 Particles on Leaf Surface to Terrestrial Vertebrate Wildlife

Ingestion of plant materials generally results in the ingestion of the particles that have settled on the plant surfaces. In some areas under some conditions, the coating of plants with particulate matter (*e.g.*, dust or soil particles) can be substantial. The general transfer factor for particles on leaf surfaces to a specific bird or mammal is given by:

$$T_{LeafP \rightarrow Twl} = \frac{p_{Plant} \times IN_D \times AE_S}{V_{LeafP} \times \rho_{LeafP}} \qquad \text{(TF 7-24)}$$

where:

$T_{LeafP \rightarrow Twl}$ = transfer factor for transfer of chemical from particles-on-leaf compartment to bird or mammal compartment via ingestion (/day);
AE_S = assimilation efficiency of chemical from soil (unitless);
V_{LeafP} = volume of the particles-on-leaf compartment (m^3); and
ρ_{LeafP} = density of dust particles (kg[particles]/m^3[particles]).

7.4.2.5 Earthworm to Terrestrial Vertebrate Wildlife

The general transfer factor for earthworms to a specific bird or mammal is given by:

$$T_{Worm \rightarrow Twl} = \frac{\rho area_{Twl}}{\rho area_{Worm}} \times p_{Worm} \times IN_D \times AE_{Worm} \qquad \text{(TF 7-25)}$$

where:

$T_{Worm \rightarrow Twl}$ = transfer factor for transfer of chemical from earthworm to bird or mammal (/day);
$\rho area_{Worm}$ = areal biomass density of earthworms (kg[worm wet wt]/m^2 [soil]);
p_{Worm} = proportion of earthworm in diet (unitless); and

AE_{Worm} = assimilation efficiency of chemical from earthworm in diet (unitless).

This transfer factor is relevant in cases where the specific bird or mammal of interest is known to consume earthworms. Examples of species that ingest earthworms include the raccoon, short-tailed shrew, woodcock, and American robin.

7.4.2.6 Soil Arthropod to Terrestrial Vertebrate Wildlife

The general transfer factor for soil arthropods to a specific bird or mammal is given by:

$$T_{Arth \rightarrow Twl} = \frac{\rho area_{Twl}}{\rho area_{Arth}} \times p_{Arth} \times IN_D \times AE_{Arth} \qquad \text{(TF 7-26)}$$

where:

$T_{Arth \rightarrow Twl}$ = transfer factor for transfer of chemical from soil arthropods to bird or mammal (/day);
$\rho area_{Arth}$ = areal biomass density of soil arthropods (kg[arthropod wet wt]/m^2[soil]);
p_{Arth} = proportion of soil arthropods in diet (unitless); and
AE_{Arth} = assimilation efficiency of chemical from arthropods in diet (unitless).

This transfer factor is relevant in cases where the specific bird or mammal of interest is known to consume soil arthropods. Soil arthropods are invertebrates with segmented bodies and jointed limbs as adults, such as ants, beetles, spiders, grasshoppers, and centipedes and include their larval forms that dwell in the soil as well (*e.g.*, beetle grubs). Examples of wildlife species that consume soil arthropods include the shrew, woodcock, and white-footed mouse.

7.4.2.7 Terrestrial Vertebrate to Terrestrial Vertebrate Wildlife

The general transfer factor for bird or mammal ingestion of chemical in avian or mammalian prey is given by:

$$T_{prey-i \rightarrow Twl} = \frac{\rho area_{Twl}}{\rho area_{Tprey-i}} \times p_{Tprey-i} \times IN_D \times AE_{Twl} \qquad \text{(TF 7-27)}$$

where:

$T_{prey-i \rightarrow Twl}$ = transfer factor for the transfer of chemical from the i^{th} terrestrial vertebrate prey species to the bird or mammal predator species (/day);
$\rho area_{Twl}$ = areal biomass density of the consumer wildlife (*i.e.*, bird or mammal) species (kg[predator wet wt]/m^2[soil]);
$\rho area_{Tprey-i}$ = areal biomass density of the prey wildlife (*i.e.*, bird or mammal) species (kg[prey wet wt]/m^2[soil]);
$p_{Tprey-i}$ = proportion of i^{th} terrestrial vertebrate prey species in diet (unitless); and
AE_{Twl} = assimilation efficiency of chemical from birds or mammals in diet (unitless).

The transfer factor for terrestrial vertebrate to terrestrial vertebrate is only applicable to birds and mammals that are classified as terrestrial omnivores, carnivores, and predators/scavengers. Examples of species to which this transfer factor would apply include the red-tailed hawk, long-tailed weasel, and mink. Note that the assimilation efficiencies for a chemical in either avian or mammalian prey consumed by avian or mammalian predators are likely to be similar; hence, a single AE_{Twl} is specified.

7.4.2.8 Fish to Terrestrial Vertebrate Wildlife

The transfer factor for ingestion of a chemical in fish by a terrestrial vertebrate is relevant in cases where the bird or mammal of interest is known to consume fish species (*i.e.*, the bird or mammal is classified as a piscivore or an omnivore). Several types or species of fish can be represented in TRIM.FaTE, including benthic herbivores, omnivores, and carnivores, and water column herbivores, omnivores, and carnivores (see Chapter 6). Different species of piscivorous wildlife are more likely to catch certain types and sizes of fish than others (*e.g.*, the belted kingfisher is more likely to eat small water column herbivores and omnivores such as minnows and bluegill than larger carnivorous species of fish). The general transfer factor for fish to a specific bird or mammal is given by:

$$T_{fish-i \rightarrow Twl} = \frac{Biomass_{Twl}}{A_{SW} \times \rho area_{fish-i}} \times p_{fish-i} \times IN_D \times AE_{fish} \qquad \text{(TF 7-28)}$$

where:

$T_{fish-i \rightarrow Twl}$ = transfer factor for transfer of chemical from i^{th} type of fish to bird or mammal (/day);
p_{fish-i} = proportion of i^{th} type of fish in diet (unitless);
AE_{fish} = assimilation efficiency of chemical from fish in diet (unitless);
A_{SW} = area of surface of surface water body compartment (m^2); and
$\rho area_{fish-i}$ = areal biomass density of the i^{th} type of fish (kg[fish wet wt]/m^2[surface water]).

7.4.2.9 Benthic Invertebrate to Terrestrial Vertebrate Wildlife

Benthic invertebrates include mayflies, dragonfly nymphs, crayfish, clams, and aquatic snails, which dwell primarily at the bottom of water bodies. Examples of wildlife species that consume benthic invertebrates are the mallard, raccoon, and belted kingfisher. The general transfer factor for ingestion of a chemical in benthic invertebrates by a specific bird or mammal is given by:

$$T_{BI \rightarrow Twl} = \frac{Biomass_{Twl}}{A_{Sed} \times \rho area_{BI}} \times p_{BI} \times IN_D \times AE_{BI} \qquad \text{(TF 7-29)}$$

where:

$T_{BI \rightarrow Twl}$ = transfer factor for transfer of chemical from benthic invertebrates to bird or mammal (/day);
p_{BI} = proportion of benthic invertebrates in diet (unitless);
AE_{BI} = assimilation efficiency of chemical from benthic invertebrates in diet (unitless);
A_{Sed} = area of the sediment compartment (m^2); and
$\rho area_{BI}$ = areal biomass density of benthic invertebrates (kg[invertebrates wet wt]/m^2 [sediment]).

The same transfer factor is used to represent flying insects consumed by birds (or bats) for species of insects with aquatic larval stages. For purposes of the model, the flying insects are assumed to have the same chemical concentrations in their tissues as they had when living underwater before metamorphosis into flying adults. Representative species that consume flying insects include the black-capped chickadee and tree swallow.

7.4.2.10 Air to Terrestrial Vertebrate Wildlife

The general transfer factor for inhalation of a chemical in air (vapor- and particulate-phase) to a specific bird or mammal is given by:

$$T_{Air \rightarrow Twl} = Biomass_{Twl} \times \frac{IN_{Air} \times AE_{Air}}{V_{Air}} \qquad \text{(TF 7-30)}$$

where:

$T_{Air \rightarrow Twl}$ = transfer factor for transfer of chemical from air to bird or mammal (/day);
IN_{Air} = inhalation rate normalized to body weight (m^3[air]/kg[body wet wt]-day);
AE_{Air} = assimilation efficiency of chemical from air (unitless); and
V_{Air} = volume of air compartment (m^3).

The inhalation rates for birds and mammals are estimated from allometric equations that relate inhalation rates of captive animals to body weight, as described in Section 3.3 of EPA's (1993) *Wildlife Exposure Factors Handbook.* The allometric equation for inhalation rate (*IR*) by mammals is from Stahl (1967). For mammals:

$$IR = 0.5458 \times BW^{0.80} \qquad \text{(Eq. 7-76)}$$

where:

IR = inhalation rate (m^3[air]/day); and
BW = body weight (kg[body wet wt]).

The allometric equations for inhalation rate by birds are from Lasiewski and Calder (1971). For nonpasserine birds (*i.e.*, birds other than the perching songbirds):

$$IR = 0.4089 \times BW^{0.77} \qquad \text{(Eq. 7-77)}$$

However, adjustments are required to estimate the inhalation rates of free-living animals from these estimates, which are based on conditions used to measure standard metabolic rate of captive animals. For example, it may be appropriate to multiply the predicted *IR* from these allometric equations by a factor of 2 to 3 (USEPA 1993). The value used in initial TRIM.FaTE applications is 2.5.

Also, the inhalation rate for birds is for nonpasserine species only. Passerines tend to have a higher metabolic rate than nonpasserines for a given body weight. For example, the equations for basal metabolic rate (*BMR*) developed by Lasiewski and Dawson (1967) from almost 100 species of birds revealed the following differences:

For passerine birds: $$BMR = 128 \times BW^{0.724} \qquad \text{(Eq. 7-78)}$$

For nonpasserine birds: $$BMR = 77.6 \times BW^{0.723} \qquad \text{(Eq. 7-79)}$$

where:

BMR = basal metabolic rate (kcal/day);
BW = body weight (kg[body wet wt]/day).

In other words, the BMR of passerine birds is about 1.65 times higher than that of nonpasserine birds. Similarly, the equations for free-living metabolic rate (FMR) developed by Nagy (1987) for passerines (N = 26) and nonpasserines (N = 24) indicated that the FMR of passerine birds is about 1.85 times higher than that of nonpasserine birds.

Thus, the equations for estimating the free-living inhalation rate (*FIR*) in m^3/day for birds and mammals may be derived as:

For all mammals: $$FIR = 0.5458 \times BW^{0.80} \times 2.5 \qquad \text{(Eq. 7-80)}$$

For nonpasserine birds: $$FIR = 0.4089 \times BW^{0.77} \times 2.5 \qquad \text{(Eq. 7-81)}$$

For passerine birds: $$FIR = 0.4089 \times BW^{0.77} \times 2.5 \times 1.75 \qquad \text{(Eq. 7-82)}$$

Thus, IN_{Air} (in m^3/kg[body wet wt]-day) in equation TF 7-30 is estimated by:

$$IN_{Air} = \frac{FIR}{BW} \qquad \text{(Eq. 7-83)}$$

where:

FIR = free-living inhalation rate (m^3/day).

7.4.2.11 Terrestrial Vertebrate Wildlife to Surface Soil

The general transfer factor for elimination of a chemical from a bird or mammal to surface soil is given by:

$$T_{Twl \rightarrow Ss} = f_{fuSs} \times k_{ET} \qquad \text{(TF 7-31)}$$

where:

$T_{Twl \rightarrow Ss}$ = transfer factor for transfer of chemical from bird or mammal to surface soil (/day);
f_{fuSs} = fraction eliminated to surface soil (instead of surface water) (unitless); and
k_{ET} = first-order rate constant for total elimination of chemical in urine and feces (E_{uf}) plus feathers or fur (E_{ff}) (/day), *i.e.*,
= $k_{uf} + k_{ff}$.

This single first-order elimination rate refers to the parent chemical (*i.e.*, undegraded, untransformed chemical). In addition to excretion in urine and feces, chemicals also can be excreted by birds into feathers and eggs and by mammals into hair, or fur, and milk. For the chemicals modeled in TRIM.FaTE to date, with the exception of methylmercury, this single elimination rate constant will be dominated by elimination in urine and feces. For the excretion of methylmercury from birds, feathers and eggs is similar in importance to urine and feces (see Table A-17 in Appendix A). Thus, in the case of birds and methylmercury, the rate constant for chemical elimination that reaches the soil, k_{ET}, is set equal to the rate constant for elimination in urine and feces plus the rate constant for elimination in feathers. Note that in the current TRIM.FaTE compartment design, excretion to eggs does not constitute movement of the chemical out of the bird population compartment, nor does milk represent movement out of mammal population compartment. A discussion of estimating elimination rate constants from metabolic studies is presented in the TRIM.FaTE user guidance.

7.4.2.12 Semi-aquatic Vertebrate Wildlife to Surface Water

The general transfer factor for elimination of a chemical from semi-aquatic wildlife to surface water is given by:

$$T_{Twl \rightarrow SW} = f_{fuSW} \times k_{ET} \qquad \text{(TF 7-32)}$$

where:

$T_{Twl \rightarrow SW}$ = transfer factor for transfer of chemical from bird or mammal to surface water (/day);
f_{fuSW} = fraction eliminated to surface water (unitless); which
= $1 - f_{uSs}$.

7.4.3 TRANSFORMATIONS AND DEGRADATION

Transformations of organic chemicals into metabolic by-products that are no longer tracked in TRIM.FaTE are modeled as transfers to the wildlife degradation/reaction sinks. See the TRIM.FaTE user guidance for discussion of identifying rate constants for metabolism separately from rate constants associated with chemical excretion and elimination back to the environment. Equation 2-64 (Chapter 2) is used to estimate the first-order metabolic degradation (in TRIM.FaTE, called "general degradation") rate constant, $k_{degradation}$, for an organic chemical. The transfer-factor algorithm for transfer of metabolic by-products to the wildlife degradation/reaction sink is simply equal to $k_{degradation}$.

It has been observed that first-order degradation rate constants generally scale as a function of body weight (BW) to a negative one quarter power (U.S. EPA 1992). Thus, $k_{degradation}$ for a species of interest may be derived from $k_{degradation}$ for a reference species using the following equation:

$$k_{degradation}(Twl) = k_{degradation}(ref) \times \frac{BW(Twl)^{-0.25}}{BW(ref)^{-0.25}} \qquad \text{(Eq. 7-84)}$$

where:

$k_{degradation}(Twl)$ = metabolic degradation rate constant for the terrestrial wildlife species in TRIM.FaTE (/day);
$k_{degradation}(ref)$ = metabolic degradation rate constant for the reference laboratory animal (/day);
$BW(Twl)$ = body weight for the terrestrial wildlife species in TRIM.FaTE (kg[body wet wt]); and
$BW(ref)$ = body weight for the reference laboratory animal (kg[body wet wt]).

Metabolic transformations of chemicals among different compounds containing the same core chemical (*e.g.*, transformation among mercury species) are included in the TRIM.FaTE wildlife models. See Appendix A, Section A.3, for a discussion of mercury transformations in birds and mammals.

7.4.4 SEASONALITY

Seasonality of diet is partially reflected in the current TRIM.FaTE library algorithms. Herbivorous or omnivorous wildlife consume leaves of deciduous trees, grasses/herbs, and possibly agricultural crops only during the growing season, when such leaves are available. During the non-growing season, those types of vegetation are no longer available to wildlife for consumption. Applications to date have not included alternative dietary items (containing the modeled chemical) for herbivorous wildlife in winter. Wildlife species could migrate out of the area for the winter (*e.g.*, American robin) or switch to other foods during the winter (*e.g.*, deer begin stripping bark and move from deciduous areas to coniferous forest).

To reflect winter sleep, hibernation, or migration, the user may turn off wildlife algorithms during relevant seasons. Additionally, it may be appropriate to seasonally vary the diet of particular wildlife species.

7.4.5 USE OF TERRESTRIAL WILDLIFE COMPARTMENTS

The TRIM.FaTE model has been parameterized for many functional trophic groups of wildlife species. These are listed in Table 7-1. The parameters for which input is needed in a TRIM.FaTE simulation for these compartment types are presented in Appendix D.

Discussion on the selection of wildlife species for a TRIM.FaTE scenario and the association of different species with appropriate volume elements is provided in the TRIM.FaTE users guidance. The addition of wildlife populations to a TRIM.FaTE scenario will depend on the goals and objectives of the project as well as the ecosystem being modeled. In addition, the

Table 7-1
Terrestrial and Semi-aquatic Vertebrate Compartment Types in Current TRIM.FaTE Library

Functional Trophic Group	Compartment Type
Semi-aquatic piscivore[a]/predator	Belted kingfisher Common loon (water-based)[b] Mink
Semi-aquatic predator/scavenger	Bald eagle
Semi-aquatic aerial insectivore (*i.e.*, feeding on adults of emergent insects such as mayflies)	Tree swallow
Semi-aquatic omnivore	Mallard (water-based)[b] Raccoon
Terrestrial omnivore	American robin White-footed mouse
Terrestrial insectivore	Black-capped chickadee
Terrestrial predator/scavenger	Long-tailed weasel Red-tailed hawk
Terrestrial herbivore	Black-tailed deer Bobwhite quail Long-tailed vole Meadow vole Mule deer White-tailed deer
Terrestrial ground-invertebrate feeder	Short-tailed shrew Trowbridge shrew Woodcock

[a] Consumes fish.

[b] The containing volume element is associated with surface water, and the species' population density represents the number of individuals per unit surface water area.

distribution of chemical mass (and transfers) across wildlife biomass and trophic levels in the ecosystem needs consideration.

Exclusively terrestrial wildlife species may be associated with terrestrial surface volume elements depending on the plant community represented by the volume element (*e.g.*, deciduous forest, coniferous forest, herbs/grasses). The containing volume element for semi-aquatic wildlife species can either be a surface water volume element (*i.e.*, water-based species, such as loons, that spend most of their time on the water and feed entirely on aquatic organisms) or a surface soil volume element (*i.e.*, land-based species, such as mink that spend most of their time on land and consume both aquatic and terrestrial foods) (see Table 7-1).

Several semi-aquatic wildlife species have been included in the current TRIM.FaTE library. Each of these species must be linked to a specific surface water body from which they can obtain their aquatic prey or food (*e.g.*, fish, benthic invertebrates, macrophytes). This generally is accomplished by including the wildlife species' compartment in a land parcel that is adjacent to the surface water body and estimating the density and numbers of individuals present based on the area of the land parcel. Alternatively, it might be appropriate to create two different compartment types for these semi-aquatic wildlife (*e.g.*, raccoons consuming aquatic prey and raccoons consuming terrestrial prey), particularly for applications where aquatic species play a substantive role (*e.g.*, as focus in assessment, or significant source of pollutant to predators). The densities of the land-based semi-aquatic wildlife in the containing surface soil volume element should reflect only those individuals with foraging ranges that might realistically include the water body. For species that defend feeding territories, the number of individuals per unit length of shoreline would be the relevant density measure for those consuming aquatic prey. The density of that species per unit area of the containing surface soil volume element would equal the number of individuals that might forage along the interface between the surface water compartment and containing surface soil volume element divided by the area of the surface soil volume element. Otherwise, the simulation might reflect an unrealistic consumption of aquatic organisms by their land-based predators. For species that forage in flocks or herds far from nesting or breeding sites, such as tree swallows, the number of individuals per unit area of the terrestrial environment generally would be the relevant density measure.

Predators/scavengers with large home ranges (*e.g.*, bald eagle) can be modeled as consuming prey from a number of different surface parcels or volume elements. A TRIM.FaTE variable called *TheLink.Fraction-SpecificCompartmentDiet* in the transfer factor algorithm used for the ingestion link from the prey (and its associated surface parcel) to the predator would be used to partition the diet among different surface parcels.

7.4.6 ASSIMILATION EFFICIENCY AND ELIMINATION

The TRIM.FaTE user guidance discusses the types of data from published studies that may be appropriate to use for chemical assimilation (absorption) efficiencies from the diet (AE_D), from drinking water (AE_W), from air via inhalation (AE_{Air}), and for elimination rate constants (k_{ET}). Nonetheless, some explanation is warranted here to assist the user in understanding differences in the fish and wildlife values for AE and k_{ET} properties in the current TRIM.FaTE library. A simplified explanation of AE_D, AE_W, and k_{ET} for mammals and birds is presented in Section 7.4.6.1. A simplified explanation of AE_{Air} is provided in Section 7.4.6.2.

7.4.6.1 Efficiency of Chemical Assimilation from the Diet

An AE_D for dietary intake of a chemical (or an AE_W for intake of a chemical with drinking water) of 1.0 implies complete absorption from the diet/drinking water, while an AE_D of 0.2, for example, indicates that 80 percent of the chemical passed through the wildlife unabsorbed and hence, must have been eliminated in the feces. For the chemical that was absorbed (*e.g.*, 20 percent in the current example), there are several possible elimination routes listed below, the first three of which may be considered "excretory processes":

- excretion in urine (via the kidney);
- excretion in bile, which is eliminated in the feces;
- transfer to fur or feathers, to eggs, or to milk;
- exhalation via the lungs (considered a diffusive process of negligible magnitude for compounds of interest and not included in the current TRIM.FaTE library); and
- metabolic degradation to other chemicals.

Depending on the organism, available data by which to estimate one or more of these processes might be predominantly of one type or another. Many toxicokinetic studies using birds or mammals, where both feces and urine are fairly easy to collect and analyze, estimate "elimination" rates or rate constants based on those data. Those data account for (a) fecal elimination of the unabsorbed chemical, and excretion of the absorbed chemical (b) in urine and (c) in the bile. Many such studies also measure dose as the concentration of the chemical in the diet multiplied by the quantity of food eaten. With these types of measurements, one would not need to estimate an AE_D (or AE_W) for the chemical. Instead, all of the chemical ingested with food (and water) would represent the chemical gain rate for the wildlife compartment and chemical elimination in urine and feces would represent the loss rate. In this case, the AE_D (or AE_W) would be set equal to 1.0. Given that the mercury loss (elimination) rates for wildlife modeled in an initial mercury application were based on measurements of the quantity of chemical in urine and feces compared with the quantity in the diet and water, we set AE_D and AE_W to 1.0 for that test case.

Toxicokinetic studies of organic compounds often use radioactive labels to track the elimination of metabolites of organic compounds in urine and feces as well as elimination of the parent compound. In TRIM.FaTE, if the metabolites are not tracked further by the model, the mass of parent chemical that was degraded into metabolites should be transferred to a wildlife sink. Only the parent chemical that is excreted in urine and feces should be transferred back to the environment (either surface soil or surface water) via the “elimination” transfer factors. Thus, only those studies in which the investigator quantifies the radioactive metabolites separately from the radioactive parent chemical can be used to set a rate constant for transfer to the degradation sink separately from the rate constant for elimination to the environment.

Another type of data often reported in the literature are elimination rate constants based on measurements of body burdens of a chemical over time following a single administration. Suppose that a group of animals were administered an organic chemical one time by intravenous injection. Suppose further that the body burdens of the chemical in different subsets of those animals were measured at weekly intervals after that. From those data (*i.e.*, body burden at time 0, 7 days, 14 days, etc.), the estimated elimination rate constant would account for (a) excretion in urine, (b) excretion in bile (in feces), and (c) metabolic degradation to other chemicals. That is, these data (from an intravenous injection study) do not provide information on assimilation or absorption from the diet that is needed to estimate $AE_{D.}$ For additional discussion of these topics, see the TRIM.FaTE user guidance.

7.4.6.2 Efficiency of Chemical Assimilation from Air

In a very simple inhalation model, the efficiency of assimilation of a chemical from air can be calculated from the estimated inhalation dose (*i.e.*, the chemical concentration in air multiplied by the animal's inhalation rate, measured in volume of air per unit time) compared with the body burden of the chemical in the animal after a specified exposure duration. The estimated AE_{Air}, representing a net absorption, would account for transfers from the air in the lungs to the bloodstream and from the bloodstream to the air in the lungs.

8. REFERENCES

Ambrose, R.A., Jr., T.A. Wool, and J.L. Martin. 1995. The water quality analysis simulation program, WASP5. Part A: Model documentation. Athens, GA: U.S. EPA National Exposure Research Laboratory, Ecosystems Division.

ARS (Agricultural Research Service). 1982. Analytical Solutions of the One-dimensional Convective-dispersive Solute Transport Equation. Washington, D.C.: U.S. Department of Agriculture.

