TRIM.FaTE USER'S GUIDE
MODULE 13: OPERATION OF TRIM.FaTE IN STEADY-STATE MODE[1]

Most of the initial test case applications of TRIM.FaTE have been executed in the dynamic mode, which accepts time-varying input data and generates time-series results (e.g., hourly or monthly concentrations for a 30-year time span). However, TRIM.FaTE can also be configured to run in the steady-state mode, which calculates a steady-state solution for the chemical amount in each compartment. Scenario runs in the steady-state mode have a *much* shorter run time than dynamic runs (e.g., a few minutes vs. hours or even days, depending on the duration of the simulation, complexity in terms of numbers of compartments, and frequency of time-varying input data). The steady-state mode is therefore useful for testing new approaches and conducting sensitivity or Monte Carlo analyses that can require numerous iterations.

A technical description of TRIM.FaTE's steady-state mode is presented in **Volume II of the TRIM.FaTE TSD, Appendix C** (EPA 2002). That appendix includes discussion on how a steady-state run should be configured, along with technical reasons for why these changes from the dynamic set-up are necessary. A summary of potential applications for the steady-state mode is also included in that appendix. The user is encouraged to review Appendix C prior to setting up and executing a steady-state run. In addition, information on a test case application of TRIM.FaTE in the steady-state mode is presented in the TRIM.FaTE Evaluation Report, Volume II (EPA 2005).

To run TRIM.FaTE in the steady-state mode, the user creates a project and scenario in the same way as they would for a dynamic simulation, with a few exceptions. A summary is presented here of the steps the user must complete that are *different* for a steady-state run compared with a dynamic run. Note that these steps could also be applied to create a steady-state simulation from an existing dynamic simulation.

(1) ***Ensure that no time-varying input data are used in the scenario.*** While essentially all properties may be represented by time-varying data, the ones listed in Table 1 are those that have been most commonly represented by time-varying data in test applications to date (the current TRIM.FaTE library name and location of each property is provided in the table).

For each time-varying property, the user must replace the time-varying input data with constant values. The user should be especially careful in developing constant values for inputs such as precipitation rate, which are either "on" (non-zero) or "off" (zero) at different times. Implications of different approaches – for example, setting a property as "on" or "off" all the time – should be considered, and it may even be useful to perform multiple iterations with different settings.

[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.

Table 1
Common Time-Varying Properties

Object	Property	TRIM.FaTE Library Name
Scenario	Air temperature	*AirTemperature_K*
	Horizontal wind speed	*horizontalWindSpeed*
	Rain	*Rain*
	Wind direction	*windDirection*
Volume elements containing air compartments	Height (set equal to atmospheric mixing height)	*top*
Leaf compartment	Litterfall rate	*LitterFallRate*
Surface water compartment	Current velocity of waterbody	*currentVelocity*
	Flush rate of waterbody to sink	*Flushes_per_year*
Surface water to surface water sink	Flow rate of waterbody	*BulkWaterFlowRate_Volumetric*

It is noted that calculating an arithmetic mean may not be an appropriate approach for estimating a representative value for some time-varying properties (e.g., wind direction). It is the user's responsibility to ensure that suitable steady-state inputs have been developed for his or her application.

It is important to note that the current library has separate dynamic and steady state properties controlling properties depending on the growing season (i.e., *AllowExchange*) and the exchange of chemical mass between leaves and air (i.e., *isDay*). The *AllowExchange_Dynamic* leaf compartment property and the *isDay_Dynamic* scenario property are typically time-varying and are used when a dynamic scenario is run. For steady-state scenarios (i.e., when *simulateSteadyState* is set to "true"), constant values are entered for *AllowExchange_SteadyState_forAir* and *AllowExchange_SteadyState_forOther* leaf compartment properties and *isDay_SteadyState_forAir* and *isDay_SteadyState_forOther* scenario properties.

(2) ***Disable dynamic air advection algorithms and enable steady-state air advection algorithms.*** Once the scenario has been created, the user should disable the air advection algorithms that use time-varying data and enable the steady-state air advection algorithms by changing the appropriate *enabled* properties as described in Table 2. To accomplish this, the user should complete the following steps:

Algorithms for Steady-state Air Advective Transfer in the TRIM.FaTE Public Reference Library

The TRIM.FaTE public reference library currently includes steady-state air advection algorithms that can be used in place of the dynamic horizontal air advection algorithms that are dependent on wind speed and wind direction. The transfer factor associated with the steady-state algorithm references a link property – *SteadyState_AdvectiveTransfer* – that is defined as a constant real number value for each interface between air compartments (and between air compartments and sinks). This constant transfer factor must be calculated off-line by the user (see Step 3). The steady-state air advection algorithms are necessary because using a constant wind speed and direction with the air-to-air transfer algorithms that were developed for the dynamic mode can result in a much different spatial distribution of chemical mass than is estimated when wind speed and direction are allowed to vary.

- Go to the Algorithms view in the scenario and be sure that "Links" is selected from the drop-down menu at the top of the Outdoor Environment pane on the left.

- In the Outdoor Environment pane, find any air compartment and select a link from that compartment to an adjacent air compartment. Click the "Show Algs" button at the bottom of this pane to display the algorithms on that link (i.e., steady-state and dynamic advection between air compartments).

- In the "Algorithms in Links" pane, select the dynamic air advection algorithm and click the "Properties" button at the bottom of the pane. Change the *enabled* property to "false." Then, enable the steady-state algorithm via the same process, changing the *enabled* property to "true." **Note that the *enabled* property for any algorithm controls the status of that algorithm throughout the entire scenario (not just on the selected link);** therefore, this process only needs to be completed for a single air-to-air link to affect all air advection algorithms in the scenario.

