# 5. CURRENT STATUS OF TRIM.FaTE

As discussed in Chapter 4, EPA has implemented many changes and additions to TRIM.FaTE since May 1998. This chapter summarizes the current status of the TRIM.FaTE module, including the compartment types that are addressed and the links and processes that are represented by the algorithms included in Prototype V.

**TRIM.FaTE HISTORY**

**Prototype I** was designed in 1997 to test the mass transfer methodology and the Livermore Solver for Ordinary Differential Equations (LSODE) utility. Air, soil, ground water, surface water, and fish compartment types were included. Chemical reaction was not simulated. The runs produced estimates of benzene mass throughout the system.

**Prototype II**, also developed in 1997, included more spatial detail in the types and number of compartments. It included multiple volume elements for soil and air compartment types and included plant and sediment compartments. Prototype II was developed using benzo(a)pyrene (B(a)P) as an example chemical. The links between compartments had multiple-phase (*i.e.*, gas, liquid, solid) mass transfers.

**Prototype III**, developed later in 1997 using B(a)P as an example chemical and greater complexity than previous prototypes, included a focus on code and input data structure refinements. This prototype was primarily developed to incorporate lessons learned from earlier prototypes, including a refined set of algorithms, and to set up the module for a case study model run using Prototype IV.

**Prototype IV**, developed in 1998 using B(a)P as an example chemical, was designed to be applied to an actual site rather than for evaluation simulations with generic inputs like the earlier prototypes. Prototype IV was used to evaluate the likely limits of TRIM.FaTE with respect to the number of land parcels and the length of time steps used.

**Prototype V**, the current prototype, addresses the issues identified by the SAB in their May 1998 advisory and includes additional and revised fate and transport algorithms. This prototype was designed to be applied to an actual site for a metal contaminant (*i.e.*, mercury) rather than an organic contaminant, as was the case for Prototype IV.

**Version 1.0** is a computer framework that is intended to support all of TRIM, although only TRIM.FaTE is currently implemented. While the prototype versions of TRIM.FaTE were developed using Microsoft Visual Basic™, Fortran, and Microsoft Excel™ software, Version 1.0 was developed using Java, C, and Fortran in a manner that allows it to run on multiple operating systems, including Windows and UNIX. Version 1.0 also provides improved management of multiple modeling scenarios and is more user-friendly and reliable. Version 1.0 is designed for assessments of any chemical, although it includes some specific algorithms for B(a)P and mercury.

## 5.1 COMPARTMENT TYPES

The TRIM.FaTE module includes both abiotic and biotic compartment types. The seven abiotic compartment types that are included in Prototype V of TRIM.FaTE are air, surface soil, root zone soil, vadose zone soil, surface water, sediment, and ground water. Biotic compartment types are generally defined by trophic group. Terrestrial plant compartment types include leaves, stems, leaf surfaces, and roots. Table 5-1 lists the 24 biotic compartment types that currently are included in TRIM.FaTE.

## 5.2 LINKS AND ALGORITHMS

Algorithms are used to model the transport of chemicals from one compartment to another (*i.e.*, through links) and the transformation of chemicals from one form to another within a compartment. Prototype V of TRIM.FaTE includes abiotic, biotic, and chemical- and chemical class-specific algorithms. Many algorithms are currently included in the algorithm library of TRIM.FaTE, and users can add algorithms to the library as needed.

### 5.2.1 ABIOTIC LINKS AND ALGORITHMS

Abiotic algorithms in TRIM.FaTE represent the transfer of chemicals from one abiotic compartment to other compartments of the same or different compartment type. The links between abiotic compartment types and the processes modeled by abiotic algorithms are provided in Table 5-2. The major changes and additions to abiotic algorithms since May 1998 are discussed in Chapter 4, and detailed information on abiotic algorithms is provided in Chapters 3 through 7 of the TRIM.FaTE TSD Volume II.

**KEY TERMS**

A **chemical** is a unit whose mass is being modeled. A chemical can be any element or compound, or even group of compounds, assuming the necessary parameters (*e.g.*, molecular weight, diffusion coefficient in air) are defined.

