5. APPLICATION OF TRIM.FaTE

This chapter illustrates the application of the concepts presented in Chapters 3 and 4 by briefly explaining each of the main steps necessary to set up and perform a simulation with TRIM.FaTE. It explains the methods associated with key steps in the modeling process, provides a general sense of the level of effort associated with performing a TRIM.FaTE simulation, and summarizes the inputs and outputs of the model. Note that the text here is simply a summary based on the applications of TRIM.FaTE to date and the associated chemicals, algorithms, compartment specifications, and properties. Future applications may expand upon these or implement alternatives. However, it is expected that the basic framework for model application will remain as presented here.

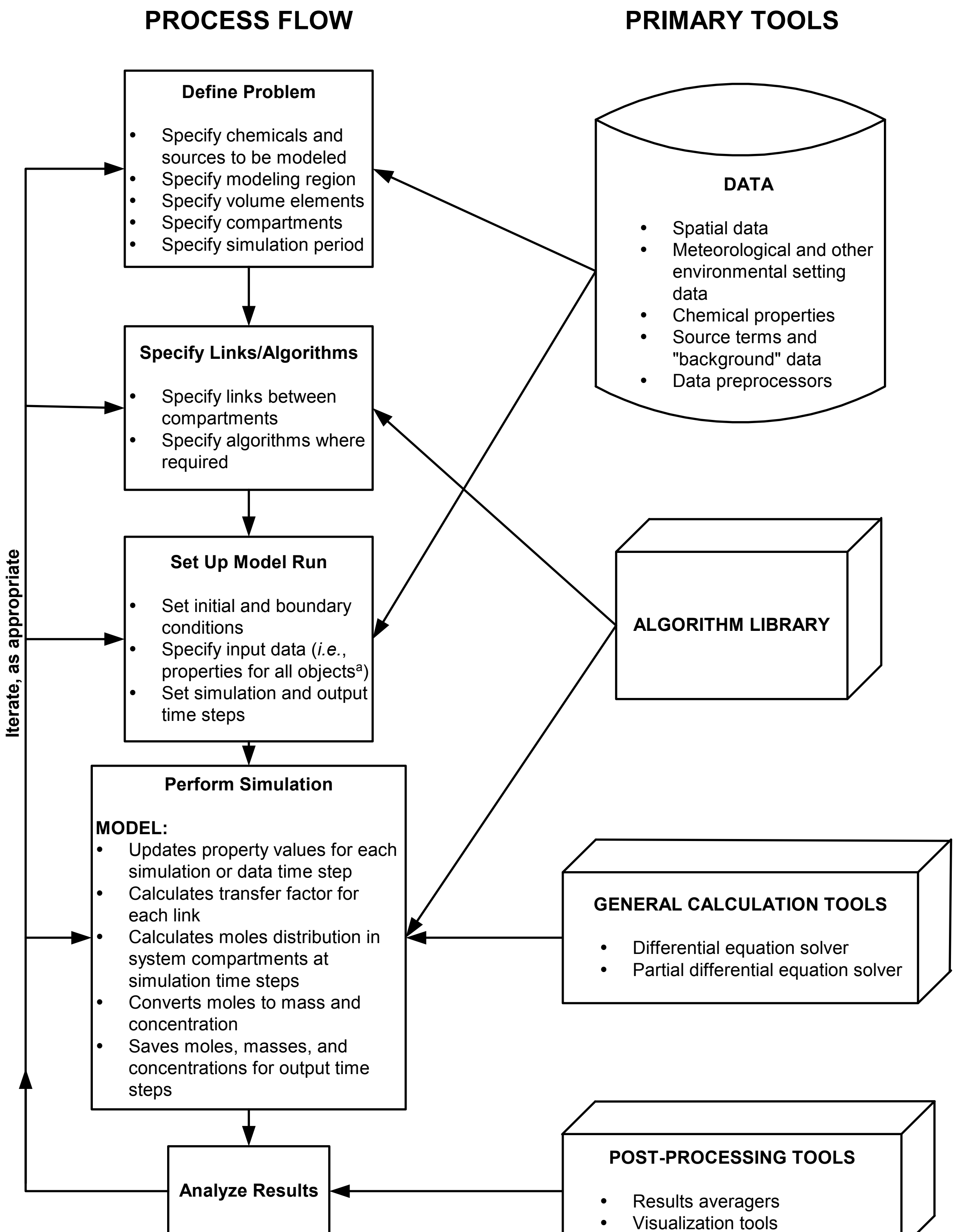
This chapter is not intended to serve as a user's guide to the model; rather, it provides a broad understanding of how TRIM.FaTE works by explaining in general terms how it is used to simulate the multimedia fate and transport of air emissions from one or more sources. For detailed information on installing and navigating TRIM.FaTE software, applying the model for a specific scenario, and other aspects of operating TRIM.FaTE, refer to the TRIM.FaTE User Guidance.