Baes, C.F., III, R.D. Sharp, A.L. Sjoreen, and R.W. Shor. 1984. A Review and Analysis of Parameters for Assessing Transport of Environmentally Released Radionuclides Through Agriculture. ORNL-5786. Oak Ridge, TN: Oak Ridge National Laboratory.

Baines, S. B., and M.L. Pace. 1994. Relationships between suspended particulate matter and sinking flux along a trophic gradient and implications for the fate of planktonic primary production. Canadian Journal of Fisheries and Aquatic Sciences. 51:25-36.

Bennett, D.H., T.E. McKone, M. Matthies, and W.E. Kastenberg. 1998. General formulation of characteristic travel distance for semivolatile organic chemicals in a multimedia environment. Environmental Science and Technology. 32:4023-4030.

Beyer, W.N., E.E. Connor, and S. Gerould. 1994. Estimates of soil ingestion by wildlife. Journal of Wildlife Management. 58:375-382.

Briggs, G.G., R.H. Bromilow, A.A. Evans, and M.R. Williams. 1983. Relationships between lipophilicity and the distribution of non-ionised chemicals in barley shoots following uptake by the roots. Pesticide Science. 14:492-500.

Briggs, G.G., R.H. Bromilow, and A.A. Evans. 1982. Relationship between lipophilicity and root uptake and translocation of non-ionised chemicals by barley. Pesticide Science. 13:495-504.

Calder, W.A., and E.J. Braun. 1983. Scaling of osmotic regulation in mammals and birds. American Journal of Physiology. 244:R601-R606.

Chamberlain, A.C. 1970. Interception and retention of radioactive aerosols by vegetation. Atmospheric Environment 4: 57-78.

Connell, D.W., and R.D. Markwell. 1990. Bioaccumulation in the soil to earthworm system. Chemosphere. 20:91-100.

Covar, A.P. 1976. Selecting the proper reaeration coefficient for use in water quality models. Presented at the U.S. EPA Conference on Environmental Simulation Modeling, April 19-22, Cincinnati, OH.

Crank, J., N.R. McFarlane, J.C. Newby, G.D. Paterson, and J.B. Pedley. 1981. Diffusion processes in environmental systems. In: Paterson et al. 1991. London: Macmillan Press, Ltd.

Di Toro, D.M., and J.P. Connolly. 1980. Mathematical Models of Water Quality in Large Lakes, Part 2: Lake Erie. Washington, D.C.: U.S. Environmental Protection Agency. EPA-600/3-80-056; pp. 28-30.

Efroymson, R.A., B.E. Sample, and G.W. Suter II. 2001. Bioaccumulation of inorganic chemicals by soil from plants: regressions of field data. Environ. Toxicol. Chem. 20:2165-2571.

Gobas, F.A.P.C. 1993. A model for predicting the bioaccumulation of hydrophobic organic-chemicals in aquatic food-webs – application to Lake Ontario. Ecological Modeling. 69:1-17.

Gobas, F.A.P.C., E.J. McNeil, L. Lovettdoust, and G.D. Haffner. 1991. Bioconcentration of chlorinated aromatic-hydrocarbons in aquatic macrophytes. Environmental Science & Technology. 25:924-929.

Hargrove, W.W. 1999. Personal communication. University of Tennessee. January.

Harner and Bidleman. 1998. Octanol-air coefficient for describing particle/gas partitioning of aromatic compounds in urban air. Environmental Science and Technology. 32:1494-1502.

Hsu, F.C., R.L. Marxmiller, and A.Y.S. Yang. 1990. Study of root uptake and xylem translocation of cinmethylin and related compounds in detopped soybean roots using a pressure chamber technique. Plant Physiology. 93:1573-1578.

Junge, C.E. 1977. Basic considerations about trace constituents in the atmosphere as related to the fate of global pollutants. In: Suffet, I.H., ed. Fate of Pollutants in the Air and Water Environments. New York, NY: Wiley and Sons; pp. 7-26.

Jury, W., W. Spencer, and W. Farmer. 1983. Behavior assessment model for trace organics in soil: I. Model description. Journal of Environmental Quality. 12:558-564.

Karickhoff, S.W. 1981. Semi-emperical estimation of sorption of hydrophobic pollutants on natural sediments and soils. Chemosphere. 10:833-846.

Lasiewski, R.C., and W.A. Calder. 1971. A preliminary allometric analysis of respiratory variables in resting birds. Respiration Physiology. 11:152-166.

Lasiewski, R.C., and W.R. Dawson. 1967. A reexamination of the relation between standard metabolic rate and body weight in birds. Condor. 69:12-23.

Leonard, T.L., G.E. Taylor, Jr., M.S. Gustin, and G.C. J. Fernandez. 1998. Mercury and plants in contaminated soils: 2. Environmental and physiological factors governing mercury flux to the atmosphere. Environmental Toxicology and Chemistry. 17:2072-2079.

Lindberg, S. 1999a. Personal communication. Oak Ridge National Laboratory. January.

Lindberg, S. 1999b. Personal communication. Oak Ridge National Laboratory. September.

Lindberg, S.E., T.P. Meyers, G.E. Taylor, Jr., R.R. Turner, and W.H. Schroeder. 1992. Atmosphere-surface exchange of mercury in a forest: results of modeling and gradient approaches. Journal of Geophysical Research. 97:2519-2528.

Mackay, D. 1991. Multimedia Environmental Models: The Fugacity Aproach. Chelsea, MI: Lewis Publishers.

Mackay, D., M. Joy, and S. Paterson. 1983a. A quantitative water, air, sediment interaction (QWASI) fugacity model for describing fate of chemicals in lakes. Chemosphere. 12:981-997.

Mackay, D., S. Paterson, and M. Joy. 1983b. A quantitative water, air, sediment interaction (QWASI) fugacity model for describing fate of chemicals in rivers. Chemosphere. 12:1193-1208.

Mackay, D., and P.J. Leinonen. 1975. Rate of evaporation of low-solubility contaminants from water bodies to atmospheres. Environmental Science and Technology. 7:611-614.

Mackay, D., and A.T.K. Yeun. 1983. Mass transfer coefficients correlations of volatilization of organic solutes from water. Environmental Science and Technology. 17:211-216.

McCune, D.C., and T.L. Lauver. 1986. Experimental modeling of the interaction of wet and dry deposition on conifers. In: Lee, S. F., T. Schneider, L. D. Grant, and P. J. Verkerk, eds. Aerosols: Research, Risk Assessment, and Control Strategies. Proceedings of the Second U.S.-Dutch International Symposium, Williamsburg, VA; pp. 871-878. May 1985.

McKone, T.E. 1993a. CalTOX, A Multimedia Total-exposure Model for Hazardous-wastes Sites, Part I: Executive Summary. UCRL-CR-111456PtI. Livermore, CA: Lawrence Livermore National Laboratory.

McKone, T.E. 1993b. CalTOX, A Multimedia Total-exposure Model for Hazardous-wastes Sites, Part II: The Dynamic Multimedia Transport and Transformation Model. UCRL-CR-111456PtII. Livermore, CA: Lawrence Livermore National Laboratory.

McKone, T.E. 1993c. CalTOX, A Multimedia Total-exposure Model for Hazardous-waste Sites, Part III: The Multiple-pathway Exposure Model. UCRL-CR-111456PtIII. Livermore, CA: Lawrence Livermore National Laboratory.

Mill, T., W.R. Mabey, P.C. Bomberger, T.W. Chou, D.G. Herdy, and J.H. Smith. 1982. Laboratory Protocols for Evaluating the Fate of Organic Chemicals in Air and Water. EPA-600/3-82-0220. Athens, GA: U.S. Environmental Protection Agency.

Millington, R.J. and J.M. Quirk. 1961. Permeability of porous solids. Transactions of the Faraday Society. 57:1200-1207. In: Wallach, R., W.A. Jury, and W.F. Spencer. 1989. The concept of convective mass transfer for prediction of surface-runoff pollution by soil surface applied chemicals. Transactions of the American Society of Agricultural Engineers. May-June. 1989.

Muller, H., and G. Prohl. 1993. Ecosys-87: A dynamic model for assessing radiological consequences of nuclear accidents. Health Physics. 64:232-252.

Nagy, K.A. 1987. Field metabolic rate and food requirement scaling in mammals and birds. Ecological Monograph. 57: 111-128.

Nobel, P.S. 1999. Physiochemical and Environmental Plant Physiology. Second Edition. New York, NY: Academic Press.

O'Connor, D.J. 1983. Wind effects on gas-liquid transfer coefficients. Journal of Environmental Engineering. 109(9):731-752.

Paterson, S., and D. Mackay. 1995. Interpreting chemical partitioning in soil-plant-air systems with a fugacity model. In: Trapp, S. and J.C. McFarlane, eds. Plant Contamination: Modeling and Simulation of Organic Chemical Processes. Boca Raton, FL: Lewis Publishers; pp. 191-214.

Paterson, S., D. Mackay, and A. Gladman. 1991. A fugacity model of chemical uptake by plants from soil and air. Chemosphere. 23:539-565.

Post, W.M. 1999. Personal communication. Oak Ridge National Laboratory. January.

Prohl, G., Hoffman, F.O. 1996. Radionuclide interception and loss processes in vegetation. In: Modeling of Radionuclide Interception and Loss Processes in Vegetation and of Transfer in Semi-natural Ecosystems. Vienna. IAEA-TECDOC-857, pp. 9-46.

Ribeyre, F., and A. Boudou. 1994. Experimental study of inorganic and methylmercury bioaccumulation by 4 species of fresh-water rooted macrophytes from water and sediment contamination sources. Ecotoxicology and Environmental Safety. 28(3):270-286.

Riederer, M. 1995. Partitioning and transport of organic chemicals between the atmospheric environment and leaves. In: S. Trapp and J.C. McFarlane, eds. Plant Contamination: Modeling and Simulation of Organic Chemical Processes. Boca Raton, FL: Lewis Publishers; pp. 153-190.

Sample, B.E., G.W. Suter II, J.J. Beauchamp, and R.A. Efroymson. 1999. Literature-derived bioaccumulation models for earthworms: development and validation. Environmental Toxicology and Chemistry. 18:2110-2120.

Schnoor, J.L. 1981. Fate and transport of dieldrin in Coraville Reservoir: residues in fish and water following a pesticide ban. Science. 211:840-842.

Schnoor, J.L., and D.C. McAvoy. 1981. A pesticide transport and bioconcentration model. Journal of Environmental Engineering. 107:1229-1246.

Simonich, S.L,. and R.A. Hites. 1995. Global distribution of persistent organochlorine compounds. Science. 269:1851-1854.

Smith, S.M. 1993. Black-capped chickadee. In: A. Poole, P. Stettenheim, and F. Gill, eds., The Birds of North America. No. 39. Philadelphia, The Academy of Natural Sciences; Washington D.C., The Ornithologists Union.

Stahl, W.R. 1967. Scaling of respiratory variables in mammals. Journal of Applied Physiology. 22:453-460.

Suter, G.W., II, R.A. Efroymson, B.E. Sample, and D.S. Jones. 2000. Ecological Risk Assessment for Contaminated Sites. Boca Raton, FL: Lewis Publishers.

Thomann, R.V. 1989. Bioaccumulation model of organic-chemical distribution in aquatic food-chains. Environmental Science and Technology. 23:699-707.

Thomann, R.V., J.P. Connolly, and T.F. Parkerton. 1992a. An equilibrium-model of organic-chemical accumulation in aquatic food webs with sediment interaction. Environmental Toxicology and Chemistry. 11:615-629.

Thomann, R.V., J.P. Connolly, and T.F. Parkerton. 1992b. Modeling accumulation of organic chemicals in aquatic food webs. In: Gobas, F.A. and J.A. McCorquodale, eds. Chemical Dynamics in Fresh Water Ecosystems. Boca Raton, FL: Lewis Publishers; pp. 153-186.

Trapp, S. 1995. Model for uptake of xenobiotics into plants. In: Trapp, S. and J.C. McFarlane, eds. Plant Contamination: Modeling and Simulation of Organic Chemical Processes. Boca Raton, FL: Lewis Publishers; pp. 107-151.

Trapp, S., and M. Matthies. 1995. Generic one-compartment model for uptake of organic chemicals by foliar vegetation. Environmental Science and Technology. 29:2333-2338.

Trudel, M., and J.B. Rasmussen. 1997. Modeling the elimination of mercury by fish. Environmental Science and Technology. 31:1716-1722.

Tsivoglou, E.E., and J.R. Wallace. 1972. Characterization of Stream Reaeration Capacity. EPA-R3-72-012. Washington, DC: U.S. Environmental Protection Agency.

Turner, R. 1998. Personal communication. Frontier Geosciences. August.

U.S. EPA (U.S. Environmental Protection Agency). 2002a. TRIM.FaTE Technical Support Document Volume I: Description of Module. EPA-453/R-02-011a. Research Triangle Park, NC: Office of Air Quality Planning and Standards. September.

U.S. EPA (U.S. Environmental Protection Agency). 2002b. Evaluation of TRIM.FaTE Volume I: Approach and Initial Findings. EPA-453/R-02-0012. Research Triangle Park, NC: Office of Air Quality Planning and Standards. September.

U.S. EPA (U.S. Environmental Protection Agency). 1999a. The Total Risk Integrated Methodology: TRIM.FaTE Technical Support Document. Volume I: Description of Module. External Review Draft. EPA-453/D-99-002A. Research Triangle Park, NC: Office of Air Quality Planning and Standards. November.

U.S. EPA (U.S. Environmental Protection Agency). 1999b. The Total Risk Integrated Methodology: TRIM.FaTE Technical Support Document. Volume II: Description of Chemical Transport and Transformation Algorithms. External Review Draft. EPA-453/D-99-002B. Research Triangle Park, NC: Office of Air Quality Planning and Standards. November.

U.S. EPA (U.S. Environmental Protection Agency). 1999c. Bioaccumulation and Aquatic System Simulator (BASS) User's Manual Beta Test Version 2.0. Internal Draft as supplied by Craig Barber. Research Triangle Park, NC: Office of Research and Development.

U.S. EPA (U.S. Environmental Protection Agency). 1998a. The Total Risk Integrated Methodology: Technical support document for the TRIM.FaTE module. Draft. EPA-452/D-98-001. Office of Air Quality Planning and Standards.

U.S. EPA (U.S. Environmental Protection Agency). 1998b. AQUATOX for Windows: A Modular Toxic Effects Model for Aquatic Ecosystems. Internal Draft. Washington, D.C.: Office of Pollution Prevention and Toxics.

U.S. EPA (U.S. Environmental Protection Agency). 1997. Mercury Study Report to Congress. Volume III: Fate and Transport of Mercury in the Environment. EPA-452/R-97-005. Research Triangle Park, NC, and Washington, D.C.: Office of Air Quality Planning and Standards and Office of Research and Development.

U.S. EPA (U.S. Environmental Protection Agency). 1993 Wildlife Exposure Factors Handbook, Volume I. EPA/600/R-93/187a. Washington, D.C.: Office of Water and Office of Research and Development. December.

U.S. EPA (U.S. Environmental Protection Agency). 1992. Draft Report: A Cross-Species Scaling Factor for Carcinogen Risk Assessment Based on Equivalence of mg/kg3/4/day; Notice. Federal Register. June 5. 57(109): 24152-24173.

van der Leeden, F., F.L. Troise, and D.K. Todd. 1991. The Water Encyclopedia. Chelsea, MI: Lewis Publishers.

van de Water, R.B. 1995. Modeling the transport and fate of volatile and semi-volatile organics in a multimedia environment. Ph.D. Dissertation. Chemical Engineering, University of California, Los Angeles.

Wallach, R., W.A. Jury, and W.F. Spencer. 1989. The concept of convective mass transfer for prediction of surface-runoff pollution by soil surface applied chemicals. Transactions of the American Society of Agricultural Engineers. May-June. 1989.

Wania, F., J. Axelman, and D. Broman. 1998. A review of processes involved in the exchange of persistent organic pollutants across the air-sea interface. Environmental Pollution. 102:3-23.

Whicker, F.W., and T.B. Kirchner. 1987. Pathway: A dynamic food-chain model to predict radionuclide ingestion after fallout deposition. Health Physics. 52:717-737.

Whitby, K.T. 1978. The physical characteristics of sulfur aerosols. Atmospheric Environment. 12:135-159.

Whitman, R.G. 1923. A preliminary experimental confirmation of the two-film theory of gas adsorption. Chemical and Metallurgical Engineering. 29:146-148.

Wilmer, C., and M. Fricker. 1996. Stomata. Second ed. New York, NY: Chapman and Hall. p. 121.

Wilson, R., and J.D. Spengler, eds. 1996. Particles in Our Air: Concentrations and Health Effects. Cambridge, MA: Harvard School of Public Health.

[This page intentionally left blank.]

APPENDIX A

DERIVATION OF MERCURY-SPECIFIC ALGORITHMS

[This page intentionally left blank.]

APPENDIX A
DERIVATION OF MERCURY-SPECIFIC ALGORITHMS

This appendix contains derivations of mercury-specific transfer algorithms (Section A.1) and transformation algorithms (Section A.2).

A.1 MERCURY-SPECIFIC TRANSFER ALGORITHMS

The algorithms/equations included in the current TRIM.FaTE library that are specific to mercury are described below. These include:

- dry deposition of divalent mercury vapors to surface water, plants, and soil (Section A.1.1);
- exchange of mercury between algae and surface water (Section A.1.2);
- mercury excretion by fish (Section A.1.3);
- time-to-equilibrium-based mercury accumulation by fish (Section A.1.4); and
- resistance of the plant leaf mesophyll to diffusion of elemental mercury (Section A.1.5).

A.1.1 DRY VAPOR DEPOSITION OF DIVALENT MERCURY

Some of the algorithms used to transfer mercury from air to surface water, surface soils, and plants (and the algorithms used for transfers in the opposite direction) depend on the mercury species. The algorithms for diffusion between air and surface water, surface soils, and plant leaves apply only to Hg(0) and CH_3Hg, but not Hg(2). The net diffusion of Hg(2) vapors from air to surface water, surface soils, and plant leaves is described in a single algorithm called dry vapor deposition to distinguish it from the other diffusion algorithms noted above. The dry-vapor algorithm uses an empirical value for net Hg(2) vapor deposition velocity to account for diffusive processes, as described below. Thus, the net dry transfer factors for diffusion of Hg(2) vapors in air to the compartments listed above and are expressed as:

$$T_{Air \rightarrow SW}^{DVdep} = \frac{v_{vapor}^{dry\_dep} \times A_{ASW}}{V_{Air}} \times f_{MV} \qquad \text{(TF A-1)}$$

$$T_{Air \rightarrow Ss}^{DVdep} = \frac{v_{vapor}^{dry\_dep} \times I_{dry} \times A_{ASs}}{V_{Air}} \times f_{MV} \qquad \text{(TF A-2)}$$

$$T_{Air \rightarrow Leaf}^{DVdep} = \frac{v_{vapor}^{dry\_dep} \times (1 - I_{dry}) \times A_{ASs}}{V_{Air}} \times f_{MV} \qquad \text{(TF A-3)}$$

where:

$T_{Air \rightarrow SW}^{DVdep}$ = transfer factor for dry deposition of Hg(2) vapor from air to surface water (/day);
$T_{Air \rightarrow Ss}^{DVdep}$ = transfer factor for dry deposition of Hg(2) vapor from air to surface soil (/day);
$T_{Air \rightarrow Leaf}^{DVdep}$ = transfer factor for dry deposition of Hg(2) vapor from air to plant leaf (/day);
$v_{vapor}^{dry\_dep}$ = dry vapor deposition velocity for Hg(2) based on empirical studies of net diffusion/dry vapor deposition rates (m/day);
A_{ASW} = area of air/surface water interface (m^2);
A_{ASs} = area of air/surface soil interface (m^2);
V_{Air} = volume of air compartment (m^3[air]);
I_{dry} = fraction of dry-depositing chemical that is intercepted and initially retained by the plant canopy (unitless, see Section 7.2.1.1); and
f_{MV} = mass fraction of the chemical that is in the vapor phase divided by the volume fraction of the air compartment that is vapor/gas phase (close to 1.0 of the volume) (unitless).

A.1.2 ALGAE

The uptake of pollutants by algae is generally assumed to occur by passive diffusion. The algorithm for chemical uptake by algae in TRIM.FaTE has only been derived for mercury at this time. Because algae is treated as a phase of the surface water, instead of as a separate compartment, we do not derive a T-factor *per se* for the exchange between algae and surface water.

Passive uptake of uncharged, lipophilic chloride complexes is the principal accumulation route of both methylmercury and inorganic mercury in phytoplankton and is determined by water chemistry, primarily pH and chloride concentration (Mason et al. 1996). Mason and others (Mason et al. 1995, 1996) developed an accumulation model for a marine diatom (*Thalassiosira weissflogii*) and modified it for use with "typical" freshwater algae for the purposes of predicting mercury accumulations in fish. The model assumes that uptake via passive diffusion is determined by the overall octanol/water partition coefficient, K_{ow} (*i.e.*, the D_{ow}) for the neutral mercury complexes present in solution. The D_{ow} is given as the sum of the individual K_{ow}s for each mercury species by the following equation (Mason et al. 1996):

$$D_{ow} = \sum f_i \times \left(K_{ow}\right)_i \tag{Eq. A-1}$$

Where f_i = mole fraction of total mercury present as species *i*. The fractional amount of total mercury present as each neutral mercury species was estimated as a function of pH and chloride concentration. The predicted inorganic mercury (divalent) and methylmercury D_{ow}s for each of five pH levels (pH 4, pH 5, pH 6, pH 7, and pH 8) and for chloride concentrations ranging approximately from 0.01 mg/L to 10,000 mg/L were presented graphically in the report by

Mason et al. (1996). The D_{ow}s for divalent mercury and methylmercury in TRIM.FaTE were estimated based on those curves.

Uptake of inorganic mercury (divalent) and methylmercury by algae is given by the following equation (Mason et al. 1996):

$$Hg_{algae} = \frac{D_{ow} \times U \times 4\pi R^2}{\left(\frac{4}{3}\right)\pi R^3 \times \rho \times \mu} \times Hg_{water} \qquad \text{(Eq. A-2)}$$

where:

Hg_{algae} = total mercury concentration in algae (nmol[Hg]/g[algae wet wt]);
Hg_{water} = total dissolved mercury concentration in water (nM[Hg]);
D_{ow} = overall K_{ow} for neutral mercury complexes at specified pH and chloride concentrations (unitless);
U = algal surface area-specific uptake rate constant (nmol[Hg]/µm^2[algal surface]-day-nM[Hg]);
R = average radius of algae (µm);
ρ = average algal cell density (g[algae wet wt]/µm^3[algae]); and
μ = algal growth rate constant (/day).

Within TRIM.FaTE, the uptake of mercury by algae is characterized using the ratio of Hg_{algae} to Hg_{water}. To transform the previous equation to this ratio, the units of Hg_{water} should be converted from nM to nmol/g by dividing the right side of the equation by 1000 g/L. If both sides are then divided by Hg_{water}, the equation can be simplified to:

$$\frac{Hg_{algae}}{Hg_{water}} = \frac{D_{ow} \times U \times 3}{R \times \rho \times \mu \times 1000} \qquad \text{(Eq. A-3)}$$

Note that this equation uses moles. Gram weights are derived by multiplying the moles per gram or liter by the chemical-specific molecular weight. Table A-1 shows the molecular weights of mercury and methylmercury in the units appropriate for converting the above algae (nmol/g) and water (nM) concentrations.

Table A-1
Molecular Weights of Mercury and Methylmercury

Chemical	**Molecular Weight**		
	g/mol	µg/nmol	mg/nmol
Hg	200.59	2.0059×10^{-1}	2.0059×10^{-4}
CH_3Hg	215.62	2.1562×10^{-1}	2.1562×10^{-4}

The uptake process appears to be relatively fast, *i.e.*, hours rather than days (Mason et al. 1996). Also, uptake of elemental mercury by algae is assumed to be insignificant in TRIM.FaTE, based on the findings of (Mason et al. 1996) that the accumulation rates were less than 1 amol/cell-hr-nM, where amol equals 1×10^{-18} moles.

