

TRIM.FaTE USER'S GUIDE

MODULE 2: OVERVIEW – CREATING A NEW SCENARIO¹

1. OVERVIEW

This module summarizes the steps to be completed in setting up a new TRIM.FaTE project and scenario. A scenario is a specified set of conditions used to define the model setup for a particular simulation or set of simulations. Multiple scenarios can be stored within a project file. Each project is associated with one or more libraries that serve as the source(s) of the objects (e.g., compartments, algorithms, sources) used to populate a scenario. A user can create a new project for each *new* TRIM.FaTE application, such as a new site or area to which TRIM.FaTE will be applied. Within a project, several scenarios can be created that define ready-to-run simulations differing in any number of ways (e.g., duration, various input values, or inclusion of different compartment types). The sequence of steps presented in this module is somewhat flexible – other permutations are possible, and some iteration is usually involved in setting up a scenario. The information presented in this module is not intended to provide a comprehensive, in-depth explanation of each step or user requirement. Rather, this module provides a frame of reference for the other modules included in this user guidance and an introductory summary of the steps required to set up a scenario.

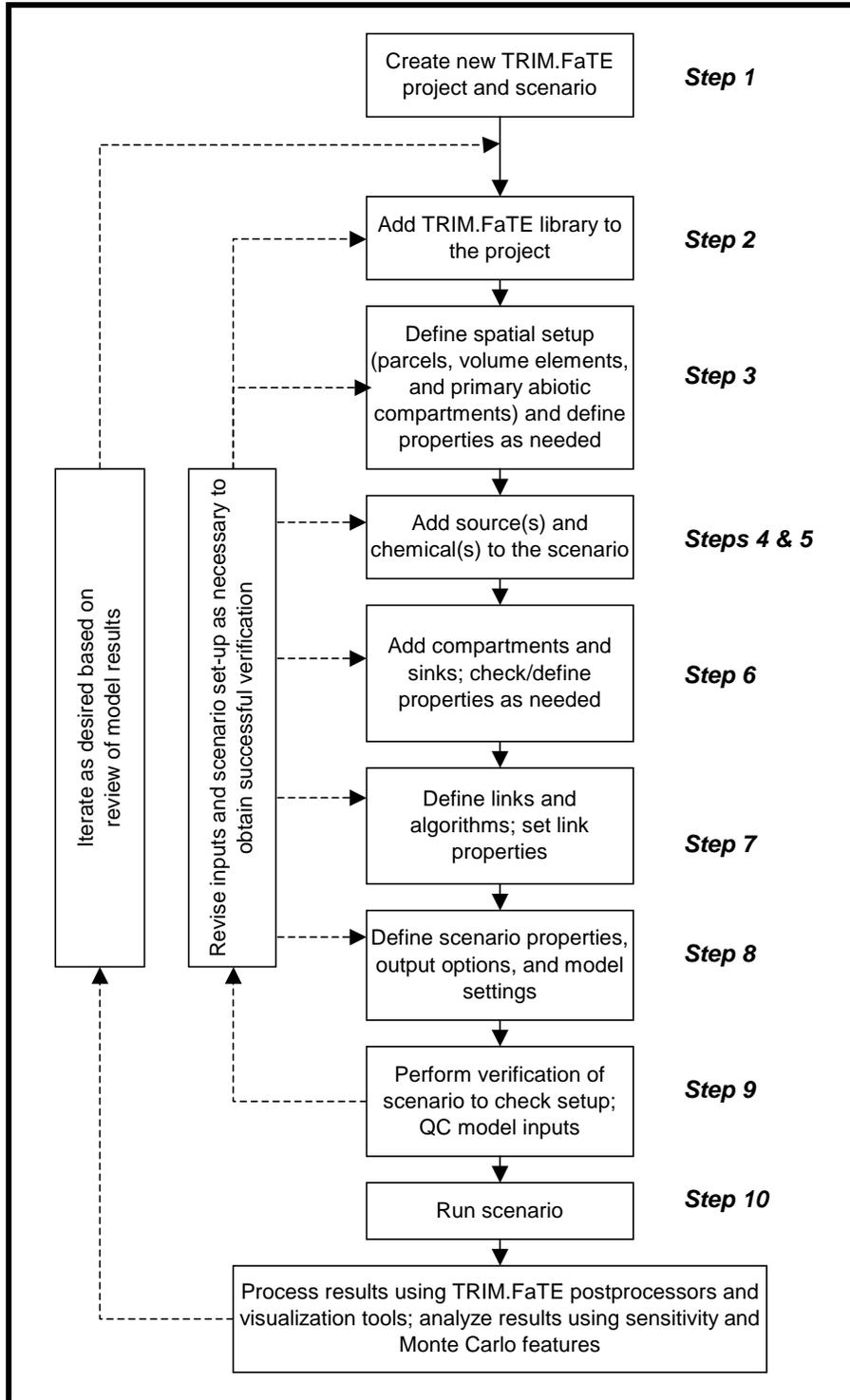
A summary of the step-wise process for setting up a TRIM.FaTE scenario is diagrammed in Figure 1. In Section 2, the purpose of each step is described (the “What” sections) along with a brief description of how the step is carried out (the “How” sections). References to specific user guidance modules are included for each step where applicable. Section 3 provides a conceptual overview of the TRIM.FaTE modeling process.