5.1 GENERAL PROCESS FOR A TRIM.FaTE SIMULATION

TRIM.FaTE is designed to be an iterative and flexible model. Although there are a number of steps that the user must include in the development and application of a TRIM.FaTE simulation, some of the order in which these steps are completed is flexible. The general process is shown in Figure 5-1. The boxes on the left side of the figure categorize the basic steps involved in the completion of TRIM.FaTE simulation: problem definition, specification of links, simulation set-up, model execution, and analysis of results. In an actual application, progression through the modeling process might not be quite as linear as that shown in the figure. However, all of the tasks identified in the basic steps must be addressed during the course of developing and executing a TRIM.FaTE simulation.

The vertical arrows linking the steps under the "Process Flow" heading represent the typical order of events in an application. The arrows to the left indicate that model application might involve multiple iterations as the modeling scenario is refined. Primary components of the analysis are illustrated under the "Primary Tools" heading and linked with arrows to the relevant steps in the "Process Flow" column. To focus on key aspects of the TRIM.FaTE approach, only selected tools are shown. There are other tools that may be relied upon that are not indicated in this figure (*e.g.*, sensitivity analysis and Monte Carlo features, steady state solver).

Figure 5-1
TRIM.FaTE Modeling Sequence



[a] The term objects refers to sources, chemicals, volume elements, compartments, and the scenario.

5.2 PROBLEM DEFINITION

TRIM.FaTE is not intended for use in assessments involving air pollutant emissions where the air is the medium of interest; rather, it is intended for applications involving air pollutant emissions where the assessment focus is on non-air media. The first step in the TRIM.FaTE modeling process is articulating a clear statement of the problem and then translating that into the TRIM.FaTE structure. In defining the problem for a TRIM.FaTE application, the chemical(s), source(s), primary spatial features of the ecosystem, and simulation period are defined. Using the nomenclature presented in Chapter 3, the volume elements and compartments within the volume elements are specified.

The TRIM.FaTE problem definition is based directly on the underlying objectives of the fate and transport/exposure/risk assessment to be performed. As recommended in recent EPA and other risk guidance, a clear problem formulation should be developed for the fate and transport/exposure/risk assessment before any modeling begins. This is particularly important for highly flexible models like TRIM.FaTE.

5.2.1 DETERMINING SOURCE(S) AND CHEMICAL(S) TO BE MODELED

The sources and chemicals to be included in the TRIM.FaTE simulation are identified in the first step of the problem definition process. Generally, this identification flows directly from the overall problem formulation for the fate and transport/exposure/risk assessment. This step must be performed first because the chemical(s) and location of the source(s) can influence how the region to be modeled is delineated and subdivided. In determining the chemicals to be modeled, the user should consider the objective of the modeling exercise, the available emissions information, and the potential effects and receptors of concern. The user must decide, given the objectives and resources available for the analysis, which sources and chemicals should be included in the modeling analysis. The process of identifying chemicals of concern and associated sources should be referenced to existing EPA guidance when possible.

5.2.2 DETERMINING SCALE AND SPATIAL RESOLUTION

This section introduces the considerations for defining the overall modeling scale and the level of spatial complexity (*i.e.*, location, size, shape, and number of parcels) in a TRIM.FaTE analysis. Definitions for the important spatial terms used in this section are discussed in more detail in Chapter 3 and are summarized in the adjacent text box. After the initial scenario is constructed and a simulation has been completed, the preliminary results

> A **parcel** is a planar (*i.e.*, two-dimensional), horizontal geographical area used to subdivide the modeling region. Parcels, which are polygons of virtually any size or shape, are the basis for defining volume elements and do not change for a given scenario. There can be separate parcels for air and for the land surface (soil or surface water).
>
> A **volume element** is a bounded three-dimensional space that defines the location of one or more compartments.
>
> A **compartment** is defined as a unit of space characterized by its homogeneous physical composition and within which it is assumed, for modeling purposes, that all chemical mass is homogeneously distributed and is in phase equilibrium.

need to be evaluated to confirm that an appropriate level of resolution has been used. An example of a general approach for determining appropriate scale and spatial resolution as well as suggestions for defining compartments are included in the TRIM.FaTE User Guidance.

It is important to note that TRIM.FaTE is designed to model the fate and transport of air pollutant emissions into non-air media. Scenarios may be created that range from general and conceptual (*e.g.*, an environment consisting of air, soil, and a water body) to more detailed and site-specific (*e.g.*, capturing major land and water topographic variation in a 25 square mile area). The compartment-based design, with its assumptions of homogeneity within compartments, is not intended to provide fine scale resolution of predicted pollutant concentrations. When such detail is desired for particular media (*e.g.*, a water body), it may be appropriate to also consider use of a detailed model specific to that medium (*e.g.*, a water quality model). As noted previously, for assessments of air pollutant emissions where the air is the medium of interest, users should rely on an air quality model.

