

TRIM.FaTE USER'S GUIDE

MODULE 12: POINTERS FOR SETTING UP A TRIM.FaTE SCENARIO¹

This module is a collection of helpful hints, warnings, quality control (QC) tips, and examples that may be useful to a user when setting up a TRIM.FaTE scenario. These pointers address a wide range of model implementation topics and are gathered here as a way to highlight them for the user. Specifics about the model set up, algorithms, and properties are not described here in significant detail. The user is instead referred to more complete documentation and discussion in companion TRIM.FaTE User's Guide modules and the TRIM.FaTE Technical Support Document (TSD), Volumes I and II (EPA 2002a,b).

The pointers are organized into three sections:

1. General Information
2. Chemical-specific Inputs
3. Interdependent Properties

1. GENERAL

1.1 Mass and Materials Balance in TRIM.FaTE. TRIM.FaTE is designed to track and balance *chemical* mass throughout the modeled system. In general, the TRIM.FaTE model architecture is not designed to explicitly model the movement of other mass (i.e., abiotic media and plants or animals) and consequently does not track overall materials balances for media like soil.

- ▶ ***Abiotic media.*** The current library has various simplifications regarding some complex inter-related processes. For example, in applications to date, the runoff property that is influential in moving pollutant among surface soil compartments or to surface water compartments has been set to a constant derived from site-specific information rather than a formula with an explicit dependency on the precipitation data used in the model simulation. The user has the flexibility to implement this simplification or to implement a new formula (or set of formulas) describing the relationship of the runoff property with other properties, including, if desired, explicit attention to water and soil balance. See Section 3 for a discussion of properties for which inter-dependencies and materials balance issues may be important to consider.
- ▶ ***Biota.*** With the exception of litterfall, the algorithms in the current library do not account for movement or changes in biotic mass. Each biotic compartment represents a stable population for which the following is true:

¹ Descriptions of library-specific algorithms and properties presented in this module pertain to the July 2005 version of the TRIM.FaTE Public Reference Library.

Reproduction + immigration = migration + predation + death by other causes

Note, however, that the current library does not include algorithms or properties describing an impact on pollutant mass in a biotic compartment as a result of immigration and migration. In other words, in applications to date, it is assumed that any immigration or migration that occurs does not impact pollutant accumulation and distribution in the scenarios. There may be applications for which the user may want to make additions/changes to the library in order to simulate pollutant loss or gains from these processes or a seasonal dependency for pollutant uptake to account for biota that come and go (e.g., migrating birds).

1.2 Groundwater Modeling. The groundwater modeling approach implemented in the current library is a highly simplified model as follows:

- ▶ The groundwater compartment type currently acts like a transfer sink for chemicals infiltrating through the soil layers; no horizontal movement of groundwater is modeled except when groundwater is adjacent to surface water (one-directional net flow into surface water). No groundwater is modeled below a surface water body. Also, no vertical movement of chemical mass from groundwater back to the overlying soil layer(s) is modeled. Thus, groundwater compartments *not* adjacent to surface water compartments act essentially as mass sinks.
- ▶ Recharge into a surface water body is currently possible only if the surface water compartment and groundwater compartments are horizontally adjacent and vertically overlapping (i.e., depth of surface water must be greater than depth to groundwater; TRIM.FaTE requires interfacial area to allow transport between groundwater and surface water).

This simple approach has been implemented because TRIM.FaTE is designed to model persistent/bioaccumulative chemicals emitted initially to air, which generally are not very mobile in soils and do not infiltrate significantly to groundwater. Thus, the groundwater compartment is unlikely to accumulate much chemical relative to other compartments.

1.3 Timing Inputs at Set-up. Because TRIM.FaTE is a dynamic model, timing concepts relating input data, calculations, and model outputs are important. TRIM.FaTE timing-related terms and concepts include the following (refer also to Section 3.5 of TSD Volume I, EPA 2002a):

- ▶ ***Simulation period***, the length of time over which the simulation occurs.
- ▶ ***Input data time step***, the interval between changes in value of any time-varying property (e.g., wind speed data may be provided in hourly intervals). Each change in an input data value dictates a point in time at which TRIM.FaTE calculates new transfer factors. The interval between changes can vary both across and within data types depending on the data provided to the model.