A **compartment** is a homogeneous unit of space characterized by its physical composition and within which it is assumed, for modeling purposes, that all chemical mass is in equilibrium.

A **compartment type** is a specific kind of compartment, such as an air compartment type or a mule deer compartment type. Compartment types are distinguished from each other by the way they exchange chemical mass with other compartment types.

An **abiotic compartment type** is one consisting primarily of a non-living environmental medium (*e.g.*, air, soil) for which TRIM.FaTE calculates chemical masses and concentrations; it may also contain biota, such as the microorganisms responsible for chemical transformation.

A **biotic compartment type** is one consisting of a population or community of living organisms (*e.g.*, bald eagle, benthic invertebrate), or in the case of terrestrial plants, portions of living organisms (*e.g.*, stems, leaves), for which TRIM.FaTE calculates chemical masses and concentrations.

A **volume element** is a bounded three-dimensional space that defines the location of one or more compartments. This term is introduced to provide a consistent method for organizing objects that have a natural spatial relationship.

A **link** is a connection that allows the transfer of chemical mass between any two compartments. Each link is implemented by an algorithm or algorithms that mathematically represent the mass transfer.

A **source** is an external component that introduces chemical mass directly into a compartment.

**Table 5-1**
**Compartment Types in TRIM.FaTE**

| Abiotic Compartment Types | Biotic Compartment Types |
|---|---|
| Air | Leaf |
| Surface soil | Leaf surface |
| Root zone soil | Stem |
| Vadose zone soil | Root |
| Surface water | Algae |
| Sediment | Macrophyte |
| Ground water | Water column herbivore |
| | Water column omnivore |
| | Water column carnivore |
| | Benthic invertebrate |
| | Benthic omnivore |
| | Benthic carnivore |
| | Terrestrial omnivore |
| | Semiaquatic piscivore |
| | Terrestrial herbivore |
| | Semiaquatic predator/scavenger |
| | Terrestrial insectivore |
| | Semiaquatic herbivore |
| | Terrestrial predator/scavenger [a] |
| | Semiaquatic insectivore |
| | Semiaquatic omnivore |
| | Terrestrial ground-invertebrate feeder |
| | Flying insect |
| | Soil detritivore |

[a] Includes terrestrial carnivores (*e.g.*, hawks).

### 5.2.2 BIOTIC LINKS AND ALGORITHMS

Biotic compartments in TRIM.FaTE are linked, using biotic algorithms, to abiotic compartments through two principal chemical processes: diffusion and advection. For example, in the process of ingestion, chemicals are advected in the air or diet to a mammal or bird. Active uptake of chemicals that mimic nutrients is possible but not represented mechanistically in TRIM.FaTE.

Examples of links between biotic compartment types and between abiotic and biotic compartment types in TRIM.FaTE are shown in Figure 4-1 in the TRIM.FaTE TSD Volume I. Many of these links also are summarized below in Table 5-3, which shows the links between biotic compartment types and between abiotic and biotic compartment types and the processes that are modeled by biotic algorithms.

## Table 5-2
## Links and Processes Addressed for Abiotic Compartment Types

| Links Between Compartment Types | | |
|---|---|---|
| **Receiving** | **Sending** | **Processes Addressed** |
| Air | Air | Bulk Advection |
| | Surface Soil | Diffusion<br>Resuspension |
| | Surface Water | Diffusion |
| Surface Soil | Surface Soil | Diffusion<br>Erosion<br>Runoff |
| | Root Zone Soil | Diffusion |
| | Air | Diffusion<br>Dry Deposition<br>Wet Deposition |
| Root Zone Soil | Root Zone Soil | Diffusion<br>Percolation |
| | Surface Soil | Diffusion<br>Percolation |
| | Vadose Zone Soil | Diffusion |
| Vadose Zone Soil | Vadose Zone Soil | Diffusion<br>Percolation |
| | Root Zone Soil | Diffusion<br>Percolation |
| Surface Water | Surface Water | Bulk Advection<br>Dispersion |
| | Surface Soil | Erosion<br>Runoff |
| | Air | Dry Deposition<br>Wet Deposition<br>Diffusion |
| | Sediment | Resuspension<br>Pore Water Diffusion |
| Sediment | Surface Water | Abiotic Solids Settling<br>Pore Water Diffusion |
| Ground Water | Surface Water | Recharge |
| | Vadose Zone Soil | Percolation |
| Air Advection Sink | Air | Bulk Advection Beyond System Boundary |
| Surface Water Advection Sink | Surface Water | Bulk Advection Beyond System Boundary |
| Sediment Burial Sink | Sediment | Solids Advection Beyond System Boundary |