2. STEPS FOR SETTING UP A SCENARIO

The basic steps that the user must complete to set up a new scenario are described below. Each step in this section includes a description of the step, a basic overview of how the user carries out the step, and references to other User's Guide modules. In addition, each step is referenced in the overview of the set-up process presented in Figure 1.

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.

Figure 1
Overview of Basic Steps: Setting up a Scenario



Step 1 – Create a new TRIM.FaTE project file and scenario

What: Create a new project file and scenario within the TRIM.FaTE modeling framework.

How: Install and start up TRIM.FaTE. Using the *File* pull-down menu, create a new project and scenario.

Reference: Module 1, Software Overview

Step 2 – Add a library to the project

What: Add a TRIM.FaTE library to the new project, making it available as a source of objects for the new scenario.

How: From the TRIM project window, select a library on the hard drive and add the project using the “Add” button. Before adding the library to the project, it is suggested that the library be “customized”² to include project-specific objects, properties, and non-spatially varying property values (e.g., source data, chemicals to be modeled, algorithms to be used, abiotic and biotic compartment types to be included in the scenarios of this project). Note that aspects of Steps 3 through 7 may relate to the data values in the library. Refer to Section 3 for additional details.

Reference: Module 1, Software Overview

Step 3 – Set up the scenario spatial layout

What: Define the air and surface parcels, volume elements, and primary abiotic compartments for the scenario (i.e., the size and basic characteristics of the area to be modeled).

How: Create and import a Volume Element Import file.

References: Module 3, Library and Scenario Data Files
Module 5, Developing the Spatial Layout

Step 4 – Add sources of chemical mass to the scenario

What: Add chemical source(s) (e.g., emission point(s) that are being modeled) to the scenario.

How: Characterize sources in the library; add sources from the library to the scenario via the Sources view in the scenario window.

Reference: Module 7, Source Characterization

Step 5 – Add chemicals to the scenario

What: Add chemicals to be modeled in the scenario.

How: Characterize chemicals in the library (modify/update existing chemical properties, if desired); add chemicals to the scenario via the Chemicals view in the scenario window.

² This can be done by duplicating an existing library and then editing it to include project-specific information.

Reference: The existing TRIM.FaTE library includes data and algorithms for several different chemicals; any of these can be added to a scenario. Additional chemicals can be added by the user provided that the required input data and algorithms are available; see Module 4, Adding New Components to the Library. Note that any chemicals for which transformation is modeled (including chemicals not emitted from any sources or entering as boundary contributions, but formed *only* through transformation) must be added to a scenario during this step (i.e., before compartments and links are created).

Step 6 – Add compartments and degradation or flush rate sinks to the scenario and define compartment properties

What: Add biotic compartments to the scenario (note that the abiotic compartments are added via the volume elements file in Step 3); set compartment properties to application-specific values; add degradation and flush rate sinks as necessary.

How: Compartments can be added to a scenario from the library either manually via the Compartments view in the scenario or by importing a compartments import file into TRIM.FaTE. Compartment properties can then be modified as desired, either via the Compartments view in the scenario (i.e., manually) or via an import file. Degradation sinks (i.e., for any abiotic or biotic compartments in which chemical degradation will be modeled) and flush rate sinks (i.e., for surface water bodies that release water out of the modeled region) can be added by the user either manually via the Compartments view or by including them in a compartments import file. Note, however, that advection sinks (i.e., sinks that will be linked to those air and surface soil compartments comprising the outside border of the modeling region to account for chemical mass transported horizontally out of the modeled region, or sinks linked to sediment compartments that account for burial beneath the sediment compartment) will be added automatically by TRIM.FaTE where they are needed if the Smart Link tool is used in Step 7. It is *not* possible to add advection sinks manually.