- ▶ **Output time step**, the frequency at which results are provided by the model (i.e., the time interval between outputs). The results at each output time are those derived for that time point (i.e., a “snapshot” at the end of the time step), not an average. The output time step is determined by two user-specified inputs (both are scenario properties):

Output time step = simulation time step * number of simulation steps per output step

- The **simulation time step** is the fixed time interval at which the model recalculates the moles distribution for the full set of compartments and sinks being modeled (also recalculated when input data change, which may differ); this time step defines the successive points in time at which a “snapshot” is taken of the moles distribution in the system. For a given simulation time step, TRIM.FaTE calculates a new transfer factor matrix (i.e., the complete set of transfer factors for every compartment pair) if the transfer factors have changed since the last recalculation (e.g., due to a change in time-varying input data).
- The **number of simulation steps per output step** is a factor that determines the time points at which values are reported as output. This parameter does not affect calculation of the output.

Two simple examples in Table 1 illustrate these concepts.

Pointers related to timing properties and inputs are listed below.

- ▶ When setting the simulation time step, the user should consider its relationship to the time steps in the input data being used (i.e., there may not be a benefit to setting the simulation time step smaller than the input data time step).
- ▶ Run time is affected by both the simulation time step value and the input data time step value(s), with the latter believed to be more important, because at every point a time-varying input changes, both the affected transfer factors and the moles distribution must be recalculated.
- ▶ For TRIM.FaTE runs in the steady-state mode in which there are no time-varying inputs or outputs, only one transfer factor matrix is calculated, one set of output values is generated, and the scenario time step properties are not relevant.
- ▶ The value of the output time step can have a major effect on the size of the output files (i.e., small values for this time step increase size of output files). To reduce file size, the user can specify the largest output time step that suits the user’s needs. Additionally, if averages of multiple time points (rather than instantaneous values) are of interest, output file size can be reduced by generating only average

values over the periods of interest using the scenario properties *averageResultsFiles* and *averagingInterval* (see Module 9, Scenario Properties).

Table 1
Examples Illustrating How Input Time Step and Simulation Time Step
Can Affect Model Calculations and Output

Example A	Example B
<ul style="list-style-type: none"> • Input data time step = 1 hour (e.g., meteorological data measured at 1-hour increments) • Simulation time step = 2 hours • Simulation steps per output step = 1 	<ul style="list-style-type: none"> • Input data time step = 2 hours (e.g., 2-hour averaged meteorological data) • Simulation time step = 1 hour • Simulation steps per output step = 1
<p><i>Model calculation:</i> Model recalculates transfer factors and moles distribution at 1-hour intervals</p>	<p><i>Model calculation:</i> Model recalculates transfer factors at 2-hour intervals and moles distribution at 1-hour intervals</p>
<p><i>Output:</i> Output time step = 2 hours Results are reported at 2-hour intervals</p>	<p><i>Output:</i> Output time step = 1 hour Results are reported at 1-hour intervals</p>

1.4 Time Scale for Model Results. Although TRIM.FaTE can provide outputs in time increments as small as one hour, and input data values may also change frequently (e.g., when using hourly meteorological data), **the user should be aware that the smallest time scale appropriate for interpreting results of a given process depends on all of the scenario-specific input data for the parameters involved in algorithms describing that process.** For example, when long-term average values (e.g., annual averages) are used in estimating erosion/runoff properties, outputs impacted by those properties (e.g., soil, water, and related compartments) will be limited in their ability to provide useful information on a smaller temporal scale. In the current library, uncertainty in deriving site-specific estimates at smaller scales has resulted in the use of several such simplifications that limit the user’s ability to draw interpretations for various compartment types at smaller time scales.

1.5 Specifying Initial Concentrations. Before running a TRIM.FaTE scenario, the user has the option of specifying an initial concentration for each chemical in each compartment. This option is useful when the user knows the starting concentration of a chemical in the environment (e.g., the background concentration of mercury present in a surface soil due to non-modeled sources).

If the user does not specify an initial concentration, the default value used in all compartments will be zero. Running a scenario with the default values (i.e., initial concentrations of zero) can be useful as it may give some indication of the impact of

sources in the absence of background on predicted chemical concentrations in environmental media.

There are three primary properties used in specifying initial concentrations for each compartment:

- ▶ ***initialConcentration [units]_UserSupplied*** is a user-specified Compartment Property that contains the value for the initial concentration of a chemical that the user wants to use for a particular compartment. The user should make sure that **[units]** is replaced with the actual units of concentration (e.g., mg/L).
- ▶ ***FractionInitialConcentrations*** is a user-specified Scenario Property that specifies the fraction of ***initialConcentration [units]_UserSupplied*** that should be used in the simulation (e.g., 0.5 if the user wants to include 50 percent of the user-specified initial concentrations for a particular simulation, 1 if the user wants to use 100 percent of the user-specified initial concentrations in a simulation). This property can be set to zero if desired (doing so will result in no initial concentrations for that simulation).
- ▶ ***initialConcentration [units]*** is a formula Compartment Property that calculates the initial concentration that the model that will be use in the simulation. This value is calculated by multiplying ***initialConcentration [units]_UserSupplied*** for that compartment by ***FractionInitialConcentrations*** for the scenario. Because this is a formula property calculated by TRIM.FaTE, the user does *not* need to specify a value for this property. The user should make sure that **[units]** is replaced with the actual units of concentration (e.g., mg/L).