**Table 5-3**
**Links and Processes Addressed For Biotic Compartment Types**

| Links Between Compartment Types | | Processes Addressed |
|---|---|---|
| **Receiving** | **Sending** | |
| Leaf Surface | Air (Particulates) | Dry Deposition [b] |
| | Air (Rain Water) | Wet Deposition [b] |
| | Leaf | Diffusion/Advection |
| Surface Soil | Leaf Surface | Particle Washoff [b]<br>Litterfall [b] |
| | Leaf | Litterfall [b] |
| | Terrestrial Ground-Invertebrate Feeder | Excretion [a] |
| | Terrestrial Herbivore | |
| | Terrestrial Omnivore | |
| | Terrestrial Insectivore | |
| | Semiaquatic Omnivore | |
| | Predator/Scavenger | |
| | Semiaquatic Insectivore | |
| | Semiaquatic Herbivore | |
| | Semiaquatic Piscivore | |
| Leaf | Leaf Surface<br>Air<br>Stem | Uptake [a] |
| Air<br>Stem | Leaf | Diffusion/Advection |
| Root | Root Zone Soil | Uptake [a] |
| Stem | Root Zone Soil (Water Phase)<br>Leaf | Uptake [a] |
| Soil Detritivore | Root Zone Soil | Uptake [a] |
| Root Zone Soil | Root | Equilibrium Partitioning |
| | Soil Detritivore | |
| Flying Insect | Sediment | Uptake [a] |
| Terrestrial Ground-Invertebrate Feeder | Soil Detritivore<br>Surface Soil | Diet [b] |
| | Air | Inhalation [b] |

| Links Between Compartment Types | | Processes Addressed |
|---|---|---|
| Receiving | Sending | |
| Terrestrial Herbivore | Leaf<br>Leaf Surface<br>Surface Soil | Diet [b] |
| | Air | Inhalation [b] |
| Terrestrial Omnivore | Leaf<br>Leaf Surface<br>Soil Detritivore<br>Surface Soil | Diet [b] |
| | Air | Inhalation [b] |
| Terrestrial Insectivore | Soil Detritivore | Diet [b] |
| | Air | Inhalation [b] |
| Semiaquatic Omnivore | Benthic Invertebrate<br>Soil Detritivore<br>Herbivorous Fish<br>Omnivorous Fish<br>Carnivorous Fish<br>Surface Soil | Diet [b] |
| | Air | Inhalation [b] |
| Predator/Scavenger | Terrestrial Herbivore<br>Terrestrial Omnivore<br>Terrestrial Insectivore<br>Soil Detritivore<br>Benthic Invertebrate (Insect) | Diet [b] |
| Semiaquatic Insectivore | Benthic Invertebrate (Insect) | Diet [b] |
| Semiaquatic Herbivore | Benthic Invertebrate<br>Leaf | Diet [b] |
| Semiaquatic Piscivore | Terrestrial Omnivore<br>Terrestrial Herbivore<br>Terrestrial Insectivore<br>Herbivorous Fish<br>Omnivorous Fish<br>Carnivorous Fish | Diet [b] |
| Surface Water | Semiaquatic Omnivore | Excretion |
| | Semiaquatic Insectivore | |
| | Semiaquatic Herbivore | |
| | Semiaquatic Piscivore | |
| | Algae | Equilibrium Partitioning [a] |
| | Macrophyte | |
| | Water Column Herbivorous Fish | Equilibrium Partitioning [ac] |
| | | Elimination [bd] |

