

TRIM.FaTE USER'S GUIDE

MODULE 7: SOURCE CHARACTERIZATION¹

This module provides information on how chemical mass can be added to a TRIM.FaTE scenario. There are three ways that chemical mass can be added to a scenario:

- By specifying *initial concentrations* for a compartment (i.e., chemical concentrations present at the start time of a scenario);
- By defining a *boundary contribution* for an air compartment located on the outside edge of the modeling region (i.e., ambient air concentrations present at the edge of the modeling region); or
- By defining a *source* that releases mass directly into an air compartment in a TRIM.FaTE scenario (e.g., an entity representing stack or fugitive emissions of one or more chemicals at a facility).

Although any of these methods for adding chemical mass could potentially be referred to as a “source” outside the context of TRIM.FaTE, the term *source* is used in this module and elsewhere in this User’s Guide to refer to sources as defined in the third bullet – that is, a particular source of chemical mass other than background or initial conditions, such as a facility with stack and fugitive emissions of mercury. This approach is used for consistency with the terminology used in the TRIM.FaTE software. An overview of TRIM.FaTE concepts related to modeling sources and other ways that chemical mass can be added to a scenario is presented in Section 1.

Initial concentrations are useful if the user is aware of the starting concentration in a compartment or compartments (such as background levels of mercury in surface soil at a site) and wants to account for fate and transport of this mass in the assessment. The process for specifying initial concentrations is explained in Section 1.5 of Module 12 (Pointers for Setting up a Scenario). Boundary contributions to air compartments can be used to model levels of chemicals in ambient air (unrelated to the sources being modeling) that are blown into the modeling region (e.g., what is often referred to as “background” concentrations in air). Instructions for setting boundary contributions are described in Section 2 of this chapter.

The majority of the information presented this module is focused on how to model a chemical source as defined in the third bullet above. In general, one or more sources will be the focus of a TRIM.FaTE scenario – it is expected that users will usually be carrying out a TRIM.FaTE simulation to model fate and transport of emissions from the source(s). A summary of the data needed to set up a source for a TRIM.FaTE scenario is described in Section 3. Instructions on how to add source data to a scenario are presented in Section 4, and a description of how to change source data that has been added to a scenario is included in Section 5. Note that this module does not address the estimation of air emission rates based on measurements or

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.

assumptions, a topic covered extensively in other Agency documentation (see, for example, <http://www.epa.gov/ttn/chief>).

1. CONCEPTUAL BACKGROUND

1.1 TRIM.FaTE Model Configuration

TRIM.FaTE was designed by EPA to focus on distribution of a pollutant in the environment as a result of air emissions. Modeling of environmental releases to media other than air (e.g., releases to surface water bodies) is conceptually possible due to the flexibility of the modeling system. However, the current version of TRIM.FaTE has not been evaluated for other types of releases and is recommended for modeling sources of air emissions only at this time. Likewise, only boundary contributions to air have been evaluated (and the algorithms in the public reference library are relevant only for air boundary contributions).

A TRIM.FaTE simulation can include a single source, multiple sources, or even no sources (e.g., simulations for which the source of chemical to the modeling area is from boundary contributions only), and can include or exclude initial concentrations and boundary contributions. Multiple sources can emit to the same compartment (often, they can be modeled as one source; see Section 3.4.1 of this module) or can emit to different compartments. Any time pattern of emissions can be modeled: constant or time-varying, continuous or intermittent.

1.2 Adding Chemical Mass to a TRIM.FaTE Scenario from a Source

Within a TRIM.FaTE scenario, a source introduces chemical mass into a specified air compartment. Each modeled source is located at a discrete point in three-dimensional space. The model uses this spatial information to place the source emissions “inside” the air compartment associated with the volume element that encompasses this location in the scenario. All chemical mass released by that source is added directly to this compartment.

Because *each* emission point must be assigned to a discrete point, TRIM.FaTE does not differentiate between true point source emissions (i.e., releases from stacks, vents, or other distinct sources) and non-point source emissions (i.e., emissions from fugitive equipment leaks, area source emissions from a building, or other diffuse types of sources). Within the TRIM.FaTE framework, all sources are referred to as “sources.” However, large area sources could be treated as multiple emission points in TRIM.FaTE and could emit to different compartments if spatial distribution of the emissions is desired.