Instructions for setting initial concentrations for specific compartment types are provided below:

- (1) For the compartment for which initial concentrations are to be set, check to see if the required pair of properties (identified in the table below) already exist. If the properties do not exist for the compartment, add them.

Compartment Type	Property Pair
Biota	<i>initialConcentration_g_per_kg;</i> <i>initialConcentration_g_per_kg_UserSupplied</i>
Abiotic media, except for surface water and groundwater	<i>initialConcentration_g_per_m3;</i> <i>initialConcentration_g_per_m3_UserSupplied</i>
Surface water and groundwater	<i>initialConcentration_g_per_L;</i> <i>initialConcentration_g_per_L_UserSupplied</i>

- (2) Input the desired initial concentration for each chemical by assigning a number value to the ***initialConcentration [units]_UserSupplied*** property.

- (3) Set the *initialConcentration* *[units]* property to the appropriate formula (if the property has already been added, it should be set to the correct formula).

Compartment Type	Property Specifications for <i>initialConcentration</i> <i>[units]</i>
Biota	<i>containingScenario.FractionInitialConcentrations;</i> <i>compartment.Chemical.initialConcentration_g_per_kg_UserSupplied</i>
Abiotic media, except for surface and ground water	<i>containingScenario.FractionInitialConcentrations;</i> i
Surface and ground water	<i>containingScenario.FractionInitialConcentrations;</i> <i>compartment.Chemical.initialConcentration_g_per_L_UserSupplied</i>

1.6 Specifying Fixed Concentrations.² Before running a TRIM.FaTE scenario, the user has the option of specifying the chemical concentrations (in one or more compartments of any type) that will be maintained by TRIM.FaTE throughout the duration of the scenario. Because this option does not allow for normal movement of chemical mass through the model system and will disrupt the overall mass-balance of the simulation, the fixed concentration feature is used primarily for evaluation or diagnostic purposes.

To specify the concentration for a compartment throughout the simulation, the user should complete the following two steps:

- (1) Add the property *useSpecifiedConcentration* to the compartment(s) and set it to “true.” When prompted to select a chemical to which this property will apply, select “<None>” (this property should not be set as a chemical-specific property).
- (2) Add one of the following properties (specifying the chemical with which it will be associated) and set the value to the appropriate concentration level. Note that if more than one of *concentration* *[units]* property for the same chemical is added for a single compartment, they will all be ignored. Also, if the user wants the value at the first time step to be the same as the specified concentration value, they must also specify the initial concentration (see Section 1.5).

² For this section, “fixed concentrations” are compartment concentrations that are specified by the user as unaffected by *model-calculated fluxes*. The mass in a compartment with fixed concentrations will not change according to the transfer and transformation rates generated by the transition matrix solved by TRIM.FaTE. However, the “fixed concentrations” can be time-varying. To specify a time-varying concentration for a compartment, the user should set the property form for the concentration property to unevenly time stepped real number. Refer to Modules 2 (Software Overview) and 3 (Library and Scenario Data Files) for more information on setting time-varying property values in TRIM.FaTE.

Compartment Type	Property to be Added
Biota	<i>concentration_g_per_kg</i>
Abiotic media, except for surface and ground water	<i>concentration_g_per_m3</i>
Surface and ground water	<i>concentration_g_per_L</i>

1.7 Adding and Linking Sinks in a Scenario. There are three types of sinks in the current library. The process for adding sinks to a scenario differs depending on the type of sink.

- (1) **Advection sinks** (i.e., air advection sinks, surface soil advection sinks, and sediment burial sinks) capture chemical mass advected out of the modeling region. These sinks are automatically added by TRIM.FaTE wherever they are needed when Smart Link is used to create links in a scenario. Smart Link will add advection sinks to the volume element containing the sending compartment. Note that any advection sinks that are added by Smart Link will *not* appear as compartments in the Compartments view of the scenario; however, they will appear on the link names displayed in the Links and Algorithms views. Furthermore, the chemical mass that is transferred to each sink is included in the results of a simulation (e.g., mass and moles results files). TRIM.FaTE assigns a name and number to advection sinks that are added by Smart Link (e.g., “Sink in Sink 23 for Air_NE2”). If Smart Link is not used to create any links in a scenario, advection sinks will not be added.
- (2) **Flush rate sinks** capture chemical mass in surface water compartments that is transported outside the modeled region via flowing water (see Appendix A for more information on flush rate sinks). These sinks must be added by the user for each surface water compartment manually or via an import file.
- (3) **Degradation sinks** capture the mass of chemicals that are degraded or transformed into another chemical not tracked within TRIM.FaTE. These sinks must be added by the user to the scenario manually or via an import file.