| | | |
|---|---|---|
| Surface Water (continued) | Water Column Omnivorous Fish | Equilibrium Partitioning [ac] |
| | | Elimination [bd] |
| | Water Column Carnivorous Fish | Equilibrium Partitioning [ac] |
| | | Elimination [bd] |
| | Benthic Omnivorous Fish | Equilibrium Partitioning [ac] |
| | | Elimination [bd] |
| | Benthic Carnivorous Fish | Equilibrium Partitioning [ac] |
| | | Elimination [bd] |
| Algae | Surface Water | Uptake [a] |
| Macrophyte | Surface Water | Uptake [a] |
| Benthic Invertebrate | Sediment | Uptake [a] |
| Sediment | Benthic Invertebrate | Equilibrium Partitioning [a] |
| Water Column Herbivorous Fish [c] | Algae | Diet [b] |
| Water Column Herbivorous Fish [d] | Algae | Diet [b] |
| | Surface Water | Gill filtration [a] |
| Water Column Omnivorous Fish [c] | Herbivorous Fish | Diet [b] |
| Water Column Omnivorous Fish [d] | Herbivorous Fish | Diet [b] |
| | Surface Water | Gill filtration [a] |
| Water Column Carnivorous Fish [c] | Water Column Omnivorous Fish | Diet [b] |
| Water Column Carnivorous Fish [d] | Water Column Omnivorous Fish | Diet [b] |
| | Surface Water | Gill filtration [a] |
| Benthic Omnivorous Fish [c] | Benthic Invertebrate | Diet [b] |
| Benthic Omnivorous Fish [d] | Benthic Invertebrate | Diet [b] |
| | Surface Water | Gill filtration [a] |
| Benthic Carnivorous Fish [c] | Benthic Omnivorous Fish | Diet [b] |
| Benthic Carnivorous Fish [d] | Benthic Omnivorous Fish | Diet [b] |
| | Surface Water | Gill filtration [a] |

[a] Uptake, filtration, or partitioning which includes diffusion, advection, and/or active accumulation by organism.
[b] Advection processes.
[c] Equilibrium model for bioaccumulation by fish.
[d] Bioenergetic model for bioaccumulation by fish.

An alternative way to describe the chemical transfer processes and types of links handled by TRIM.FaTE is as follows:

- Diffusion of gaseous forms of elements into and out of plants following the concepts of conductance and resistance;

- Deposition of particles to the leaf surface;

- Equilibrium partitioning of chemicals from one environmental medium to another, using the time-to-equilibrium (*e.g.*, plant roots, soil detritivores, benthic invertebrates, algae, macrophytes, herbivorous fish, omnivorous fish, carnivorous fish); and

- Ingestion, inhalation, and excretion by terrestrial and semiaquatic wildlife.

All biotic transfer algorithms in TRIM.FaTE represent first-order chemical transfers between compartments. As for the abiotic compartments, there is no gradient of mass within a single compartment. For example, all of the plant leaves or benthic invertebrates within a single volume element have a homogeneous chemical concentration at any simulation time step. In addition, EPA developed mechanisms in TRIM.FaTE that allow the user to turn off or on particular algorithms at certain times (*e.g.*, at night, on a certain date such as the date of first or last frost).

### 5.2.3 CHEMICAL-SPECIFIC ALGORITHMS

As discussed in Chapter 4, TRIM.FaTE Prototype V includes some chemical- and chemical class-specific fate and transport algorithms for processes that are specific to particular chemicals and chemical classes. For such chemical classes, TRIM.FaTE can substitute the specific algorithms for certain of the more generic abiotic or biotic algorithms. Currently, TRIM.FaTE includes chemical-specific algorithms for three forms of mercury (elemental, divalent, methyl). Appendix A of the TRIM.FaTE TSD Volume II provides detailed information on these algorithms. In addition, TRIM.FaTE is designed to allow users to add chemical- and chemical class-specific algorithms to the algorithm library, as necessary.

Chemical-specific algorithms can also represent the transformation of chemicals from one form to another within a compartment. At this time, these algorithms consist of using input transformation rates.