5.2.2.1 Specifying the Modeling Region

The first step in determining the scale and spatial resolution of a TRIM.FaTE scenario is to determine the scale of the modeling region (*i.e.,* external spatial boundaries of the analysis). In this step, the user specifies the geographical extent of the area to be modeled. A user should consider factors such as mobility of the modeled chemical(s), location of source(s), location of sensitive populations, and background concentrations of the chemical(s). A scoping step using air dispersion modeling may be appropriate to evaluate the predicted spatial pattern of deposition. When the predominant wind direction is variable, the modeling region may need to extend beyond the region of primary interest to account for the possibility of pollutant mass leaving and re-entering the system. After the scale of the modeling region has been chosen, one must consider whether that scale is appropriate when compared to other sources of model uncertainty.

5.2.2.2 Specifying Parcels

Once the scale of the analysis is determined, the next step is to specify the spatial resolution of the modeling region using two-dimensional parcels—essentially polygons—that subdivide the modeling region. **Parcels** need to be defined for the air and for the land surface (*i.e.*, soil and surface water); these two sets of parcels do not need to have the same spatial layout (*i.e.*, their individual and combined boundaries do not need to line up). A larger number of parcels in a given scenario can be used to provide higher spatial resolution and/or greater areal coverage. It is noted however, that more parcels correspond to greater resource requirements, both in terms of model set-up and data collection as well as model run time.

Beyond complexity and resource considerations, there are three principal technical considerations for determining the parcels for a TRIM.FaTE scenario:

- The likely pattern of transport and transformation of each chemical of concern (*i.e.,* where significant concentration gradients are likely to be);

- The locations of natural and land use boundaries; and

- The locations of important environmental or biological receptors. These can include populations of receptors (*e.g.*, human or ecological cohorts) or landscape components (*e.g.*, lake, agricultural area) of interest.

For the chemical(s) of interest, three important factors in determining the likely pattern of transport and transformation are the atmospheric transport of chemical mass, rapidity of chemical transport in media other than air, and transformation or degradation of the chemical(s) in the environment. Understanding the atmospheric transport of the chemical(s) of interest is useful in developing both the modeling scale and spatial resolution. Because air pollutants travel more rapidly in air than any other medium, insight into atmospheric transport can provide the user with a general idea of the extent of chemical transport and thus can be useful in determining the modeling scale. Furthermore, this information can provide the user with a picture of the general path of chemical transport, helping the user determine where higher spatial resolution may be beneficial.

Information about the mobility and transformation or degradation of the chemical(s) of interest in soils and water, when combined with information on land use, can provide additional insight into the transport in media other than air. It can be helpful in refining the scale of the scenario as well as providing additional input to help determine the spatial resolution of the modeling region.

Natural boundaries are also an important consideration in developing the parcel layout. For example, an airshed boundary can be defined by a combination of geographical and meteorological conditions such as large valleys where inversion layers and diurnal wind patterns may result in a confined and relatively well mixed air mass within the area for extended periods of time. Airshed boundaries can also include smaller valleys when meteorological conditions produce a long residence time for the air mass in the bounded region. Airshed boundaries are useful in providing information about the scale of the overall modeling region (*i.e.*, external boundaries of the system).

Watersheds are also useful in determining the scale of the system as well as the size and location of surface parcels within the system, especially if chemical concentrations in a particular lake or stream are of interest. Watershed boundaries can be identified from existing references (*e.g.*, United States Geological Survey (USGS) applications) or approximated from topographical maps by tracing ridgelines and noting the origin and direction of flow for streams and rivers. The size and location of a watershed can influence the transfer of chemical to water bodies within it.

Land use and land cover data should be considered in defining land parcels. That is, it may be appropriate for the parcel layout to capture the pattern of land use and cover, including forest type, rangeland, or agriculture lands,[1] as land use homogeneity can be desirable within

[1] For example, it is useful to consider variation in vegetation type which may be important for the subsequent step of assigning vegetation and other biotic compartments.

parcels. Land use or land cover can also correspond with a particular receptor of interest (*e.g.*, ecological receptor(s) in a coniferous forest, or residents on small farms). The location of the receptor(s) is important because it allows the user to focus the analysis on the area(s) of interest, thus allowing resolution to be coarse in areas that are not expected to affect the chemical concentrations near the receptor(s) and resolution to be finer in areas that may have a greater impact.

The illustrative approach to specifying parcels described in the TRIM.FaTE User Guidance provides a starting point for any given analysis objective for which TRIM.FaTE is used. The approach is intended to impart some consistency and transparency into the spatial set-up process while maintaining an adequate level of flexibility.

5.2.2.3 Specifying Volume Elements

After the parcels have been determined for a scenario, the volume elements corresponding to those parcels are specified. This step involves specifying the appropriate vertical dimension and resolution of the modeling region. Whereas parcels only represent the modeling region in two dimensions (*i.e.*, a horizontal plane), volume elements add the component of depth, thus representing the modeling region in three dimensions (the location and horizontal two-dimensional planar shape of a volume element correspond exactly to the relevant parcel). The volume elements are determined based on various factors, including knowledge of mixing heights in air, average depth of water bodies or approximate levels of stratification, and typical demarcations in the soil horizon (or demarcations of interest to a particular assessment). The specification of volume elements represents the final step in specifying the spatial dimensions of the modeling region.