1.3 Fate of Chemical Mass Released by a Source

All chemical mass present in a given compartment for each time step is assumed to be evenly distributed within that compartment. Thus, any chemical mass released by a source into an air compartment is instantaneously and homogeneously distributed within that air compartment. Furthermore, individual sources that have different coordinates but are located within the same compartment will, in effect, be modeled in TRIM.FaTE as if they are in the same place (i.e., spatial variations of sources *located within the same compartment* have no effect on chemical mass transport and fate).

2. BOUNDARY CONTRIBUTIONS

In TRIM.FaTE, boundary contributions can be used to account for ambient air concentrations of modeled chemicals present at the edge of the modeling region, such as those that might result from sources located outside of the modeling region (i.e., what are sometimes referred to as “background concentrations” in air). Setting a boundary contribution results in an addition of chemical mass to the scenario when the wind blows horizontally into the modeled region across the outside boundary of a compartment for which a boundary condition has been specified. In the current TRIM.FaTE public reference library, there is a compartment formula property that calculates the input of mass to an air compartment resulting from a boundary condition; the calculation of the mass transferred by this process is similar in concept to the approach used to calculate air-to-air advection. Technical information on boundary contributions is presented in the TRIM.FaTE Technical Support Document, Volume II, Chapter 3 (EPA 2002a).

To include boundary contributions in a TRIM.FaTE scenario, the user specifies the ambient concentration at the outer edge of each air parcel in the air parcel layout. TRIM.FaTE then uses this concentration to calculate mass inputs to the air compartments within these parcels for the time steps when contributions would be expected (i.e., times when the wind direction is blowing toward the air compartment from outside the modeling region). Although the amount of the contribution is calculated using the same equations as those for the air-to-air advection algorithm, no additional links or compartments are created in TRIM.FaTE when boundary contributions are specified. Rather, the model uses the information provided by the user for the boundary contribution to create a sort of “virtual source” within the air compartment and adds the appropriate amount of mass to that compartment for that time step.

Boundary contributions can be set up in a scenario by adding two chemical-specific properties to the compartments in the air parcels comprising the outer edge of the air parcel layout:

- *boundaryConcentration_g_per_m3* (a user-defined real number property); and
- *boundaryContribution* (a formula property).

These properties are not assigned to the air compartment type by default, so they must be added to the scenario after the air volume elements and compartments have been set up in the scenario. As with other properties, they can be added to a compartment by highlighting the compartment(s) of interest, opening the list of properties for that compartment, and clicking the “New” button to bring up a “Create New Property” window. Upon selecting these two properties (both can be added at the same time), a second window will appear allowing the user to select the chemical(s) to which the properties apply. After selecting the chemicals and clicking “OK,” the properties will be added to the designated compartments. If desired, the user could include these properties in a property import file and TRIM.FaTE will add them during the import process (see Module 3, Section 1.2.3).

The user can then specify the desired ambient air concentration for a specific chemical with the *boundaryConcentration_g_per_m3* property. This property is referenced by the formula property *boundaryContribution* that calculates the amount of mass to add to a

compartment based on the concentration at the boundary, the wind speed and direction for that time step, and the orientation of the volume element containing the air compartment. The formula property used by TRIM.FaTE to calculate boundary contributions is a locked, “built-in” formula (like the formula for the air-to-air advection transfer factor) and the actual equation cannot be viewed or edited within TRIM.FaTE by the user.

Once these two compartment properties have been added to the appropriate compartments on the border of the layout, the user must specify one additional property. The scenario property:

- *enableBoundaryContributions* (included by default with every scenario)

should be set to “true” to instruct TRIM.FaTE to have include boundary contributions in a simulation. This feature allows a user to more easily turn boundary contributions on and off.

3. SOURCE DATA NEEDED FOR A TRIM.FaTE SCENARIO

Three key types of data are needed for source characterization within a scenario: location of the source, chemicals to be modeled, and emission rates for each chemical. Details on these data inputs are discussed in Sections 3.1 through 3.3. Important user tips related to source characterization and data inputs are summarized in Section 3.4.

