3. OVERVIEW OF TRIM.FaTE CONCEPTS AND TERMINOLOGY

The TRIM.FaTE methodology integrates OAQPS' needs and multimedia modeling concepts into a unique model that serves as an integral part of the TRIM system. This chapter provides an overview of the terminology central to the TRIM.FaTE module. Note that the Glossary presented in Appendix A also provide brief definitions for key terms related to TRIM.Fate. An understanding of the terminology and concepts presented in this chapter is crucial to understanding the remainder of this report.

Because the terminology used in the world of environmental modeling can have multiple meanings and implications, it is essential in the initial steps of any model conceptualization that the terminology is clearly defined within the model framework. The terminology for multimedia modeling is particularly complicated because multimedia models are, by nature, multidisciplinary. Thus, terminology can be especially confusing because a single term can have different meanings in different disciplines. Three general modeling terms are defined, for the purposes of TRIM.FaTE, in the adjacent text box to provide a consistent basis for the discussion in this section and the remainder of the document.

GENERAL MODELING TERMS

Scenario: A specified set of conditions (*e.g.,* spatial, temporal, environmental, source, chemical) used to define a TRIM.FaTE model set-up for a particular simulation or set of simulations.

Simulation: A single application of TRIM.FaTE to estimate chemical transport and fate, based on a given scenario and any initial input values needed.

Project: A TRIM.FaTE computer framework for saving one or more scenarios and all of the data properties for the scenarios that pertain to a single model application.

The primary objective of the TRIM.FaTE module is to estimate the fate and transport of a chemical pollutant or pollutants over time through a modeled environment. Because the term "pollutant" can have various meanings, the modeled unit of chemical mass in TRIM.FaTE is referred to as a chemical. Within the context of TRIM.FaTE, a **chemical** is simply defined as a unit whose mass is being modeled by TRIM.FaTE. A chemical can be any element or compound, or even a group of compounds, assuming the necessary parameters (*e.g.*, molecular weight, diffusion coefficient in air) are defined. Examples of chemicals that may be modeled in TRIM.FaTE are polycyclic aromatic hydrocarbons (PAHs), methylmercury, elemental mercury, and benzene.

3.1 BASIC TRIM.FaTE TERMINOLOGY

In the TRIM.FaTE module, chemicals are contained within compartments. The term "compartment" is in some ways similar to what is referred to as a "medium" in environmental fate and transport modeling literature. However, the term "medium" was considered too limited in its scope because it generally invokes images of abiotic systems such as soil or air, while

TRIM.FaTE includes both abiotic and biotic systems. Therefore, the term compartment was adopted for TRIM.FaTE because it captures the flexibility of the TRIM.FaTE module in that it refers to both abiotic and biotic systems. Simply, a **compartment** is defined as the TRIM.FaTE modeling unit that contains chemical mass. Within TRIM.FaTE, chemical mass is transported between and transformed within compartments. A specific compartment is characterized by its physical and spatial composition and its relationship to other compartments. It is assumed, for modeling purposes, that all chemical mass within a compartment is homogeneously distributed and is in phase equilibrium. Multiple chemicals can exist within a compartment, and the various phases that compose a compartment (gases, liquids, solids) are generally assumed to be in equilibrium with respect to chemical partitioning (see TRIM.FaTE TSD Volume II for exceptions). Compartments can be either biotic, such as a deer compartment, or abiotic, such as a surface water compartment. Furthermore, two compartments could have identical compositions and only be distinguished by their location in the modeled environment; they are still separate compartments. It is important to note that biotic compartments do not refer to an individual organism, but instead to the population of that organism (or in some cases community, or other subgroup) within a specified spatial volume or area.

The term **compartment type** is used to denote a particular kind of compartment, such as an air compartment type or a soil detritivore compartment type. Compartment types are typically distinguished from each other by their basic characteristics and the way they exchange chemical mass with other compartment types. A compartment type can be thought of as a "template" for a specific, spatially defined and located compartment. A specific compartment is defined for a modeling scenario by first adding a copy of that "template" to the scenario and then defining its location and establishing its site-specific properties. Compartments of the same type are distinguished from each other in a given scenario by their location and sometimes also by the values that define their composition at a particular location. For example, two different surface soil compartments may have organic carbon fractions of 0.015 and 0.01, respectively, but they are both described by the compartment type called "surface soil."

SINKS

A sink is a special kind of compartment type that accounts for chemical mass no longer available for transport or uptake within a TRIM.FaTE simulation. Like other compartment types, sinks are linked to compartments, but sinks do not have a volume and, by definition, they do not have any loss processes associated with them (*i.e.*, they "receive" mass but do not "send" mass). There are three types of sinks: advection sinks, flush rate sinks, and degradation/reaction sinks. Advection sinks are linked to the outside edges of certain compartments (*e.g.*, air compartments) to account for chemical mass removed from the entire modeling region via advection from these compartments. Flush rate sinks are needed for each water body that "flushes" or releases water out of the modeled domain (*e.g.*, a river that flows across the boundary of the modeled region, or a lake that flushes its contents outside of the region). Degradation/reaction sinks are needed when modeling chemicals that degrade or are transformed into products whose fate after degradation/transformation is not tracked by the model.