EXAMPLES OF VOLUME ELEMENTS USED IN TRIM.FaTE

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

TRIM.FaTE allows the specification of multiple layers of volume elements, when the additional complexity and resource requirements of doing so are offset by the desire for greater spatial resolution. In addition, the user must ensure that algorithms to model the transfer of chemical mass between multiple layers (or multiple vertically stacked volume elements) are included in the library. Although use of a single volume element (*i.e.*, no vertical stacking of volume elements), may be sufficient for the application at hand, use of multiple vertically stacked volume elements of the same type (*e.g.*, air, surface water) may be useful in particular assessments. For example, instead of one set of volume elements for the vadose zone (*i.e.*, one layer), additional vertical resolution can be gained by dividing the vadose zone into two or more vertically stacked layers of volume elements. Without such assignment of multiple volume elements of the same type, however, TRIM.FaTE currently accommodates vertical variation in soil through the use of separate volume elements of different types for the three major soil zones (*i.e.*, surface, root zone, and vadose zone) and the availability in the TRIM.FaTE library of algorithms describing vertical transport among them.

5.2.3 DETERMINING COMPARTMENTS

5.2.3.1 Abiotic Compartments

Abiotic compartment types are assigned as appropriate to each volume element (*e.g.*, air compartments in air volume elements, surface water compartments in surface water compartments). At least one abiotic compartment must be contained within each volume element. Although not currently implemented, the model framework supports multiple abiotic compartments within a volume element. In most cases, the determination of abiotic compartments is an implied step because these compartments are simply defined by the abiotic medium designation of the volume element.

5.2.3.2 Biotic Compartments

Of the available biotic compartment types, the user is only required to run the model with those that significantly influence the overall mass balance of the chemical in the modeled scenario and those that significantly affect concentration in the compartments of interest in the assessment. In applying the model to PAHs, for example, plant biomass significantly influences the mass balance in the system. Thus, it would not be appropriate to run a PAH application of the model without the plant compartment types, even if the only results of interest for a particular application were concentrations in abiotic compartments. In addition to plants, the TRIM.FaTE scenario should include those biotic compartment types that significantly affect chemical concentrations in the compartments of interest to the assessment.

The flexibility of TRIM.FaTE can accommodate a variety of designs for compartmentalization of biota for a modeling scenario. For example, a user can perform a TRIM.FaTE assessment for a whole trophic group using parameter values for a single species selected to be representative of all of the species in the group. In addition, a user can choose particular animal species of concern (*e.g.*, threatened or endangered populations) and parameterize the model for those species.

5.2.4 DETERMINING SIMULATION PERIOD

After determining the sources and chemicals to be modeled, the user determines the appropriate simulation period by considering the modeling objectives (per the problem definition), the lifetime of the modeled source(s), the persistence and mobility of the modeled chemical(s), and the effects of concern. The user should also consider resource limitations when determining the simulation period because this parameter directly affects the computing time. In addition to the dynamic modeling mode, TRIM.FaTE includes a feature for obtaining a steady solution. This is desirable for some assessments or for parts of some assessments, and provides substantial savings in computing time over a multi-year dynamic simulation.

5.3 DETERMINING LINKS/ALGORITHMS

The second step shown in Figure 5-1 is to assign the links, as appropriate, between the compartments and sinks specified for a given scenario (the compartment types currently available in TRIM.FaTE are listed in Chapter 3). Generally, for abiotic compartment types, the user will want to link all adjacent compartments to each other and link compartments at the edge of the modeling region to advection sinks. Biotic compartment types need to be linked to the appropriate abiotic compartments, as well as to other biotic compartments, depending on their relationships to each other in terms of the transfer of chemical mass. For example, each biotic compartment should be linked to all compartments that comprise its diet or in any way provide it a source of chemical mass (*e.g.*, terrestrial biota need to be linked to air compartments for inhalation of chemical), as well as to all compartments to which that biotic compartment provides chemical mass (*e.g.*, via excretion or by acting as a dietary component). TRIM.FaTE has a "SmartLink" feature that facilitates setting links, particularly among abiotic compartments. However, it is still necessary, particularly for biotic compartments, to carefully identify what links should be in place and confirm their placement or assignment within the TRIM.FaTE scenario.

The system of links is one of the most critical components of TRIM.FaTE. This component is critical because the links provide for the assignment of the algorithms describing the processes that drive chemical transfer and transformation. By specifying a link between two compartments, it is assumed that one or more algorithms[2] exist by which to estimate the transfer of chemical through the link via the prevailing processes. If an algorithm is not in the algorithm library, then it must be "added" so that it can be accessed by the underlying software. Methods for adding additional algorithms to the library will be described in the TRIM.FaTE User Guidance. Tables 5-1 and 5-2 present examples of links between abiotic and biotic compartment types, respectively, which are supported by non-transforming mass transfer algorithms in the current TRIM.FaTE library. In addition, Table 5-3 presents links that are implemented if the user chooses to apply the equilibrium model for bioaccumulation by fish (see Volume II of the TRIM.FaTE TSD for more information regarding this model for fish). To support the modeling of chemical transformation (*i.e.*, transportation of mass between different chemicals within the same compartment), TRIM.FaTE includes a feature that automatically creates links for each compartment with itself. At this time, the TRIM.FaTE library includes transformation algorithms for mercury species.