- Then, in the Outdoor Environment pane, find an air compartment on the outside edge of the layout and select the link to an air advection sink (this sink will usually be numbered; for example, the link may be entitled "to Sink in Sink 42 for Air_ESE5"). Click the "Show Algs" button to display the algorithms on that link (i.e., steady-state and dynamic advection between an air compartment and an air advection sink).

- In the "Algorithms in Links" pane, select each algorithm and change the *enabled* property to "true" or "false" as appropriate. Again, note that changing the status of an algorithm on just one link affects the *enabled* status of the algorithm throughout the scenario.

This process and other details related to controlling TRIM.FaTE algorithms is described in more detail in Module 8. If desired, this process can be done in the library before the scenario has been created, by making the changes to the air advection algorithms via the "Algorithms" tab in the library and then using that library to create the steady-state scenario.

Table 2
Air Advection Algorithm Settings

Algorithm Type	Air Algorithm Name	*enabled* Property Setting for Steady-state Scenario
Dynamic	Advection from Air to Air, Horizontal	*false*
	Advection from Air to Air, Vertical	*false*
	Bulk Advection from Air to Advection Sink, General	*false*
Steady-state	Advection from Air to Air, Steady-state Approx	*true*
	Bulk Advection from Air to Advection Sink, Steady-state Approx	*true*

(3) ***Import steady-state advective air transfer link properties***. Once the appropriate air advection algorithms have been disabled/enabled, the user should set the steady-state air advective link properties to constant values. Although this can be accomplished by entering the values directly to the scenario via the GUI (i.e., by typing in the values for each *SteadyState_AdvectiveTransfer* property on each air link), it can be simpler and more accurate to import these values using a property import file (i.e., using "File/Load Properties" from the *File* option on the menu bar). When the import file with the advective link properties is selected, the user should make sure to click "override" first, and then click "ok" when the import has been successful.

It is the user's responsibility to develop an appropriate method for calculating steady-state advective transfers. In the TRIM.FaTE mercury test case (EPA 2005), steady-state air transfers were estimated by arithmetically averaging the hourly air-to-air and air-to-sink advective transfers (for each interface, in each direction). The averaged transfers were calculated using results from a dynamic application of TRIM.FaTE for this site over the five-year meteorological input data period. Other approaches to developing representative steady-state transfers may also be possible. It is the user's responsibility to ensure that an appropriate method is employed.

(4) ***Disable all links FROM groundwater compartments by setting the "enabled" property for these links to "false."*** Links from groundwater compartments could include links to adjacent surface water compartments (referred to as "recharge" in TRIM.FaTE) and links "from/to self" (i.e., the links on which transformation occurs.) This step is required because the processes within and transfers from ground water for many chemicals of interest tend to be so slow that these compartments act as virtual sinks and prevent the solver used in TRIM.FaTE from successfully finding a steady-state solution.

Links in a scenario must be turned off individually by changing the *enabled* property on the link to "false." However, to turn off all of the individual links from groundwater at once (i.e., without having to manually find each link), the user can complete the following steps:

- Go to the Algorithms view in the scenario and select "Links" from the drop-down menu above the Outdoor Environment pane on the left. Click the "Select" button at the bottom of the Outdoor Environment pane. A dialog box will appear entitled "Select Links."

  Note that the user must use the "Select" function on the Algorithms view – ***not*** on the Links view – in order to select only those links going ***from*** groundwater. If the "Select" function on the Links view is used, all links involving groundwater (both to and from) will be selected. For a steady-state scenario, processes that transfer chemical mass ***to*** groundwater compartments should remain enabled.

- For "Type is:," select "Link" from the drop-down menu. Under the "For Sending Compartment" box, type "groundwater" for Name Contains. Click the "Select" button and all of the links from groundwater for that scenario will be highlighted.

- Click the "Properties" button to display the properties for all links from groundwater in the scenario and change the *enabled* property to "false."

(5) ***Set the value of the scenario property "simulateSteadyState" to "true."*** If the user has set *simulateSteadyState* to "true" in a property import file used to create the scenario, this step will be completed upon importing that file to the scenario.

The simulation can then be initiated by selecting "Run Scenario" from the *Run* pull-down menu in the Scenario window (or pressing Control + R).

Note that there are three scenario properties related to the operation of LSODE (the differential equation solver used by TRIM.FaTE) in steady state mode. These properties and their default values (as included in the current version of the library) are:

- *SteadySimAbsoluteTolerance* (the absolute error tolerance for the linear equation solver; default value is 1.0 x 10^{-12});
- SteadySimMaxSolverIterations (the maximum number of iterations the linear equation solver should cycle through in seeking a solution before failing; default value is 10,000); and
- *SteadySimRelaxationParam* (the relaxation parameter for the Jacobi linear equation solver; default value is 1.2).

The user should not change these properties from their default values without fully considering the impacts of the changes. For information on LSODE that would be relevant to this consideration, refer to Radhakrishnan and Hindmarsh (1993).

REFERENCES

Radhakrishnan, K., and A. Hindmarsh. 1993. Description and Use of LSODE, the Livermore Solver for Ordinary Differential Equations. National Aeronautics and Space Administration, Office of Management, Science and Technical Information Program. NASA Reference Publication 1327. Lawrence Livermore National Laboratory Report UCRL-ID-113855.

U.S. EPA. 2002. 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.

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