A.1.3 MERCURY EXCRETION BY FISH

The mercury excretion rate constant (k_E) (*i.e.*, transfer of absorbed mercury back to surface water) is given by the following bioenergetic model (Trudel and Rasmussen 1997):

$$\ln(k_E) = 0.066 \times T - 0.20 \times \ln(m_f) + 0.73 \times ED - 6.56 \qquad \text{(Eq. A-4)}$$

where:

k_E = total mercury excretion rate constant (/day);
T = temperature (°C);
m_f = body mass fish (**g**[fish wet wt], note units are not kg); and
ED = exposure duration; 0 = acute (<90 days), 1 = chronic (>90 days).

For the chronic exposures for which TRIM.FaTE may be most frequently applied, the mercury excretion rate constant is reduced to:

$$\ln(k_E) = 0.066 \times T - 0.20 \times \ln(m_f) - 5.83 \qquad \text{(Eq. A-5)}$$

The transfer factor for mercury from fish to the surface water is simply:

$$T^{Hg}_{fish \to SW} = k_E \qquad \text{(TF A-4)}$$

Trudel and Rasmussen (1997) based the excretion rate on the clearance of methylmercury only, because greater than 95 percent of mercury in fish is methylmercury and the elimination of methylmercury is much slower than that of inorganic mercury (*i.e.*, the overall rate is dominated by the elimination of methylmercury). Trudel and Rasmussen (1997) found the clearance of inorganic mercury by fish to be about three times faster than the clearance of methylmercury. Thus, to estimate k_E for elemental and divalent mercury, the equation to estimate k_E for methylmercury is multiplied by a factor called *HowMuchFasterHgElimination IsThanForMHg*, which is set equal to three in the current TRIM.FaTE library.

A.1.4 ACCUMULATION OF MERCURY BY FISH

Mercury concentrations in fish are ultimately determined by methylmercury accumulation at the base of the food chain (Mason et al. 1995, 1996). Therefore, one algorithm for the uptake of mercury in fish based on the general equation for the time-to-equilibrium food-chain model is presented in Section 6.4.2. Intertrophic level concentration ratios ($K_{receptor\text{-}diet}$) were obtained from studies of natural populations of fish, zooplankton, and phytoplankton. Based on studies using methylmercury/nitrogen ratios in whole fish, the concentration ratio between two adjacent trophic levels was found generally to be around 3 to 4 (studies cited in Lindqvist et al. (1991)). As noted in Section 6.4.2, mercury transfers from algae to water-column herbivores in TRIM.FaTE implicitly include the intermediate transfer from algae to zooplankton. Concentration ratios between planktivorous fish and phytoplankton were between 9 and 16 (Lindqvist et al. 1991, Watras and Bloom 1992). That is, zooplankton were an intermediate trophic level and the transfers between each trophic level were approximately equal. Taking the geometric mean results in approximate concentration ratios for methylmercury of 3.5 for one trophic-level transfer and 12 for two trophic-level transfers (Mason et al. 1996).

Inorganic mercury (divalent) transfer factors between phytoplankton and zooplankton and between zooplankton and planktivorous fish are given by Watras and Bloom (1992). In the absence of similar factors for fish-to-fish transfers of inorganic mercury, the zooplankton-to-planktivorous-fish transfer factor was used to estimate the concentrations in the water-column omnivore, water-column carnivore, benthic omnivore, and benthic carnivore compartment types. In other words, in the current TRIM.FaTE library, the mercury partition coefficient between adjacent trophic levels in the time-to-equilibrium model for bioaccumulation by fish is set as follows:

$$K_{fish\text{-}diet} \quad = \quad 3.5.$$

A.1.5 PLANT MESOPHYLL RESISTANCE

A general plant algorithm for mesophyll resistance was added to TRIM.FaTE to accommodate the behavior of mercury in plants. For most organic chemicals and most plant species, the stomatal or cuticular conductance is the rate-limiting pathway (Riederer 1995). Therefore, for many chemicals, there is no need to consider mesophyll (inner tissue) conductance. However, some work with mercury cited in Lindberg et al. (1992) suggests that "resistance on or within mesophyll surfaces dominates the atmosphere-leaf diffusive path of Hg(0)."

For herbaceous species, Lindberg et al. (1992) indicate that this mesophyll resistance for elemental mercury is a factor of 2.5 × stomatal resistance and that mesophyll conductance is a factor of 1/2.5 or 0.4 × stomatal conductance. TRIM.FaTE therefore uses the following equation for elemental mercury (only):

$$g_m = g_{stomata} \times 0.4 \qquad \text{(Eq. A-6)}$$

where:

g_m = conductance of chemical through mesophyll (m/day); and
$g_{stomata}$ = conductance of chemical through stomata (m/day).

Note that the high mesophyll resistance of elemental Hg might be due to its assimilation in mesophyll tissue (Lindberg et al. 1992). It has previously been assumed that the mesophyll resistance for divalent mercury is 0.0 (U.S. EPA 1997a); *i.e.*, that g_m is infinite.

A.2 MERCURY TRANSFORMATION ALGORITHMS

Since there are three species of mercury, there are six possible transformation routes from one species to another. All but one of these routes will be considered:

• Reduction	Hg(2)→ Hg(0);
• Oxidation	Hg(0) → Hg(2);
• Methylation	Hg(2)→ CH_3Hg;
• Demethylation	CH_3Hg → Hg(2); and
• Mer cleavage demethylation	CH_3Hg → Hg(0).

The route not considered is methylation of Hg(0), for which little information has been reported.

In the case of mercury, the transformation from one chemical species to another is modeled using a first-order rate constant. In particular, the following general equations may be used to model transformation:

$$\textit{Reduction}, Hg^{2+} \rightarrow Hg^{0}: \quad \frac{dM_1}{dt} = k_R \times M_2(t) \qquad \text{(Eq. A-7)}$$

$$\textit{Oxidation}, Hg^{0} \rightarrow Hg^{2+}: \quad \frac{dM_2}{dt} = k_O \times M_1(t) \qquad \text{(Eq. A-8)}$$

$$\textit{Methylation}, Hg^{2+} \rightarrow CH_3Hg: \quad \frac{dM_3}{dt} = k_M \times M_2(t) \qquad \text{(Eq. A-9)}$$

$$\textit{Demethylation}, CH_3Hg \rightarrow Hg^{2+}: \quad \frac{dM_2}{dt} = k_{Dm} \times M_3(t) \qquad \text{(Eq. A-10)}$$

$$\textit{Mer cleavage demethylation}, CH_3Hg \rightarrow Hg^{0}: \quad \frac{dM_1}{dt} = k_{MC} \times M_3(t) \qquad \text{(Eq. A-11)}$$

where:

M_1 = mass of elemental mercury in a compartment type (g[Hg(0)]);
M_2 = mass of divalent mercury in a compartment type (g[Hg(2)]);
M_3 = mass of methylmercury in a compartment type (g[CH_3Hg]);
k_R = reduction rate in compartment type (/day);
k_O = oxidation rate in compartment type (/day);
k_M = methylation rate in compartment type (/day);
k_{Dm} = demethylation rate in compartment type (/day); and
k_{MC} = mer cleavage demethylation rate in compartment type (/day).

The transformation rates may be input directly or calculated based on other parameters. If both algorithms and input values are available, then the user will be able to choose which method to use. The corresponding transfer factors for Equations A-7 through A-10, respectively, are listed below:

$$T^{reduction}_{Hg(2)\rightarrow Hg(0)} = k_R \qquad \text{(TF A-5)}$$

$$T^{oxidation}_{Hg(0)\rightarrow Hg(2)} = k_O \qquad \text{(TF A-6)}$$

$$\begin{aligned} T^{methylation}_{Hg(2)\rightarrow CH_3Hg} &= k_M \\ T^{demethylation}_{CH_3Hg\rightarrow Hg(2)} &= k_{Dm} \end{aligned} \qquad \text{(TF A-7)}$$

A.2.1 ABIOTIC MERCURY TRANSFORMATION RATE CONSTANTS

The information in Tables A-2 through A-13 is taken primarily from the 1997 Mercury Report to Congress (U.S. EPA 1997a) and model documentation for EPRI's R-MCM Mercury Cycling Model (Hudson et al. 1994).

Table A-2
Issues Related to Reduction of Hg(2) to Hg(0) in Soil, Surface Water, and Sediment

Soil	Surface Water	Sediment
Decreases in decreasing sunlight	Decreases with decreasing sunlight and temperatures	Sparse literature on subject
Abiotic reduction (transfer of electrons from humic acid to Hg(2)) is dependent on pH	Has been observed to increase with decreasing dissolved organic carbon (DOC) conditions (Amyot et al. 1997), and vice versa, due to reduced light penetration and increased complexation of Hg(2)	
Strong stability complex between Hg(2) and humic acid		

Table A-3
Reduction (k_R) in Surface Water: Inputs

Input Values (1/day)	Comment	Reference(s)
5E-1to 3.5	Experimental value using simulated sunlight, after normalizing to sunlight in Stockholm, Sweden	U.S. EPA (1997a), Xiao et al. (1995)
5E-3 to 1E-1	Based on mass balances in Wisconsin seepage lakes	U.S. EPA (1997a), Mason et al. (1994)
2E-2 to 4E-2	Epilimnion	Mason et al. (1995)
1E-2	9 m depth	Mason et al. (1995)
<5E-3	17 m depth	Mason et al. (1995)
1.4E-1	high Arctic lake during 24 hour sunlight period	Amyot et al. (1997)
2E-1 to 4E-1	high Arctic lake, low DOC conditions	Amyot et al. (1997)
2E-2 to 1.4E-1	high Arctic lake, high DOC conditions	Amyot et al. (1997)
1E-1	July-August, upper 3 m	Vandal et al. (1995)
5E-2	July August, upper 6 m	Vandal et al. (1995)
7.5E-3	Value in current TRIM.FaTE library	U.S. EPA (1997a)

Table A-4
Reduction (k_R) in Sediment: Inputs

Input Values (1/day)	Comment	Reference(s)
1E-6	Inferred value calculated based on presence of Hg(0) in sediment porewater	U.S. EPA (1997a), Vandal et al. (1995)
0.216	Derived from humic acid from farm pool sediment. pH did not appear to affect the rate of reaction, but does seem to influence the amount of mercury reduced	Alberts et al. (1974)
1E-6	Value in current TRIM.FaTE library	U.S. EPA (1997a), Vandal et al. (1995)

Table A-5
Reduction (k_R) in Soil: Inputs

Equations to Calculate Input Values	Comment	Reference(s)
$k_R^{soil} = k_{norm} \times \theta \times d_{Ss} \times d_S$ where k_{norm} = reduction rate constant normalized by soil water content in the surficial 5 mm of soil (L[soil]/L[water]-day); values range from 1E-4 for forest site to 1.3E-3 for field site; θ = soil water content (L[water]/L[soil]); d_{Ss} = depth of soil surface layer to which reduction rate is normalized, 5E-3 (m); and d_S = soil layer depth (m).	Formula is derived from evasion flux measurements	U.S. EPA (1997a), Carpi and Lindberg (1997)

Table A-6
Issues Related to Methylation in Soil, Surface Water, and Sediment

Soil	Surface Water	Sediment
Anaerobic conditions favor higher methylation rates[a]	Anaerobic conditions favor higher methylation rates[a]	Anaerobic conditions favor higher methylation rates[a]
Biotic methylation may occur due to bacteria; abiotic methylation may occur by transmethylation from other organometals or by humic substances[b]	Photodegradation at surface can lower the gross methylation rate[c]	Highest rates may occur at the sediment surface (sulfate-reducing bacteria may be important mediators of the reaction), Gilmour and Henry (1991)
Increases with increasing organic carbon content and BHT[f]	Positively correlated with DOC[d] (dissolved organic carbon)	Positively correlated with TOC (total organic carbon)[d]
Generally occurs for Hg(2) dissolved in soil pore water	Generally occurs for Hg(2) dissolved in water column[d]	Generally occurs for Hg(2) dissolved in sediment pore water[d]
Abiotic methylation is proportional to temperature and Hg(2) concentration. Also, it is inversely proportional to pH (at pH > 5)[g]	Positively correlated with temperature[d]	Positively correlated with temperature[d]
	Potentially positively correlated with sulfate concentration in water column[e]	Potentially positively correlated with sulfate concentration in sediment pore water[e]

a This is generally due to increased bacterial reactions in anaerobic conditions.
b: U.S. EPA (1997a), Gilmour and Henry (1991).
c: Initial reference is Bob Ambrose's discussion of methylation in water column in U.S. EPA (1997a).
d: Hudson et al. (1994).
e: Watras et al. (1995).
f: Nagase et al. (1984); BHT = 2,6, di-tert-butyl-methyl phenol.
g: Bodek et al. (1988).

Table A-7
Methylation (k_M) in Surface Water: Inputs

Input Values (1/day)	Comment	Reference(s)
1E-4 to 3E-3	reported as maximum potential methylation rate	Gilmour and Henry (1991)
6E-4 to 6E-3	Depth of 3 - 9m	U.S. EPA (1997a), based on Henry et al. (1995a, 1995b) and Jacobs et al. (1995)
5E-4 to 1E-3	Oxic portion of four forest lakes in Finland	Matilainen (1995)
1E-2 to 3E-2	At seasonally-anoxic depth of 15 m	U.S. EPA (1997a), based on Henry et al. (1995a, 1995b) and Jacobs et al., (1995)
4E-3 to 1E-2	Anaerobic layers of hypolimnion	Matilainen (1995)
1E-2 to 4E-2	0.5 - 1.0 m layer of bacterioplankton near the top of the anoxic hypolimnion	Watras et al. (1995)
1E-3	Value in current TRIM.FaTE library	U.S. EPA (1997a)

Table A-7
Methylation (k_M) in Surface Water: Inputs (cont.)

Equations to Calculate Input Values	Comment	Reference
$k_M^{SW} = \frac{k_{MW} \times Q_{10m}^{(T-Tb)\times 0.1} \times C_{DOC} \times f_{ma}^{Hg(2)} \times f_{dissolved}^{Hg(2)} \times C_{Su}}{C_{Su} + K_{Su}}$ where: k_{MW} = methylation rate constant in the water column, based on DOC (L/mg[DOC]-day); Q_{10m} = term to adjust methylation rate for temperature (implied value in R-MCM documentation is 2, so that methylation rate doubles for every 10 degree increase in temperature above the base temperature); T = water column temperature (degrees Celsius); Tb = base temperature at which methylation rate constant k_{MW} applies (degrees Celsius); C_{DOC} = DOC concentration in water column (mg[DOC]/L); f_{ma} = fraction of the dissolved Hg(2) in the water column available for methylation (unitless); $f_{dissolved}$ = fraction of the Hg(2) in the water column that is dissolved (unitless); C_{Su} = concentration of sulfate in the water column (μeq[sulfate]/L[water]); and K_{Su} = half-saturation constant for the effect of sulfate on methylation (μeq[sulfate]/L[water[).		Hudson et al. (1994)].

Table A-8
Methylation (k_M) in Sediment: Inputs

Input Values (1/day)	Comment	Reference(s)
1E-5 to 1E-3	Reported as maximum potential methylation rate	Gilmour and Henry (1991)
8E-4 to 2.5E-2	Above intact sediment cores	Stordal and Gill (1995)
8E-5 to 2E-5	Upper 4 cm of Little Rock Lake sediments	Calculated in U.S. EPA (1997a) from methylation rates in units of ug/m^2/day (Gilmour and Riedel 1995) and assumed dry density of 1.2 g/cm^3
1E-4	Value in current TRIM.FaTE library	U.S. EPA (1997a)
Equations To Calculate Input Values	**Comment**	**Reference(s)**
$k_M^{Sed} = k_{MS} \times Q_{10m}^{(T-Tb)\times 0.1} \times C_{TOC} \times f_{ma}^{Hg(2)} \times f_{dissolved}^{Hg(2)} \times ((\theta_i - \theta_b) \times 0.5) \times C_{SPWSu} \div \left(C_{SPWSu} + K_{Su}\right)$ where: k_{MS} = methylation rate constant in the sediment, based on TOC (m^3/g[TOC]-day); Q_{10m} = term to adjust methylation rate for temperature (implied value in R-MCM documentation is 2, so that methylation rate doubles for every 10 degree increase in temperature above the base temperature); T = sediment temperature (degrees Celsius); Tb = base temperature at which methylation rate constant K_{MS} applies (degrees Celsius); C_{TOC} = TOC concentration in water column (g[organic carbon]/m^3); f_{ma} = fraction of the dissolved Hg(2) in the sediment pore water available for methylation (unitless); $f_{dissolved}$ = fraction of the Hg(2) in the sediment that is dissolved (unitless); θ_i = volume fraction water of the sediment at the sediment/water interface (unitless); θ_b = volume fraction water of the bottom of the sediment (unitless); C_{SPWSu} = concentration of sulfate in the sediment pore water (μeq/L); and K_{Su} = half-saturation constant for the effect of sulfate on methylation (μeq/L).		Hudson et al. (1994), p.5-22

Table A-9
Methylation (k_M) in Soil: Inputs

Input Values (1/day)	Comment	Reference(s)
2E-4	minimum value for average maximum potential methylation rate constant under aerobic conditions for 120-day experiment	Porvari and Verta (1995)
1E-3	maximum value for average maximum potential methylation rate constant under anaerobic conditions for 120-day experiment	Porvari and Verta (1995)
7E-5 to 9.7E-4	Range for median aerobic reaction rate (from peat, humus layer, and soil samples, respectively)	Verta et al (1994)
9.2 E-3	Anaerobic median rate of four inundated soil samples (range = 4.2E-3 to 1.2E-2/day)	Verta et al. (1994)
1E-3	Value in current TRIM.FaTE library	Porvari and Verta (1995)

Table A-10
Issues Related to Demethylation in Soil, Surface Water, and Sediment

Soil	Surface Water	Sediment
May increase with increasing anaerobic conditions	Negatively correlated with light	May depend on bacteria processes
		Has been reported as maximal at the sediment/water interface (Gilmour et al. 1992)

Table A-11
Demethylation (k_{Dm}) in Surface Water: Inputs

Input Values (1/day)	Comment	Reference(s)
1E-3 to 2.5E-2 Value in current TRIM.FaTE library = 0.013	Maximum potential demethylation rate constants	Gilmour and Henry (1991)
Equations Used to Calculate Input Values	**Comment**	**Reference(s)**
$k_{Dm}^{SW} = (k_{ds} / L_{ext}) \times \left(1 - e^{-L_{ext} \times d_{SW}}\right) / d_{SW}$ where: k_{ds} = demethylation rate constant at the lake surface (/day) L_{ext} = light extinction coefficient for use in demethylation calculations (/m) d_{SW} = mean depth of water column (m)		Hudson et al. (1994)

Table A-12
Demethylation (k_{Dm}) in Sediment: Inputs

Input Values (1/day)	Comment	Reference(s)
2E-4 to 1E-1 Value in current TRIM.FaTE library = 0.0501	Reported maximum potential demethylation rate constants	Gilmour and Henry (1991)
Equations to Calculate Input Values	**Comment**	**Reference(s)**
$k_{Dm}^{Sed} = k_{DmS} \times C_{TOC} \times f_{dissolved}^{MHg} \times \left((\theta_i + \theta_b) \times 0.5\right)$ where k_{DmS} = demethylation rate in the sediment, based on TOC (m^2/g[TOC]-day) C_{TOC} = TOC concentration in sediment (g[organic carbon]/m^2) $f^{MHg}_{dissolved}$ = fraction of the methylmercury in the sediment that is dissolved (unitless) θ_i = porosity of the sediment at the sediment/water interface (unitless) θ_b = porosity of the bottom of the sediment (unitless)		Hudson et al. (1994)

Table A-13
Demethylation (k_{Dm}) in Soil: Inputs

Input Values (1/day)	Comment	Reference(s)
3E-2	Average of maximum potential demethylation rate constants in aerobic conditions	Porvari and Verta (1995)
6E-2	Average of maximum potential demethylation rate constants in anaerobic conditions	Porvari and Verta (1995)
3.6E-2, 7.6E-2, 1.1E-1	Median aerobic rates for 15 inundated soil samples, 15 humus layer samples, and five peat samples, respectively.	Verta et al. (1994)
8.9E-2	Median anaerobic rate for 15 inundated soil samples.	Verta et al. (1994)
6E-2	Value in current TRIM.FaTE library	Porvari and Verta (1995)

A.2.2 BIOTIC MERCURY TRANSFORMATION RATE CONSTANTS

A.2.2.1 Plants

Fortmann et al. (1978) observed that some plants can change the mercury species accumulated from the environment. However, few studies are available from which to determine transformation rates.

Hg(0) → Hg(2)

The oxidation of elemental mercury to divalent mercury (transformation listed above) occurs in leaves; elemental mercury is probably not taken up by the root. This oxidation rate is apparently very rapid and may be assumed to be instantaneous (U.S. EPA 1997a). No instances have been found where elemental mercury was measured in plants (*e.g.*, Cappon 1987). Thus, elemental mercury in air or on the surface of the leaf can be directly transferred to divalent mercury in the leaf.

Hg(2) → CH_3Hg

It is assumed that the methlyation of Hg(2) to methylmercury (CH_3Hg) does not occur in plants. Although the *in vivo* transformation of inorganic mercury to methylmercury was observed in *Pisum sativum* (peas) in one study (Gay 1975), the chemical was ephemeral and quickly (several hours) decayed to low parts per billion levels. Methylmercury residues were not detected in mature crops following the addition of mercuric chloride to soil (Bache et al. 1973). Indeed, most mercury in plants is usually in inorganic form (Lindberg 1998).

CH_3Hg → Hg(2)

It is assumed that demethylation of methylmercury to Hg(2) (above) occurs in leaves and stems, but not in roots (because transformations interfere with the equilibrium assumption in roots). We assume that methylmercury is transformed to Hg(2) according to first-order kinetics, where the first-order rate constant is 0.03 /day, based on the following information.

Only one study is available in which methylmercury was added to soil and the forms of mercury (methyl and total) were measured after a defined period of exposure (Bache et al. 1973). In the few other studies of speciation of mercury within plants, either it is not known which species were present in soil (*e.g.*, Heller and Weber 1998), or multiple Hg species were present in soil and it is not known which were initially taken up by the plant (Cappon 1987).

Using data from Bache et al. (1973) (see Table A-14 below), we assume that the methylmercury is readily taken up through the roots or foliage, that equilibrium between soil and plant is achieved quickly, that methylmercury is not appreciably transformed in soil during a crop season, that all methylmercury is only transformed to ionic mercury, and that crops were harvested after 40 days. Under these assumptions, 1^{st}-order rate constants for the transformation of methylmercury to Hg(2) vary by almost two orders of magnitude in a single study. No mechanistic explanation is available for

Table A-14
Concentrations of Methylmercury in Foliage and Stems of Crops from Bache et al. (1973) and Associated First-order Rate Constants, Using Assumptions in Text

Plant Species	Soil	Application to Soil (mg/kg)	Total Mercury in Foliage and Stem	Methylmercury in Foliage and Stem	1st Order Rate Constant (d^{-1})
Bush bean (*Phaseolus vulgaris*)	gravelly loam	1	52	46	0.003
Bush bean (*Phaseolus vulgaris*)	gravelly loam	10	90	28	0.03
Carrot (*Daucus carota*)	gravelly loam	10	214	1	0.1
Potato (*solanum tuberosum*)	silt loam	1	86	27	0.03
Potato (*solanum tuberosum*)	silt loam	10	58	17	0.03
Tomato (*Lycopersicon esculantum*)	gravelly loam	10	341	3	0.1

this high degree of variability. The default value of 0.03 /day in the TRIM.FaTE library for demethylation of methylmercury to Hg(2) in plants is one of the mid values in the range.

A.2.2.2 Soil Detritivores

No information is available for transformations of mercury in soil detritivores. In addition, transformation algorithms cannot be implemented if the mercury in these organisms is in equilibrium with mercury in root-zone soil.

A.2.2.3 Terrestrial and Semi-aquatic Wildlife

Little quantitative information is available on the transformation of mercury in mammals and birds. Where information is available, calculations of rate constants assume first-order transformations and are calculated on the basis of the total mercury ingested by the organism but not necessarily absorbed. (The exception is the inhalation pathway, where rate constants are derived based on the absorbed fraction.)

Hg(0) → Hg(2)

No information is available from which to derive transformation rate constants for the oxidation of elemental mercury to the mercuric ion. Based on the following information, we assume that the rate is rapid, and 1.0 /day is a rough estimate of the first-order rate constant. Elemental mercury is readily oxidized to the inorganic divalent species in most tissues via the hydrogen peroxidase-catalase pathway. This oxidation primarily occurs in the red blood cells, and hydrogen peroxide is probably the rate-limiting reactant (ATSDR 1997, U.S. EPA 1997b).