TRIM.FaTE also has the flexibility to use model results from single-medium models (*e.g.*, ISC) in place of some of the internal links and algorithms. In this case, the output from the external model would replace the calculations of fate and transport within the specific medium. It is noted, however, that this could have ramifications on the mass balance feature of

[2] Where multiple process operate to transport chemical across a link (*e.g.*, deposition and diffusion between an air compartment and a soil compartment), multiple algorithms may be active (*i.e.*, enabled) on a single link. Additionally, there may be more than one algorithm, derived by different methods, which could be used to describe chemical movement across a link via the same process. In that case, the user must identify the algorithm preferred for the process in the current scenario and disable the other(s).

Table 5-1
Abiotic Compartment Type Links and Mass Transfer Processes

(Table includes non-transformation related examples supported by the current TRIM.FaTE algorithm library.)

Links Between Compartment Types		Mass Transfer Processes Addressed
Sending	**Receiving**	
Air	Air	Bulk Advection
	Surface Soil	Dry Deposition (of particles) Wet Deposition (of particles and vapors) Diffusion
	Surface Water	Dry Deposition (of particles) Wet Deposition (of particles and vapors) Diffusion
	Air Advection Sink	Bulk Advection Beyond System Boundary
Surface Water	Air	Diffusion [a]
	Surface Water	Bulk Advection Dispersion
	Sediment	Suspended Sediment Deposition Pore Water Diffusion
	Surface Water Advection Sink	Bulk Advection Beyond System Boundary
Sediment	Surface Water	Resuspension Pore Water Diffusion
	Sediment Burial Sink	Solids Advection Beyond System Boundary
Surface Soil	Air	Diffusion [a] Resuspension
	Surface Soil	Erosion Runoff
	Root Zone Soil	Percolation Diffusion
	Surface Water	Erosion Runoff
	Surface Soil Advection Sink	Erosion Beyond System Boundary Runoff Beyond System Boundary
Root Zone Soil	Surface Soil	Diffusion
	Root Zone Soil	Percolation (if multiple root zone layers)
	Vadose Zone Soil	Percolation Diffusion

Links Between Compartment Types		Mass Transfer Processes Addressed
Sending	**Receiving**	
Vadose Zone Soil	Root Zone Soil	Diffusion
	Vadose Zone Soil	Percolation (if multiple vadose zone layers)
	Ground Water	Percolation
Groundwater	Surface Water	Bulk Advection (recharge)

[a] Includes volatilization.

Table 5-2
Biotic Compartment Type Links and Mass Transfer Processes

(Table includes non-transformation related examples supported by the current TRIM.FaTE algorithm library.[a])

Links Between Compartment Types		Mass Transfer Processes Addressed
Sending	**Receiving**	
Air	Plant Leaf	Uptake [b]
	Terrestrial and Semi-aquatic Wildlife (birds and mammals)	Inhalation [c]
Air (Particulates)	Particle on Leaf	Wet Deposition [c] Dry Deposition [c]
Air (Rain Water)	Leaf	Wet Deposition [c]
Plant Leaf	Particle on Leaf	Diffusion
	Surface Soil	Litterfall [c]
	Air	Diffusion/Advection
	Terrestrial Vertbrate Herbivore and Omnivore	Diet [c]
	Semi-aquatic Herbivore	Diet [c]
	Plant Stem	Uptake [b] (advection only)
Particle on Leaf	Surface Soil	Particle Washoff [c] Litterfall [c]
	Plant Leaf	Uptake [b] (diffusion only)
	Terrestrial Herbivore and Omnivore	Diet [c]
	Semi-aquatic Herbivore and Omnivore	Diet [c]
Plant Stem	Plant Leaf	Uptake [b] (advection only)
Plant Root	Root Zone Soil	Equilibrium Partitioning

Links Between Compartment Types		Mass Transfer Processes Addressed
Sending	**Receiving**	
Surface Soil	Terrestrial Ground-invertebrate Feeder	Diet [c]
	Terrestrial Vertebrate Herbivore and Omnivore	Diet [c]
	Semi-aquatic Herbivore	Diet [c]
	Plant Stem	Uptake [b] (advection only)
Root Zone Soil	Plant Root	Uptake [b] (equilibrium partitioning)
	Soil Detritivore	Uptake [b]
	Plant Stem	Uptake [b] (advection only)
Surface Water	Macrophyte	Equilibrium Partitioning [b]
	Fish [e]	Gill Exchange [bd]
	Water-column Herbivore	Diet (algae as phase of surface water) [c]
Macrophyte	Surface Water	Equilibrium Partitioning [b]
Sediment	Benthic Invertebrate (Flying Insect) Herbivore [f]	Uptake [b]
Terrestrial and Semi-aquatic Predator/Scavenger	Surface Soil	Excretion [b]
Terrestrial Vertebrate Herbivore	Semiaquatic Omnivore	Diet [c]
	Terrestrial and Semi-aquatic Predator/Scavenger	Diet [cg]
	Surface Soil	Excretion [b]
Terrestrial Omnivore, Insectivore, and Ground-invertebrate Feeder	Terrestrial Predator/Scavenger	Diet [c]
	Semi-aquatic Piscivore	Diet [c]
	Surface Soil	Excretion [b]
Soil Detritivore	Surface Soil (soil arthropod)	Equilibrium Partitioning
	Root Zone Soil (earthworms)	Equilibrium Partitioning
	Terrestrial Ground-invertebrate Feeder (earthworms)	Diet [c]
	Terrestrial Insectivore (arthropods)	Diet [c]
	Terrestrial Omnivore, Semi-aquatic Omnivore, and Terrestrial Predator/Scavenger (worms and arthropods)	Diet [c]