In general, compartment types are classified as either abiotic or biotic (see also the text above describing sinks). An abiotic compartment type consists primarily of a non-living environmental medium[1] (*e.g.*, air, soil) for which TRIM.FaTE calculates chemical masses and concentrations. A biotic compartment type consists 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. Abiotic and biotic compartment types are discussed in more detail in Section 3.2.

Each compartment is associated with (contained within) a volume element. 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 locating and organizing objects that have a natural spatial relationship. In applications of TRIM.FaTE thus far, one (and only one) abiotic compartment is contained within any one volume element, and each volume element is identified by the abiotic compartment type it contains (*e.g.*, surface soil volume element, ground water volume element). In addition to the abiotic compartment, numerous biotic compartments may be contained within a single volume element (*e.g.*, multiple terrestrial biota compartment types along with a surface soil compartment may be contained within a surface soil volume element). Animals are typically associated with surface soil or surface water compartment types depending on where they usually reside and/or feed. For example, mallards generally feed in the water, so the mallard compartment type, when included in modeling, is placed along with the surface water compartment in one or more surface water volume elements. Terrestrial biota included in modeling are placed with the surface soil compartment in one or more surface soil volume elements. It should be noted, however, that animals are not restricted to feeding only in the volume element where they are located. The user may designate that a particular biotic compartment (*e.g.*, bald eagle) obtains its diet from compartments (*e.g.*, mouse) in more than one volume element.

The size and shape of volume elements for a given TRIM.FaTE application depend on the needs of the user. For example, if the user is most interested in the range of impacts of a chemical over a given water body, the water body could be divided into a number of volume elements with depth, length, and width. Typically, the higher the desired resolution, the greater the number and more complicated the shapes of the volume elements.

Figure 3-1 shows the basic spatial relationships between chemicals, compartments, and volume elements. This figure shows that chemicals are contained within compartments, and compartments are associated with volume elements. Figure 3-2 demonstrates how multiple compartments can exist within a single volume element. Because the air compartment is the only abiotic compartment within the volume element in Figure 3-1, this volume element is referred to as an air volume element. Likewise, the volume element in Figure 3-2 is referred to as a surface water volume element. Figure 3-3 applies the concepts presented in Figures 3-1 and 3-2 by dividing a hypothetical environment into volume elements and defining the compartments to be modeled within this framework.

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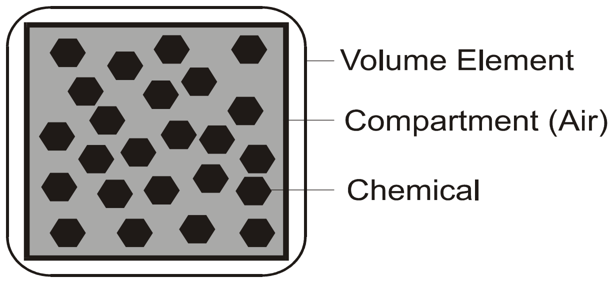
[1] When chemical transformation or degradation is modeled, an abiotic compartment may implicitly contain biota in the form of the microorganisms responsible for chemical transformation.

Figure 3-1
Simple TRIM.FaTE System[a]



[a] Chemicals shown in this figure, and all subsequent similar figures, are units of mass of the same chemical instead of multiple chemicals.