Hg(2) → Hg(0)

Mercuric salts primarily remain in their divalent form. However, a small fraction of the inorganic divalent cation can be reduced to elemental mercury and exhaled as a vapor (ATSDR 1997). Given the lack of information on the rate of this transformation, the transformation is assumed not to occur.

Organic mercury → Hg(2)

Forms of organic mercury are the most studied species of mercury. The short-chain alkyl mercury compounds (*e.g.* methylmercury) are relatively stable and are more slowly metabolized to the inorganic form than the longer-chain compounds (U.S. EPA 1997b) The longer-chain compounds may be more readily metabolized to the mercuric ion (U.S. EPA 1997b). Takeda and Ukita (1970) dosed Donryu rats with 20 µg Hg/kg body weight as ethyl-mercuric chloride via intravenous injection. After 8 days, 58.1 percent of the mercury excreted in the urine was inorganic mercury and 35 percent of the mercury excreted in feces was inorganic (Table A-15). If it is assumed that (1) the excreted chemicals reflect the transformation rate in the animal (transformation occurred immediately prior to excretion) and (2) the first-order transformation rate reflects a weighted average of the amount of dose excreted in urine (10.52 percent) and that excreted in feces (6.01 percent), then the transformation rate may be estimated to be 0.09 /day.

Table A-15
Transformation Rate (/day) of Organic Mercury to the Inorganic Divalent Form in Mammals (Takeda and Ukita 1970)

Elimination Type	Dose Route	% Organic after 8 days	% Inorganic after 8 days	Transform Rate Constant
urine	injection	41.9	58.1	0.1084
feces	injection	65.0	35.0	0.0539
assumed transformation for whole animal				0.09

Hg(2) → organic mercury

No information is available on this transformation. Therefore it is assumed to be zero.

A.2.2.4 Aquatic Species

Transformations of mercury in algae, macrophytes, and benthic organisms are assumed not to occur with one exception. It is assumed that elemental is transformed to divalent mercury in macrophytes, and the transformation is described as a rapid (almost instantaneous) first-order rate constant (*i.e.*, 10^6 to 10^9). Thus, it is assumed that elemental mercury can be taken up by macrophytes but is not accumulated in macrophytes (*i.e.*, data showing Hg(0)) in macrophytes were not found). Data demonstrating methylation of divalent mercury or demethylation of methylmercury in macrophytes also were not found.

$Hg(2) \rightarrow CH_3Hg$

Very little is known about the rate at which transformation of mercury species occurs in aquatic organisms. A large body of field data suggests that most (> 90 percent) of mercury in fish is in the form of methylmercury and other organic species (represented here simply as CH_3Hg); however, methylation of inorganic mercury has not been demonstrated in fish. For this reason, it is assumed that methylation of divalent mercury does not to occur in fish.

$Hg(0) \rightarrow Hg(2)$

Oxidation of elemental mercury is assumed to occur instantaneously in fish.

$Hg(0) \rightarrow CH_3Hg$

Methylation of inorganic mercury is assumed not to occur directly in fish.

$Hg(2) \rightarrow Hg(0)$

Reduction of divalent mercury is assumed not to occur in fish.

$CH_3Hg \rightarrow Hg(2)$

Demethylation is assumed not to occur in fish.

$CH_3Hg \rightarrow Hg(0)$

Mer cleavage demethylation is assumed not to occur in fish.

A.4 REFERENCES

Alberts, J.J., J.E. Schindler, and R.W. Miller. 1974. Elemental mercury evolution mediated by humic acid. Science. 184: 895-897.

Amyot, M., G. Mierle, D. Lean, and D.J. McQueen. 1997. Effect of solar radiation on the formation of dissolved gaseous mercury in temperate lakes. Geochemica et Cosmochimica Acta. 61(5):975987.

ATSDR. 1997. Agency for Toxic Substances and Disease Registry. Toxicological Profile for Mercury. Draft for public comment (Update). ATSDR-7P-97-7 (Draft). U.S. Department of Health and Human Services.

Bache, C.A., W.J. Gutenmann, L.E. St. John, Jr., R.D. Sweet, H.H. Hatfield, and D.J. Lisk. 1973. Mercury and methylmercury content of agricultural crops grown on soils treated with various mercury compounds. J. Agr. Food Chem. 21:607-613.

Bodek, I., W.J. Lyman, W.F. Reehl, et al. 1988. Environmental Inorganic Chemistry: Properties, Processes, and Estimation Methods. Elmsford, NY: Pergammon Press.

Cappon, C.J. 1987. Uptake and speciation of mercury and selenium in vegetable crops grown on compost-treated soil. Water, Air, Soil Pollut. 34:353-361.

Carpi, A.., and S.E. Lindberg. 1997. Sunlight mediated emission of elemental mercury from soil amended with municipal sewage sludge. Environmental Science and Technology. 31(7):2085-2091.

Fortmann, L.C., D.D. Gay, and K.O. Wirtz. 1978. Ethylmercury: Formation in Plant Tissues and Relation to Methylmercury Formation. EPA600/378 037. U.S. EPA Ecological Research Series.

Gay, D.D. 1975. Biotransformation and chemical form of mercury in plants. International Conference on Heavy Metals in the Environment. Symposium Proceedings, pp. 87-95. Vol. II, Part 1. October 1975.

Gilmour, C.C. and G.S. Riedel. 1995. Measurement of Hg methylation in sediments using high specific activity 203Hg and ambient incubation. Water, Air, and Soil Pollution. 80:747-756.

Gilmour, C.C, E.A. Henry, and R. Mitchell. 1992. Sulfate stimulation of mercury methylation in freshwater sediments. Environmental Science and Technology. 26(11):2281-2287.

Gilmour, C.C. and E.A. Henry. 1991. Mercury methylation in aquatic systems affected by acid deposition. Environmental Pollution. 71:131-169.

Heller, A.A., and J.H. Weber. 1998. Seasonal study of speciation of mercury(II) and monomethylmercury in *Spartina alternaflora* from the Great Bay Estuary, NH. Science of the Total Environment. 221:181-188.

Henry, E.A., L.J. DodgeMurphy, G.N. Bigham, S.M. Klein, and C.C. Gilmour. 1995a. Total mercury and methylmercury mass balance in an alkaline, hypereutrophic urban lake (Onondaga Lake, NY). Water, Air, and Soil Pollution. 80:509-518.

Henry, E.A., L.J. DodgeMurphy, G.N. Bigham, and S.M. Klein. 1995b. Modeling the transport and fate of mercury in an urban lake (Onondaga Lake, NY). Water, Air, and Soil Pollution. 80:489-498.

Hudson, R., S.A. Gherini, C.J. Watras, and D. Porcella. 1994. Modeling the biogeochemical cycle of mercury in lakes: the Mercury Cycling Model (MCM) and its Application to the

MTL Study Lakes. In: C.J. Watras and J.W. Huckabee, eds. Mercury Pollution Integration and Synthesis. Lewis Publishers; pp. 473-523.

Jacobs, L.A., S.M. Klein, and E.A. Henry. 1995. Mercury cycling in the water column of a seasonally anoxic urban lake (Onondaga Lake, NY). Water, Air, and Soil Pollution. 80:553-562.

Lindberg, S.E. 1998. Personal communication. Oak Ridge National Laboratory. December.

Lindberg, S.E., T.P. Meyers, G.E. Taylor, Jr., R.R. Turner, and W.H. Schroeder. 1992. Atmosphere-surface exchange of mercury in a forest: Results of modeling and gradient approaches. Journal of Geophysical Research. 97:2519-2528.

Lindqvist, O., K. Johansson, M. Aastrup, A. Andersson, L. Bringmark, G. Hovsenius, L. Hakanson, A. Iverfeldt, M. Meili and B. Timm. 1991. Mercury in the swedish environment - recent research on causes, consequences and corrective methods. Water Air and Soil Pollution. 55(1-2):R11.

Mason, R.P., J.R. Reinfelder and F.M.M. Morel. 1996. Uptake, toxicity, and trophic transfer of mercury in a coastal diatom.. Environmental Science & Technology. 30(6):1835-1845.

Mason, R.P., J.R. Reinfelder and F.M.M. Morel. 1995. Bioaccumulation of mercury and methylmercury. Water Air and Soil Pollution. 80(1-4):915-921.

Mason, R.P., W.F. Fitzgerald, and F.M.M. Morel. 1994. The biogeochemical cycling of elemental mercury: Anthropogenic influences. Geochemica et Cosmochimica Acta. 58(15):3191-3198.

Matilainen, T. 1995. Involvement of bacteria in methymercury formation in anaerobic lake waters. Water, Air, and Soil Pollution. 80:757-764.

Nagase, H, Y Ose, T Sato, et al. 1984. Mercury Methylation by Compounds in Humic Material. The Science of the Total Environment. 32: 147-156.

Porvari, P. and M. Verta. 1995. Methylmercury production in flooded soils: a laboratory study. Water, Air, and Soil Pollution. 80:765-773.

Riederer, M. 1995. Partitioning and transport of organic chemicals between the atmospheric environment and leaves. In: Trapp, S. and J. C. McFarlane, eds. Plant Contamination: Modeling and Simulation of Organic Chemical Processes. Boca Raton, FL: Lewis Publishers; pp. 153-190.

Stordal, M.C. and G.A. Gill. 1985. Determination of mercury methylation rates using a 203Hg radiotracer technique. Water, Air, and Soil Pollution. 80:529-538.

Takeda, Y. and T. Ukita. 1970. Metabolism of ethylmercuric chloride-203Hg in rats. Toxicol. Applied Pharm. 17:181-188.

Trudel, M., and J.B. Rasmussen. 1997. Modeling the elimination of mercury by fish. Environmental Science and Technology. 31:1716-1722.

U.S. EPA (Environmental Protection Agency). 1997a. Mercury Study Report to Congress. Volume III: Fate and Transport of Mercury in the Environment. EPA-452/R-97-005. U.S. EPA Office of Air Quality Planning and Standards, and Office of Research and Development.

U.S. EPA (Environmental Protection Agency). 1997b. Mercury Study Report to Congress. Volume V: Health effects of mercury and mercury compounds. EPA-452/R-97-007. U.S. EPA Office of Air Quality Planning and Standards, and Office of Research and Development.

Vandal, G.M., W.F. Fitzgerald, K.R. Rolfhus, and C.H.Lamborg. 1995. Modeling the elemental mercury cycle in Pallette Lake, Wisconsin, USA. Water, Air, and Soil Pollution. 80:789-798.

Verta, M, T Matilainen, P Porvari, et al. 1994. Methylmercury sources in boreal lake ecosystem. In: C.J. Watras and J.W. Huckabee, eds. Mercury Pollution Integration and Synthesis. Lewis Publishers Inc., MI; pp.119-136.

Watras, C.J. and N.S. Bloom. 1992. Mercury and methylmercury in individual zooplankton - Implications for bioaccumulation. Limnology and Oceanography. 37(6):1313-1318.

Xiao, Z.F., D. Stromberg, and O. Lindqvist. 1995. Influence of humic substances on photolysis of divalent mercury in aqueous solution. Water, Air, and Soil Pollution. 80:789-798.

APPENDIX B

DERIVATION OF PAH-SPECIFIC ALGORITHMS

[This page intentionally left blank.]

APPENDIX B
DERIVATION OF PAH-SPECIFIC ALGORITHMS

This appendix contains includes derivations of algorithms and parts of algorithms specific to polyaromatic hydrocarbons (PAHs). Section B.1 covers exchanges of PAHs between benthic invertebrates and sediments. Section B.2 includes provides a note about bioaccumulation in fish which can metabolize PAHs. Section B.3 provides a note about dry deposition of PAHs sorbed to airborne particles to plant leaves. The references are provided in Section B.4.

B.1 EXCHANGES BETWEEN SEDIMENT AND BENTHIC INVERTEBRATES

Uptake of contaminants from water by benthic invertebrates (*e.g.*, mayfly nymphs, amphipods) is primarily based on respiratory processes. Stehly et al. (1990) found that the clearance rate of benzo-a-pyrene (B(a)P) and phenanthrene from water by the mayfly (*i.e.*, mayfly net uptake of the chemical from water) is analogous to the clearance rate (*i.e.*, net uptake rate) of oxygen during mayfly respiration. The uptake of these two PAHs can, therefore, be estimated similarly to the ratio of oxygen clearance to the volume of water passing over respiratory surfaces. With a known or assumed volume of water passing over respiratory membranes with known concentrations of B(a)P and phenanthrene, the extraction efficiency of these PAHs can be calculated. The following concentration algorithms and mass derivatives were adopted from the model of Stehly et al. (1990) for estimating PAH uptake and loss for benthic invertebrates. The equations are based on the clearance rate driven by the volume of water cleared and the bioconcentration factor (BCF). Uptake rates, as measured by a clearance constant (*CLu*), as well as the BCF for 30-, 60-, and 120-day-old mayflies for B(a)P and phenanthrene were provided by Stehly et al. (1990).

$$\frac{dC_{Mayfly}}{dt} = CL_u \times C_W - CL_u \times \frac{C_{Mayfly}}{p_C} \qquad \text{(Eq. B-1)}$$

where:

C_{Mayfly} = concentration of chemical compound in the organism expressed on a wet weight basis (ng[chemical]/g[mayfly wet wt] = mg[chemical]/kg[mayfly wet wt]);

CL_u = clearance constant (equivalent to k_u) (mL[water cleared]/g[mayfly wet wt]-hour = L[water cleared]/kg[mayfly wet wt]-(day/24);

C_W = concentration of the chemical in the interstitial water (ng[chemical]/mL[water] = mg[chemical]/L[water]); and

p_C = proportionality constant that relates the concentration of chemical in the organism to the concentration in the exposure water (equivalent to the bioconcentration factor (BCF)) (mg[chemical]/kg[mayfly wet wt] per mg[chemical]/L[water] = L[water]/kg[mayfly wet wt]).

We substitute generic benthic invertebrates (BI) for the mayflies in Stehly et al. (1990). Thus, an estimation of the PAH concentrations in benthic invertebrate populations (*i.e.*, compartments) is as follows:

$$\frac{dN_{BI}}{dt} = \left(n_{BI} \times m_{BI} \times CL_u \times \frac{N_W}{V_W} \times \frac{24}{1000} \right) - \left(CL_u \times \frac{N_{BI}}{p_C} \times 24 \right) \tag{Eq. B-2}$$

where:

N_{BI} = mass of chemical in benthic invertebrates (g[chemical]);
n_{BI} = number of benthic invertebrates (unitless);
m_{BI} = mass of individual benthic invertebrate organisms (g[BI wet wt]/individual);
N_W = mass of chemical dissolved in interstitial pore water (g[chemical]);
V_W = volume of the interstitial pore water (L[water]);
1/1000 = units conversion factor (kg/g); and
24 = units converstion factor (hr/day).

Note that:

$$V_{SedW} = V_{Sed} \times \theta \tag{Eq. B-3}$$

where:

V_{SedW} = volume of the pore water in the sediment compartment (m^3);
V_{Sed} = volume of the sediment compartment (m^3);
θ = volume fraction of the sediment compartment that is liquid (*i.e.*, water) (unitless).

Also note that:

$$Fraction\_Mass\_Dissolved = N_W \times N_{Total} \tag{Eq. B-4}$$

where:

$Fraction\_Mass\_Dissolved$ = the fraction of the chemical mass in the sediment compartment that is dissolved in the interstitial water (unitless);
N_W = chemical inventory dissolved in the interstitial water (g[chemical]); and
N_{Total} = total chemical inventory in the sediment compartment, both dissolved and associated with sediment particles (g[chemical]).

As described in Chapter 2, Equation 2-81:

$$f_{ML} = \frac{Fraction\_Mass\_Dissolved}{\theta} \qquad \text{(Eq. B-5)}$$

Note that for sediments:

$$\theta = 1 - Volume\_Fraction\_Solid \qquad \text{(Eq. B-6)}$$

where:

$Volume\_Fraction\_Solid$ = fraction of sediment compartment that consists of solid sediment particles (unitless),

because the fraction of the sediment compartment that is vapor/gas-phase is assumed to be zero. From those equations, transfer factors can be derived as:

$$T_{SedW \rightarrow BI} = n_{BI} \times m_{BI} \times \frac{CL_u}{V_{SedW}} \times \frac{1}{1000} \times 24 \times f_{ML} \qquad \text{(TF B-1)}$$

$$T_{BI \rightarrow SedW} = \frac{CL_u}{p_C} \times 24 \qquad \text{(TF B-2)}$$

where:

$T_{SedW \rightarrow BI}$= transfer factor for PAHs from sediment pore water to benthic invertebrates (/day); and

$T_{BI \rightarrow SedW}$= transfer factor for PAHs from benthic invertebrates to sediment pore water (/day).

B.2 BIOACCUMULATION BY FISH

It is possible to use the time-to-equilibrium-based model (Section 6.4.2) for estimating bioaccumulation of nonionic organic chemicals in fish. As described in Section 2.5, some algorithms that represent steady-state equilibrium relationships can be turned into time-dependent ones for use in TRIM.FaTE if an estimate of the time required for the concentration to reach some fraction of the equilibrium value is known. In this case, the concentration of a nonionic organic chemical in a fish compartment at one trophic level (e.g., water-column carnivore, F_{wcc}) can be related to the concentration of the chemical in the next lower trophic level (e.g., water-column omnivore F_{wco}) by the equilibrium relationship of the form $C_{Fwcc} = K \times C_{Fwco}$. The value of K, also known in this context as the bioacumulation factor (BAF), and the time t_α required to reach 100α percent of the equilibrium must be known or estimated (default $\alpha = 0.95$).

For PAHs, which are readily metabolized by fish, it is appropriate to use a measured wet-weight *BAF* for the PAH chemicals and a measured time to reach $100\times\alpha$ percent of the equilibrium ratio of concentrations in the transfer factor equations TF 6-9 and 6-10. *BAF* values for PAHs can be estimated from K_{OW} values only if the empirical model used (*i.e.*, regression equation) for relating *BAF* to K_{OW} values was derived for fish from a series of PAHs.

B.3 REFERENCE

Stehly, G. R., Landrum, P. F., Henry, M. G. & Klemm, C. (1990). Toxicokinetics of PAHs in Hexagenia. Environmental Toxicology and Chemistry, 9, 167-174.

APPENDIX C

STEADY-STATE MODE

[This page intentionally left blank.]

APPENDIX C
STEADY-STATE MODE

TRIM.FaTE can be run in two modes: dynamic or steady-state. This appendix describes implementation of the TRIM.FaTE steady-state mode (Section C.1) and potential user applications of that feature (Section C.2). The advantage of the steady-state mode is that the run time is very short compared with typical dynamic runs that use hourly-to-daily simulation time steps over the course of many years (*e.g.*, 30-year). The short run-time allows the user to quickly test new approaches and to conduct sensitivity or Monte Carlo analyses that would be require much greater run times if the dynamic mode were used.

C.1 STEADY-STATE SOLUTION FEATURE

The description of TRIM.FaTE in Chapters 1 through 8 apply to both dynamic and steady-state modes except where noted below. The remainder of this section describes important differences between the steady-state and dynamic modes.

Section C.1.1 describes how to develop constant values for time-varying model inputs. Section C.1.2 describes changing the air transfer factors in the dynamic mode to implement the steady-state mode. Section C.1.3 notes changes that are needed with respect to the ground-water transfer factors. Finally, Section C.1.4 describes other differences in the TRIM.FaTE code setup for the steady-state versus dynamic modes.

C.1.1 CHANGING TIME-VARYING INPUT DATA TO CONSTANTS

Generating steady-state results with the model requires representative steady-state values for the time-varying inputs in the current version of the TRIM.FaTE library. The primary time-varying inputs include:

- wind speed;
- wind direction;
- mixing height;
- rain;
- *IsDay* (0 at night; = 1 during the day);
- *AllowExchange* (0 during non-growing season; = 1 during growing season);
- litter fall (*e.g.*, deciduous forest and grasses/herbs); and
- river flow.

Many of these time-varying inputs combine and interact to influence specific transfer factors within TRIM.FaTE, and the different time-varying inputs interact/combine in different ways when used in different algorithms. For example, wind speed and direction influence the relative magnitude of the advective air transfers along the interfaces between air compartments. Other transfer factors are influenced in a discontinuous fashion, as for example the transfer factors that include the variable I_{wet}, the proportion of the wet deposition of chemical sorbed to dust particles (or in vapor phase) that is intercepted and retained on the plants. The variable I_{wet} is a function of the leaf area index (*LAI*), mixing height, rain, and *AllowExchange*. When

AllowExchange is zero, the wet interception fraction is zero. Thus, it is not appropriate to simply assign an average value for each of the time varying inputs and assume that would result in appropriate values for the calculated transfer factors. In addition to providing representative values for the time-varying inputs, a number of calculated transfer factors need to be assigned steady-state values.

The calculated steady-state variables (or distributions) that need to be considered include:

- Advective transfers across each air-to-air interface including external boundaries of the system (calculated as function of wind speed, wind direction, mixing height, and parcel coordinates) (Section C.1.1.1);
- Dry interception fraction for vegetation (calculated as function of *AllowExchange*, mixing height, and the wet biomass of the vegetation per unit area) (Section C.1.1.2);
- Wet interception fraction (calculated as function of *AllowExchange*, rain, mixing height, and *LAI*) (Section C.1.1.3);
- Diffusive transfer across air/stomata interface (calculated as function of *LAI*, *IsDay*, and mixing height) and diffusive transfer across air/cuticle interface (calculated as function of *LAI* and mixing height) (Section C.1.1.4);
- Litter fall (*e.g.*, deciduous forest and grasses/herbs) and river flow (Section C.1.1.5); and
- Plant intake rates for wildlife, which are modified by the *AllowExchange* variable (Section C.1.1.6).

Steady-state models have typically used long-term arithmetic mean (*AM*) values for the inputs, but we are not aware of any research that has evaluated whether those *AM* inputs are more appropriate than other indications of central tendency (*e.g.*, median, geometric mean, etc.) for estimating steady-state output in a spatially segmented dynamic model. Fortunately, this problem should not affect a steady-state uncertainty or sensitivity analysis because the user is generally most interested in the *relative* propagation of uncertainty/variability through the model for a given set of inputs. To maintain consistency with the other TRIM.FaTE inputs, we recommend using the *AM* input values (and distributions) for the calculated time-varying inputs and for the transfer factors in the steady-state scenario. For hourly meteorological data, the *AM* value for each year of meteorological data can be calculated. The annual average values can then be used to estimate a long-term average, and an appropriate statistical model can be used to describe the set of annual average values.

C.1.1.1 Advective Air-to-air Transfers

A challenge that arises in calculating steady-state inputs for use in the advective air transfers is that the time-varying inputs from the meteorological data files per unit time are not normally distributed. As a result, the long-term average transfer factor estimated at the simulation time steps from the transfer factors may differ from that estimated from the long-term average inputs for a given mass-transfer process. We use an example to illustrate this challenge below.

In its simplest form, the advective transfer factor (/day) across an interface between two neighboring air parcels is given by:

$$T_{As\rightarrow Ar} = \frac{flux_{s\rightarrow r}}{V_s} \tag{TF C-1}$$

where $flux_{s\rightarrow r}$ is the flux of air across the interface (m^3/d) from sending compartment *s,* to receiving compartment *r*, and V_s is the volume of the sending compartment. Assuming that the long-term arithmetic mean (*AM*) transfer factor is a good surrogate for steady state, we can calculate the $AM[T_{As\rightarrow Ar}]$ in two ways. The first way calculates a value of $T_{As\rightarrow Ar}$ for each hour of meteorological data and then estimates the long-term average transfer factor from this set of hourly values:

$$AM\left[T_{As\rightarrow Ar}\right] = \frac{1}{n} \times \sum_{j=1}^{n} T_{As\rightarrow Ar} \tag{Eq. C-1}$$

where *j* represents the hour and *n* is the total number of hours (*i.e.*, $n = 8760$ for one year of meteorological data). The second way calculates the average values of $flux_{s\rightarrow r}$ and V_s from the set of hourly values for these variables, then estimates the steady state $T_{As\rightarrow Ar}$ as the quotient of the two average values such that:

$$AM\left[T_{AS\rightarrow Ar}\right] = \frac{AM\left[f_{s\rightarrow r}\right]}{AM\left[V_s\right]} \tag{Eq. C-2}$$

However, if the hourly values for flow and/or volume are not normally distributed (which they are not) then the two approaches give different answers:

$$\frac{1}{n} \times \sum_{j=1}^{n} T_{As\rightarrow Ar} \neq \frac{AM\left[f_{s\rightarrow r}\right]}{AM\left[V_s\right]} \tag{Eq. C-3}$$

In other words, the arithmetic mean (*AM*) of the set of hourly transfer factors does not equal the quotient of the $AM\ [flux_{s\rightarrow r}]$ and the $AM\ [V_s]$.