Links Between Compartment Types		Mass Transfer Processes Addressed
Sending	**Receiving**	
Water-column Herbivore and Omnivore	Semi-aquatic Omnivore	Diet [c]
	Semi-aquatic Piscivore	Diet [c]
	Water-column Carnivore	Diet [cd]
	Surface Water	Elimination [cd]
	Semi-aquatic Predator/Scavenger	Diet [c]
Water-column Carnivore	Semi-aquatic Omnivore	Diet [c]
	Semi-aquatic Piscivore	Diet [c]
	Surface Water	Elimination [cd]
	Semi-aquatic Predator/Scavenger	Diet [c]
All Semi-aquatic Wildlife	Surface Soil	Excretion [b]
	Surface Water	Excretion [b]
Benthic Omnivore	Benthic Carnivore	Diet [cd]
	Surface Water	Elimination [cd]
Benthic Carnivore	Surface Water	Elimination [cd]
Benthic Invertebrate	Semi-aquatic Omnivore	Diet [c]
	Sediment	Equilibrium Partitioning [b]
	Benthic Omnivore	Diet [c]
Flying Insect (emerged from benthic larval insect) [f]	Semiaquatic Predator/Scavenger	Diet [c]
	Semi-aquatic Insectivore	Diet [c]

[a] Examples of links among aquatic fish compartments that are supported by the time-to-equilibrium model for bioaccumulation by fish are not shown here; they are presented in Table 5-3.
[b] Uptake, filtration, or partitioning which includes diffusion, advection, and/or active accumulation and elimination by organism.
[c] Advection processes.
[d] Bioenergetic model for bioaccumulation by fish.
[e] “Fish” include the following compartment types: benthic omnivore, benthic carnivore, water-column herbivore, water-column omnivore, and water-column carnivore.
[f] The flying insect compartment is modeling an insect with an aquatic benthic larval phase; assumes insect emerges and becomes a flying adult invertebrate with the same body concentration as aquatic larval phase.
[g] The presence of the terrestrial herbivore to terrestrial predator/scavenger link will depend on the species or groups selected to represent these compartment types for particular site (*e.g.*, a mouse could be prey for red-tailed hawks or mink, but a deer might not be prey for any predators).

Table 5-3
Biotic Compartment Type Links and Mass Transfer Processes:
Time-to-Equilibrium Model for Bioaccumulation by Fish [a]

(Table includes non-transformation related examples supported by the current TRIM.FaTE algorithm library.)

Links Between Compartment Types		Mass Transfer Process Addressed
Sending	**Receiving**	
Surface Water (algae as phase of surface water)	Water-column Herbivore	Equilibrium Partitioning
Water-column Herbivore	Surface Water (algae as phase of surface water)	(Equilibrium Partitioning)
Sediment	Benthic Invertebrate (Flying Insect) Herbivore [b]	Equilibrium Partitioning
Benthic Invertebrate (Flying Insect) Herbivore [b]	Sediment	Equilibrium Partitioning
Water-column Herbivore	Water-column Omnivore	Equilibrium Partitioning
Water-column Omnivore	(Water-column Herbivore)	(Equilibrium Partitioning)
	Water-column Carnivore	Equilibrium Partitioning
Water-column Carnivore	(Water-column Omnivore)	(Equilibrium Partitioning)
Benthic Invertebrate	Benthic Omnivore	Equilibrium Partitioning
Benthic Omnivore	(Benthic Invertebrate)	(Equilibrium Partitioning)
	Benthic Carnivore	Equilibrium Partitioning
Benthic Carnivore	(Benthic Omnivore)	(Equilibrium Partitioning)

[a] In the current library, the algorithms implementing this model are limited to use with mercury species.

[b] The flying insect compartment represents an insect with an aquatic benthic larval phase; assumes insect emerges and becomes a flying adult with the same body concentration as aquatic larval phase.

TRIM.FaTE. A description of how external models can be integrated with TRIM.FaTE is presented in Appendix B.