Flush rate and degradation sinks can be added to a scenario manually via the Compartments view in the Scenario window by following the same basic steps as those followed to add a biotic or abiotic compartment:

- Select the volume element to which to add the sink by highlighting a volume element in the “Outdoor Environment” pane.
- Select the desired sink type from the library by highlighting the sink in the “Compartments in Lib” pane of the Compartments view.
- Click the “<<Add” button below the “Compartments in Lib” pane to add the sink to the scenario.

Alternatively, flush rate and degradation sinks can be added to a scenario via a Compartment Import file in the same manner than abiotic and biotic compartments are added. Refer to Module 3, Library and Scenario Data Files, for information on using Compartment Import files.

Separate sinks do not need to be added for different chemicals (i.e., multiple chemicals can be transferred to a single sink of any type). In TRIM.FaTE test cases, flush rate sinks have been added to the volume element containing the sending surface water compartment. Degradation sinks have been added to each volume element containing any compartments in which chemical degradation occurs. Only one degradation sink has been added to each volume element – therefore, all degradation that occurs in compartments in that volume element is tracked by a single degradation sink, regardless of the type of compartment in which the degradation occurs. For example, if a surface soil compartment, a mouse compartment, and an eagle compartment are all placed in the same volume element, one degradation sink has been added to that volume element to account for any chemicals that degrade. Other approaches may be appropriate depending on the purpose of the application.

As mentioned above, the Smart Link tool will add any needed advection sinks and create all links between advection sinks and the sending compartment (e.g., air). Once the user has added flush rate and degradation sinks, Smart Link will create the necessary links between the sink and the sending compartment(s) *if the sinks have been added to the volume element containing the sending compartment*. If the user wants to link a sink and a compartment associated with separate volume elements, the link must be created manually via the Links view (i.e., Smart Link will not create this link). Regardless of how the links are created, the appropriate algorithms will be added by TRIM.FaTE automatically when the links are created.

If the Smart Link tool is not used, the user will need to create all links to flush rate and degradation sinks manually via the Links view in the scenario window.

1.8 Sediment Burial. The burial rate of chemical mass below the sediment volume element (i.e., to a sediment burial sink) is a function of the sediment deposition and sediment resuspension rates. Conceptually, as sediment particles suspended in the surface water settle with their associated chemical mass to the top sediment layer, there is a simultaneous burial of sediment particles and associated chemical from the bottom sediment layer into a sediment burial sink. Such burial can be accomplished in TRIM.FaTE using a sediment burial sink and the sediment burial algorithm.

The formula properties in the July 2005 version of the TRIM.FaTE public reference library, however, dictate that the net chemical mass transferred “down” to the benthic sediment via sediment deposition is equal to the chemical mass transferred “up” to the suspended sediment via resuspension. Consequently, there is no net burial of chemical mass in the sediments (i.e., the mass transfer from a sediment compartment to the linked sediment burial sink is zero). If the user wishes to model burial of chemical mass in the

sediment, values for some of the properties describing the deposition and resuspension processes (listed below) would need to be modified.

Properties involved in describing the deposition and resuspension processes:

- ▶ Suspended sediment deposition velocity (*SedimentDepositionVelocity*; a property of the surface water compartment),
- ▶ Benthic sediment resuspension velocity (*SedimentResuspensionVelocity*; a property of the sediment compartment),
- ▶ Concentration of suspended sediment (*SuspendedSedimentconcentration*; a property of the surface water compartment),
- ▶ Suspended sediment solid material density (*rho*; a property of the surface water compartment), and
- ▶ Benthic solids concentration (*Benthic_Solids_Concentration*; a property of the sediment compartment),
- ▶ Benthic sediment solid material density (*rho*; a property of the sediment compartment), and
- ▶ Sediment porosity (*Porosity*; a property of the sediment compartment)

Refer to Section 4.2.2 of the TRIM.FaTE TSD Volume 2 (EPA 2002b) for a complete description of the conceptual basis of transfers between surface water and sediment. Additional information on the interdependency and sensitivities of surface water and sediment properties is also presented in the TRIM.FaTE Evaluation Report, Volume 2 (EPA 2005).