3.1 Location of Source

For each source to be included in a simulation, the user must define the following data inputs that designate the location of the emission point:

- **X-Y coordinates** of the geographic location of the emission point, using the same units selected for defining the spatial layout of the scenario (e.g., latitude/longitude, UTM coordinates). Refer to Module 5, Developing the Spatial Layout, for additional details regarding definition of geographic coordinates in TRIM.FaTE.
- **Elevation** of the emission source in meters, relative to the X-Y-Z coordinate system used to define the spatial setup of the modeling region (e.g., for a region consisting of a flat ground surface defined at $Z = 0$, the source elevation in TRIM.FaTE will be equivalent to the height above ground level).

These data are used by TRIM.FaTE to determine the air compartment to which chemical emissions will be released. Because emissions are assumed to be instantaneously and homogeneously mixed within a compartment, it is suggested that TRIM.FaTE users set the parcel area containing one or more facility sources to be relatively small (e.g., approximately equivalent to the area of the facility) in order to minimize the resulting “artificial dispersion” immediately on chemical introduction to the system. For additional guidance on configuration of the source parcel, refer to Module 5.

In reality, of course, most air emission sources do not occupy one specific point in space. This is especially true for volume or area sources, such as fugitive emissions from a building or equipment leaks, where emissions can be released over a large area. In order to define a source within TRIM.FaTE, these “non-point” sources must be assigned to a single point (or, multiple single points modeled as separate sources). The user can select the centroid of an area or other specific point to locate the source if site-specific details warrant.

3.2 Chemicals to be Modeled

For each source location that is defined within a TRIM.FaTE scenario, the user must specify the emitted chemicals to be modeled. These chemicals are added to the scenario from the library associated with that scenario. Note that any chemicals that are included in a simulation must have been previously defined in the TRIM.FaTE library (and all relevant chemical-specific properties defined). If transformation with subsequent tracking of reaction products is being modeled, then all reaction products must be added to the scenario from the library as well, even if they are not emitted.

3.3 Emission Rates

Emission rates for each emitted chemical being modeled are assigned as chemical-specific properties of the source. Rates must be defined in TRIM.FaTE using the units of grams per day (g/day). However, this rate is assumed to be an instantaneous rate for whatever time interval the user specifies. In other words, rates can be defined by the user as a constant or time-varying value (as with other TRIM.FaTE properties), and emissions can start and stop any time within the modeling period. Thus, the user can account for facility-specific cyclical variations in emission rate (e.g., due to the daily process schedule, seasonal variations, or process start/stop cycles). If time-specific variations are not known by the user, an overall, average emission rate can be used (applying the appropriate unit conversions to obtain the rate in g/day).

3.4 User Tips for Source Characterization and Data Inputs

3.4.1 Modeling Multiple Emission Points

If multiple points at a facility, or multiple facilities, will be grouped for release into a single compartment within a scenario, the user can combine various emission points into a single TRIM.FaTE source if desired. Note that chemical-specific speciation and emission rates must be preserved if sources are combined (i.e., the combined source must accurately represent emissions of the various chemicals). However, the user should be aware of situations where combining sources is inappropriate or undesirable. For example:

- Scenarios that include sources with widely varying emission heights, where the elevation of one or more emission points may exceed the mixing height (see Section 3.4.2).
- Scenarios that include multiple emission points that are not located so close to each other that they should occur in the same compartment and for which preservation of significant spatial differences is warranted.

- Scenarios where the user will be running multiple single-source scenarios to investigate relationships between specific sources and exposure levels.

3.4.2 Relationship Between Emission Source Height and Air Compartment Height

The height of the air volume elements in a scenario (including the height of the volume element in the source air parcel) can be defined by the atmospheric mixing height (this has been done for test cases to date). The mixing height is a meteorological parameter that varies over time (see Module 10 on meteorological data processing for more information). If the emission height of the source exceeds the mixing height at a given time (e.g., hours when the mixing height is low), then the emissions during that time will be released *above* the air volume element and, if there is no volume element on top of that one, will not be included in the subsequent fate and transport modeling. Note that if chemical mass is emitted above the mixing height, it may be more appropriate to focus on long-range transport than local-scale fate and transport analysis.