Figure 3-2
Multiple Compartments within a Single Volume Element

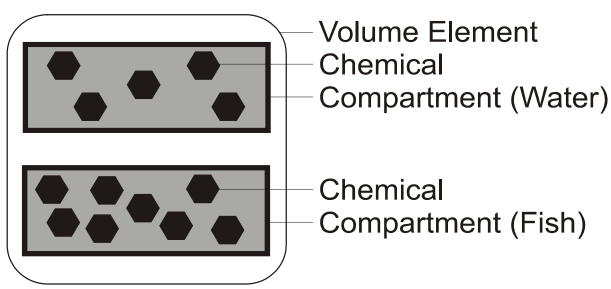
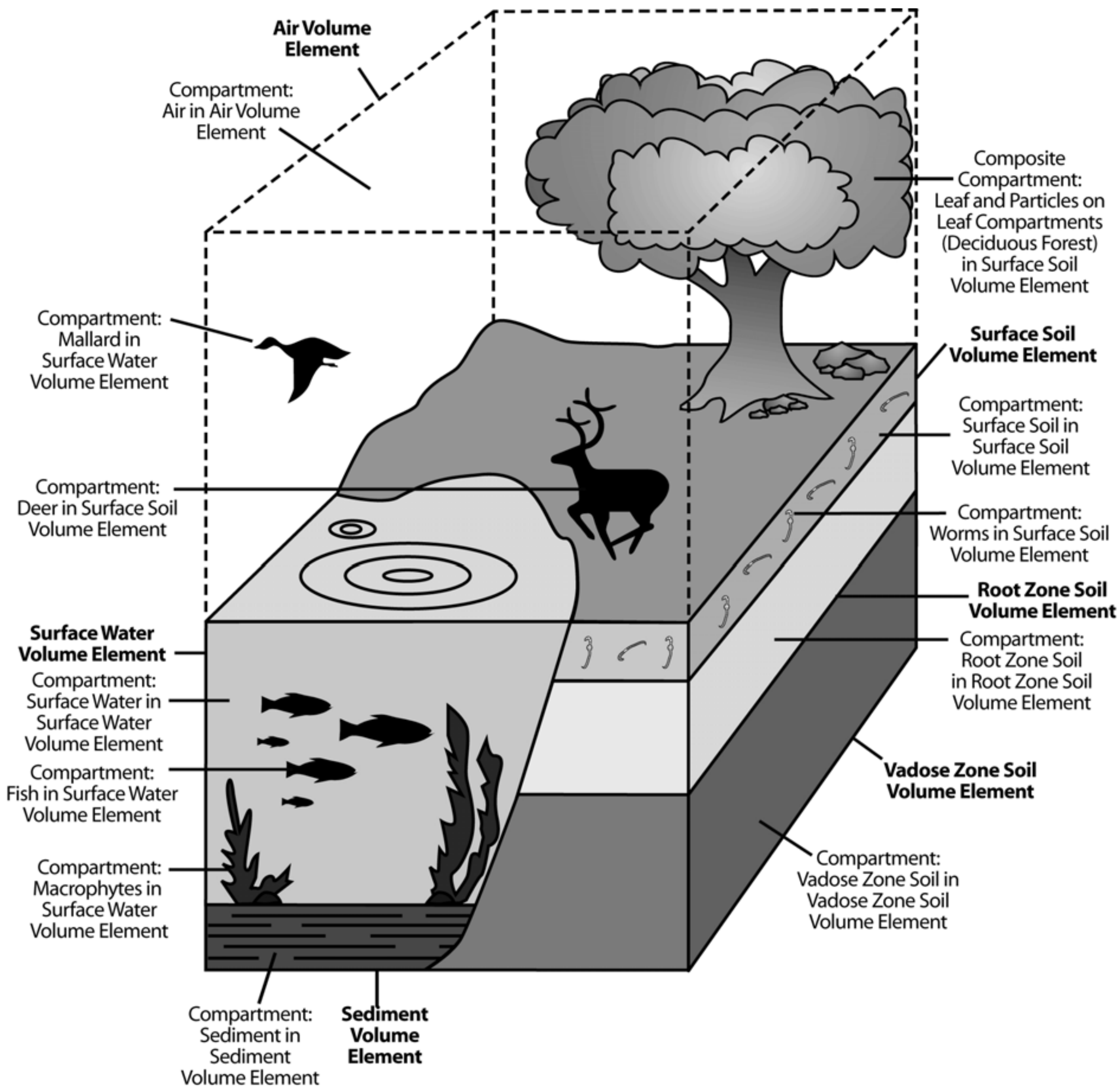


Figure 3-3
Example of a Hypothetical Environment (Multiple Volume Elements, Multiple Compartments)



Abiotic compartments (*e.g.*, surface soil, air) generally possess the same dimensions (*i.e.*, height, length, and width), and hence the same volume, as the containing volume element. Note that a sediment compartment may include both the sediment particles and the interstitial pore water, with the chemical in phase equilibrium between them. The total volume of this sediment compartment would consist of water (with a volume fraction equal to *x*) and sediment particles (with a volume fraction equal to (1 ! *x*)). Similarly, surface water compartments include both particulate and dissolved phases, and air compartments contain particulate and vapor phases (see Section 4.3).

Biotic Compartments and Volume Elements: Examples from Figure 3-3

The **fish compartment** is associated with the Surface Water Volume Element and is assumed to exist as a population evenly spread throughout the surface water compartment within that volume element. Characteristics for the fish population are defined by the user (*e.g.*, average body weight, number of fish per square meter of water body). However, the volume occupied by the biomass of the fish is not calculated, and the volume fraction of the surface water compartment that consists of fish is not estimated or subtracted from the volume of water in the compartment for any of the calculations in TRIM.FaTE.

The **mallard compartment** is also associated with the Surface Water Volume Element, and some of the same population characteristics (*e.g.*, average body weight, number of individuals per area) are defined by the user. The mallard population is assumed to feed on both aquatic invertebrates (associated with the same volume element) and terrestrial plants (associated with one or more neighboring volume elements). Thus, in terms of feeding habits, the mallard population is not physically restricted to the volume element with which it is associated.

Although biotic compartments are associated with volume elements as a part of the TRIM.FaTE modeling structure, they do not "take up space" within a volume element. Concentrations in biotic compartments are calculated on the basis of biomass (refer to TRIM.FaTE TSD Volume II for more detailed information). For the purposes of estimating chemical mass and concentration in the abiotic compartment, the volumes associated with biotic compartments are considered insignificant compared with the volumes of the associated abiotic compartment (*e.g.*, air, soil, water). See the text box above for two examples of the conceptual relationship between biotic compartments and volume elements for the hypothetical environment shown in Figure 3-3.