2. CHEMICAL-SPECIFIC INPUTS

2.1 First-Order Half-Life Versus First-Order Rate Constant. TRIM.FaTE applies one or the other, depending on the process being modeled; the user must understand the difference to select and input appropriate data. Rate constants in TRIM.FaTE are specific to the process (e.g., oxidation of elemental to divalent mercury, elimination of absorbed chemical from an animal via urine and feces), and the data selected should match the specific process(es) covered. Half-lives in TRIM.FaTE are used to estimate general degradation rates of chemicals in specific compartments to compounds whose subsequent fate is not modeled because (1) the reaction products are not of major interest in the analysis, (2) adequate data to model the reaction products are not available, or (3) the nature of the chemical reaction processes is too complex to model using a single (or few) first-order equation(s). The degradation rate constant (calculated from the input half-life) is used in transferring the chemical to a degradation sink for that compartment (i.e., removing it from the modeled system). The half-life input to TRIM.FaTE to

estimate degradation can cover all degradation processes that apply to the chemical in that compartment (e.g., bacterial degradation, photolysis, and oxidation of a chemical in surface soils).

2.2 Degradation Versus Transformation. Measures of the rate of **degradation** (i.e., half-life or rate constants) are used in TRIM.FaTE to calculate the transfer of the parent compound to a degradation sink, in which the mass of the degradation product(s) are no longer tracked in the scenario. Degradation measures are used when the user's interest is limited to the fate of the parent chemical. TRIM.FaTE models all degradation/transformation processes as first-order processes.

Measures of the rate of **transformation** are used in TRIM.FaTE to calculate the quantity of chemical to transform into another chemical being modeled in the scenario. Process-specific transformation rate constant data for the transformed chemical are needed when the user is interested in tracking the fate of transformation products of the parent chemical in each compartment. Note that the transformation of the daughter compound may include transformation back to the parent.

2.3 Chemical Fate in Biota. In the current library, a biotic compartment is designed to consist of a single "container" for chemical mass; chemicals can be taken up into, released from, or degraded within this container.

- For terrestrial plants, compartment types are defined as plant subparts – stem, root, leaf, and particle on leaf – and the chemical is distributed among these four subparts. For animals, however, the current library does not include subparts such as organs (e.g., liver, muscle).
- The current library includes transformation algorithms for three mercury species. To track movement of transformation products of other pollutants, the new chemicals and algorithms describing their production and transfers among the compartments would need to be implemented in the library.

2.4 Elimination Versus Degradation. The user should note the difference in TRIM.FaTE between elimination (i.e., excretion of the parent via urine or feces from animal to abiotic media, where it continues to be tracked in TRIM.FaTE) and degradation (i.e., chemical transformation to a chemical species not tracked by the model and transferred to a sink). The user needs to ensure that the literature values obtained for this information denote the specific fate (either elimination or degradation) of a chemical consumed by biota, and the appropriate rate constants/half-lives are implemented in TRIM.FaTE. It is important for the TRIM.FaTE user to check the specific data type because some biotic research is focused on general *removal* of a chemical from an organism rather than the specific mechanism (i.e., either degradation or elimination).

3. INTERDEPENDENT PROPERTIES

Some environmental setting parameters that are interdependent in natural systems are treated as independent parameters in the current library. It is up to the user to ensure consistency between any independent parameters whose values may have inter-dependencies. Some specific parameters that the user should consider are listed here.

3.1 Precipitation. Precipitation rate is entered as a scenario-level property that references the hourly (or other time step) precipitation rates contained in a meteorology data file. Processes that depend directly on precipitation rate (e.g., wet deposition rate) reference these data. Processes that are dependent on precipitation occurrence and rate in a natural system, but for which values are input directly by the user to the library or scenario, include:

- Runoff and erosion rates (generally entered as long-term averages, but could be time-dependent).
- Infiltration rate (generally entered as long-term average, but could be time-dependent).
- Streamflow (can be entered as long-term average; more specific time-varying data, such as monthly or daily, can be used if available). See also the following surface water paragraph.

The user can calculate runoff and infiltration, for example, by applying coefficients to the precipitation data being used. At a minimum, users should always check to make sure values being used are internally consistent (e.g., the sum of runoff and infiltration should not be greater than precipitation).

User Tip

The user should confirm that wind direction data in the TRIM.FaTE meteorological data input file represents the direction wind is blowing FROM.

3.2 Surface Water. The user should ensure consistency between (1) the movement of water between individually modeled water bodies, and (2) the water inputs and outflows from each, in order to give an approximate overall water balance for the modeled scenario. For rivers, the user should ensure consistency between streamflow or flush rate (i.e., bulk flow of water to another compartment or sink) and the current velocity given the dimensions of the containing surface water volume element.