References: Module 3, Library and Scenario Data Files
Module 6, Implementing Biota in a TRIM.FaTE Scenario
Module 12, Pointers for Setting Up a TRIM.FaTE Scenario
Module 16, Tables of TRIM.FaTE Input Parameters

Step 7 – Link compartments and implement associated algorithms; set link properties

What: Create connections (i.e., links) between compartments (and between compartments and sinks); confirm or specify algorithms to direct chemical mass transfer, degradation, and transformation across the links; set required properties of the links between compartments (e.g., runoff fraction, bulk water flow).

How: Links can be created between compartments (and sinks) manually via the Links view in the Scenario, automatically using the Smart Link tool, or by using a combination of manual and automatic methods. Algorithms will be added automatically when the links are created (the available algorithms for a

scenario are stored in the library). Site-specific modifications related to implementation of algorithms (e.g., turning on or off specific algorithms, choosing alternate algorithms from the library) can be accomplished via the Algorithms view in the Scenario. Link properties can be set manually via the Links view in the Scenario or an import file. If the Smart Link tool is used, air, surface soil, and sediment advection sinks will be added automatically by TRIM.FaTE where appropriate during this step (this is the *only* way that advection sinks can be added to a scenario).

References: Module 3, Library and Scenario Data Files
Module 8, Links and Algorithms
Module 11, Estimating Runoff and Erosion Fractions for Surface Soil
Module 12, Pointers for Setting Up a TRIM.FaTE Scenario

Step 8 – Set scenario properties

What: Define the basic settings for the run (e.g., start/stop time, location for results files) and other properties as desired (e.g., meteorological data).

How: Scenario properties can be set manually via the Scenario view or by including these properties in a Properties file to be imported. Some other properties, such as meteorological properties, can be set at the “scenario level” (i.e., via the Scenario view) if desired.

References: Module 9, Scenario Properties
Module 10, Compiling and Processing Meteorological Data Inputs
Module 12, Pointers for Setting Up a TRIM.FaTE Scenario
Module 14, Simulation Results and Analyses

Step 9 – Verify scenario setup

What: Ensure that most required properties and links have been set; TRIM.FaTE also performs some simple checks for selected property values (e.g., diet fractions must sum to 1 for biotic compartments).

How: The Verify function can be initiated via the *Run* pull-down menu on the TRIM.FaTE scenario window. Based on the results of the verification, the user may need to revise certain compartment properties, links, or other aspects of the scenario set-up. Note that the Verify function does *not* check for reasonableness for all property values; the user is responsible for this type of QA/QC. This function also does not necessarily verify that the scenario will run to completion successfully (not all properties are checked).

Reference: Module 1, Software Overview

Step 10 – Run scenario

What: Run model for the scenario and save the specified results to files on the user’s computer.