In order to track the emissions released above the mixing height, the user could implement a second upper-air “layer.” This layer could consist of a separate set of volume elements representing the air space above the mixing height, where the mixing height is used as the lower bound of the second layer of volume elements.² To prevent errors resulting from a negative volume element thickness, the upper bound of this upper “layer” of volume elements (i.e., the maximum height) should be set above the maximum mixing height in the meteorology data set being used. An alternative approach to simply account for the total mass of chemical emissions released above the mixing height is the implementation of a single volume element that overlies all other air volume elements to function as a “reservoir” or sink. To achieve this function, no links should be enabled between the upper air layer and any other compartments or sinks. Refer to Module 5, Developing the Spatial Layout, for more information on defining the air volume elements in a TRIM.FaTE scenario.

3.4.3 Emission Phase Fractionation

TRIM.FaTE uses chemical parameters to calculate phase fractions of emitted chemicals (e.g., vapor vs. particle-bound); this fractionation is not specified manually by the user as a characteristic of the source. Note that, using this approach, modeling of emissions is different in TRIM.FaTE compared to the setup for ISC modeling, where the user specifies *a priori* parameters such as vapor fraction and fraction sorbed to particles (EPA 1995). As a part of the source modeling simplification that is currently set up in TRIM.FaTE, the fractionation in the emissions plume is not explicitly specified by the user; instead, the model assumes that the plume takes on the physical characteristics of the chemical species according to the user-defined chemical and receiving air compartment properties. This fractionation of emissions occurs instantaneously (i.e., immediately following emission from the source) in the air compartment containing the source. Note that the user has the flexibility to accommodate some source-specific factors that influence chemical phase fractionation in the receiving air (e.g., through the

² See Volume I of the TRIM.FaTE Evaluation Report (EPA 2002b) for an evaluation of pollutant transport involving a second layer of air volume elements and discussion regarding the limitations of the approach.

values chosen for certain parameters of the air compartment containing the source). In designing an approach, the user will need to consider its scientific defensibility.

4. CONFIGURING THE SOURCE IN A TRIM.FaTE SCENARIO

To define a source for a TRIM.FaTE scenario, the user must complete four steps:

- (1) Create the new source in the project library;
- (2) Enter site-specific spatial information into the library for the source;
- (3) Enter chemical-specific information into the library for the source, including chemicals emitted and emission rates; and
- (4) Add the source from the library to the modeling scenario.

A full explanation of these four steps is provided below. Steps 1 through 3, which describe how to set up and define the source in the library, can be carried out manually (i.e., via the TRIM.FaTE GUI) or by using a library import file (see Module 3, Library and Scenario Data Files, for more information on import files). The manual method is presented below. Note that Steps 1 through 3 must be repeated for *each* source that is included in a TRIM.FaTE scenario. In addition, note that Step 4, adding sources to a scenario, must be completed manually (i.e., this step cannot be completed using an import file).

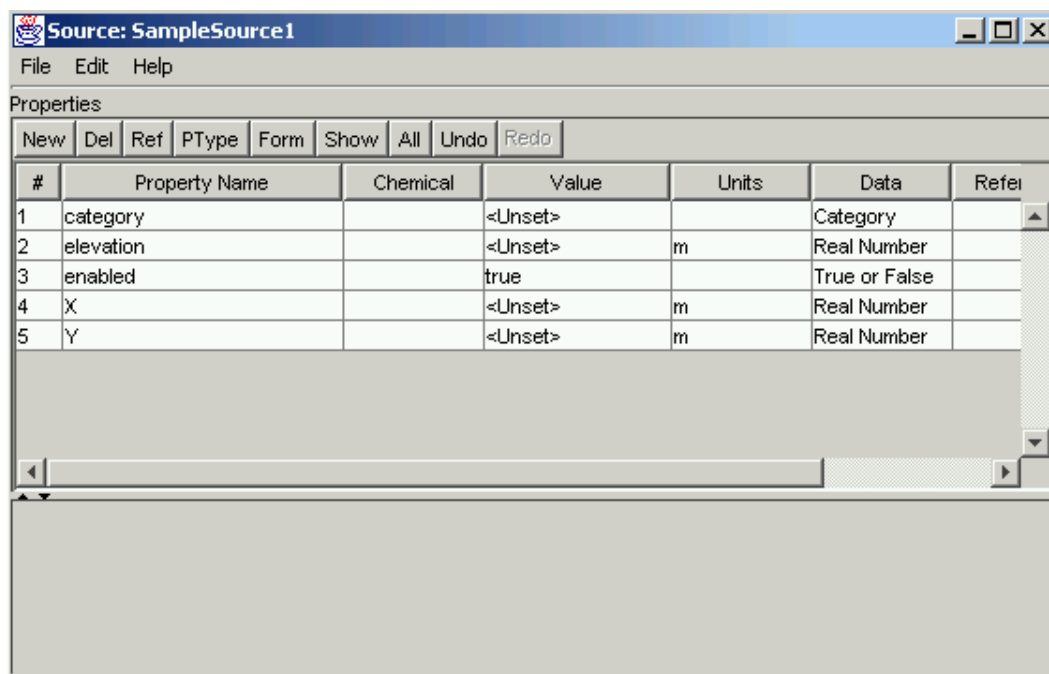
Step 1: Create the New Source in the Library