Depending on the water bodies modeled, two surface water flow properties need to be defined by the user for a scenario:

- ▶ The link property *BulkWaterFlowRate_Volumetric* for any water bodies that are modeled as connected to each other; and

- ▶ The surface water compartment property *Flushes_per_year* (i.e., volumetric turnovers per unit time) for any water body that is modeled as connected to a flush rate sink.³

For many of the relatively small flowing and non-flowing water bodies of potential interest in TRIM.FaTE applications, measured data for flows (e.g., U.S. Geological Survey (USGS) gauging station data) and flush rates are not expected to be available. An approach for estimating surface water flow values that has been used for previous TRIM.FaTE test cases applies an *overall runoff ratio* for the whole watershed (e.g., a runoff value based on total watershed area and local river flow data (USGS) for that watershed) to determine flows for the smaller watersheds modeled within the scenario. A demonstrative example of this approach is described in Appendix A. Note that this example is not meant to describe a particular real system (i.e., the numbers are illustrative and may not necessarily represent realistic input values) and the responsibility rests with the user for ensuring the scientific defensibility of the approach employed for their application. In addition, as with all input parameters, the user would need to check the units of any input data to ensure they are correctly configured for TRIM.FaTE.

3.3 Soil and Sediment Particle Properties. Porosity and density properties are used for soil and sediment in TRIM.FaTE; the user should be aware of what is calculated and what is a user input.

For sediment, the following three TRIM.FaTE parameters are related and interdependent (the TRIM.FaTE property name is provided in italics):

- ▶ Solid material density in sediment (*rho*), in kg[dry sediment]/m³[dry sediment particle]
- ▶ Benthic solids concentration (*Benthic_solids_concentration*), in kg[total sediment]/m³[sediment compartment]
- ▶ Porosity (*Porosity*), in m³[water]/m³[sediment compartment]

As it is assumed that water completely fills the sediment pore spaces, these parameters are related as follows:

$$Benthic_solids_concentration = rho * (1 - Porosity)$$

or:

$$Porosity = 1 - ([Benthic_solids_concentration]/[rho])$$

For sediment compartments in TRIM.FaTE, the user enters number values for rho and porosity, and the benthic solids concentration is calculated. The user should check to

³ A single water body can be treated both ways if part of its total flow is modeled as going to a connected water body and the rest of the flow to a flush rate sink.

make sure that the calculated benthic solids concentration is reasonable and consistent with any site-specific data that are available.

For soil, the basic relationship is essentially the same. However, instead of entering a numeric value for porosity, the user is required to enter values for the volume fractions of the soil compartment that are liquid and vapor (i.e., *VolumeFraction_Liquid* and *VolumeFraction_vapor*). The sum of these fractions is the equivalent “porosity” of the soil. The solid material density in the soil (sometimes referred to as the “soil bulk density”) is not used in TRIM.FaTE calculations and therefore is not actually calculated by the model. However, it may be useful for the user to calculate this property offline for comparisons to site-specific measurement data (which may be available as soil bulk density rather than porosity or liquid/vapor fractions). The equation for this relationship is analogous to that for sediment:

$$\text{Soil bulk density} = \rho * (1 - [\text{volume fraction liquid} + \text{volume fraction vapor}])$$

3.4 Soil Compartment Vertical Dimensions. When using the soil diffusion algorithm in the current library, the normalized thickness of each soil layer (i.e., surface, root zone, vadose zone soil in the current version) should increase with increasing distance from the upper surface of the soil. In other words, the normalized thickness of the soil layers should increase with depth. The normalized depth of a soil layer is represented by the following expression:

$$\text{Normalized soil layer depth} = \gamma_{Si} * (\text{depth of soil layer in meters})$$

where γ_{Si} is the gradient of soil concentration change in the soil compartment i in units of (1/m). γ_{Si} is equal to the inverse of the characteristic soil depth. The algorithm used to model diffusion between vertically stacked soil compartments was developed based on the assumption that the normalized soil thickness of the higher soil layers is smaller than that of the lower ones. For additional information, refer to the discussion of Transfer Factor (TF) 5-8 in the TRIM.FaTE TSD Volume II (EPA 2002b).

3.5 Average Vertical Velocity of Water in Soil. The soil compartment property *AverageVerticalVelocity* (units of m/day) represents the average velocity of the moving liquid phase in the soil column. This is a property of surface soil, root zone soil, and vadose zone soil compartments that is used to calculate the effective advection velocity of chemical moving vertically through the soil compartment (see Chapter 5 of TSD Volume II; EPA 2002b). In the current library, this property is entered as a constant value and is intended to be representative of the range of velocities occurring over all times due to various factors (e.g., precipitation rate, soil characteristics). The parameter is designed to be inclusive of zero flow periods; it is *not* limited only to the velocity during rainfall events. In other words, although there are factors that can affect the *instantaneous* velocity of water infiltrating through soil, in the current library this parameter represents the overall *average* velocity of water in soil at any given time.