5.4 SIMULATION SET-UP

The third step shown in Figure 5-1 is providing the relevant input data for the simulation. This involves specifying the chemical properties of each modeled chemical, the initial distribution of chemical mass in the compartments, the data for each modeled source, environmental data needed by the selected algorithms, and the simulation and output time steps. Note that some properties must be specified before links can be made. The role of these inputs in estimating the chemical fate and transport is briefly explained in this section. A complete list of all the parameters for the currently implemented algorithms is presented in Appendix D of Volume II of the TRIM.FaTE TSD.

5.4.1 CHEMICAL PROPERTIES

To estimate the fate and transport of chemical mass through the system, certain properties for each modeled chemical must be specified. The list of chemical properties that are necessary for a given simulation varies depending on the chemical (*e.g.*, organic chemicals differ from metals) and the media and biota modeled. Several examples of abiotic and biotic chemical properties are listed in the adjacent text box.

ILLUSTRATIVE EXAMPLES OF ABIOTIC CHEMICAL PROPERTIES

- half-life or degradation rate (in each environmental medium)
- Henry's Law constant
- melting point
- molecular weight

ILLUSTRATIVE EXAMPLES OF BIOTIC CHEMICAL PROPERTIES

- half-life or rate of metabolic degradation (for each modeled animal or plant species)
- chemical transformation rates (in modeled plant leaves and animal species)
- elimination rate (for modeled animal species)

5.4.2 INITIAL AND BOUNDARY CONDITIONS

For each compartment and chemical in a scenario, the user has the option of specifying an initial concentration. In addition, the user can specify boundary concentrations for volume elements that include an external interface (*e.g.*, air volume elements located around the outer edge of the modeled domain). Boundary contribution algorithms for air compartments in outer volume elements can then be applied to account for continuing contribution of chemical to the modeled region from external sources (*e.g.*, the cumulative effect of non-local sources). Default values of zero may be assumed for boundary concentrations for pollutants that have a relatively short half-life in the air or if the objective of the simulation is to assess the effects of a modeled source (or sources) in the absence of "background." If the objective is to assess "cumulative" exposures, or if results of the analysis are to be compared with measurement data, however, the initial concentration and boundary contribution features may be essential. Refer to Section 3.5 for additional discussion of initial and boundary conditions in TRIM.FaTE.

Additionally, the user can specify concentrations (in one or more compartments of any type) to be held constant (or fixed) throughout the simulation period. This feature is useful for evaluation or diagnostic simulations.

5.4.3 SOURCE DATA

Source data must be specified for each source modeled in the scenario. Conceptually, there is no limit on the number of different sources that can be modeled. The adjacent text box lists the variables that must be defined for each source.

SOURCE INPUTS

- source location
- emission height
- chemical-specific emission rate

5.4.4 ENVIRONMENTAL SETTING DATA

Whereas initial and boundary conditions and source data specify the location and influx of chemical mass in the system, environmental setting data are needed to estimate the fate and transport of that mass throughout the modeled system. There are two general types of environmental data necessary for TRIM.FaTE to estimate mass transfers in abiotic media: meteorological data and other environmental setting data. The level of desired refinement in the simulation dictates the appropriate data (*i.e.,* ranging from site-specific data to default values). Each general type of input data is briefly described below.

5.4.4.1 Meteorological Data

Meteorological data are required for many of the transport-related algorithms. For example, the air advection algorithms rely on wind data, and some of the deposition algorithms from air to surface soil and surface water rely on precipitation data. The meteorological and related inputs needed for TRIM.FaTE are listed in the adjacent text box (vertical wind velocities are also needed when modeling multiple air layers). Meteorological data at any (or various) time intervals can be used in TRIM.FaTE (*e.g.*, hourly wind speed and direction data). Preprocessors are available to convert the available meteorological data to the format required for TRIM.FaTe. For example, TRIMet is a data preprocessor developed for use with TRIM.FaTE to process the necessary meteorological data and convert them into a single, specifically formatted, meteorological input file.

METEOROLOGICAL INPUTS

- horizontal wind speed
- horizontal wind direction
- air temperature
- precipitation rate
- mixing height
- day/night
- beginning and end of litter fall
- frost date

5.4.4.2 Other Environmental Setting Data

Other environmental setting data are needed to define the characteristics of the biotic and abiotic compartment types that TRIM.FaTE uses to estimate the transport and transformation of chemical mass in the system. For example, data on atmospheric dust load are needed for TRIM.FaTE to estimate dry deposition of airborne particles to soils and surface water; data on sediment porosity (*i.e.*, water content) are required to estimate mass transfers between a sediment compartment and its overlying surface water compartment. In addition, some data are also required to define properties of links between compartments, such as the fraction of total surface runoff from one soil compartment that enters into an adjacent soil or water compartment. Input data values can be provided to TRIM.FaTE as point estimates, or, when using the stochastic sampling feature for uncertainty analyses, as distributions (with appropriate associated characteristics such as mean and standard deviation). The adjacent text box presents some examples of both biotic and abiotic environmental setting data that may be necessary for a TRIM.FaTE simulation.