In the first step of source characterization, the user needs to create a new source in the library as follows.

- (1) From the library window, select “Sources” on the pull-down menu at the top of the object browser. Any existing sources will appear in the object browser.
- (2) Click the “New” button at the bottom of the object browser to bring up a dialog box asking the user to “Name new Source.”
- (3) Enter a name for the emission source.
- (4) Click on OK in the source window. This will add the source to the library and automatically open an object window for the new source with five properties. See Figure 1 for an object window that has opened for a new source named “SampleSource1.”
- (5) If desired, the user can add a description to the source by selecting the *Edit* pull-down menu from the menu bar at the top of the object window and selecting the “Description” command. A description dialog box will appear. The user can type in a description and click the “Accept” button to save changes.

Each source that will be modeled independently must be created as a new object in the library using the process described in Step 1. However, a single source can emit multiple chemicals (see Step 3 below).

Figure 1
Object Window for a New Source Created in the Library



Step 2: Enter Spatial Information for the Source

After the new source has been created in the library, site-specific spatial information must be added as properties of the source.

- (1) Continuing directly from Step 1, the object window listing the properties for the new source will be open (see Figure 1). If this window has been closed, go to the object browser window in the library and select the "Sources" option on the pull-down menu. From the list that appears, double-click on the name of the new source that was added in Step 1. The object window listing the source properties will reappear.³

³ Alternatively, the user can highlight the name of the new source in the object browser and click the "Properties" button to open a property editor for the new source in the library window. The source properties can be edited in the *property editor* of the library window in the same manner that they can be edited in the *object window*; the only difference is that the source description cannot be edited as described in item (5) of Step 1. The instructions provided in this module are presented in the framework of the object window; however, they apply equally to the property editor. See Module 1, Software Overview, for a complete description of the object window and the property editor in TRIM.FaTE.

- (2) Enter the coordinates of the source location for the appropriate properties (i.e., X and Y) in the *Value* column. A reference can be added in the *Reference* column if desired. Remember to hit the Enter key after typing in any property values to store the data in the library.
- (3) Enter the source elevation in meters for the *elevation* property in the *Value* column. Hit the Enter key to store the data in the library.
- (4) Leave the *category* property as “<unset>” (this property appears for every object in TRIM.FaTE but does not pertain to the source characterization).
- (5) Leave the *enabled* property as “true” (this property informs TRIM.FaTE that the new source should be activated in the scenario).

See Figure 2 for an example of the object window after the user has added spatial data. In this example, the source is located at UTM coordinates (513770.4, 4955600.8) and has an elevation of 55 meters.

Figure 2
Object Window with Spatial Data

#	Property Name	Chemical	Value	Units	Data	Refer
1	category		<Unset>		Category	
2	elevation		55.0	m	Real Number	
3	enabled		true		True or False	
4	X		513770.4	m	Real Number	
5	Y		4955600.8	m	Real Number	

Step 3: Enter Chemical-specific Information for the Source

Next, information on the chemical(s) emitted and their corresponding emission rates needs to be added to the library. Each emitted chemical is added as a new property of the source. Note that more than one chemical and emission rate can be added to a single source during this step.