3.2 COMPARTMENT TYPES

The openness and flexibility of TRIM.FaTE give the user wide latitude in defining the compartment types for any particular modeling scenario. The discussion in the two sections that follow describes compartment type implementations that have been used and evaluated thus far. TRIM.FaTE provides the user the capability to define scenarios using these or alternate compartment type strategies. With this flexibility, however, comes the responsibility to consider the ramifications of the selected strategy. Observations of complexity evaluations described in the TRIM.FaTE Evaluation Report (USEPA 2002b) and discussion in TRIM.FaTE User Guidance (USEPA 2002a) may be of assistance, particularly in considering the strategy for including biota in a TRIM.FaTE scenario.

3.2.1 ABIOTIC COMPARTMENT TYPES

Abiotic compartment types consist primarily of a non-living environmental medium. The adjacent text box lists the abiotic compartment types currently included in TRIM.FaTE. Within the TRIM.FaTE system, chemical mass is initially transported to biotic compartments based on their relationships with abiotic compartment types. In addition to the abiotic compartment types listed here, compartment types defined within the TRIM.FaTE system that are not associated with biota also include advection and flush rate sinks (to account for mass transported outside of the modeled region) and reaction/degradation sinks (to account for the results of chemical transformation reactions when the fate of the reaction product is no longer tracked by TRIM.FaTE). Sinks are described in more detail in the text box in Section 3.1 and in the discussion of the TRIM.FaTE mass balance framework (Chapter 4).

ABIOTIC COMPARTMENT TYPES IN TRIM.FaTE

Air	Ground Water
Surface Soil	Surface Water
Root Zone Soil	Sediment
Vadose Zone Soil	

The properties of abiotic compartment types are set by the user who can give them differing or identical values throughout the modeling region. For example, parameter values for all surface soil compartments in a modeling scenario can be assumed to be the same. However, if site-specific data are available for different compartments in a scenario, these data can be entered as compartment-specific properties. For example, where multiple water bodies are represented in a scenario, the user may need to specify differing values for the surface water and sediment compartment properties (*e.g.*, current velocity, water pH, sediment particle density).

3.2.2 BIOTIC COMPARTMENT TYPES

Biotic compartment types generally are differentiated from one another based on their links with other compartment types. Thus, each biotic compartment type represents a different trophic/taxonomic group or has a different route of uptake. The compartment types are further distinguished by the ecosystem (*i.e.*, terrestrial or aquatic) in which the biotic compartment feeds or is located. Mammalian and avian wildlife, soil detritivores, fish, aquatic (benthic) invertebrates, and aquatic plants are considered different compartment types because they belong to unique trophic groups and/or occupy different ecosystems. Those groups can be further subdivided based on their habitat (*e.g.*, terrestrial, semi-aquatic) and/or general feeding patterns (*e.g.*, herbivore, omnivore). For example, some wildlife species are considered to be entirely terrestrial (*e.g.*, deer), while others are considered to be semi-aquatic (*e.g.*, mink), feeding on prey from both aquatic and terrestrial habitats. The different biotic compartment types that have been used to date in TRIM.FaTE are listed in Table 3-1.

For terrestrial and semi-aquatic wildlife (*i.e.*, birds and mammals), one or more species can represent each trophic/functional group. For example, a single species, the short-tailed shrew, might represent terrestrial ground invertebrate feeders for the terrestrial portions of the modeling region. For a terrestrial predator trophic group, both the red-tailed hawk and the

Table 3-1
Biotic Compartment Types Defined for TRIM.FaTE

Biotic Compartment Type	Representative Subgroup or Species
Aquatic Plants	
Macrophyte	[User input] [a]
Benthic Fauna	
Benthic invertebrate	[User input] [a]
Benthic omnivore	[User input] [a]
Benthic carnivore	[User input] [a]
Water-Column Fauna	
Water-column herbivore	[User input] [a]
Water-column omnivore	[User input] [a]
Water-column carnivore	[User input] [a]
Semi-Aquatic Fauna	
Semi-aquatic piscivore	Belted kingfisher Common loon Mink
Semi-aquatic predator/scavenger	Bald eagle
Semi-aquatic aerial insectivore (*i.e.*, feeding on adults of emergent insects such as mayflies, mosquitos, damselflies)	Tree swallow
Semi-aquatic omnivore	Mallard Raccoon
Terrestrial Plants [b]	
Plant leaf	Defined as appropriate for coniferous or deciduous forest, grass/herb fields, or agricultural systems.
Particle on leaf	
Plant stem	
Plant root	
Terrestrial Fauna	
Terrestrial omnivore	American robin White-footed mouse
Terrestrial insectivore	Black-capped chickadee
Terrestrial predator/scavenger	Long-tailed weasel Red-tailed hawk

Biotic Compartment Type	Representative Subgroup or Species
Terrestrial vertebrate 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 American woodcock
Flying insect [c]	Mayfly
Soil detritivore	Earthworm Soil arthropod