4. REFERENCES

U.S. EPA. 2002a. U.S. Environmental Protection Agency. TRIM.FaTE Technical Support Document Volume I: Description of Module. EPA 453/R-02-011a. Office of Air Quality Planning and Standards.

U.S. EPA. 2002b. U.S. Environmental Protection Agency. TRIM.FaTE Technical Support Document Volume II: Description of Chemical Transport and Transformation Algorithms. EPA 453/R-02-011b. Office of Air Quality Planning and Standards.

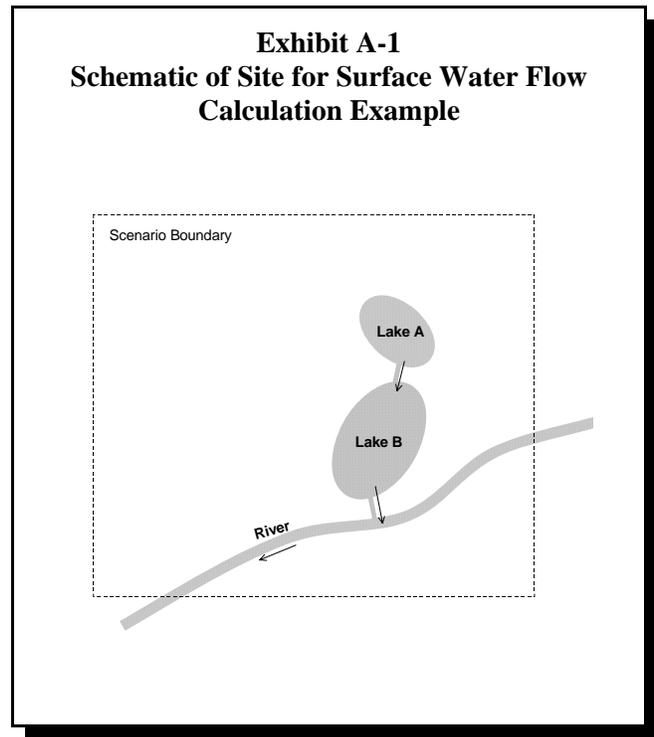
U.S. EPA. 2005. U.S. Environmental Protection Agency. Evaluation of TRIM.FaTE Volume II: Model Performance Focusing on Mercury Test Case. EPA 453/R-05-002. Office of Air Quality Planning and Standards.

APPENDIX A

DESCRIPTION OF SURFACE WATER FLOW CALCULATION EXAMPLE

For this example, assume that there are two lakes (A and B) and one river to be modeled (see Exhibit A-1). The following assumptions apply to this example.

- ▶ Lake A empties into Lake B.
- ▶ Lake B empties into the river.
- ▶ Lake A and Lake B are connected via a short stream that is not explicitly modeled (i.e., chemical mass in the water flowing out of Lake A is assumed to be instantaneously transferred to Lake B).
- ▶ Lake B and the river are connected via a short stream that is not explicitly modeled.
- ▶ The river does not originate nor end within the modeled scenario (i.e., it flows through it).



The steps to calculate surface water flow values are described below as applied to the example described above.

- (1) **Calculate or obtain overall runoff rate for the region** (i.e., overland water flow rate per area of watershed). Measured data (based on precipitation rates and local measurements) may be available. Alternatively, the user can find the overall watershed (e.g., see U.S. EPA's Find Your Watershed Web site at <http://cfpub.epa.gov/surf/locate/index.cfm>) and then find corresponding flow data for the stream/river that drains this watershed (e.g., from the USGS water resources Web site at <http://water.usgs.gov/>). For this example, assume these or similar sources provide the following data:

- ▶ Total watershed area (i.e., encompassing modeled region and other nearby regions; all land and water surface area included): 500 mi² (1,295 km²); and
- ▶ Mean flow for river flowing out of total watershed (measured at boundary of watershed): 750 feet³/second (cfs) (1.83 × 10⁶ m³/day).

Based on these numbers, the mean ratio of water flow to watershed area is 750/500, which results in an overall runoff rate of 1.5 cfs/mi² or 1,413 m³/km²-day (0.001413 m³/m²-day, or m/day).

Alternatively, if site-specific data are available for a runoff coefficient (e.g., percent of precipitation that is surface runoff), the user may apply this coefficient to site-specific precipitation data to estimate local surface water flows.

Note: The property for total runoff rate (i.e., *TotalRunoffRate_m3_m2_day*) is a property of the surface soil compartment in the current library. Depending on the size and nature of the regional watershed relative to the modeled region (and availability of other data), it may be appropriate to use the runoff rate described above for the total runoff rate parameter.