- (1) In the object window for the source, click the “New” button above the data table to insert a new property. A window labeled “Create new property” will appear that lists all the property types included in the library.

- (2) From the list of properties that appears in this window, scroll down to *emissionRate*. Highlight this property and click “OK.”
- (3) A new window (also labeled “Create new property”) will appear that lists all of the chemicals included in the library. Select the chemical(s) that are emitted by the source from this list (note that any emitted chemicals must already be added to the library). Use the Control or Shift keys with the mouse to select multiple chemicals for an individual emission point. Click “OK” after selecting all of the chemicals that are released from the source.

For each chemical emitted, a new *emissionRate* property will appear in the table in the object window. The chemical names will appear in the *Chemical* column in the object window. See Figure 3 for an example of the object window after emitted chemicals have been added. In this example, benz(a)anthracene and chrysene have been added to the source as emitted chemicals.

Figure 3
Object Window with Emitted Chemicals Added

#	Property Name	Chemical	Value	Units	Data	Ref
1	category		<Unset>		Category	
2	elevation		55.0	m	Real Number	
3	emissionRate	Benz(a)anthracene	<Unset>	g/day	Real Number	
4	emissionRate	Chrysene	<Unset>	g/day	Real Number	
5	enabled		true		True or False	
6	X		513770.4	m	Real Number	
7	Y		4955600.8	m	Real Number	

At this point, the chemicals emitted will be added to the source in the library but not the emission rates. The values for each chemical-specific *emissionRate* property will be “<unset>” by default. The user can assign chemical-specific emission rates that are either constant or time-varying (i.e., changing in magnitude or starting and stopping at any time interval) over the course of the simulation.

To set constant emission rates:

- (1) For each chemical released from the source, place the cursor in the *Value* cell for the *emissionRate* property in the object window.

- (2) Enter the appropriate emission rate in units of g/day in the value cell and hit the Enter key to store the data in the library.
- (3) Repeat this process for each chemical emitted from the source and save the changes to the library by hitting Ctrl-S, or by clicking on File from the library menu and then selecting the “Save Library” command.

To set time-varying emission rates:

- (1) For a chemical released from the source, place the cursor into the *Value* cell for *emissionRate* for that chemical.
- (2) Click on the “Form” button located above the data table in the object window. A window labeled “Change Property Form” will appear. The user can either set time-varying emission rates directly into the library or reference an external data file containing time-varying data as follows.
 - ▶ To input time-varying emission data directly into the library (i.e., without storing the data in an external data file), select “Unevenly Time Stepped Real Number.” A value editor will appear with date, time, time zone, information, and value columns, along with a series of buttons (i.e., insert, delete, store, import, sort, and help) at the top of the value editor. These buttons can be used to enter time-varying data for the *emissionRate* properties that have been added. Refer to Section 3.3.3 of Module 1, Software Overview, for more information on the value editor in TRIM.FaTE.
 - ▶ To use time-varying emission data stored in a separate file, select “Unevenly Time Stepped Real Number From File.” A value editor will appear that allows the user to reference time-varying data in a file. Refer to Section 2.3 of Module 3, Library and Scenario Data Files, for instructions on how to format and use time-varying data input files in TRIM.FaTE.
- (4) Repeat this process for each chemical emitted from this source and save the changes to the library by hitting Ctrl-S or by clicking on File from the library menu and then selecting the “Save Library” command.

Step 4: Adding Source Data from the Library to the Scenario

After the sources and chemical-specific emission rates have been entered and saved in the TRIM.FaTE library and a scenario has been created, the source characterization information can be added to a scenario as follows.