ILLUSTRATIVE EXAMPLES OF ABIOTIC ENVIRONMENTAL SETTING DATA

- atmospheric dust load (for air compartment type)
- soil density (for all soil compartment types)
- current flow velocity (for surface water compartment type)

ILLUSTRATIVE EXAMPLES OF BIOTIC ENVIRONMENTAL SETTING DATA

- population per area (for all animal compartment types)
- biomass per area (for all plant compartment types)
- food ingestion rate (for all animal compartment types)

5.4.5 DEFINING TIME STEPS

The final inputs necessary to begin a TRIM.FaTE simulation are the time steps. The simulation time step specifies a minimum frequency at which the model will calculate transfer factors and chemical mass exchange between (and transformation within) compartments.[3] The output time step (defined by a combination of the simulation time step and the number of simulation steps per output) determines the points in time at which the amount of chemical in each compartment will be reported as an output as moles, mass, or concentration. Post-processors may be used to aggregate these results over specified averaging periods. For example, the results using an output time step of one hour may be averaged to produce the mean daily or monthly concentrations of the pollutant in each compartment. Refer to Section 3.2 for a more detailed discussion of basic timing issues and Section 5.6 for more information on analysis of results.

5.5 SIMULATION IMPLEMENTATION

The next step is the actual running of the model, where the movement of the chemical(s) through the compartments is simulated for each calculation time step for the specified simulation period. The exact manner in which this is performed depends on the algorithms selected. For each link, a call is made by the model to the algorithm library to determine the transfer factors that mathematically describe the potential exchange of chemical mass across an interface between two compartments or a compartment and a sink. If all algorithms involve only first-order processes, then movement of the chemical will be simulated with a system of linked differential equations, the solution of which is found using a differential equation solver (*e.g.,* LSODE). For more complicated algorithms, other tools would be necessary (*e.g.*, a method of solving partial differential equations).

[3] As described in Section 3.5.1, the model also calculates the chemical inventory at each time point when a new value is encountered for any inputs.

TYPES OF OUTPUTS

TRIM.FaTE provides several different types of output to a user. The main TRIM.FaTE outputs are the moles, mass, and concentration in each compartment at each reporting time step. TRIM.FaTE can also output all algorithms used, all input values, and transfer factors for each transfer of mass. In addition, TRIM.FaTE can output certain intermediate calculated values, such as the calculated chemical mass moving across the interface between two volume elements, that can be used for evaluating the performance of the model.

The basic TRIM.FaTE outputs are described in the adjacent text box. The concentration estimates in the abiotic compartments and uptake rates (*i.e.*, doses) for biotic compartments can be used to estimate ecological risks (see Section 2.3.6). The concentration estimates in the abiotic and biotic compartments can be output to an exposure model (*e.g.,* TRIM.Expo) to estimate human exposure.

A separate part of the application of TRIM.FaTE at a site involves analysis of uncertainty and variability for a simulation. The concepts and processes involved with that analysis are discussed in Chapter 6, Treatment of Uncertainty and Variability.

5.6 ANALYSIS OF RESULTS

After completion of a simulation, the user must interpret the model output. This can be a daunting task because of the quantity of output data TRIM.FaTE produces. For example, for an analysis that models the fate and transport of three chemicals in 100 compartments for 30 years, with simulation and reporting time steps of one hour, the model would produce nearly 79 million values each for moles, mass, and concentration (3 × 100 × 30 × 8,760). Even using a reporting time of once per day (*i.e.*, 24-hour reporting time step) would result in over three million output values. If the user wanted to also examine the intermediate model calculations, the output data set could grow even larger. Because output data from a multimedia fate and transport model can be used in many ways, different users will have different needs for the model's output. Post-processors can be used to present the output in forms that are useful to the decision-makers, such as the maximum concentration in the modeling region or in specific compartments, the average concentration in an environmental medium, and long-term time trends of environmental concentrations.

TRIM.FaTE also includes tools that facilitate analysis of results by summarizing and condensing output data through spatial, tabular, and graphical methods. Examples of three tools currently implemented in TRIM.FaTE are presented here.

- The **Averager** can generate averages of TRIM.FaTE outputs in any multiple of the output time step as well as in monthly and annual increments. It can also limit the compartments included in the averaged file by excluding selected results columns (each column represents the results for a single compartment). These functions are useful for reducing the size of output files for further off-line analysis in a separate program (*e.g.*, spreadsheet or other quantitative analysis program).

- The **Graphical Results Viewer** presents model results (moles, mass, or concentration) for each compartment type on a map of the parcels by using different colors to represent incremental gradations in the results for a specific chemical. Results can be presented for any time increment that is output by the model or generated using the Averager. The results can also be animated over a time series (*e.g.*, to show changes in monthly average concentration over the course of a multi-year run).

- The **Aggregator** can produce tables in HTML, text, or comma-delimited formats that combine columns of output data in different ways for producing combined or comparative statistics. Functions available for combining results columns include sum, average, difference, ratio, and percent difference. For example, the user can use this tool to combine columns for similar chemicals (*e.g.*, to calculate total mercury for a particular compartment type) or to compare two columns (*e.g.*, to compare results for two PAHs and calculate differences in concentration).