(2) **Determine watershed and water body surface areas** for the water bodies to be modeled in the scenario. These can be calculated using Geographic Information System (GIS) tools from site-specific watershed data, or estimated manually from maps. For the lakes in this example, assume:

- ▶ Lake A: watershed = 5 km²; lake = 0.5 km²; total area = 5.5 km².
- ▶ Lake B: watershed = 7 km²; lake = 1 km²; total area = 8 km².

**Major Assumptions/Simplifications of Approach to Derive
Surface Water Flow Inputs Described in Example**

- ▶ Assumes that the only water inputs for a water body are runoff and bulk flow from a separate water body (or water bodies). Other factors (e.g., recharge to water bodies from groundwater) are not accounted for.
- ▶ Assumes that the overall runoff rate for a watershed can be used to find surface water flows for that watershed via runoff based on the land surface plus water surface area (i.e., the runoff rate is assumed to apply equally to the water body and the surrounding watershed).
- ▶ In real systems, the water flow parameters described here will be dependent on, or at least related to, other parameters that are included in the TRIM.FaTE library. Connections between the flow parameters and these additional parameters are not discussed exhaustively in this section. Parameters that may be related to water flow and that the user may decide to employ in customizing the library to their modeling purposes include:
 - Runoff, precipitation, infiltration, and other related parameters, and
 - Current velocity of flowing water bodies (e.g., rivers, streams).

NOTE: The user is reminded of their responsibility for assuring appropriateness and scientific defensibility of the approach employed for their application.

In addition, the dimensions of the river segment being modeled are needed along with an estimate of flow (based on USGS monitoring data from a point in or near the modeled segment, or, if not available, estimated following the basic method described here for the lakes):

- ▶ Dimensions of segment modeled for this scenario: length = 5,000 m; width = 25 m; depth = 0.5 m (volume of segment = 62,500 m³).

- ▶ Flow rate at USGS station near modeled segment: 60,000 m³/day.

(3) **Combine data from steps (1) and (2) to calculate flow data for each lake.** For this method, it is assumed that the water flow into a lake (i.e., from overland runoff and any bulk flow from a connected water body) is equal to the flow leaving a lake (i.e., via bulk flow to another water body or flushed to a sink).⁴ To calculate the flow, multiply the total area (lake + watershed) by the average runoff rate (assume the runoff rate applies equally to land and water surfaces for the purposes of calculating water flows). In addition, the water flowing in from other water bodies must be accounted for (i.e., accumulative water flow must be considered).

- ▶ *For flow from Lake A to Lake B:*

Runoff into Lake A (from Lake A watershed) is equal to flow out of Lake A and into Lake B:

$$5.5 \text{ km}^2 * 1,413 \text{ m}^3/\text{km}^2\text{-day} = 7,771 \text{ m}^3/\text{day}$$

- ▶ *For flow from Lake B to river:*

Runoff into Lake B from Lake B watershed:

$$8 \text{ km}^2 * 1,413 \text{ m}^3/\text{km}^2\text{-day} = 11,304 \text{ m}^3/\text{day}$$

Add flow into Lake B from Lake A to get total flow out:

$$11,304 + 7,771 = 19,075 \text{ m}^3/\text{day} \text{ total water flowing into river from Lake B}$$

This flow is less than total flow of the river, so it appears to be relatively reasonable.

(4) **Calculate flush rate for river emptying to flush rate sink.** The flush rate for the river can be calculated from the flow and the compartment volume (see data values presented in Step 2):

$$60,000 \text{ m}^3/\text{day} \div 62,500 \text{ m}^3 = 0.96/\text{day} \text{ (just less than once per day, or roughly 350 times per year)}$$

(5) **Enter values into scenario as compartment or link properties** (see also Note in the text box below).

- ▶ For the *link* between Lake A and Lake B: bulk water flow rate = 7,771 m³/day
- ▶ For the *link* between Lake B and river: bulk water flow rate = 11,304 m³/day

⁴ This assumption is a broad simplification of the actual system because it does not address other gains or losses (e.g., via evaporation or groundwater recharge); however, these other processes may be partly accounted for by the overall runoff rate that is used.

- ▶ For the lake surface water *compartment*: flush rate = 350/year

Note: If dispersive water flow is modeled for surface water compartments that are directly connected, the links between the connected water bodies will also require the following link properties:

- ▶ Distance between water body midpoints in meters; and
- ▶ Diffusive exchange coefficient between surface water compartments in m^2/day .

If the surface water compartments are not directly connected but chemical mass is moved from one to the other (e.g., by using a “pipeline” connection), the algorithm for dispersive water flow should be *removed* from the link between the two water bodies.