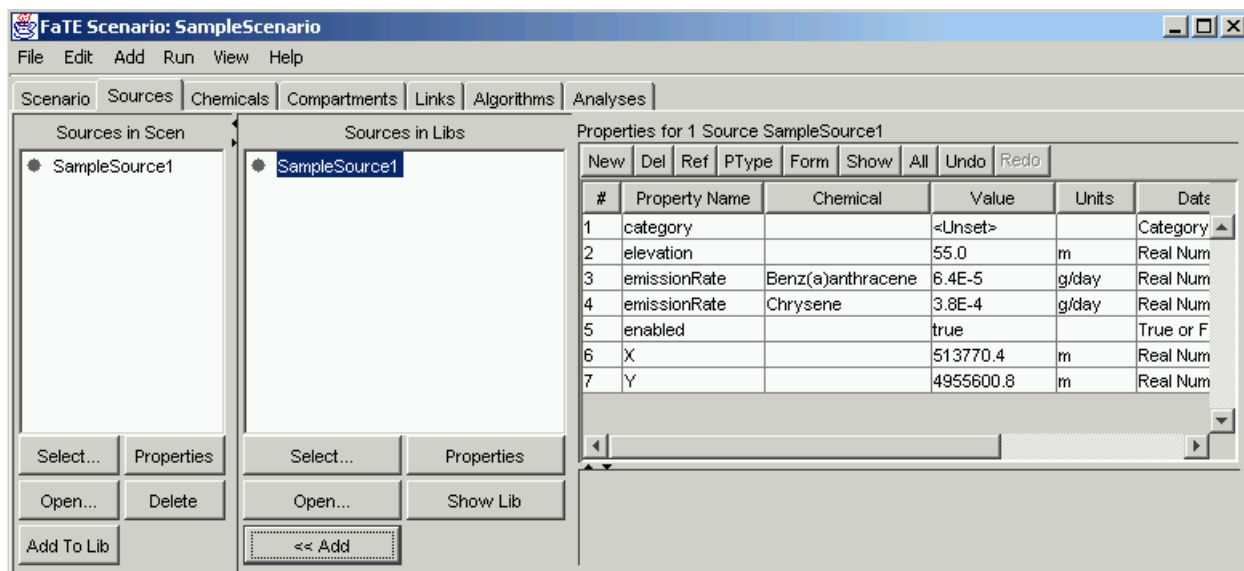
- (1) Within the scenario window, click on the Sources tab to access the Sources view. Two panes will appear on the left portion of this view. The “Sources in Scen” pane (farthest to the left) will list the sources that already exist in the scenario; the

“Sources in Libs” pane will list all of the sources that are available in the library. For a new scenario, the “Sources in Scen” pane should be blank because no sources have been added to the scenario. Any sources added to the library in Steps 1 through 3 will appear in the “Sources in Libs” list.

- (2) Add source(s) to the scenario from the library by highlighting one or more sources in the “Sources in Libs” window and then clicking the “<< Add” button. Note that only sources saved to the library can be added to the scenario.

The sources that have been added to the scenario will appear as a bulleted list in the “Sources in Scen” pane on the left side of the scenario window. See Figure 4 for an example of the Sources view after the source named “SampleSource1” has been added to the scenario. Changes to the scenario should be saved by opening the File pull-down menu on the Scenario window and then selecting “Save Project” from the scenario menu commands (or by pressing Ctrl-S).

Figure 4
Sources View in Scenario Window with “SampleSource1” Added to the Scenario



5. EDITING SOURCE DATA

To remove a source that has been added to a scenario, go to the Sources view in the Scenario window. Highlight the source name in the “Sources in Scen” list and click the “Delete” button below the list.

Although changes to source property values (e.g., emission rate) can be made directly in the scenario, it may be more efficient to make the changes in the library associated with the scenario if the source will be relevant to multiple scenarios included in the project. After property values for the sources have been changed in the library, the old sources can be removed from the scenario via the Sources view in the Scenario window. Then, the revised source(s) in

the library can be added via the Sources view by following the directions under Step 4. In addition, note that it is possible to save several different configurations for the same source using different names in the library (e.g., “Source A, constant emissions,” “Source A, time-varying emissions”). This allows the user to simulate the same source using different property values in different scenarios by selecting one of the configurations when adding the source to the scenario.

6. REFERENCES

U.S. EPA. 2002a. 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. Research Triangle Park, NC.

U.S. EPA. 2002b. Evaluation of TRIM.FaTE. Volume I: Approach and Initial Findings. EPA 453/R-02-012. Office of Air Quality Planning and Standards. Research Triangle Park, NC.

U.S. EPA. 1995. User’s Guide for the Industrial Source Complex (ISC3) Dispersion Models. Volumes I and II. EPA 454/B-95-003a,b. Office of Air Quality Planning and Standards. Research Triangle Park, NC.

[This page intentionally left blank.]