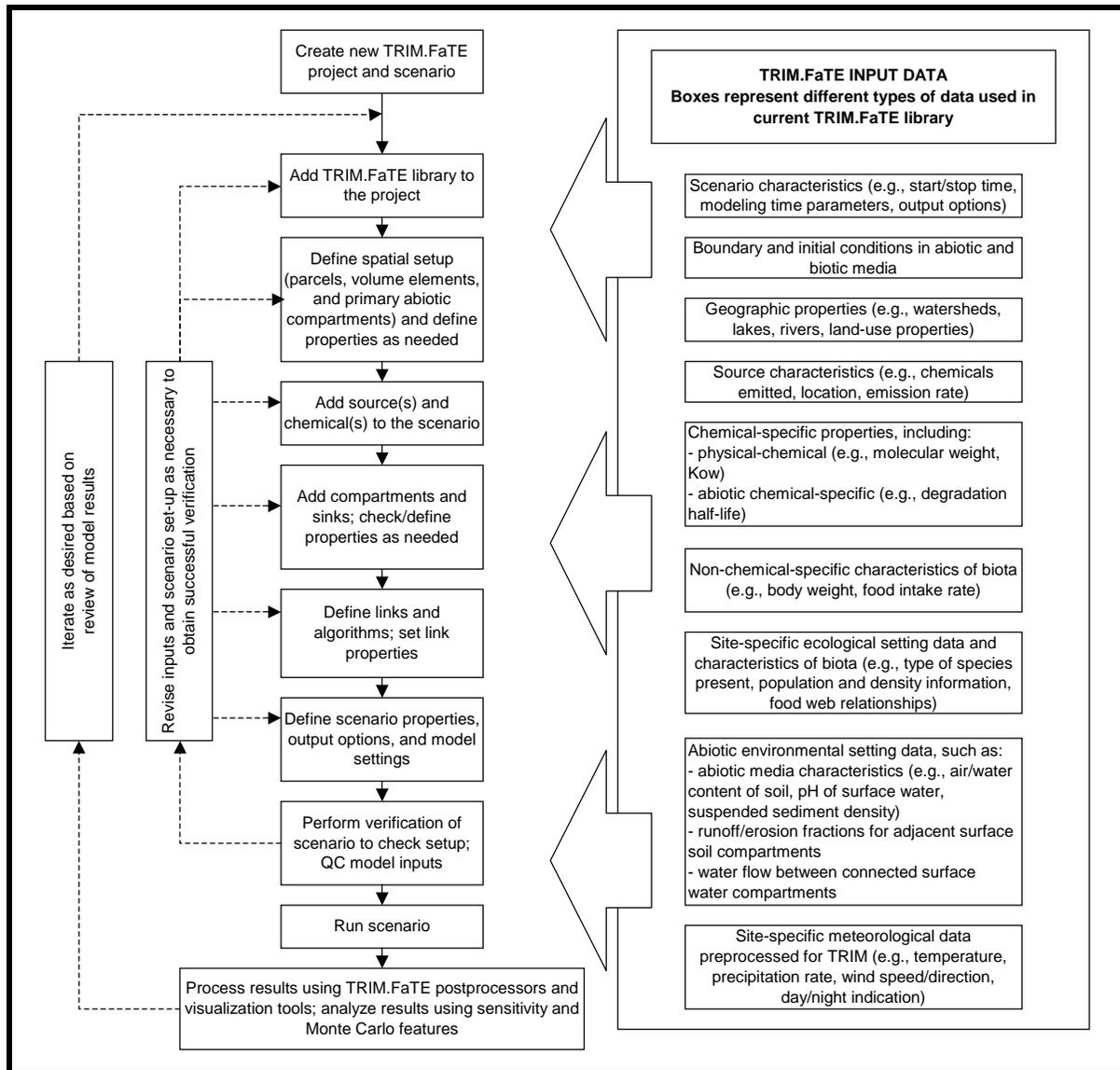
How: A TRIM.FaTE scenario can be run from the Scenario window using the “Run Scenario” command on the *Run* pull-down menu.

References: Module 1, Software Overview
Module 9, Scenario Properties

3. THE TRIM.FaTE MODELING PROCESS

A conceptual overview of the TRIM.FaTE modeling process is presented in Figure 2. This flow chart builds on the diagram presented in Figure 1 by including a summary of the main types of input data used in a scenario. As mentioned in the previous sections, these data are used to define the properties of the objects included in the scenario (i.e., the compartments, volume elements, links, and other components that comprise the scenario). For a specific scenario, it will be necessary to obtain application-specific values for at least some of these parameters. The extent to which new data gathering is required will depend on the scenario being modeled and the objectives of the particular model application.

Figure 2
Conceptual Overview of the TRIM.FaTE Modeling Process



Entering Data for a TRIM.FaTE Scenario

There are several files that the user can use to provide data to TRIM.FaTE for a simulation. These include:

- the **library or libraries** for the scenario;
- **scenario import files** (volume element, compartment, & property import files); and
- **input data files** (most frequently used to provide time varying input data sets)

These items can be used to systematically create a scenario via the steps outlined in Section 2. If desired, the user can create scenario-specific input data tables similar to the tables presented in Module 16 and use the tables to record site-specific values and data sources and to facilitate creation of the TRIM.FaTE scenario.

Customizing the Library. When a scenario is created, the user can add objects and their associated properties (see text box) to the scenario from the library (or libraries) associated with the project. Consequently, prior to populating a scenario with objects, the user may want to customize a copy of the TRIM.FaTE reference library according to the particular specifications of their application. This library can then be used for any scenarios created in that project file. Once a copy of the reference library is made and assigned a name relevant to the project, the library can be customized by revising the values of the different object properties in the library as appropriate for an application.

LIBRARY COMPONENTS

Libraries are comprised of different types of objects, including:

- Algorithms,
- Chemicals,
- Compartments, and
- Sources.

Each object in a library has associated properties that are used to describe characteristics of that object. For example, water temperature and suspended sediment concentration may be properties of a surface water compartment, and number of individuals per square meter may be a property of a deer compartment.

To set or change a property value for any object in the library, the user can use the TRIM.FaTE graphical user interface (GUI) to find and select a property and the keyboard to type in an appropriate value (see Module 1). Alternatively, the user can use library import files to make changes to the library (see Module 3).