To illustrate the difference, we use the first year's hourly meteorological data prepared for the mercury test case to calculate advective transfer across one of the segments of the parcel that included the source facility. The $AM[T_{As\rightarrow Ar}]$ calculated from the 8760 hourly transfer factors (excluding the zeros) was 19.9 /hr. The transfer factor calculated from the quotient of average flow and volume was 12.7 /hr, a difference of about 40 percent.

The steady-state input for transfer across an air-to-air interface is dependent on wind speed, wind direction, mixing height, and the coordinates of the interface (length and angle). In addition, the actual transfer also depends on the volume of the sending compartment, which in turn depends on the atmospheric mixing height. In the mercury test case, we actually calculated the transfer factor for each interface using both of the methods described earlier (*i.e.*, Equations C-1 and C-2).

For Eq. C-2, the value of $T_{As \to Ar}$ for the j^{th} hour of the meteorological data is given by:

$$Tj_{As \to Ar} = \frac{u}{\sqrt{(y_2 - y_1)^2 + (x_2 - x_1)^2}} \times \left[(y_2 - y_1)\sin\vartheta - (x_2 - x_1)\cos\vartheta\right] \times \frac{A_i}{V_{sj}} \qquad \text{(TF C-2)}$$

where u is the wind speed (m/day) towards the direction ϑ across the compartment boundary during the j^{th} hour, A_i is the area of the interface given by the time-varying mixing height h_j (m), and length of compartment interface, L_i (m). The volume of the sending compartment, V_{sj}, is also a function of the time-varying mixing height. The L_i is constant over time and is defined by two Cartesian coordinates ($P_1 = (x_1, y_1)$, $P_2 = (x_2, y_2)$) where the coordinates of each segment of a polygon are evaluated in clockwise order and the length is:

$$L_i = \sqrt{(y_2 - y_1)^2 + (x_2 - x_1)^2} \qquad \text{(Eq. C-4)}$$

TF C-2 can be simplified for each hourly time step to give the following transfer-factor algorithm:

$$Tj_{As \to Ar} = \frac{u}{A_i}\left[(y_2 - y_1)\sin\vartheta - (x_2 - x_1)\cos\vartheta\right] \qquad \text{(TF-C-3)}$$

Evaluating the coordinates in clockwise order around a given polygon results in a negative value for transfer out of the polygon and a positive value for transfer into the polygon (wind direction is also reported as degrees clockwise from North). In estimating steady-state transfer factors, the user is only interested in transfers out of a given polygon across a given interface. Thus, the positive values can be ignored and the absolute values of transfers out of the polygon (*i.e.*, from the sending compartment) are used. In the example for the mercury test case, we calculated values of $AM[T_{As \to Ar}]$ for each of the five years of meteorological data, which resulted in a distribution of $AM[T_{As \to Ar}]$ values for each line segment and direction.

We also calculated the transfer factor for each year by summing the annual volumetric flux across the interface and using the long-term average mixing height and constant area of the

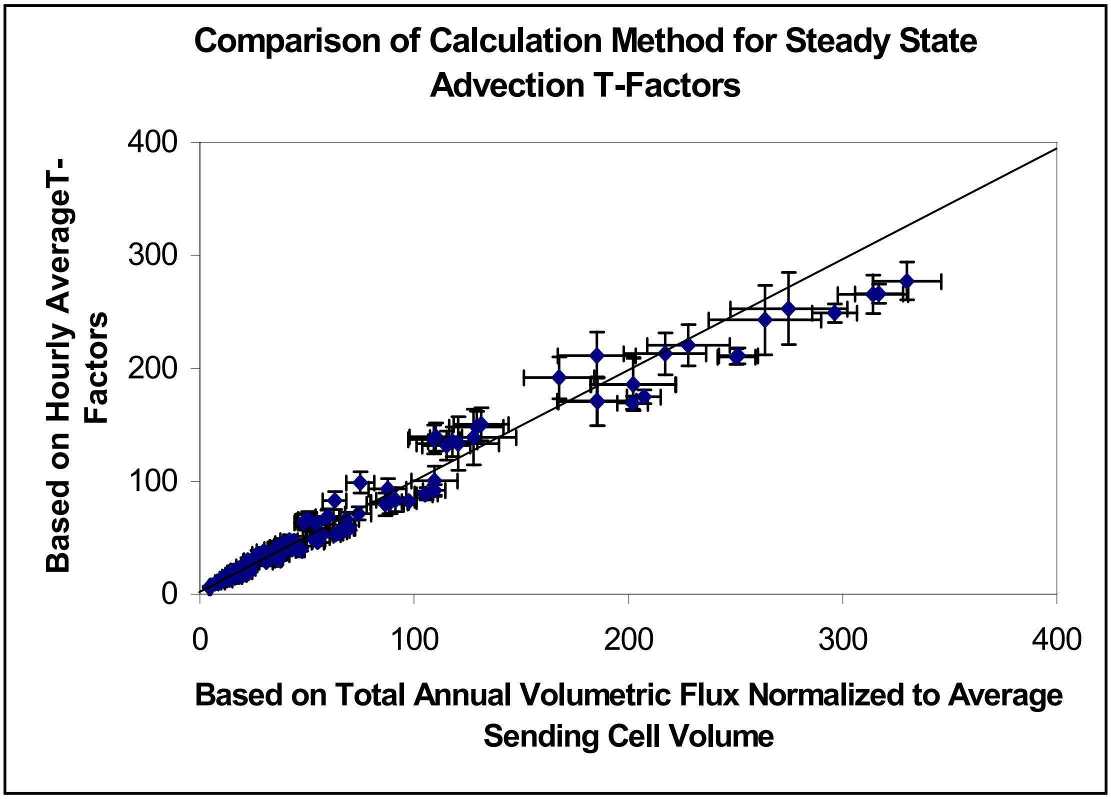


Figure C-1. Comparison of long-term average advective transfer factors calculated using the daily average volumetric flux normalized to sending compartment (cell) volume (x-axis) and the average of the hourly transfer factors (y-axis).

sending compartment to estimate the transfer factor using Eq. C-2. The difference between the two methods is illustrated in Figure C-1. The overall difference in the results of the two methods was not great. (In the mercury test case, we combined the two sets of results to provide a single estimate of the transfer factor for each interface).

It is important to remember that the steady-state value (or distribution) for a given transfer factor represents a long-term average transfer, not day-to-day or hour-to-hour variation in the transfer.

C.1.1.2 Dry Interception Fraction

For deciduous plants and grasses/herbs, the dry interception fraction is a function of *AllowExchange*, mixing height, and biomass (wet wt) of the vegetation per unit area. For coniferous plants that do not loose their leaves seasonally, the dry interception fraction is assumed to be a constant value throughout the year.

The dry interception fraction, $I_{dry,}$ is calculated for deciduous plants and grasses/herbs as receiving compartments per Eq. 7-2 of TSD Volume II, as modified to accommodate a steady-state *AllowExchange* variable:

$$I_{dry} = 1 - \exp\left[\left(1 - fW_{Leaf}\right)\left(-\alpha_{VAF} \times AllowExchange \times \rho area\right)\right] \qquad \text{(Eq. C-5)}$$

where, for both grasses/herbs and deciduous plants, fW_{Leaf} is the water content of the plant (0.8, unitless), α_{VAF} is the vegetation attenuation factor (-2.9 m2[leaf]/kg[plant dry wt]), and $\rho area$ is the areal density of above-ground non-woody vegetation (0.6 kg[plant wet wt]/m^2[surface soil]). *AllowExchange* is used as a seasonal on/off switch for the interception fraction. When *AllowExchange* is one, I_{dry} is calculated by Eq. C-5, but when *AllowExchange* is zero, I_{dry} is zero.

The volume of the sending air compartment, V_s, is also used to calculate the transfer factor for dry deposition (see TF 7-1 in TSD Volume II). Due to hourly changes in the mixing height, the long-term average V_s can differ during times when *AllowExchange* is on and when it is off, as illustrated in Figure C-2. Therefore, the steady-state value of I_{dry} needs to be normalized to a sending compartment volume that is relevant to the time when leaves are intercepting particles (*i.e.*, when *AllowExchange* = 1). The factor used to normalize the steady-state interception fraction is the long-term (annual) average mixing height divided by the average mixing height when *AllowExchange* is equal to 1. In summary, the steady-state I_{dry} value for each of the five years is given by:

$$SS.I_{dry,j} = \frac{\bar{h}(AE = 1{,}0)}{\bar{h}(AE = 1)} \times \frac{1}{n} \times \sum_{j=1}^{n} I_{dry,j} \qquad \text{(Eq. C-6)}$$

where *h (AE=1,0)* represents the average over the full year and *h (AE=1)* represents average mixing height when *AllowExchange* is set to 1.

C.1.1.3 Wet Interception Fraction

The wet interception fraction, I_{wet}, is a function of total rain for each rain event, the seasonal LAI (calculated from the average leaf area interface and the *AllowExchange* variable) and, as with the dry interception fraction, a normalization factor to the appropriate average air mixing height. Wet interception is calculated by Equation 7-4 of the TSD Volume II as modified to accommodate the *AllowExchange* variable and the cumulative rain for a given rainfall event. We define a rainfall event as the cumulative time over which rain occurs, which is bracketed (before and after) by at least one hour with no rain. Given this definition of *rain*, the wet interception fraction for rain event *k* is:

$$I_{wet,k} = \frac{AllowExchange \times LAI \times S}{rain} \times \left[1 - \exp\left(\frac{-\ln(2)}{3 \times S} \times rain\right)\right] \qquad \text{(Eq. C-7)}$$

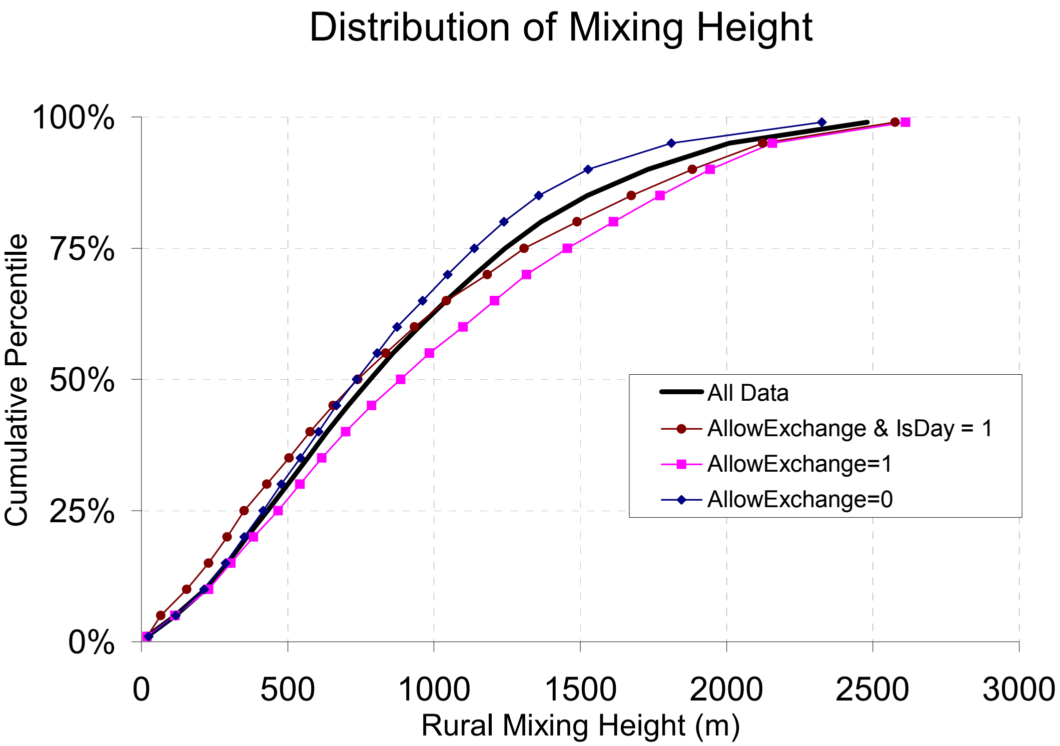


Figure C-2: Distributions of hourly mixing height reported for different conditions where *AllowExchange* controls seasonality and *IsDay* is used in the model to modify stomata diffusion.

where k indicates the k^{th} rain event, S is the leaf wetting factor (0.0003 m) and LAI is the leaf area index (grasses/herbs = 5, deciduous forest = 3.4 and coniferous forest = 5). The I_{wet} for the k^{th} event is multiplied by the cumulative amount of rain for that event to give the volume of intercepted rain. The event-specific volume of intercepted rain is summed over the year to give the total volume of "intercepted" rain. The long-term interception fraction is then estimated as the intercepted volume for the given year divided by the cumulative rain for that year.

As with I_{dry}, the final steady-state value for wet interception (for each year) is normalized to account for differences between the overall average mixing height of the sending compartment and the average mixing height when it is both raining and the *AllowExchange* variable is 1 such that:

$$SS.I_{wet} = \frac{\bar{h}(AE = 1{,}0)}{\bar{h}(AE = 1 \& rain > 0)} \times \frac{1}{n} \times \sum_{j=1}^{n} I_{wet,j} \qquad \text{(Eq. C-8)}$$

where AE=1&$rain$>0 indicates that both the *AllowExchange* variable = 1 and it is raining.

C.1.1.4 Diffusive Transfer Across Air/Stomata Interface and Across Air/Cuticle Interface

This diffusive transfer combines two process where the stomata transfer is controlled by the *LAI* (*AllowExchange*), *IsDay*, and the relative mixing height during exchange (*i.e.*, when *LAI* and *IsDay* are both 1) and where the cuticle transfer is influenced only by *LAI* (*AllowExchange*) and relative mixing height. The two parts of the equation need to be treated separately so that each mass transfer process can be independently modified by either the *AllowExchange* variable (cuticle) or the combined *AllowExchange.IsDay* variable (stomata).

The first *AllowExchange* variable, the one that modifies cuticle exchange, is the same height-normalized value that is used for I_{dry}. In this case, we derive a single steady-state value for *AllowExchange* that modifies both I_{dry} and the cuticle side of the air-to-plant diffusion equation.

The steady-state modification factor for the stomata diffusion is calculated as the long-term average of the product of *IsDay*, input as a fraction representing the average number of daylight hours per 24-hr period, and *AllowExchange*, adjusted for height of the sending compartment, using the following normalization factor:

$$NormalizationFactor = \frac{\bar{h}(AE = 1,0)}{\bar{h}(AE = 1\&\,ID = 1)} \qquad \text{(Eq. C-9)}$$

where AE=1&ID=1 indicates that both *AllowExchange* and *IsDay* are equal to one.

These two steady-state modification factors are incorporated into the equation for total diffusive transfer across the air/plant interface so that both the stomata pathway and the cuticle pathway are transformed to steady state.

C.1.1.5 Litter Fall and River Flow

In the current TRIM.FaTE library, the litter-fall rate constant, k_L, for deciduous forests and for grasses/herbs is set such that 99 percent of the mass is transferred to soil in approximately one month.[1] To run TRIM.FaTE in the steady-state mode, this litter-fall rate is transformed such that 99 percent of the mass is transferred to soil on an annual basis (365 days):

$$0.01 = \exp(-k_L \times 365) \qquad \text{(Eq. C-10)}$$

Solving Equation C-10 for k_L gives a steady-state litter-fall rate constant of 0.013 /day. The litter-fall rate for coniferous plants does not change from the rate used for TRIM.FaTE in the dynamic mode. The user can set a date for harvest of agricultural plants or allow them to become litter.

---

[1] In the current TRIM.FaTE library, the litter-fall rate constant for coniferous forest is set to a value that is constant throughout the year. For the agricultural plants, the user can set the date of harvest, and the chemical mass in the harvested biomass can be transferred to a sink.

The steady-state flow of a river is simply the time-weighted average flow (or velocity).

C.1.1.6 Wildlife Plant Ingestion Rates

The wildlife plant ingestion rates (i.e., total ingestion rate × fraction of diet that consists of plants on a wet weight basis) are multiplied by *AllowExchange* to ensure that wildlife only consume plant leaves during the growing season. For a steady-state run, *AllowExchange* is set to a fractional value equal to the number of days it is equal to 1 divided by 365 days per year to get an annual average.

C.1.2 SWITCHING ADVECTIVE AIR TRANSPORT ALGORITHMS

Switching from the dynamic to the steady-state advective air transport algorithms involves three steps:

(1) Enabling the steady-state algorithms;
(2) Disabling the dynamic algorithms; and
(3) Setting up the steady-state advective transfer factors.

The steady-state air advective transfer factors are used to calculate air advection (see Section C.1.1.1). Two transfer factors (two directions) are calculated for each interface between one air volume element and an adjacent air volume element. In addition, the user should calculate transfer factors across each interface from air volume elements bounding the exterior of the modeling domain to the air sinks (*i.e.*, moving chemical mass from the boundary air volume elements into the air sinks). These transfer factors can be calculated by hand (in a spreadsheet) using the meteorological data set and information about the spatial relationships of the air volume elements. The number of years of meteorological data to average for each interface depends on the number of years associated with any apparent cycle or pattern of meteorologic conditions that is repeated at intervals (e.g., five years in the mercury test case). The steady-state air advective transfer factors are simply set equal to the calculated value for a particular link.

The use of the steady-state air advection transfer factors for each air/air compartment interface results in a more accurate representation of the average advective flows between air compartments than simply using average values for all of the meteorological properties and allowing the model to use those values in the existing dynamic air advection transfer algorithms. The use of steady-state air advection transfer factors (see Section C.1.1) retains information on correlations among the meteorological properties (e.g., a certain wind direction may be associated with higher wind speeds) that would be lost in an overall averaging process.

At the moment, the steady-state air advection transfer factors for each air/air compartment interface must be calculated outside of TRIM.FaTE (e.g., using spreadsheets). We expect that future versions of TRIM.FaTE will include the ability to calculate these transfer factors internally, thus reducing the time required of the user to set up a steady-state simulation.

C.1.3 DISABLING LINKS WITH GROUND WATER

A limitation of applying the steady-state mode is the inability to accommodate ground water. Thus, the final step in setting up a steady-state simulation is disabling all of the links from groundwater to other compartments (*i.e.*, vadose-zone soil and surface water). This step is required because the groundwater compartments lose mass so slowly that the steady-state solver cannot find a solution. After disabling the dynamic-mode links to and from groundwater, the ground-water compartment basically acts as a sink for chemical mass. Then, the steady-state solver is able to calculate a solution.

C.2 APPLICATIONS OF THE STEADY-STATE MODE

The speed of the steady-state solution makes it attractive for several types of applications (*e.g.*, diagnostic and uncertainty analyses).

As a diagnostic tool, the steady-state mode, with its short run time, can be used in evaluating the impact of changes to the set-up of a simulation, as well as parameter values and algorithms. The ability to perform a large number of realizations in reasonable run time (as provided in the steady-state mode) gives the user the opportunity to investigate model behavior. If the results from TRIM.FaTE appear inconsistent with expectations or with existing data, the user can quickly test different hypotheses about how those results were produced. During this exercise, the user can modify certain input parameters or assess different formulas for transfer factor algorithms (or for various compartment properties) and quickly assess the response of the model results to those changes.

In uncertainty and sensitivity analyses, the steady-state mode is also a valuable tool. For large and/or complex parcel layouts, sensitivity analyses of the many property values in a simulation when run in dynamic mode (*e.g.*, involving simulations of many years) can involve substantial run times. Similarly, dynamic simulations involving Monte Carlo assignment of key property values can also be time consuming. The steady-state mode can be used to provide a Monte Carlo sampling-based sensitivity analysis of many properties in a reasonable run time. This enables examination of the sensitivity of the model results to a much larger number of variables than would be possible using the sensitivity analysis feature in the dynamic mode in the same amount of run time.

Information from sensitivity/Monte Carlo analyses conducted using the steady-state mode can then be used to select a small number of input parameters for which the user can run a dynamic-mode uncertainty analysis. The final uncertainty analysis could then be a set of fully dynamic runs that produce a family of time-series curves (or an uncertainty band around an outcome curve). Results from the steady-state uncertainty/sensitivity analysis might also be evaluated as to their use to predict the outcome variance in the dynamic runs.

Appendix D

TABLES OF TRIM.FaTE INPUT PARAMETERS

Appendix D
TABLES OF TRIM.FaTE INPUT PARAMETERS

This appendix contains the following sets of tables listing and describing the input parameters used in TRIM.FaTE:

- non-chemical-dependent parameters for abiotic compartment types;
- non-chemical-dependent parameters for biotic compartment types;
- chemical-dependent (i.e., value varies by chemical) parameters independent of compartment type;
- chemical-dependent parameters for abiotic compartment types;
- chemical-dependent parameters for biotic compartment types; and
- source, meteorological, and other input parameters.

For each parameter listed, the parameter name and symbol, exact TRIM.FaTE code name, input units, and a brief description are given; for chemical-specific parameters, the applicable chemicals (*e.g.* , all, organics, mercury) also are given. Values for parameters are not listed here, but the values used should be documented for individual model applications.

Within the framework of the TRIM.FaTE computer model, several different kinds of “properties” are defined and used. The input parameters described in this appendix fall into the following categories of TRIM.FaTE properties:

- compartment properties (includes by far the largest number of input parameters);
- volume element (VE) properties;
- link properties;
- chemical properties;
- source properties; and
- scenario properties.

In the following tables, the property type is identified for all input parameters that are not compartment properties.

This appendix is intended to document only input parameters that are TRIM.FaTE computer model properties, *i.e.,* those parameters for which a user needs to supply a value (or confirm that an existing TRIM.FaTE library value is appropriate) in order to apply TRIM.FaTE. There are many other parameters, described throughout this Technical Support Document (TSD), that are calculated from these inputs and used in various chains of equations in the model. These intermediate parameters are not listed in the following tables, but they are described in the other parts of this document.

In addition to the input parameters listed here, the transfer factor algorithms and other equations described in the body of this document also include some parameters for which the user may want to set different values (e.g., gill assimilation efficiency in fish, or "overall K_{ow}" (D_{ow}) in surface water). Although these parameters are considered part of the TRIM.FaTE algorithms/equations, rather than TRIM.FaTE properties, they and the algorithms/equations themselves are available to the user to modify as appropriate and scientifically defensible for the application at hand. These parameters are described along with the transfer factor algorithms and other equations in the other parts of this document, and are not listed in this appendix.

Finally, for a TRIM.FaTE application, “off-line” calculations generally are needed to develop some of the input parameters listed in these tables (e.g., meteorological data preprocessing, calculation of surface water flows, calculation of runoff fractions for overland flow). Inputs for such “off-line” calculations, which may vary considerably across model applications, are not listed in this appendix.

Note that the units listed in these tables are the units in which model input values need to be expressed. In a few cases, these computer model input units do not match the units used for the same parameter in equations and derivations in the other parts of this TSD. In such cases, there are internal units conversions in the computer model that account for the differences.

For most of the input parameters listed in the following tables, the symbol used in the other parts of this TSD is included. For a few input parameters (e.g., initial concentration of a chemical, boundary concentration of a chemical), no symbol is included because no symbol is used in the other parts of this TSD.

Non-Chemical-Dependent -- Abiotic

Air Compartment Type

Parameter Name (TSD Symbol)	TRIM FaTE Code Name	Input Units	Description
Atmospheric dust particle load (D_L)	DustLoad	kg[dust particles]/m^3[air compartment]	Concentration of atmospheric dust particles in the air compartment
Density of air (ρ_a)	AirDensity_g_cm3	g/cm^3	Mass of air per unit volume of air
Density of dust particles (ρ_p)	DustDensity	kg[dust particles]/m^3[dust particles]	Mass of atmospheric particulate per unit volume of atmospheric particulate
Fraction organic matter on particulates (f_{om})	FractionOrganicMatteronParticulates	unitless (wet wt)	Mass fraction of air particulates that is organic material
Height [VE Property][a]	top, bottom[a]	m	Height (i.e., vertical dimension) of the air volume element
Particulate washout ratio (w_r)	WashoutRatio	m^3[air]/m^3[rain]	Precipitation scavenging ratio for particles in air (ratio of concentration of particles in rain to concentration of particles in air); used in estimating wet deposition of particles

[a] Height of air volume elements is set in TRIM.FaTE using two properties named "top" and "bottom."