[a] In applications to date, the fish compartments have been employed to represent trophic niches arising either from a benthic (*i.e.*, sediment-based) or water-column contaminant source. In addition, the term omnivore has been a misnomer in the applications to date, because the water-column "omnivore" has fed only on the water-column herbivore, and the benthic "omnivore" only on benthic invertebrates. Thus, these compartment types have not been parameterized using the concept of a single representative species that might feed on organisms from more than one trophic level or from both the benthic and water-column environments. Rather, the total biomass for a single representative fish species that feeds from both benthic and water-column sources has been divided into two compartments for that species: one that feeds from benthic sources and one that feeds from water-column sources, respectively. The water-column "herbivore" also is a misnomer in that zooplankton are implicitly included in the diet and represent an intermediate trophic level between the phytoplankton and the fish herbivore. Further discussion of this is provided in the TRIM.FaTE Evaluation Report and the TRIM.FaTE TSD, Volume II, Chapter 6. As mentioned previously, however, alternate strategies may be evaluated and employed, as appropriate.
[b] Terrestrial plant parts constitute different compartment types even though they are not different trophic groups.
[c] For applications thus far, flying insects have been represented by the benthic invertebrate compartment type, thus essentially assuming that the concentration of chemical in the adult flying insect is the same as the concentration of chemical in the aquatic nymph from which it emerged.

long-tailed weasel might be included in one or more surface soil volume elements of the modeling region. In that case, the diet of each of those species would be specified and compartments representing the prey species would also need to be included in the model. The diet of fish and wildlife can range from a single diet item (*e.g.*, 100 percent algae for an herbivorous fish) to multiple diet items (*e.g.*, 5 percent shrews, 20 percent mice, 25 percent ducks, 25 percent benthic invertebrates, and 25 percent water-column herbivorous fish for mink). The selection of wildlife compartments and assignment of corresponding diet, biomass, and other parameter values will depend on the location of the site, the habitat types found at the site, the area covered by the modeling region, and other factors as described in the TRIM.FaTE User Guidance.

There are similarities between constructing an aquatic food web and constructing a food web for terrestrial wildlife. The user can specify fish compartments appropriate to the site and can specify the diet for each fish compartment. A given fish compartment might be parameterized to represent an entire trophic group, or one or more species considered representative of that group can be used to assign values to the parameters for one or more compartments. Biomass relevant to the distribution of the pollutant being modeled should be accounted for. For example, the entire biomass of aquatic organisms in the surface water body being modeled should be accounted for in the set of aquatic compartments implemented to ensure appropriate chemical partitioning in the aquatic ecosystem.

In some cases, composite compartment types may be implemented within the TRIM.FaTE framework. A **composite compartment type** is a group of different compartment types that are consistently interconnected. Each individual compartment within a composite compartment requires the presence of other compartments. Conceptually, a composite compartment type may be considered as a term of convenience for the user rather than a structural component of the TRIM.FaTE system; that is, TRIM.FaTE distributes mass between the individual compartments, not into the compartment type as a single unit. Currently, plant composite compartment types have been defined within TRIM.FaTE, with root, stem, leaf, and particle on leaf [2] compartments comprising the plant composite compartment type (given the difficulty in modeling woody stems and roots, only the leaf and particle on leaf compartments are currently included in the coniferous and deciduous forest composite compartments). Note that different types of plant communities (*e.g.*, deciduous forest, grass and herb community) may be represented by separate composite compartments.

Given the flexibility of the TRIM.FaTE framework, the user can design and implement their own approach to modeling pollutant movement through biotic compartments. This can include custom definitions of compartment types, feeding habits, biomass densities, and other parameters. As mentioned previously, with this flexibility comes an inherent responsibility to consider the ramifications of a given design and consequently its appropriateness for the objectives of the assessment. For example, although the animals in an ecosystem are not considered to play a large role in the distribution of pollutant mass within that ecosystem (*i.e.*, the balance will occur in abiotic media), distribution of pollutant mass among the various animals in TRIM.FaTE is influenced by the relationships among them (*e.g.*, predator-prey, relative abundance, dietary preferences).

3.3 LINKS

There are two general processes that can affect the presence of chemical mass within a given compartment:

(1) the transfer of chemical mass from and/or to another compartment; and

(2) the transformation of one chemical to another chemical within a compartment.

In order to evaluate the occurrence and magnitude of these processes, the relationships, or links, between and within the compartments must be determined. A **link** is defined as a "connection" between compartments (for transfer processes) or within a compartment (for

[2] The "particle on leaf" compartment type represents those particles deposited from air onto a leaf surface via wet and dry deposition. The chemical mass that is associated with the "particle on leaf" compartment can be transferred into the leaf or blown off the leaf surface, or can remain associated with the particles on the surface of the leaf.

transformation processes[3]) that allows one of these processes to occur. Each link contains an algorithm or multiple algorithms that mathematically represent the mass transfer or transformation. Figure 3-4 expands on the concepts presented in Figure 3-2 by showing links representing transfers between compartments in different volume elements. The figure demonstrates that chemicals in the air compartment can be transferred to the water compartment via a link.