Using Scenario Import Files. In addition to the library, the user can use scenario import files to feed data to a TRIM.FaTE scenario (see Module 3). This is the only way that the spatial layout data (i.e., parcel and volume element coordinates) can be entered into a scenario. Additionally, these files can be used to designate the compartments to be associated with the scenario's volume elements, the links between the scenario

compartments, the overall settings for the scenario (e.g., simulation start date and duration), and the particular property values for volume elements, compartments, links, and sources.

Using Input Data Files. For properties whose values will vary with time during the simulation (e.g., hourly meteorological conditions, seasonal changes), external data files can be used to store values “off-line” from the TRIM.FaTE project file (see Module 3). To specify that these data are used in the simulation, the value for these properties in the scenario must be set to reference the data file on the user’s computer.

With the exception of a few restrictions and some specifications for different file types (e.g., volume element import files must be used to feed volume element specifications to a TRIM.FaTE scenario), how the data employed in a TRIM.FaTE simulation are stored and provided to a TRIM.FaTE scenario is the prerogative of the user. Table 2 summarizes the different ways that particular types of input data can be provided to a TRIM.FaTE scenario.

Creating Additional Scenarios for a Project

The data acquisition process can begin before the TRIM.FaTE scenario has been created and may continue after execution of several simulations. If property values are to be revised from their original settings in a scenario, it is up to the user to determine the way in which the revisions will be made. For example, the user could simply make the revision to the property value directly in the scenario (e.g., via the GUI), which would mean that the scenario differs from the associated library for this property value. Or, the user could revise the value in a duplicate of the original scenario, where the duplicated scenario is given a different name and a description is added that clarifies the deviation from the original scenario. The new scenario would also differ from the associated library for this value. Alternatively, the user could revise the property value in the library and then create a new, revised scenario, using the updated object property. The new scenario would reflect the revised property value.

Because parcels and volume elements are integral parts of a scenario, a change to the spatial layout for a modeling application (e.g., in order to compare results using a different layout) will require the creation of a new scenario (to be saved in either the same project or a new project file).

User Responsibility

The user is reminded that they have the responsibility for confirming that a created scenario (including spatial and temporal design and all input data) is appropriate and scientifically defensible for their needs.³

³ As described in Step 9 of Section 2, the scenario set-up process includes a verification step that uses the TRIM.FaTE “verify scenario” command. The user should be aware that this step, which checks for required TRIM.FaTE properties from a computer operating perspective (i.e., to ensure that values exist for all properties), is separate from the steps that the user will need to take to ensure that a simulation contains the *appropriate* data values.

Table 2
Methods for Providing Input Data to Set Up a Scenario

Type of Input Data	Examples of Input Data	How to Provide Data ^a	Reference (TRIM.FaTE User Guidance)
Basic spatial properties	X and Y coordinates for surface and air parcels; temporally constant volume element depths	Volume element import file	Module 5
Chemical properties	Molecular weight; Henry's Law constant	Library file	Modules 3 and 4
Properties of emission source(s)	Chemical-specific emission rate; emission release height	Library file	Modules 3 and 7
Volume element properties that are to be modeled as constants	Boundary concentrations	Property import file	Modules 3 and 5
Compartment properties that are to be modeled as <i>constant</i> spatially and temporally	Air density; particle dry deposition velocity; chemical half-life within biota	Library file	Modules 1, 3, 6, and 7
Compartment properties that are to be modeled as <i>varying spatially</i>	pH for individual surface water bodies; soil properties for a non-homogeneous modeling region; animal population density	Property import file	Modules 3 and 6
Compartment and volume element properties that are to be modeled as <i>varying temporally</i>	Meteorological data (e.g., wind speed, ambient temperature, height of air layer); plant litterfall rate	External data file(s)	Module 3, 5, and 10
Links that are created manually (i.e., those links <i>not</i> created by the Smartlink process)	Food web links (where multiple links are possible); links between non-adjacent surface water bodies	Property import file	Modules 3 and 8
Link properties	Surface water flow, for two connected river compartments; diet fractions for biota that feed on a given food type located in multiple compartments	Link property import file	Modules 3, 8, and 11
Scenario properties	Scenario properties (e.g., simulation start/stop time; output file directory)	Property import file	Modules 3 and 9

^a Where different types of input data are designated as being saved in the same type of data file, it is possible to save all the input data in one data file if desired. For example, values for volume element properties and scenario properties can be saved to a single property import file.

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