Non-Chemical-Dependent -- Abiotic

Soil Compartment Types

Parameter Name (TSD Symbol)	TRIM FaTE Code Name	Input Units	Description
Surface Soil Compartment Type			
Air content (ε_{Ss})[a]	VolumeFraction_vapor	volume[air]/volume[compartment]	Volumetric pore space occupied by air in surface soil compartment (fraction of total volume that is air)
Average vertical velocity of water (percolation) (V_i)[b]	AverageVerticalVelocity	m/day	Average speed of water movement in downward vertical direction through soil column
Boundary layer thickness above surface soil (δ_{Ss})	AirSoilBoundaryThickness	m	Boundary layer thickness above surface soil
Density of soil solids (dry weight) (ρ)[a]	rho	kg[soil]/m^3[soil]	Dry soil density (or dry weight of surface soil particles per unit volume of surface soil particles)
Depth [VE Property] (d_{Ss})[c]	top, bottom[c]	m	Depth (i.e., vertical dimension) of the surface soil volume element
Erosion fraction ($f_{erosion}(Ssi \rightarrow Ssj)$) [Link property]	FractionofTotalErosion	unitless	Fraction of total eroded soil mass moving from a given sending compartment to a given receiving compartment or sink
Fraction of area available for erosion ($f_{avail\_erosion}$)	Fractionofareaavailableforerosion	m^2[area available]/m^2[total]	Fraction of the total surface area for which erosion can occur
Fraction of area available for runoff (f_{avail_runoff})	FractionofAreaAvailableforRunoff	m^2[area available]/m^2[total]	Fraction of the total surface area for which runoff can occur
Fraction of area available for vertical diffusion (f_A)	Fractionofareaavailableforverticaldiffusion	m^2[area available]/m^2[total]	Fraction of the total surface area for which vertical diffusion can occur
Organic carbon fraction (f_{oc})	OrganicCarbonContent	kg [organic carbon]/kg[soil wet wt]	Organic carbon mass fraction for surface soil
Runoff fraction ($f_{runoff}(Ssi \rightarrow Ssj)$) [Link property]	FractionofTotalRunoff	unitless	Fraction of total runoff volume moving from a given sending compartment to a given receiving compartment or sink
Total erosion rate *(erosion)* [b]	TotalErosionRate_kg_m2_day	kg[soil solids]/m^2[surface soil]-day	Mass of eroded surface soil particles per unit surface area per day
Total runoff rate *(runoff)* [b]	TotalRunoffRate_m3_m2_day	m^3[water]/m^2[surface soil]-day	Volume of liquid runoff from surface soil per unit surface area per day

Non-Chemical-Dependent -- Abiotic

Soil Compartment Types

Parameter Name (TSD Symbol)	TRIM FaTE Code Name	Input Units	Description
Water content (θ_{Ss})[a]	VolumeFraction_Liquid	volume[water]/volume[compartment]	Volumetric pore space occupied by water in surface soil compartment (fraction of total volume that is water)
Root Zone Soil Compartment Type			
Air content (ϵ_{Sr})[a]	VolumeFraction_vapor	volume[air]/volume[compartment]	Volumetric pore space occupied by air in root zone soil compartment (fraction of total volume that is air)
Average vertical velocity of water (percolation) (V_i)[b]	AverageVerticalVelocity	m/day	Average speed of water movement in vertical direction through soil column (downward)
Density of soil solids (dry weight) (ρ)[a]	rho	kg[soil]/m^3[soil]	Dry soil density (or dry weight of root zone soil particles per unit volume of root zone soil particles)
Depth [VE Property] (d_{Sr})[c]	top, bottom[c]	m	Depth (i.e., vertical dimension) of the root zone soil volume element
Organic carbon fraction (f_{oc})	OrganicCarbonContent	kg [organic carbon]/kg [soil wet wt]	Organic carbon mass fraction for root zone soil
Water content (θ_{Sr})[a]	VolumeFraction_Liquid	volume[water]/volume[compartment]	Volumetric pore space occupied by water in root zone soil compartment (fraction of total volume that is water)
Vadose Zone Soil Compartment Type			
Air content (ϵ_{Sv})[a]	VolumeFraction_vapor	volume[air]/volume[compartment]	Volumetric pore space occupied by air in vadose zone soil compartment (fraction of total volume that is air)
Average vertical velocity of water (percolation) (V_i)[b]	AverageVerticalVelocity	m/day	Average speed of water movement in vertical direction through soil column (downward)
Density of soil solids (dry weight) (ρ)[a]	rho	kg[soil]/m^3[soil]	Dry soil density (or dry weight of vadose zone soil particles per unit volume of vadose zone soil particles)
Depth [VE Property] (d_{Sv})[c]	top, bottom[c]	m	Depth (i.e., vertical dimension) of the vadose zone soil volume element
Organic carbon fraction (f_{oc})	OrganicCarbonContent	kg [organic carbon]/kg [soil wet wt]	Organic carbon mass fraction for vadose zone soil

Non-Chemical-Dependent -- Abiotic

Parameter Name (TSD Symbol)	TRIM FaTE Code Name	Input Units	Description
Soil Compartment Types			
Water content (θ_{Sv})[a]	VolumeFraction_Liquid	volume[water]/volume[compartment]	Volumetric pore space occupied by water in vadose zone soil compartment (fraction of total volume that is water)
Ground Water Compartment Type			
Depth [VE Property][c]	top, bottom[c]	m	Depth (i.e., vertical dimension) of the ground water volume element
Organic carbon fraction (f_{oc})	OrganicCarbonContent	kg [organic carbon]/kg [soil wet wt]	Organic carbon mass fraction for ground water
Porosity (Φ)	Porosity	volume[total pore space]/volume[compartment]	Ratio of pore space volume to total ground water compartment volume
Recharge rate to surface water *(recharge)* [Link property]	RechargeRate	m^3[water]/m^2[area]-day	Volume of ground water moving into surface water per unit interfacial area per day
Solid material density in aquifer (ρ)	rho	kg[soil]/m^3[soil]	Dry particle density (or dry weight of solid material in ground water compartment per unit volume of solid material in ground water compartment)

[a] Interdependent parameters - user is responsible for making sure input values are consistent (also interdependent with soil bulk density, which is not an input parameter in TRIM.FaTE but for which data are often available).

[b] Interdependent parameters with precipitation - user is responsible for making sure input values are consistent.

[c] Set using the volume element properties named "top" and "bottom."

Non-Chemical-Dependent -- Abiotic

Surface Water Compartment Type

Parameter Name (TSD Symbol)	TRIM FaTE Code Name	Input Units	Description
Algae carbon content (fraction) (Al_{TOC})	AlgaeCarbonContentDryWt	g[carbon]/g[algae dry wt]	Mass fraction of algae that is carbon (dry wt basis)
Algae density in water column (AC)	AlgaeDensityinWaterColumn_g_L	g[algae wet wt]/L[water]	Mass of algae per unit volume of surface water
Algae growth rate constant (μ)	AlgaeGrowthRate	1/day	First-order rate constant for increase of algae mass
Algae radius (R)	AlgaeRadius	um	Average size of algae cell
Algae water content (fraction) (fW_{Algae})	AlgaeWaterContent	unitless	Mass fraction of algae that is water
Average algae cell density (per vol cell, not water) (ρ_{Algae})	AlgaeDensity_g_m3	g[algae]/m^3[algae]	Weight of algae per unit volume of algae cells
Boundary layer thickness above sediment (δ_{Sed})	BoundaryLayerThicknessAboveSediment	m	Thickness of surface water above sediment within which molecular diffusion between media can be significant (defines boundary between the well mixed portion, where turbulent mixing is rapid and continuous, and the stable portion at the very edge of the interface)
Bulk water flow (flow) [Link property][a,b,c]	BulkWaterFlowRate_Volumetric	m^3[water]/day	Volume of water movement per unit time across a link (i.e., at a compartment-compartment interface)
Chloride concentration	ChlorideConcentration_mg_L	mg/L	Concentration of chloride ion in surface water compartment
Chlorophyll concentration (CC)	ChlorophyllConcentration_mg_L	mg[chlorophyll]/L[water]	Concentration of chlorophyll in surface water compartment
Current velocity (μ)[c,d]	CurrentVelocity	m/s	Average speed of moving water in flowing surface water compartments
Depth (d_W) [VE property][c,e]	top, bottom[e]	m	Depth (i.e., vertical dimension) of the surface water volume element
Dispersion coefficient for exchange between surface water compartments (DSPij) [Link property][a]	DiffusiveExchangeCoefficient	m^2/day	Coefficient used to calculate dispersive transport between two horizontally adjacent surface water compartments

Non-Chemical-Dependent -- Abiotic

Surface Water Compartment Type

Parameter Name (TSD Symbol)	TRIM FaTE Code Name	Input Units	Description
Dimensionless viscous sublayer thickness (λ_2)	DimensionlessViscousSublayerThickness	unitless	Parameter used in calculating gas and liquid phase transfer coefficients, which are used in calculating volatilization transfers between surface water and air
Distance between midpoints (L_{ij}) [Link property][a]	DistanceBetweenMidpoints	m	Linear distance between the midpoints of two connected surface water compartments; used as characteristic mixing length for dispersion calculations
Drag coefficient for water body (C_d)	DragCoefficient	unitless	Coefficient used to calculate the shear velocity of wind, which is used in calculating volatilization transfers between surface water and air
Flush rate *(flushes/yr)* [f]	Flushes_per_year	1/year	Number of times surface water compartment volume is completely turned over (flushed) in a year
Generic diffusive exchange coefficient with sediment (DSP_{Sed})	GenericDiffusiveExchangeCoefficientWithSediment	m^2/day	Coefficient used to calculate diffusive exchange between adjacent surface water and sediment compartments
Organic carbon fraction in suspended sediments (f_{oc})	OrganicCarbonContent	unitless	Organic carbon mass fraction for suspended sediment
pH	pH	unitless	Negative logarithm (base 10) of concentration of hydrogen ion in surface water compartment
Suspended sediment density (ρ_{Sed})	rho	kg[sediment particles]/m^3[sediment particles]	Dry suspended sediment density (or dry weight of suspended sediment particles per unit volume of suspended sediment particles)
Suspended sediment deposition velocity (v_{dep})	SedimentDepositionVelocity	m/day	Speed that suspended sediment moves downward through water column
Total suspended sediment concentration (TSS)	SuspendedSedimentconcentration	kg[suspended sediment particles]/m^3[surface water compartment]	Concentration of suspended sediment in water column
Water temperature (T) [VE property]	WaterTemperature_K	degrees K	Average water temperature of the surface water compartment

[a] Applies to all surface water compartments connected to other surface water compartments.

[b] Interdependent parameters with precipitation - user is responsible for making sure input values are consistent.

[c] Interdependent parameters - user is responsible for making sure input values are consistent.

Non-Chemical-Dependent -- Abiotic

Surface Water Compartment Type

Parameter Name (TSD Symbol)	TRIM FaTE Code Name	Input Units	Description

[d] Applies to flowing water bodies only (i.e., rivers, streams).

[e] Set using the volume element properties named "top" and "bottom."

[f] Applies to all surface water compartments connected to a flush rate sink (i.e., all or part of discharge modeled to a sink).

Non-Chemical-Dependent -- Abiotic

Sediment Compartment Type

Parameter Name (TSD Symbol)	TRIM FaTE Code Name	Input Units	Description
Depth (d_{Sed}) [VE Property][a]	top, bottom[a]	m	Depth (i.e., vertical dimension) of the sediment volume element
Organic carbon fraction (f_{oc})	OrganicCarbonContent	kg[organic carbon]/kg[soil wet wt]	Organic carbon mass fraction for bottom sediment
Porosity of the sediment zone (Φ)[b]	Porosity	m^3[pore water]/m^3[sediment compartment]	Ratio of pore space volume to total sediment compartment volume
Solid material density in sediment (ρ_{Sed})[b]	rho	kg[sediment particles]/m^3[sediment particles]	Dry sediment density (or dry weight of bottom sediment per unit volume of bottom sediment)

[a] Set using the volume element properties named "top" and "bottom."

[b] Interdependent parameters with benthic solids concentration (kg[sediment]/m^3[sediment compartment]; not a TRIM.FaTE input parameter) - user is responsible for making sure input values are consistent.

Non-Chemical-Dependent -- Biotic

Terrestrial Plant Compartment Types[a]

Parameter Name (TSD Symbol)	TRIM FaTE Code Name	Input Units	Description
Leaf Compartment Type			
Allow exchange[b]	AllowExchange	1=yes, 0=no	1 if exchange can occur with another compartment, 0 if not (can be made seasonal by setting allow exchange start and stop dates)
Average leaf area index (LAI)[c]	AverageLeafAreaIndex_No_Time_Dependence	m^2[total leaf area]/m^2[underlying soil area]	Average area of leaf per unit surface area (no time dependence)
Calculate wet dep interception fraction	CalculateWetDepInterceptionFraction_1_Means_Yes_Else_No	1=yes, 0=no	Switch used to allow use of input value or model calculations
Correction exponent, octanol to lipid (b)	CorrectionExponent	unitless	Correction exponent for the differences between octanol and lipids
Degree stomatal opening (α_s)	DegreeStomatalOpening	unitless	Mean degree of opening of stomatal pores, between 0 and 1
Density of wet leaf (ρ_{Leaf})[c]	WetDensity	kg[leaf wet wt]/m^3[leaf]	Density of wet plant leaf
Leaf wetting factor (S)	LeafWettingFactor	m	Vegetation-dependent leaf-wetting factor (retention coefficient)
Length of leaf (l)	LengthofLeaf	m	Length of flat leaf
Lipid content (fL_{Leaf})	LipidContent	kg[lipid]/kg[leaf wet wt]	Mass fraction of leaf that is lipid (wet wt basis)
Litter fall rate (K_L)[b]	LitterFallRate	1/day	First-order rate constant for fall of plant leaves to soil (can be made seasonal by setting litter fall start and stop dates)
Stomatal area, normalized for effective diffusion path length (S_N)	StomatalAreaNormalizedEffectiveDiffusionPathLength	1/m	Portion of total leaf surface area comprised of stomatal pores divided by the effective path length for a diffusing molecule through a pore; value is relatively similar across plant species
Vegetation attenuation factor (α_{VAF})	AttenuationFactor	m^2/kg	Effective attenuation by plant leaves of dry depositing particles per unit dry weight of the plant species; used to calculate interception fraction
Water content (fW_{Leaf})	WaterContent	unitless (kg[water]/kg[leaf wet wt])	Mass fraction of leaf that is water (wet wt basis)

Non-Chemical-Dependent -- Biotic

Terrestrial Plant Compartment Types[a]

Parameter Name (TSD Symbol)	TRIM FaTE Code Name	Input Units	Description
Wet dep interception fraction (I_{wet})	WetDepInterceptionFraction_Input_Used_Only_If_OptionSet	unitless	Fraction of wet deposition intercepted by leaves (input used only if option set)
Wet mass of leaf per unit area ($\rho area_{Leaf}$)[c]	WetMassperArea	kg[fresh leaf]/m^2[area]	Freshweight mass of leaf per unit surface area
Particle-on-Leaf Compartment Type			
Allow exchange[b]	AllowExchange	1=yes, 0=no	1 if exchange can occur with another compartment, 0 if not (can be made seasonal by setting allow exchange start and stop dates)
Volume particle per area leaf	VolumeParticlePerAreaLeaf	m3 [leaf particles]/m2 [leaf]	Volume of leaf particles per unit area of leaf; used to calculate compartment volume
Root Compartment Type - Nonwoody Plants Only[d]			
Allow exchange[b]	AllowExchange	1=yes, 0=no	1 if exchange can occur with another compartment, 0 if not (can be made seasonal by setting allow exchange start and stop dates)
Correction exponent, octanol to lipid (b)	CorrectionExponent	unitless	Correction exponent for the differences between octanol and lipids
Lipid content of root (fL_{Root})	LipidContent	kg[lipid]/kg [root wet wt]	Mass fraction of root that is lipid (wet wt basis)
Water content of root (fW_{Root})	WaterContent	kg[water]/kg[root wet wt])	Mass fraction of root that is water (wet wt basis)
Wet density of root (ρ_{Root})	WetDensity	kg[leaf wet wt]/m^3[root]	Density of wet plant root
Wet mass per area ($\rho area_{Root}$)	WetMassperArea	kg[root wet wt]/m^2[soil]	Freshweight mass of root per unit surface area

Non-Chemical-Dependent -- Biotic

Terrestrial Plant Compartment Types[a]

Parameter Name (TSD Symbol)	TRIM FaTE Code Name	Input Units	Description
Stem Compartment Type - Nonwoody Plants Only[d]			
Allow exchange[b]	AllowExchange	1=yes, 0=no	1 if exchange can occur with another compartment, 0 if not (can be made seasonal by setting allow exchange start and stop dates)
Correction exponent, octanol to lipid (b)	CorrectionExponent	unitless	Correction exponent for the differences between octanol and lipids
Density of phloem fluid (ρ_{Ph})	PhloemDensity	kg[phloem]/m^3[phloem]	Density of phloem fluid
Density of xylem fluid (ρ_{Xy})	XylemDensity	kg[xylem]/m^3[xylem]	Density of xylem fluid
Flow rate of transpired water per leaf area	FlowRateofTranspiredWaterperAreaofLeafSurface	m^3[water]/m^2 [leaf]-day	Empirical factor used to estimate total flow of transpired water based on leaf surface area
Fraction of transpiration flow rate that is phloem rate	FractionPhloemRatewithTranspirationFlowRate	unitless	Fraction of total transpiration flow rate that is the phloem rate
Lipid content of stem (fL_{Stem})	LipidContent	kg[lipid]/kg [stem wet wt]	Mass fraction of stem that is lipid (wet wt basis)
Water content of stem (fW_{Stem})	WaterContent	kg[water]/kg[stem wet wt]	Mass fraction of stem that is water (wet wt basis)
Wet density of stem (ρ_{Stem})	WetDensity	kg[stem wet wt]/m^3[root]	Density of wet plant stem
Wet mass per area ($\rho area_{Stem}$)	WetMassperArea	kg[stem wet wt]/m^2[soil]	Freshweight mass of stem per unit surface area

[a] TRIM.FaTE currently includes four kinds of terrestrial plants: deciduous forest, coniferous forest, grasses/herbs, and agricultural.
[b] If modeled as seasonal processes, on/off dates are interdependent - user is responsible for making sure input values are consistent.
[c] Interdependent parameters - user is responsible for making sure input values are consistent.
[d] Roots and stems are not modeled for deciduous and coniferous forest in the current version of TRIM.FaTE.

Non-Chemical-Dependent -- Biotic

Aquatic Plants Compartment Type

Parameter Name (TSD Symbol)	TRIM FaTE Code Name	Input Units	Description
Macrophyte Compartment Type			
Biomass per water area	BiomassPerArea_kg_m2	kg/m^2	Mass of macrophytes per unit surface water area (wet wt basis)
Density of macrophytes (ρ_{Mp})	Density	kg/L	Mass of macrophytes per unit volume of macrophytes (wet wt basis)

Non-Chemical-Dependent -- Biotic

Terrestrial Animal Compartment Types

Parameter Name (TSD Symbol)	TRIM FaTE Code Name	Input Units	Description
Soil Detritivore Compartment Type - Earthworm			
Density	Density_Freshweight	kg[worm]/L[worm]	Density of worm (wet wt basis); used to calculate compartment volume
Density per soil area ($parea_{Worm}$)	ArealDensity_Freshweight	kg[worm wet wt]/m^2[soil]	Mass of worm per unit surface area of soil
Water content of worm (fW_{worm})	Water_content	unitless	Mass fraction of worm that is water
Soil Detritivore Compartment Type - Soil Arthropod			
Biomass per soil area ($parea_{Arth}$)	BiomassPerArea_kg_m2	kg[arthropod wet wt]/m^2[soil]	Mass of soil arthropods per unit surface area of soil
Body weight (BW)	BW	kg	Mass of individual animal
All Other Terrestrial Animal Compartment Types[a]			
Body weight (BW)	BW	kg	Mass of individual
Food ingestion rate (IN_D)	FoodIngestionRate	kg[diet wet wt]/kg BW-day	Total amount of food eaten per day, scaled to body weight
Fraction diet - american robin ($P^{American}_{robin}$)	FractionDietAmericanRobin	unitless	Fraction of food diet comprised of american robin
Fraction diet - black-capped chickadee ($P^{Chickadee}$)	FractionDietChickadee	unitless	Fraction of food diet comprised of black-capped chickadee
Fraction diet - bobwhite quail ($P^{Bobwhite}_{quail}$)	FractionDietBobwhiteQuail	unitless	Fraction of food diet comprised of bobwhtie quail
Fraction diet - mallard ($P^{Mallard}$)	FractionDietMallard	unitless	Fraction of food diet comprised of mallard
Fraction diet - mouse (P^{Mouse})	FractionDietMouse	unitless	Fraction of food diet comprised of mouse
Fraction diet - plants (P^{Plants})	FractionDietPlant	unitless	Fraction of food diet comprised of plant
Fraction diet - short-tailed shrew ($P^{Short-}_{tailed\ shrew}$)	FractionDietshorttailedshrew	unitless	Fraction of food diet comprised of short-tailed shrew

Non-Chemical-Dependent -- Biotic

Terrestrial Animal Compartment Types

Parameter Name (TSD Symbol)	TRIM FaTE Code Name	Input Units	Description
Fraction diet - soil (f_{intake_soil})	FractionDietSoil[b]	unitless, dry wt basis	Fraction of total dry weight intake comprised of soil (used to calculate soil ingestion rate, when necessary)
Fraction diet - soil arthropod (P^{Arth})	FractionDietSoilArthropod	unitless	Fraction of food diet comprised of soil arthropod
Fraction diet - vole (P^{Vole})	FractionDietvole	unitless	Fraction of food diet comprised of vole
Fraction diet - worm (P^{Worm})	FractionDietWorm	unitless	Fraction of food diet comprised of worm
Fraction excretion to soil (f_{uSs})	FractionExcretiontoSoil	unitless	Fraction of total excretion that goes to surface soil
Fraction excretion to water (f_{uSW})	FractionExcretiontoWater	unitless	Fraction of total excretion that goes to surface water
Fraction specific compartment diet [Link property]	FractionSpecificCompartmentDiet	unitless	Fraction of food diet originating from a specific compartment; must sum to 1.0 across all links
Population per soil area (PN_{area})	NumberofIndividualsPerSquareMeter	$\#/m^2$	Number of individuals per unit surface area
Scaling constant A - inhalation rate	InhalationProps_A	unitless	Allometric scaling constant used to calculate inhalation rate based on body weight
Scaling constant B - inhalation rate	InhalationProps_B	unitless	Allometric scaling constant used to calculate inhalation rate based on body weight
Scaling constant A - water ingestion rate	WaterIngProps_A	unitless	Allometric scaling constant used to calculate water ingestion rate based on body weight
Scaling constant B - water ingestion rate	WaterIngProps_B	unitless	Allometric scaling constant used to calculate water ingestion rate based on body weight
Soil ingestion rate (IN_{Ss})	SoilIngestionRate	kg[soil]/kg BW-day	Total amount of soil eaten per day, scaled to body weight (used if data available - otherwise calculated from fraction diet-soil and food ingestion rate)

[a] TRIM.FaTE currently includes the following terrestrial animal compartment types: Terrestrial Ground-invertebrate Feeder - American Woodcock, Terrestrial Ground-invertebrate Feeder - Black-capped Chickadee, Terrestrial Ground-invertebrate Feeder - Short-tailed Shrew, Terrestrial Ground-invertebrate Feeder - Trowbridge Shrew, Terrestrial Herbivore - Bobwhite Quail, Terrestrial Herbivore - Cow, Terrestrial Herbivore - Long-tailed Vole, Terrestrial Herbivore - Meadow Vole, Terrestrial Herbivore - Mule Deer/Black-tailed Deer, Terrestrial Herbivore - White-tailed Deer, Terrestrial Insectivore - Tree Swallow, Terrestrial Omnivore - American Robin, Terrestrial Omnivore - Mouse, Terrestrial Predator/Scavenger - Long-tailed Weasel, and Terrestrial Predator/Scavenger - Red-tailed hawk.