The algorithms that mathematically represent mass transfer or transformation are assigned to links which specify the compartments involved in the transfer and the direction of transfer. This concept is demonstrated in Figure 3-5 where chemical mass is transferred between the water and air compartments and between the water and fish compartments, but not between the fish and air compartments. For a transformation process, the link exists within a compartment to allow transformation between two chemicals (parent chemical and reaction product) within the same compartment (see Figure 3-6).

In the TRIM.FaTE framework, links provide for the organization and application of algorithms that describe chemical mass transfer among, and transformation within, compartments. Links "contain" the algorithms describing the one or more processes governing mass transfer across that link, as well as any properties specific to the link itself (but *not* those properties of the compartments or chemicals involved). For example, a link between two particular surface soil compartments may contain algorithms for advection of mass via erosion and runoff processes as well as information on the fraction of overland advective flow from one soil compartment to another. A soil-to-shrew link may contain an algorithm for intake of chemical mass via soil ingestion by the shrew. The algorithms contained on both of these links would also use properties of the sending and receiving compartments and the chemicals being modeled (*e.g.*, erosion rate, liquid volume of soil, ingestion rate of soil by the shrew, chemical partition factors) to calculate transfer factors.

3.4 SOURCES

The set of all compartments in a TRIM.FaTE modeling scenario is assumed to contain all of the chemical mass within the system being modeled, excluding sources and boundary contributions. A **source** is an external component that introduces chemical mass directly into an abiotic compartment. A common example of a source would be the factory emissions of a chemical into an air compartment. TRIM.FaTE is designed to accommodate single or multiple source scenarios. Currently, sources in TRIM.FaTE can introduce chemical mass into air compartments only.

[3] Note that in TRIM.FaTE, chemical transformations that result in degradation products or metabolites of a parent chemical whose fate will not be tracked in the modeling scenario are considered "degradation" processes (see Chapter 4). Thus, chemical mass can be lost from the system of modeled compartments in two ways: (1) mass transferred into advection or flush rate sinks, and (2) mass transferred into degradation/reaction sinks due to degradation processes.

Figure 3-4
Two Linked Compartments in Separate Volume Elements

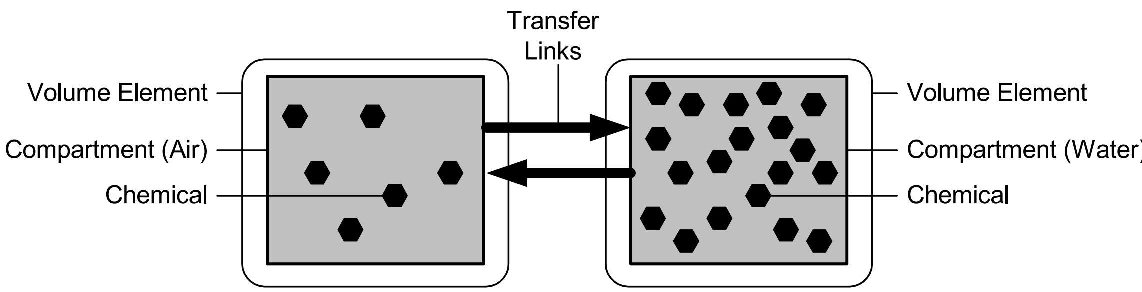


Figure 3-5
Three Linked Compartments in Two Volume Elements

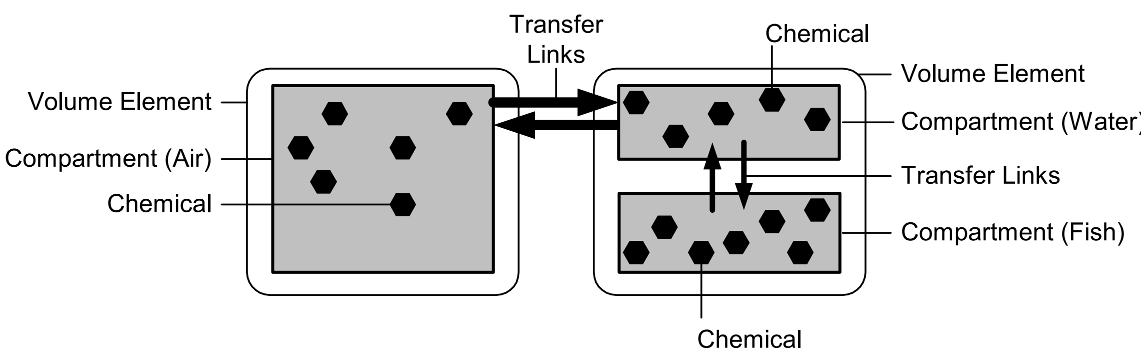
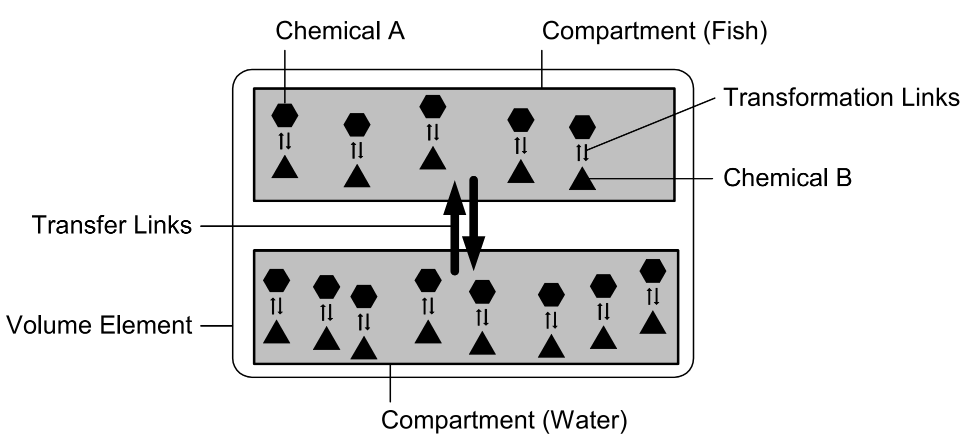


Figure 3-6
Transformation Links Between Chemicals within a Compartment

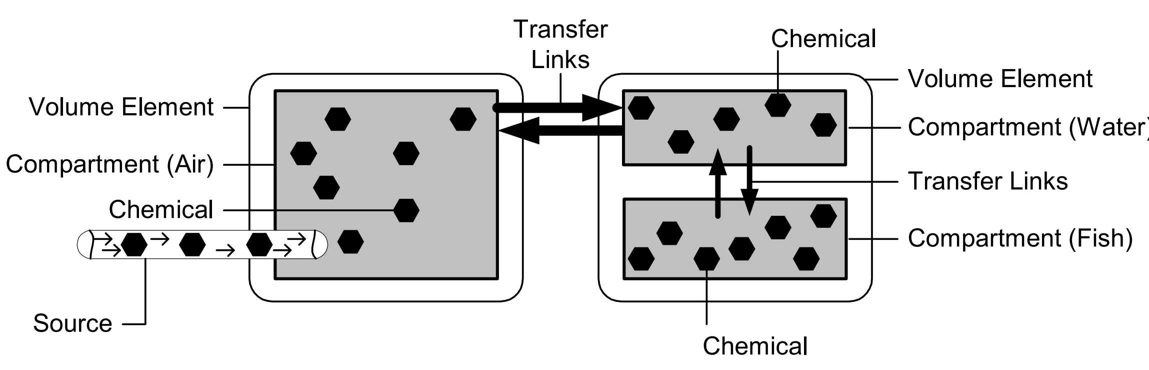


TRIM.FaTE differentiates between sources emitting within the modeling region (*e.g.*, air emissions from a facility stack) and sources of chemicals derived from outside the scenario modeling boundaries; the latter are referred to as boundary contributions (or boundary conditions) within the TRIM.FaTE framework. Sources emit chemicals directly to the primary abiotic compartment within which the source emission point(s) is located, as specified by coordinates (including height) assigned to the source. The emission rate of chemical entering this compartment (either a constant or time-varying rate) is specified by the user. A **boundary contribution** may be set for any outside interface of a compartment located on the outer sides of the modeled region. For air, a boundary concentration (which may be set by the user for the outer volume elements) establishes the concentration of a chemical in the air on the external (*i.e.*, non-modeled) side of the modeled region. Chemical mass enters the outside compartments via air advection algorithms that depend on wind speed, wind direction, and boundary concentration. Although currently implemented in TRIM.FaTE only for air compartments, boundary contributions could be set for other compartments as well (*e.g.*, flowing surface water compartments).

In addition, chemical mass can be included in the starting conditions for a scenario based on initial concentrations set by the user for abiotic or biotic compartments included in the TRIM.FaTE modeling scenario. The addition of mass to a scenario as an **initial concentration** in one or more compartments is a one-time event and represents concentrations in environmental media just before the simulation period begins. Outside of the TRIM.FaTE framework and terminology, this concept is often referred to as "background" concentrations. However, within the TRIM.FaTE framework, the word background is not used; the term "initial concentration" is used. A related TRIM.FaTE feature that can be useful for evaluation and diagnostic purposes is the ability to fix the concentration in any compartment to a user-specified value for the duration of the simulation.

Figure 3-7 adds to Figure 3-5 by showing a source emitting into the air compartment.

Figure 3-7
Linked TRIM.FaTE System with a Source



3.5 TIME-RELATED TERMS AND CONCEPTS

3.5.1 BASIC TIME TERMINOLOGY

TRIM.FaTE is a dynamic model (*i.e.*, the model accepts time-varying inputs and produces time-varying outputs), which makes it important that the time-related terminology is clearly defined and consistently used. There are three main time-related terms that are central to understanding how TRIM.FaTE relates input data, fate and transport calculations, and model outputs: **simulation period**, **input data time step**, and **output time step**. Definitions of these terms for the purposes of TRIM.FaTE are given below.

Simulation period is the length of time over which the simulation occurs.

Input data time step dictates the points in time at which TRIM.FaTE calculates a new matrix of transfer factors.