[b] Parameter and equations using it are in process of being added to TRIM.FaTE as of publication date.

Non-Chemical-Dependent -- Biotic

Semi-aquatic Animal Compartment Types

Parameter Name (TSD Symbol)	TRIM FaTE Code Name	Input Units	Description
All Compartment Types[a]			
Body weight (BW)	BW	kg	Mass of individual animal
Food ingestion rate (IN_D)	FoodIngestionRate	(kg[diet wet wt]/kg[body wet wt]-day)	Total amount of food eaten per day, scaled to body weight
Fraction diet - algae (P^{Algae})	FractionDietAlgae	unitless	Fraction of food diet comprised of algae
Fraction diet - american robin ($P^{American\ robin}$)	FractionDietAmericanRobin	unitless	Fraction of food diet comprised of american robin
Fraction diet - benthic carnivores (P^{Fbc})	FractionDietFishbenthiccarnivore	unitless	Fraction of food diet comprised of benthic carnivore
Fraction diet - benthic invertebrates (P^{BI})	FractionDietBenthicInvertebrate	unitless	Fraction of food diet comprised of benthic invertebrate
Fraction diet - benthic omnivores (P^{Fbo})	FractionDietFishbenthicomnivore	unitless	Fraction of food diet comprised of benthic omnivore
Fraction diet - black-capped chickadee ($P^{Chickadee}$)	FractionDietChickadee	unitless	Fraction of food diet comprised of black-capped chickadee
Fraction diet - bobwhite quail ($P^{Bobwhite\ quail}$)	FractionDietBobwhiteQuail	unitless	Fraction of food diet comprised of bobwhite quail
Fraction diet - macrophyte (P^{Mp})	FractionDietMacrophyte	unitless	Fraction of food diet comprised of macrophyte
Fraction diet - mallard ($P^{Mallard}$)	FractionDietMallard	unitless	Fraction of food diet comprised of mallard
Fraction diet - mouse (P^{Mouse})	FractionDietMouse	unitless	Fraction of food diet comprised of mouse
Fraction diet - plants (P^{Plants})	FractionDietPlant	unitless	Fraction of food diet comprised of plant
Fraction diet - short-tailed shrew ($P^{Short\text{-}tailed\ shrew}$)	FractionDietshorttailedshrew	unitless	Fraction of food diet comprised of short-tailed shrew
Fraction diet - soil (f_{intake_soil})	FractionDietSoil[b]	unitless, dry wt basis	Fraction of total dry weight intake comprised of soil (used to calculate soil ingestion rate, when necessary)
Fraction diet - soil arthropod (P^{Arth})	FractionDietSoilArthropod	unitless	Fraction of food diet comprised of soil arthropod

Non-Chemical-Dependent -- Biotic

Semi-aquatic Animal Compartment Types

Parameter Name (TSD Symbol)	TRIM FaTE Code Name	Input Units	Description
Fraction diet - vole (P^{Vole})	FractionDietvole	unitless	Fraction of food diet comprised of vole
Fraction diet - water-column carnivores (P^{Fwcc})	FractionDietFishcarnivore	unitless	Fraction of food diet comprised of water-column carnivore
Fraction diet - water-column herbivores (P^{Fwch})	FractionDietFishherbivore	unitless	Fraction of food diet comprised of water-column herbivore
Fraction diet - water-column omnivores (P^{Fwco})	FractionDietFishomnivore	unitless	Fraction of food diet comprised of water-column omnivore
Fraction diet - worm (P^{Worm})	FractionDietWorm	unitless	Fraction of food diet comprised of worm
Fraction excretion to soil (f_{uSW})	FractionExcretiontoSoil	unitless	Fraction of total excretion that goes to soil
Fraction excretion to water (f_{uSs})	FractionExcretiontoWater	unitless	Fraction of total excretion that goes to surface water
Fraction specific compartment diet [Link property]	FractionSpecificCompartmentDiet	unitless	Fraction of food diet originating from a specific compartment; must sum to 1.0 across all links
Population per soil area (PN_{area})	NumberofIndividualsPerSquareMeter	#/m^2	Number of individuals per unit area
Scaling constant A - inhalation rate	InhalationProps_A	unitless	Allometric scaling constant used to calculate inhalation rate based on body weight
Scaling constant B - inhalation rate	InhalationProps_B	unitless	Allometric scaling constant used to calculate inhalation rate based on body weight
Scaling constant A - water ingestion rate	WaterIngProps_A	unitless	Allometric scaling constant used to calculate water ingestion rate based on body weight
Scaling constant B - water ingestion rate	WaterIngProps_B	unitless	Allometric scaling constant used to calculate water ingestion rate based on body weight
Soil ingestion rate (IN_{Ss})	SoilIngestionRate	kg[soil]/kg BW-day	Total amount of soil eaten per day, scaled to body weight (used if data available - otherwise calculated from fraction diet-soil and food ingestion rate)

[a] TRIM.FaTE currently includes the following semi-aquatic animal compartment types: Semi-aquatic Omnivore - Mallard, Semi-aquatic Omnivore - Mink, Semi-aquatic Omnivore - Raccoon, Semi-aquatic Piscivore - Common Loon, Semi-aquatic Piscivore - Kingfisher, and Semi-aquatic Predator/Scavenger - Bald Eagle.

[b] Parameter and equations using it are in process of being added to TRIM.FaTE as of publication date.

Non-Chemical-Dependent -- Biotic

Aquatic Animal Compartment Types

Parameter Name (TSD Symbol)	TRIM FaTE Code Name	Input Units	Description
Benthic Invertebrate Compartment Type			
Biomass per water area	BiomassPerArea_kg_m2	kg/m^2	Mass of benthic invertebrates per unit surface water area
Body weight (BW) or (m_{BI})	BW	kg[inv wet wt]	Mass of individual organisms comprising the benthic invertebrate compartment
All Fish Compartment Types[a]			
Body weight (BW) OR (m_f)	BW	kg[fish wet wt]	Mass of individual fish
Fraction diet - algae (P^{Algae})	FractionDietAlgae	unitless	Fraction of food diet comprised of algae
Fraction diet - benthic carnivores (P^{Fbc})	FractionDietFishbenthiccarnivore	unitless	Fraction of food diet comprised of benthic carnivore
Fraction diet - benthic invertebrates (P^{BI})	FractionDietBenthicInvertebrate	unitless	Fraction of food diet comprised of benthic invertebrate
Fraction diet - benthic omnivores (P^{Fbo})	FractionDietFishbenthicomnivore	unitless	Fraction of food diet comprised of benthic omnivore
Fraction diet - macrophyte (P^{Mp})	FractionDietMacrophyte	unitless	Fraction of food diet comprised of macrophyte
Fraction diet - water-column carnivores (P^{Fwcc})	FractionDietFishcarnivore	unitless	Fraction of food diet comprised of water-column carnivore
Fraction diet - water-column herbivores (P^{Fwch})	FractionDietFishherbivore	unitless	Fraction of food diet comprised of water-column herbivore
Fraction diet - water-column omnivores (P^{Fwco})	FractionDietFishomnivore	unitless	Fraction of food diet comprised of water-column omnivore
Fraction lipid weight (f_{lipid})	FishLipidFraction	kg[lipid]/kg[fish wet wt]	Mass fraction of fish that is lipid (wet wt basis)
Population per water area	NumberofFishperSquareMeter	#/m^2	Number of fish per unit surface water area

[a] TRIM.FaTE currently includes the following fish compartment types: Benthic Carnivore, Benthic Omnivore, Water-column Carnivore, Water-column Herbivore, and Water-column Omnivore.

Chemical-Dependent -- Independent of Compartment Type

Parameter Name[a] (TSD Symbol)	TRIM FaTE Code Name	Input Units	Description	Applicable Chemicals
Diffusion coefficient in pure air (D_{air})	D_pureair	m^2[air]/day	Coefficient that (when combined with chemical concentration) predicts how quickly a chemical spreads out in gas phase due to diffusion	all
Diffusion coefficient in pure water (D_{water})	D_purewater	m^2[water]/day	Coefficient that (when combined with chemical concentration) predicts how quickly a chemical spreads out in aqueous phase due to diffusion	all
Henry's Law constant (H)	HenryLawConstant	Pa-m^3 /mol	Ratio of the aqueous-phase concentration of a chemical to its equilibrium partial pressure in the gas phase	all
Melting point (T_m)	MeltingPoint	°K	Temperature at which a solid becomes a liquid at standard atmospheric pressure	all
Molecular weight (M_w)	molecularWeight	g/mol	Weight of 1 mole of the chemical	all
Octanol-water partition coefficient (K_{OW})	K_ow	L[water]/kg[octanol]	Equilibrium ratio of concentration dissolved in octanol to concentration dissolved in water	all
Reference bird body weight (BW(Ref))	ReferenceBird_BodyWeight	kg	Mass of individual reference bird used for allometric scaling of degradation rate	organics
Reference bird chemical degradation rate($k_{degradation}$)	ReferenceBird_GeneralDegradationRate	1/day	First-order rate constant for chemical degradation in reference bird used for allometric scaling of degradation rate	organics
Reference bird elimination rate	TerrestrialBird_EliminationRate	1/day	First-order rate constant for elimination of chemical from the body (terrestrial birds)	organics
Reference mammal body weight (BW(Ref))	ReferenceMammal_BodyWeight	kg	Mass of individual reference mammal used for allometric scaling of degradation rate	organics
Reference mammal chemical degradation rate ($k_{degradation}$)	ReferenceMammal_GeneralDegradationRate	1/day	First-order rate constant for chemical degradation in reference mammal used for allometric scaling of degradation rate	organics
Reference mammal elimination rate	TerrestrialMammal_EliminationRate	1/day	First-order rate constant for elimination of chemical from the body (terrestrial mammals)	organics
Vapor pressure (P_{vapor})	VaporPressure	Pa	Pressure exerted by a vapor in equilibrium with its solid or liquid phase	organics
Vapor washout ratio (w_{rV})	VaporWashoutRatio	m^3[air]/m^3[rain]	Precipitation scavenging ratio for vapors (ratio of concentration in rain to concentration in vapor form in air); used in estimating wet deposition of vapors	Hg species

[a] All parameters in this table are TRIM.FaTE chemical properties.

Chemical-Dependent -- Abiotic

Air Compartment Type

Parameter Name (TSD Symbol)	TRIM FaTE Code Name	Input Units	Description	Applicable Chemicals
Initial concentration	initialConcentration_g_per_m3	g/m^3	Bulk air concentration at beginning of modeling period	all
Boundary concentration [VE property][a]	boundaryConcentration_g_per_m3	g/m^3	Air concentration at the outer boundary of the modeling region (i.e., concentration in air flowing into the modeling region)	all
Particle dry deposition velocity (V_{dry})	vdep	m/day	Speed at which chemical in particle form in air moves downward; used in estimating dry deposition of particles	all
Demethylation rate (k_{Dm})	DemethylationRate	1/day	First-order rate constant for demethylation (MHg->Hg2)	MHg
Methylation rate (k_M)	MethylationRate	1/day	First-order rate constant for methylation (Hg2->MHg)	Hg2
Oxidation rate (k_O)	OxidationRate	1/day	First-order rate constant for oxidation (Hg0->Hg2)	Hg0
Reduction rate (k_R)	ReductionRate	1/day	First-order rate constant for reduction (Hg2->Hg0)	Hg2
Half-life *(half-life)*	Halflife	day	Length of time for chemical amount to be reduced by one-half by degradation reactions	organics

[a] Only used in model runs specified as including non-zero air boundary contributions. Only applicable for air volume elements with at least one boundary on the outer edge of the modeling region (zero boundary contribution for all internal air compartments).

Chemical-Dependent -- Abiotic

Soil Compartment Types

Parameter Name (TSD Symbol)	TRIM FaTE Code Name	Input Units	Description	Applicable Chemicals
Surface Soil Compartment Type				
Initial concentration	initialConcentration_g_per_m3	g/m^3	Bulk surface soil concentration at beginning of modeling period	all
Input characteristic depth (X*)	InputCharacteristicDepth_m	m	Distance from top of the soil compartment at which soil concentration has dropped to 36.79% (1/e * 100%) of the concentration at top of compartment	all
Soil/water partition coefficient (K_d)	Kd	L[water]/kg[soil wet wt]	Equilibrium ratio of concentration sorbed to solids and concentration dissolved	all
Use input characteristic depth	UseInputCharacteristicDepth_0_MeansNo_ElseYes	0 = no , Else = yes	If = 0, use model-calculated characteristic depth, else use user-provided characteristic depth	all
Vapor dry deposition velocity (v_{vapor})	VaporDryDepositionVelocity_m_day	m/day	Speed at which chemical in vapor form in air moves downward; used in estimating dry deposition of vapors to soil	Hg2
Demethylation rate (k_{Dm})	DemethylationRate	1/day	First-order rate constant for demethylation (MHg->Hg2)	MHg
Methylation rate (k_M)	MethylationRate	1/day	First-order rate constant for methylation (Hg2->MHg)	Hg2
Oxidation rate (k_O)	OxidationRate	1/day	First-order rate constant for oxidation (Hg0->Hg2)	Hg0
Reduction rate (k_R)	ReductionRate	1/day	First-order rate constant for reduction (Hg2->Hg0)	Hg2
Half-life *(half-life)*	Halflife	day	Length of time for chemical amount to be reduced by one-half by degradation reactions	organics
Root Zone Soil Compartment Type				
Initial concentration	initialConcentration_g_per_m3	g/m^3	Bulk root zone soil concentration at beginning of modeling period	all
Input characteristic depth (X*)	InputCharacteristicDepth_m	m	Distance from top of the soil compartment at which soil concentration has dropped to 36.79% (1/e * 100%) of the concentration at top of compartment	all
Soil-water partition coefficient (K_d)	Kd	L[water]/kg[soil wet wt]	Equilibrium ratio of concentration sorbed to solids and concentration dissolved	all

Chemical-Dependent -- Abiotic

Soil Compartment Types

Parameter Name (TSD Symbol)	TRIM FaTE Code Name	Input Units	Description	Applicable Chemicals
Use input characteristic depth	UseInputCharacteristicDepth_0_MeansNo_ElseYes	0 = no , Else = yes	If = 0, use model-calculated characteristic depth, else use user-provided characteristic depth	all
Demethylation rate (k_{Dm})	DemethylationRate	1/day	First-order rate constant for demethylation (MHg->Hg2)	MHg
Methylation rate (k_M)	MethylationRate	1/day	First-order rate constant for methylation (Hg2->MHg)	Hg2
Oxidation rate (k_O)	OxidationRate	1/day	First-order rate constant for oxidation (Hg0->Hg2)	Hg0
Reduction rate (k_R)	ReductionRate	1/day	First-order rate constant for reduction (Hg2->Hg0)	Hg2
Half-life *(half-life)*	Halflife	day	Length of time for chemical amount to be reduced by one-half by degradation reactions	organics
Vadose Zone Soil Compartment Type				
Initial concentration	initialConcentration_g_per_m3	g/m^3	Bulk vadose zone soil concentration at beginning of modeling period	all
Input characteristic depth (X*)	InputCharacteristicDepth_m	m	Distance from top of the soil compartment at which soil concentration has dropped to 36.79% (1/e * 100%) of the concentration at top of compartment	all
Soil-water partition coefficient (K_d)	Kd	L[water]/kg[soil wet wt]	Equilibrium ratio of concentration sorbed to solids and concentration dissolved	all
Use input characteristic depth	UseInputCharacteristicDepth_0_MeansNo_ElseYes	0 = no , Else = yes	If = 0, use model-calculated characteristic depth, else use user-provided characteristic depth	all
Demethylation rate (k_{Dm})	DemethylationRate	1/day	First-order rate constant for demethylation (MHg->Hg2)	MHg
Methylation rate (k_M)	MethylationRate	1/day	First-order rate constant for methylation (Hg2->MHg)	Hg2
Oxidation rate (k_O)	OxidationRate	1/day	First-order rate constant for oxidation (Hg0->Hg2)	Hg0
Reduction rate (k_R)	ReductionRate	1/day	First-order rate constant for reduction (Hg2->Hg0)	Hg2
Half-life *(half-life)*	Halflife	day	Length of time for chemical amount to be reduced by one-half by degradation reactions	organics

Chemical-Dependent -- Abiotic

Soil Compartment Types

Parameter Name (TSD Symbol)	TRIM FaTE Code Name	Input Units	Description	Applicable Chemicals
Ground Water Compartment Type				
Initial concentration	initialConcentration_g_per_L	g/L	Ground water concentration at beginning of modeling period	all
Soil-water partition coefficient (K_d)	Kd	L[water]/kg[soil wet wt]	Equilibrium ratio of concentration sorbed to solids and concentration dissolved	all
Demethylation rate (k_{Dm})	DemethylationRate	1/day	First-order rate constant for demethylation (MHg->Hg2)	MHg
Methylation rate (k_M)	MethylationRate	1/day	First-order rate constant for methylation (Hg2->MHg)	Hg2
Oxidation rate (k_O)	OxidationRate	1/day	First-order rate constant for oxidation (Hg0->Hg2)	Hg0
Reduction rate (k_R)	ReductionRate	1/day	First-order rate constant for reduction (Hg2->Hg0)	Hg2
Half-life *(half-life)*	Halflife	day	Length of time for chemical amount to be reduced by one-half by degradation reactions	organics

Chemical-Dependent -- Abiotic

Surface Water Compartment Type

Parameter Name (TSD Symbol)	TRIM FaTE Code Name	Input Units	Description	Applicable Chemicals
Initial concentration	initialConcentration_g_per_L	g/L	Surface water concentration at beginning of modeling period	all
Algal surface area-specific uptake rate constant (U)	AlgaeUptakeRate	nmol/[μm^2-day-nmol]	Surface area-specific rate constant for uptake into algae of a chemical in water	Hg species
BCF-algae	RatioOfConcinAlgaeToConcDissolvedinWater	L[water]/kg[algae wet wt]	Ratio of concentration in algae to concentration dissolved in surface water (bioconcentration factor)	organics
Dow ("overall Kow") (D_{ow})	D_ow	unitless	Weighted (by mass fraction) sum of individual Kow values for all chemical species present	Hg species[a]
Soil-water partition coefficient (K_d)	Kd	L[water]/kg[soil wet wt]	Equilibrium ratio of concentration sorbed to solids and concentration dissolved	all
Vapor dry deposition velocity (v_{vapor})	VaporDryDepositionVelocity_m_day	m/day	Speed at which chemical in vapor form in air moves downward; used in estimating dry deposition of vapors to surface water	Hg2
Demethylation rate (k_{Dm})	DemethylationRate	1/day	First-order rate constant for demethylation (MHg->Hg2)	MHg
Methylation rate (k_M)	MethylationRate	1/day	First-order rate constant for methylation (Hg2->MHg)	Hg2
Oxidation rate (k_O)	OxidationRate	1/day	First-order rate constant for oxidation (Hg0->Hg2)	Hg0
Reduction rate (k_R)	ReductionRate	1/day	First-order rate constant for reduction (Hg2->Hg0)	Hg2
Half-life *(half-life)*	Halflife	day	Length of time for chemical amount to be reduced by one-half by degradation reactions	organics

[a] For Hg2 and MHg, Dow is included in TRIM.FaTE as a Formula Property (calculated within TRIM.FaTE) rather than a Constant Property (supplied as an input) because the value is dependent on surface water pH and chloride concentration. However, the relationships between Dow and pH and chloride are a user input.

Chemical-Dependent -- Abiotic

Sediment Compartment Type

Parameter Name (TSD Symbol)	TRIM FaTE Code Name	Input Units	Description	Applicable Chemicals
Initial concentration	initialConcentration_g_per_m3	g/m^3	Bulk sediment concentration at beginning of modeling period	all
Soil-water partition coefficient (K_d)	Kd	L[water]/kg[soil wet wt]	Equilibrium ratio of concentration sorbed to solids and concentration dissolved	all
Demethylation rate (k_{Dm})	DemethylationRate	1/day	First-order rate constant for demethylation (MHg->Hg2)	MHg
Methylation rate (k_M)	MethylationRate	1/day	First-order rate constant for methylation (Hg2->MHg)	Hg2
Oxidation rate (k_O)	OxidationRate	1/day	First-order rate constant for oxidation (Hg0->Hg2)	Hg0
Reduction rate (k_R)	ReductionRate	1/day	First-order rate constant for reduction (Hg2->Hg0)	Hg2
Half-life *(half-life)*	Halflife	days	Length of time for chemical amount to be reduced by one-half by degradation reactions	organics

Chemical-Dependent -- Biotic

Terrestrial Plant Compartment Types[a]

Parameter Name (TSD Symbol)	TRIM FaTE Code Name	Input Units	Description	Applicable Chemicals
Leaf Compartment Type				
Initial concentration	initialConcentration_g_per_kg	g/kg	Leaf concentration at beginning of modeling period (wet wt basis)	all
Transfer factor to leaf particle ($T_{Leaf\rightarrow LeafP}$)	TransferFactortoLeafParticle	1/day	First-order rate constant for transfer from leaf to leaf particle	all
Demethylation rate (k_{Dm})	DemethylationRate	1/day	First-order rate constant for demethylation (MHg->Hg2)	MHg
Methylation rate (k_M)	MethylationRate	1/day	First-order rate constant for methylation (Hg2->MHg)	Hg2
Oxidation rate (k_O)	OxidationRate	1/day	First-order rate constant for oxidation (Hg0->Hg2)	Hg0
Reduction rate (k_R)	ReductionRate	1/day	First-order rate constant for reduction (Hg2->Hg0)	Hg2
Half-life *(half-life)*	Halflife	day	Length of time for chemical amount to be reduced by one-half by degradation reactions	organics
Particle-on-Leaf Compartment Type				
Initial concentration	initialConcentration_g_per_kg	g/kg	Particle on leaf concentration at beginning of modeling period (dry wt basis)	all
Transfer factor to leaf ($T_{LeafP\rightarrow Leaf}$)	TransferFactortoLeaf	1/day	First-order rate constant for transfer from leaf particle to leaf	all
Demethylation rate (k_{Dm})	DemethylationRate	1/day	First-order rate constant for demethylation (MHg->Hg2)	MHg
Methylation rate (k_M)	MethylationRate	1/day	First-order rate constant for methylation (Hg2->MHg)	Hg2
Oxidation rate (k_O)	OxidationRate	1/day	First-order rate constant for oxidation (Hg0->Hg2)	Hg0
Reduction rate (k_R)	ReductionRate	1/day	First-order rate constant for reduction (Hg2->Hg0)	Hg2
Half-life *(half-life)*	Halflife	day	Length of time for chemical amount to be reduced by one-half by degradation reactions	organics

Chemical-Dependent -- Biotic

Terrestrial Plant Compartment Types[a]

Parameter Name (TSD Symbol)	TRIM FaTE Code Name	Input Units	Description	Applicable Chemicals
Root Compartment Type - Nonwoody Plants Only[b]				
Initial concentration	initialConcentration_g_per_kg	g/kg	Root concentration at beginning of modeling period (wet wt basis)	all
Alpha for root-root zone bulk soil (α)	Root_RootZonePartitioningBulkSoil_AlphaofSteadyState	unitless	Proportion of equilibrium value reached	Hg species
Alpha for root-soil water interaction (α)	RootSoilWaterInteraction_Alpha	unitless	Proportion of equilibrium value reached	organics
Root/root-zone-soil-water partition coefficient ($K_{Root-SrW}$)	Root_RootZonePartitioningBulkSoil_PartitionCoefficient	m^3[water]/m^3[root]	Equilibrium ratio of concentration in root to concentration in root zone	Hg species
talpha for root-root zone bulk soil (t_α)	Root_RootZonePartitioningBulkSoil_TimetoReachAlphaofSteadyState	day	Time to reach 100α percent of equilibrium	Hg species
Demethylation rate (k_{Dm})	DemethylationRate	1/day	First-order rate constant for demethylation (MHg->Hg2)	MHg
Methylation rate (k_M)	MethylationRate	1/day	First-order rate constant for methylation (Hg2->MHg)	Hg2
Oxidation rate (k_O)	OxidationRate	1/day	First-order rate constant for oxidation (Hg0->Hg2)	Hg0
Reduction rate (k_R)	ReductionRate	1/day	First-order rate constant for reduction (Hg2->Hg0)	Hg2
Half-life *(half-life)*	Halflife	day	Length of time for chemical amount to be reduced by one-half by degradation reactions	organics
Stem Compartment Type - Nonwoody Plants Only[b]				
Initial concentration	initialConcentration_g_per_kg	g/kg	Stem concentration at beginning of modeling period (wet wt basis)	all
Transpiration stream concentration factor (TSCF)	TSCF	g[chemical]/m^3[xylem] per g[chemical]/m^3[soil pore water])	Ratio of concentration dissolved in xylem fluid to concentration dissolved in soil pore water	Hg species
Demethylation rate (k_{Dm})	DemethylationRate	1/day	First-order rate constant for demethylation (MHg->Hg2)	MHg
Methylation rate (k_M)	MethylationRate	1/day	First-order rate constant for methylation (Hg2->MHg)	Hg2
Oxidation rate (k_O)	OxidationRate	1/day	First-order rate constant for oxidation (Hg0->Hg2)	Hg0

Chemical-Dependent -- Biotic

Terrestrial Plant Compartment Types[a]

Parameter Name (TSD Symbol)	TRIM FaTE Code Name	Input Units	Description	Applicable Chemicals
Reduction rate (k_R)	ReductionRate	1/day	First-order rate constant for reduction (Hg2->Hg0)	Hg2
Half-life *(half-life)*	Halflife	day	Length of time for chemical amount to be reduced by one-half by degradation reactions	organics

[a] TRIM.FaTE currently includes four kinds of terrestrial plants: deciduous forest, coniferous forest, grasses/herbs, and agricultural.

[b] Roots and stems are not modeled for deciduous and coniferous forest in the current version of TRIM.FaTE.

Chemical-Dependent -- Biotic

Aquatic Plant Compartment Type

Parameter Name (TSD Symbol)	TRIM FaTE Code Name	Input Units	Description	Applicable Chemicals
Macrophyte Compartment Type				
Initial concentration	initialConcentration_g_per_kg	g/kg	Macrophyte concentration at beginning of modeling period (wet wt basis)	all
Alpha for macrophyte (α)	WaterColumnDissolvedPartitioning_AlphaofEquilibrium	unitless	Proportion of equilibrium value reached	Hg species
Macrophyte/water partition coefficient ($K_{Mp\text{-}W}$)	WaterColumnDissolvedPartitioning_PartitionCoefficient	L[water]/kg[macrophyte]	Equilibrium ratio of concentration in macrophyte to concentration dissolved in water	Hg species
Oxidation rate (k_O)	OxidationRate	1/day	First-order rate constant for oxidation (Hg0->Hg2)	Hg species
talpha (t_α)	WaterColumnDissolvedPartitioning_TimeToReachAlphaofEquilibrium	day	Time to reach 100α percent of equilibrium	Hg species
Half-life *(half-life)*	Halflife	day	Length of time for chemical amount to be reduced by one-half by degradation reactions	organics

Chemical-Dependent -- Biotic

Terrestrial Animal Compartment Types

Parameter Name (TSD Symbol)	TRIM FaTE Code Name	Input Units	Description	Applicable Chemicals
Soil Detritivore - Earthworm				
Initial concentration	initialConcentration_g_per_kg	g/kg	Earthworm concentration at beginning of modeling period (wet wt basis)	all
Alpha for earthworm-soil pore water (α)	WormSoilWaterInteraction_alpha	unitless	Proportion of equilibrium value reached	organics
Alpha for worm-bulk soil (α)	WormSoilInteraction_alpha	unitless	Proportion of equilibrium value reached	Hg species
Earthworm/dry-soil partition coefficient ($K_{dworm\text{-}Sr\text{-}dry}$)	WormSoilPartitionCoefficient_dryweight	kg [soil dry wt]/kg[worm dry wt]	Equilibrium ratio of concentration in earthworm to concentration in soil (dry wt basis)	Hg species
talpha for earthworm-soil pore water (t_α)	WormSoilWaterInteraction_t_alpha	day	Time to reach 100α percent of equilibrium	organics
talpha for worm-bulk soil (t_α)	WormSoilInteraction_t_alpha	day	Time to reach 100α percent of equilibrium	Hg species
Half-life *(half-life)*	Halflife	day	Length of time for chemical amount to be reduced by one-half by degradation reactions	organics
Soil Detritivore - Soil Arthropod				
Initial concentration	initialConcentration_g_per_kg	g/kg	Soil arthropod concentration at beginning of modeling period (wet wt basis)	all
Alpha for arthropod-soil (α)	ArthropodSoilPartitioning_AlphaofEquilibrium	unitless	Proportion of equilibrium value reached	all
Arthropod/bulk-soil partition coefficient ($K_{Arth\text{-}Sr}$)	Arthropod_SoilPartitionCoefficient	kg[soil wet wt]/kg[arthropod wet wt])	Equilibrium ratio of concentration in arthropod to concentration in soil	all
talpha for arthropod-soil (t_α)	ArthropodSoilPartitioning_TimetoReachAlphaofEquilibrium	day	Time to reach 100α percent of equilibrium	all
Half-life *(half-life)*	Halflife	day	Length of time for chemical amount to be reduced by one-half by degradation reactions	organics
All Other Terrestrial Animal Compartment Types[a]				
Initial concentration	initialConcentration_g_per_kg	g/kg	Terrestrial animal concentration at beginning of modeling period (wet wt basis)	all
Assimilation efficiency for inhalation (AE_{Air})	InhalationAssimilationEfficiency	unitless	Fraction of amount of chemical breathed that is actually absorbed by the animal	all
Assimilation efficiency from arthropods (AE_{Arth})	AssimilationEfficiencyFromArthropods	unitless	Fraction of amount of chemical in arthropods eaten that is actually absorbed by the animal	all

Chemical-Dependent -- Biotic

Terrestrial Animal Compartment Types

Parameter Name (TSD Symbol)	TRIM FaTE Code Name	Input Units	Description	Applicable Chemicals
Assimilation efficiency from food (AE_{Twl})	AssimilationEfficiencyFromFood	unitless	Fraction of amount of chemical in food eaten that is actually absorbed by the animal	all
Assimilation efficiency from plants (AE_{Plant})	AssimilationEfficiencyFromPlants	unitless	Fraction of amount of chemical in plants eaten that is actually absorbed by the animal	all
Assimilation efficiency from soils (AE_{S})	AssimilationEfficiencyFromSoils	unitless	Fraction of amount of chemical in soils eaten that is actually absorbed by the animal	all
Assimilation efficiency from water (AE_{W})	AssimilationEfficiencyFromWater	unitless	Fraction of amount of chemical in drinking water that is actually absorbed by the animal	all
Assimilation efficiency from worms (AE_{Worm})	AssimilationEfficiencyFromWorms	unitless	Fraction of amount of chemical in worms eaten that is actually absorbed by the animal	all
Total elimination rate (k_{ET})	TotalExcretionRate	1/day	First-order rate constant for elimination of chemical from the body (in urine, feces, feathers, fur)	Hg species
Demethylation rate (k_{Dm})	DemethylationRate	1/day	First-order rate constant for demethylation (MHg->Hg2)	MHg
Methylation rate (k_{M})	MethylationRate	1/day	First-order rate constant for methylation (Hg2->MHg)	Hg2
Oxidation rate (k_{O})	OxidationRate	1/day	First-order rate constant for oxidation (Hg0->Hg2)	Hg0
Reduction rate (k_{R})	ReductionRate	1/day	First-order rate constant for reduction (Hg2->Hg0)	Hg2

[a] TRIM.FaTE currently includes the following terrestrial animal compartment types: Terrestrial Ground-invertebrate Feeder - American Woodcock, Terrestrial Ground-invertebrate Feeder - Black-capped Chickadee, Terrestrial Ground-invertebrate Feeder - Short-tailed Shrew, Terrestrial Ground-invertebrate Feeder - Trowbridge Shrew, Terrestrial Herbivore - Bobwhite Quail, Terrestrial Herbivore - Cow, Terrestrial Herbivore - Long-tailed Vole, Terrestrial Herbivore - Meadow Vole, Terrestrial Herbivore - Mule Deer/Black-tailed Deer, Terrestrial Herbivore - White-tailed Deer, Terrestrial Insectivore - Tree Swallow, Terrestrial Omnivore - American Robin, Terrestrial Omnivore - Mouse, Terrestrial Predator/Scavenger - Long-tailed Weasel, and Terrestrial Predator/Scavenger - Red-tailed Hawk.

Chemical-Dependent -- Biotic

Semi-aquatic Animal Compartment Types[a]

Parameter Name (TSD Symbol)	TRIM FaTE Code Name	Input Units	Description	Applicable Chemicals
Initial concentration	initialConcentration_g_per_kg	g/kg	Semiaquatic animal concentration at beginning of modeling period (wet wt basis)	all
Assimilation efficiency for inhalation (AE_{Air})	InhalationAssimilationEfficiency	unitless	Fraction of amount of chemical breathed that is actually absorbed by the animal	all
Assimilation efficiency from arthropods (AE_{Arth})[b]	AssimilationEfficiencyFromArthropods	unitless	Fraction of amount of chemical in arthropods eaten that is actually absorbed by the animal	all
Assimilation efficiency from food (AE_{Twl})(AE_{Fish})[c]	AssimilationEfficiencyFromFood	unitless	Fraction of amount of chemical in food eaten that is actually absorbed by the animal	all
Assimilation efficiency from plants (AE_{Plant})[b]	AssimilationEfficiencyFromPlants	unitless	Fraction of amount of chemical in plants eaten that is actually absorbed by the animal	all
Assimilation efficiency from soils (AE_S)	AssimilationEfficiencyFromSoils	unitless	Fraction of amount of chemical in soils eaten that is actually absorbed by the animal	all
Assimilation efficiency from water (AE_W)	AssimilationEfficiencyFromWater	unitless	Fraction of amount of chemical in drinking water that is actually absorbed by the animal	all
Assimilation efficiency from worms (AE_{Worm})[d]	AssimilationEfficiencyFromWorms	unitless	Fraction of amount of chemical in worms eaten that is actually absorbed by the animal	all
Total elimination rate (k_{ET})	TotalExcretionRate	1/day	First-order rate constant for elimination of chemical from the body (in urine, feces, feathers, fur)	Hg species
Demethylation rate (k_{Dm})	DemethylationRate	1/day	First-order rate constant for demethylation (MHg->Hg2)	MHg
Methylation rate (k_M)	MethylationRate	1/day	First-order rate constant for methylation (Hg2->MHg)	Hg2
Oxidation rate (k_O)	OxidationRate	1/day	First-order rate constant for oxidation (Hg0->Hg2)	Hg0
Reduction rate (k_R)	ReductionRate	1/day	First-order rate constant for reduction (Hg2->Hg0)	Hg2

[a] TRIM.FaTE currently includes the following semi-aquatic animal compartment types: Semi-aquatic Omnivore - Mallard, Semi-aquatic Omnivore - Mink, Semi-aquatic Omnivore - Raccoon, Semi-aquatic Piscivore - Common Loon, Semi-aquatic Piscivore - Kingfisher, and Semi-aquatic Predator/Scavenger - Bald Eagle.

[b] Parameter applies only to Semi-aquatic Omnivore - Mallard.

[c] TSD uses two symbols, one for terrestrial wildlife and one for fish.

[d] Parameter applies only to Semi-aquatic Omnivore - Raccoon.

Chemical-Dependent -- Biotic

Aquatic Animal Compartment Types

Parameter Name (TSD Symbol)	TRIM FaTE Code Name	Input Units	Description	Applicable Chemicals
Benthic Invertebrate Compartment Type				
Initial concentration	initialConcentration_g_per_kg	g/kg	Benthic invertebrate concentration at beginning of modeling period (wet wt basis)	all
Alpha (α)	SedimentPartitioning_AlphaofEquilibrium	unitless	Proportion of equilibrium value reached	Hg species
Benthic invertebrate-bulk sediment partition coefficient ($K_{BI\text{-}Sed}$)	SedimentPartitioning_PartitionCoefficient	kg[sediment wet wt]/kg[invertebrates wet wt]	Equilibrium ratio of concentration in benthic invertebrate to concentration in sediment	Hg species
Clearance constant (CL_u)	ClearanceConstant	L[water cleared]/kg[BI wet wt]-hr	Rate of water passing over respiratory surface scaled to benthic invertebrate mass	organics
talpha (t_α)	SedimentPartitioning_TimeToReachAlphaofEquilibrium	day	Time to reach 100α percent of equilibrium	Hg species
Proportionality constant (p_c)	V_d	L[water]/kg[BI wet wt]	Ratio of concentration in benthic invertebrates to concentration in water	organics
Half-life *(half-life)*	Halflife	day	Length of time for chemical amount to be reduced by one-half by degradation reactions	organics
All Fish Compartment Types[a]				
Initial concentration	initialConcentration_g_per_kg	g/kg	Fish concentration at beginning of modeling period (wet wt basis)	all
Gamma_fish (γ_{ASF})	Gamma_fish	unitless	Allometric scaling factor used in estimating gill uptake	organics
Demethylation rate (k_{Dm})	DemethylationRate	1/day	First-order rate constant for demethylation (MHg->Hg2)	MHg
Methylation rate (k_M)	MethylationRate	1/day	First-order rate constant for methylation (Hg2->MHg)	Hg2
Oxidation rate (k_O)	OxidationRate	1/day	First-order rate constant for oxidation (Hg0->Hg2)	Hg0
Reduction rate (k_R)	ReductionRate	1/day	First-order rate constant for reduction (Hg2->Hg0)	Hg2
Half-life *(half-life)*	Halflife	day	Length of time for chemical amount to be reduced by one-half by degradation reactions	organics

Chemical-Dependent -- Biotic

Aquatic Animal Compartment Types

Parameter Name (TSD Symbol)	TRIM FaTE Code Name	Input Units	Description	Applicable Chemicals
Water-column Carnivore Compartment Type				
Alpha for water-column carnivore (α)	OmnivorePartitioning_AlphaofEquilibrium	unitless	Proportion of equilibrium value reached	Hg species
Assimilation efficiency from food (AE_D)	AssimilationEfficiencyFromFood	unitless	Fraction of amount of chemical in food eaten that is actually absorbed by the fish	all
Elimination adjustment factor	HowMuchFasterHgEliminationIsThanForMHg	unitless	Factor used to adjust experimental data on elimination rate for MHg to Hg0 and Hg2	Hg species
Fish(water-column carnivore)-fish(water-column omnivore) partition coefficient ($K_{Fwcc\text{-}Fwco}$)	OmnivorePartitioning_PartitionCoefficient	kg[Fwco wet wt]/kg[Fwcc wet wt]	Equilibrium ratio of concentration in water-column carnivore to concentration in water-column omnivore	Hg species
talpha for water-column carnivore (t_α)	OmnivorePartitioning_TimeToReachAlphaofEquilibrium	day	Time to reach 100α percent of equilibrium	Hg species
Water-column Herbivore Compartment Type				
Alpha for algae (α)	AlgaePartitioning_AlphaofEquilibrium	unitless	Proportion of equilibrium value reached	Hg species
Assimilation efficiency from food (AE_D)	AssimilationEfficiencyFromFood	unitless	Fraction of amount of chemical in food eaten that is actually absorbed by the fish	all
Elimination adjustment factor	HowMuchFasterHgEliminationIsThanForMHg	unitless	Factor used to adjust experimental data on elimination rate for MHg to Hg0 and Hg2	Hg species
Fish (water-column herbivore)-algae partition coefficient ($K_{Fwch\text{-}Algae}$)	AlgaePartitioning_PartitionCoefficient	kg[algae wet wt]/kg[Fwch wet wt]	Equilibrium ratio of concentration in water-column herbivore to concentration in algae	Hg species
talpha for algae (t_α)	AlgaePartitioning_TimeToReachAlphaofEquilibrium	day	Time to reach 100α percent of equilibrium	Hg species
Water-column Omnivore Compartment Type				
Alpha for water-column herbivore (α)	HerbivorePartitioning_AlphaofEquilibrium	unitless	Proportion of equilibrium value reached	Hg species
Assimilation efficiency from food (AE_D)	AssimilationEfficiencyFromFood	unitless	Fraction of amount of chemical in food eaten that is actually absorbed by the fish	all
Elimination adjustment factor	HowMuchFasterHgEliminationIsThanForMHg	unitless	Factor used to adjust experimental data on elimination rate for MHg to Hg0 and Hg2	Hg species
Fish (water-column omnivore)-fish (water-column herbivore) partition coefficient ($K_{Fwco\text{-}Fwch}$)	HerbivorePartitioning_PartitionCoefficient	kg[Fwch wet wt]/kg[Fwco wet wt]	Equilibrium ratio of concentration in water-column omnivore to concentration in water-column herbivore	Hg species

Chemical-Dependent -- Biotic

Aquatic Animal Compartment Types

Parameter Name (TSD Symbol)	TRIM FaTE Code Name	Input Units	Description	Applicable Chemicals
talpha for water-column herbivore (t_α)	HerbivorePartitioning_TimeToReachAlphaofEquilibrium	day	Time to reach 100α percent of equilibrium	Hg species
Benthic Carnivore Compartment Type				
Alpha for benthic omnivore (α)	BenthicOmnivorePartitioning_AlphaofEquilibrium	unitless	Proportion of equilibrium value reached	Hg species
Assimilation efficiency from food (AE_D)	AssimilationEfficiencyFromFood	unitless	Fraction of amount of chemical in food eaten that is actually absorbed by the fish	all
Elimination adjustment factor	HowMuchFasterHgEliminationIsThanForMHg	unitless	Factor used to adjust experimental data on elimination rate for MHg to Hg0 and Hg2	Hg species
Fish(benthic carnivore)-fish(benthic omnivore) partition coefficient ($K_{Fbc\text{-}Fbo}$)	BenthicOmnivorePartitioning_PartitionCoefficient	kg[Fbo wet wt]/kg[Fbc wet wt]	Equilibrium ratio of concentration in benthic carnivore to concentration in benthic omnivore	Hg species
talpha for benthic omnivore (t_α)	BenthicOmnivorePartitioning_TimeToReachAlphaofEquilibrium	day	Time to reach 100α percent of equilibrium	Hg species
Benthic Omnivore Compartment Type				
Alpha for benthic omnivore (α)	BenthicInvertebratePartitioning_AlphaofEquilibrium	unitless	Proportion of equilibrium value reached	Hg species
Assimilation efficiency from food (AE_D)	AssimilationEfficiencyFromFood	unitless	Fraction of amount of chemical in food eaten that is actually absorbed by the fish	all
Elimination adjustment factor	HowMuchFasterHgEliminationIsThanForMHg	unitless	Factor used to adjust experimental data on elimination rate for MHg to Hg0 and Hg2	Hg species
Fish(benthic omnivore)-benthic invertebrate partition coefficient ($K_{Fbo\text{-}BI}$)	BenthicInvertebratePartitioning_PartitionCoefficient	kg[BI wet wt]/kg[Fbo wt wt]	Equilibrium ratio of concentration in benthic omnivore to concentration in benthic invertebrate	Hg species
talpha for benthic omnivore (t_α)	BenthicInvertebratePartitioning_TimeToReachAlphaofEquilibrium	day	Time to reach 100α percent of equilibrium	Hg species

[a] TRIM.FaTE currently includes the following fish compartment types: Benthic Carnivore, Benthic Omnivore, Water-column Carnivore, Water-column Herbivore, and Water-column Omnivore.

Source, Meteorological, and Other Input Data and Settings

Parameter Name (TSD Symbol)	TRIM FaTE Code Name	Input Units	Description
Source Inputs (all TRIM.FaTE source properties)[a]			
Emission rate (needed for each chemical emitted)	emissionRate	g/day	Quantity of chemical emitted from the source per unit time
Source location	X, Y	x and y spatial coordinates	X-and Y-coordinates of the source (can be designated as UTM or latitude/longitude)
Source height	elevation	m	Height of the emission point(s) above ground level
Meteorological Inputs (all TRIM.FaTE scenario properties)[b]			
Air temperature (T)	AirTemperature_K	degrees K	Temperature of the air
Horizontal wind speed (v or μ)[c]	horizontalWindSpeed	m/sec	Wind speed horizontally between volume elements
Wind direction (ϑ)	windDirection	degrees clockwise from N (blowing from)	Direction from which the wind is blowing (degrees clockwise from due north)
Rainfall rate (rain)	Rain	m^3[rain]/m^2[surface area]-day	Amount of precipitation per unit surface area and unit time
Day/night (IsDay)	isDay	1=day, 0=night	Day/night switch; used for certain plant algorithms
Other Settings (all TRIM.FaTE scenario properties)			
Start of simulation	simulationBeginDateTime	date/time	The starting date and time for the modeling period
End of simulation	simulationEndDateTime	date/time	The inclusive ending date and time for the modeling period
Simulation time step	simulationTimeStep	hr	The duration (hours) of each time increment at which the model calculates and stores a new moles/mass distribution; must be an integer value
Output time step[d]	N/A	hr	The time increment at which the model reports a new moles/mass distribution (based on distributions calculated at simulation time steps); must be an integer value and evenly divisible by the selected simulation time step

[a] Separate source inputs are needed for each source modeled.

Source, Meteorological, and Other Input Data and Settings

Parameter Name (TSD Symbol)	TRIM FaTE Code Name	Input Units	Description

[b] The meteorological parameter “mixing height” is not required for any algorithms, but can be used to set the vertical boundary (top) of a layer of air volume elements. The meteorological parameter “stability class” is not currently used in any algorithms, but may be in the future and is a required model input (named stabilityClass, input as an integer value of 1 through 6, representing stability classes A through F, respectively). (Because it is not currently used in any algorithms, dummy values may be used as inputs, if desired).

[c] When multiple layers of air compartments are modeled, vertical wind speed (m/sec, positive for up and negative for down) is also an input parameter. To date, the modeling of multiple air layers in TRIM.FaTE has not been fully implemented and tested.

[d] Not a direct model input, but set using the scenario property, simulationStepsPerOutput (simulationStepsPerOutput is determined by dividing the desired output time step by the selected simulation time step).

TECHNICAL REPORT DATA
(Please read Instructions on reverse before completing)

1. REPORT NO. EPA-453/R-02-011b	2.	3. RECIPIENT'S ACCESSION NO.

4. TITLE AND SUBTITLE Total Risk Integrated Methodology.TRIM.FaTE Technical Support Document. Volume II: Description of Chemical Transport and Transformation Algorithms.	5. REPORT DATE September, 2002
	6. PERFORMING ORGANIZATION CODE
7. AUTHOR(S)	8. PERFORMING ORGANIZATION REPORT NO.
9. PERFORMING ORGANIZATION NAME AND ADDRESS U.S. Environmental Protection Agency Office of Air Quality Planning and Standards Emissions Standards & Air Quality Strategies and Standards Divisions Research Triangle Park, NC 27711	10. PROGRAM ELEMENT NO.
	11. CONTRACT/GRANT NO.
12. SPONSORING AGENCY NAME AND ADDRESS	13. TYPE OF REPORT AND PERIOD COVERED Technical Report
	14. SPONSORING AGENCY CODE EPA/200/04

15. SUPPLEMENTARY NOTES

Supplements EPA-453/R-02-011A; Supercedes EPA-452/D-98-001 and EPA-453/D-99-002B.

16. ABSTRACT

This report is part of a series of documentation for the Total Risk Integrated Methodology (TRIM). TRIM is a time series modeling system, with multimedia capabilities, designed for assessing human health and ecological risks from hazardous and criteria air pollutants. The detailed documentation of TRIM's logic, assumptions, equations, and input parameters is provided in comprehensive technical support documents for each of the three TRIM modules, as they are developed. This report documents the Environmental Fate, Transport, and Ecological Exposure module of TRIM (TRIM.FaTE) and is divided into two volumes. The first volume provides a description of terminology, model framework, and functionality of TRIM.FaTE, and the second volume presents a detailed description of the algorithms used in the module.

17. KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group
Risk Assessment Multimedia Modeling Exposure Assessment Air Pollutants	Air Pollution	

18. DISTRIBUTION STATEMENT Release Unlimited	19. SECURITY CLASS *(Report)* Unclassified	21. NO. OF PAGES 298
	20. SECURITY CLASS *(Page)* Unclassified	22. PRICE

EPA Form 2220-1 (Rev. 4-77) PREVIOUS EDITION IS OBSOLETE

United States
Environmental Protection
Agency

Office of Air Quality Planning and Standards
Emissions Standards & Air Quality Strategies and Standards Divisions
Research Triangle Park, NC

Publication No. EPA 453/R-02-011b
September 2002