Output time step is the frequency at which results are provided by the model.

For a given TRIM.FaTE model run, the **simulation period** (or modeled time period) is the entire length of time over which the simulation occurs and compartment masses and concentrations are calculated – in other words, the time period from the beginning date and time of the simulation until the ending date and time. The simulation period is set by the user through specification of the simulation begin and end date and time. For most anticipated applications of TRIM.FaTE, the simulation period is expected to be one year or longer. Source emissions can occur for either all or part of the simulation period (*i.e.*, source modeling periods can be shorter than the simulation period), or even none of the simulation period if the analysis objective is to assess boundary conditions only (see Section 3.4).

The **input data time step** dictates the points in time at which TRIM.FaTE calculates new transfer factors (*i.e.*, a new transition matrix as described in Section 4.2). The input data time step refers to the interval between changes in value of any time-varying input (*e.g.*, wind speed data may be provided at hourly intervals). The input data time step (or time increments by which time-varying input data change) is recognized by the model during the run and can vary both across and within data types. That is, values for a particular data input can even be provided for erratically-spaced times during the simulation period (*e.g.*, Day 1, Day 2, Day 5, Day 7, Day 8, Day 9). In moving through the simulation time period, the model recalculates the relevant parts of the matrix of transfer factors with each occurrence of a change in input data. This up-to-date matrix is then relied on by TRIM.FaTE for its calculation of the distribution of chemical among the compartments.

The model can output results for any hourly time interval greater than or equal to one hour. The user specifies the frequency at which results are output (sometimes referred to as **"output time step"**) through the use of two model parameters: simulation time step and number of simulation steps per output. Setting the simulation time step to 12 hours and the number of simulation steps per output step at 2, the model will write out results at 24-hour intervals throughout the simulation period. Setting the number of simulation steps per output step to 1 would produce results at 12-hour intervals (*i.e.*, that specified by the simulation time step). That is, the product of the two parameters is the time interval between model outputs (*i.e.*, the output time step). The results at each output time are those derived for that time point (*i.e.*, a "snapshot"), and are ***not*** an average over any time period. The time series results output from TRIM.FaTE can also be averaged over various time periods of interest (*e.g.*, each day, month, year) using an averaging feature of TRIM.FaTE.

> For a modeling scenario with 100 compartments, a 30-year (262,800 hour) simulation period, a simulation time step of 1 hour, and the number of simulation time steps per output equal to 2, there would be 13,140,000 (100 × 262,800 ÷ 2) reported values ***each*** for moles, mass, and concentration results for ***each*** chemical modeled.

TRIM.FaTE also can be run in a steady-state mode. In this mode, there are no time-varying inputs, no simulation period, and no output time step; the model's run time is negligible compared to the dynamic modeling mode. In the steady-state mode, TRIM.FaTE calculates single values for chemical moles, mass, and concentration for each compartment. These values approximate the levels that the chemical would reach if the dynamic form of the model was run for a long enough period of time to allow all mass "inputs" and "outputs" to balance for each compartment (*i.e.*, to reach a steady-state).

3.5.2 OTHER TIME-RELATED CONCEPTS

Much of TRIM.FaTE's data are, in reality, time-varying and can be treated as such by the model, although it is expected that typically most would be treated as being constant over time. However, inputs such as meteorological data (*e.g.*, wind speed and direction), stream flow, and source emissions rate typically would be treated as time-varying in TRIM.FaTE model runs where sufficient data are available. Values for time-varying parameters can be provided to TRIM.FaTE in any time increment selected by the user, generally based on data availability and run time considerations. For example, meteorological data (*e.g.,* wind speed, precipitation measurements) may be available at hourly increments, and source emission rate data may be available at monthly increments; TRIM.FaTE can readily accommodate these different input data time increments. However, using smaller time increments for time-varying input data can increase the model's run time.

TRIM.FaTE can model certain processes that vary by season and time of day. Including seasonal changes in chemical fate and transport modeling can be advantageous for at least two reasons: (1) a seasonally dependent model can be applied to regions where below-freezing temperatures occur, and (2) model runs can be implemented for durations greater than a single growing system. However, model realism gained by accounting for seasonality must be balanced with the burden on the user to collect site-specific data on seasonal processes.

Two seasonal processes are currently implemented for plants in TRIM.FaTE: litterfall, which allows chemical mass to be transferred from the leaves to the surface soil, and growing season, which allows uptake of chemicals by plants only between the day of last and first frost.[4] These processes are implemented by enabling or disabling certain links and the associated transfer algorithms depending on the date. Additional seasonal processes may be considered in future refinements to TRIM.FaTE (*e.g.*, dynamics of snow accumulation and snowmelt, timing and rate of growth of algae during and following a bloom, dietary and habitat changes by wildlife). In addition, day-night is simulated in TRIM.FaTE to allow for different exchanges between the plants and air or soil during the day and night. These processes are implemented by enabling or disabling certain links depending on the time of day.

[4] In addition, seasonality in weather patterns is accounted for by the use of time-varying meteorological and streamflow data.