

# TRIM.FaTE USER'S GUIDE

## MODULE 5: DEVELOPING THE SPATIAL LAYOUT<sup>1</sup>

TRIM.FaTE is designed to be a tool for tracking the long-term multi-media fate and transport of chemicals. Chemicals of interest are modeled for a specified environmental domain that is subdivided into abiotic and biotic compartments. Because the relationships between the individual compartments form the basis for the movement of chemicals throughout the domain, it is important to carefully define the underlying spatial layout of the domain. This layout, comprised of parcels and volume elements, provides a framework for the location of and relationships between the compartments. Refer to the adjacent text box for a brief review of TRIM.FaTE terms. For a more complete description of TRIM.FaTE spatial concepts, refer to the TRIM.FaTE TSD Volume I, Chapters 3 and 5 (EPA 2002a).

### TRIM.FaTE SPATIAL TERMINOLOGY

**Parcel:** A planar (i.e., two-dimensional) geographical area used to subdivide a modeling region. Parcels, which can be polygons of virtually any size or shape, are the basis for defining volume elements. There can be air, land, and surface water parcels. A parcel is, essentially, a horizontal, two-dimensional representation of a volume element (i.e., a horizontal cross-section).

**Volume Element:** A bounded three-dimensional space that defines the location of an abiotic compartment, and can provide a frame of reference for one or more biotic compartments.

**Compartment:** The TRIM.FaTE modeling unit that contains chemical mass. Chemical mass is transported between and transformed within compartments; a specific compartment is characterized by its physical and spatial composition and its relationship to other compartments. Compartments can represent either abiotic or biotic media.

This module is divided into three sections. Section 1 describes the file format containing spatial data required by TRIM.FaTE (i.e., the Volume Element Import File) and presents general information on creating this file. This file specifies the spatial layout for a scenario and is imported into TRIM.FaTE as the first step in creating the scenario. By presenting this information in the first section of this module, the user should be able to gain an understanding of the data points that are needed by TRIM.FaTE, the limitations and specifications regarding the components of the spatial layout, and the mechanics of creating the import file. Section 2 presents more detailed information on the subjective aspects of developing a scenario-specific spatial layout. This section describes the steps involved in (1) defining the location and geographic extent of the overall modeling region and (2) delineating the modeling region into the set of air and surface (e.g., land, water) parcels. Section 2 should provide the user with suggestions and examples on how to set up a spatial layout for a given scenario. Section 3 provides the relevant references for the module.

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

## 1. CREATING THE VOLUME ELEMENT IMPORT FILE

The spatial layout for a TRIM.FaTE scenario is specified in the Volume Element Import File.<sup>2</sup> There are three general steps involved in creating this file:

- Specifying points;
- Specifying parcels; and
- Specifying volume elements.

Each of these steps builds on the previous step. That is, the points are used to define the parcels, and the parcels are used to define the volume elements.

The remainder of this section is divided into the following four sections:

- General overview and syntax of file format (Section 1.1);
- Points (Section 1.2);
- Parcels (Section 1.3); and
- Volume elements (Section 1.4).

In addition, an example of a complete Volume Element Import File and a graphic of the spatial layout corresponding to this file is included in Appendix A.

### 1.1 General Overview and Syntax of File Format

Each Volume Element Import File must have the following general format (text in bracketed italics indicates values that should be replaced by the user with text specific to the scenario):

```
start_volume_element_file
version [version number]

start_points
[list of points]
end_points

start_parcels
[list of parcels]
end_parcels

start_volume_elements
[list of volume elements]
end_volume_elements

end_volume_element_file
```

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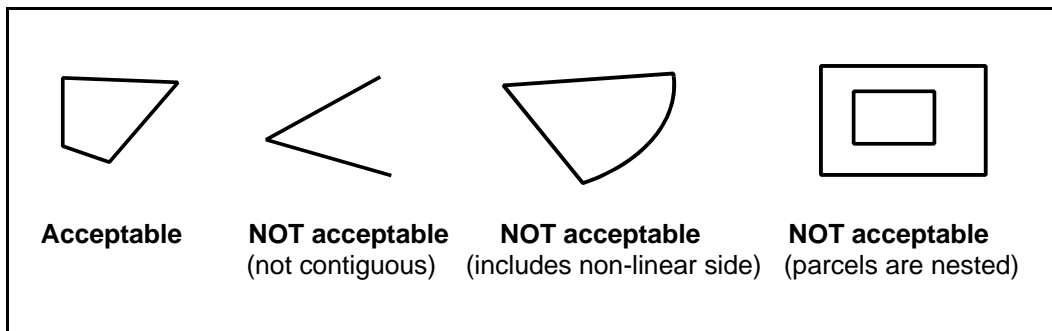
<sup>2</sup> Prior to creating the Volume Element Import File, the user should define the spatial layout using the steps described in Section 2.

General information on designing the spatial layout are presented in Section 1.1.1, keywords used in the Volume Element Import File are described in Section 1.1.2, and information on including comments in the file are described in Section 1.1.3. The formats for the lists of points, parcels, and volume elements are described in Sections 1.2, 1.3, and 1.4, respectively.

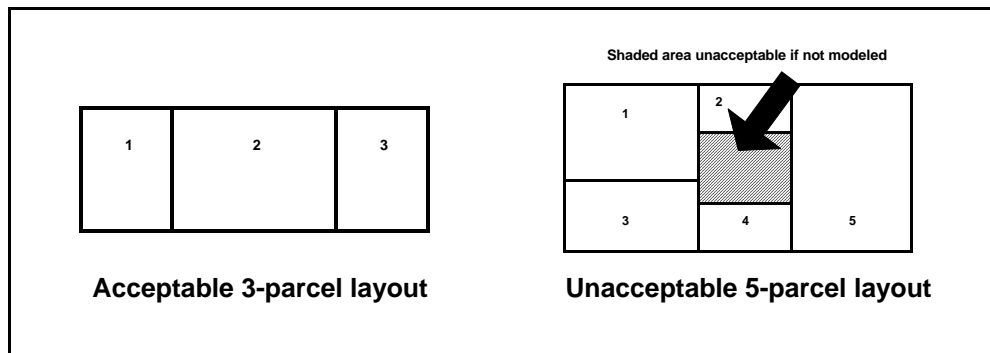
### 1.1.1 General Information on Spatial Layout

Parcels are the planar representation of the volume elements. Volume elements are the three-dimensional objects that define the modeling region. Each corner or vertex of the parcels and volume elements is identified by a set of coordinates defining a point in space. In designing the spatial layout of parcels, the user should ensure that the following general guidelines are met.

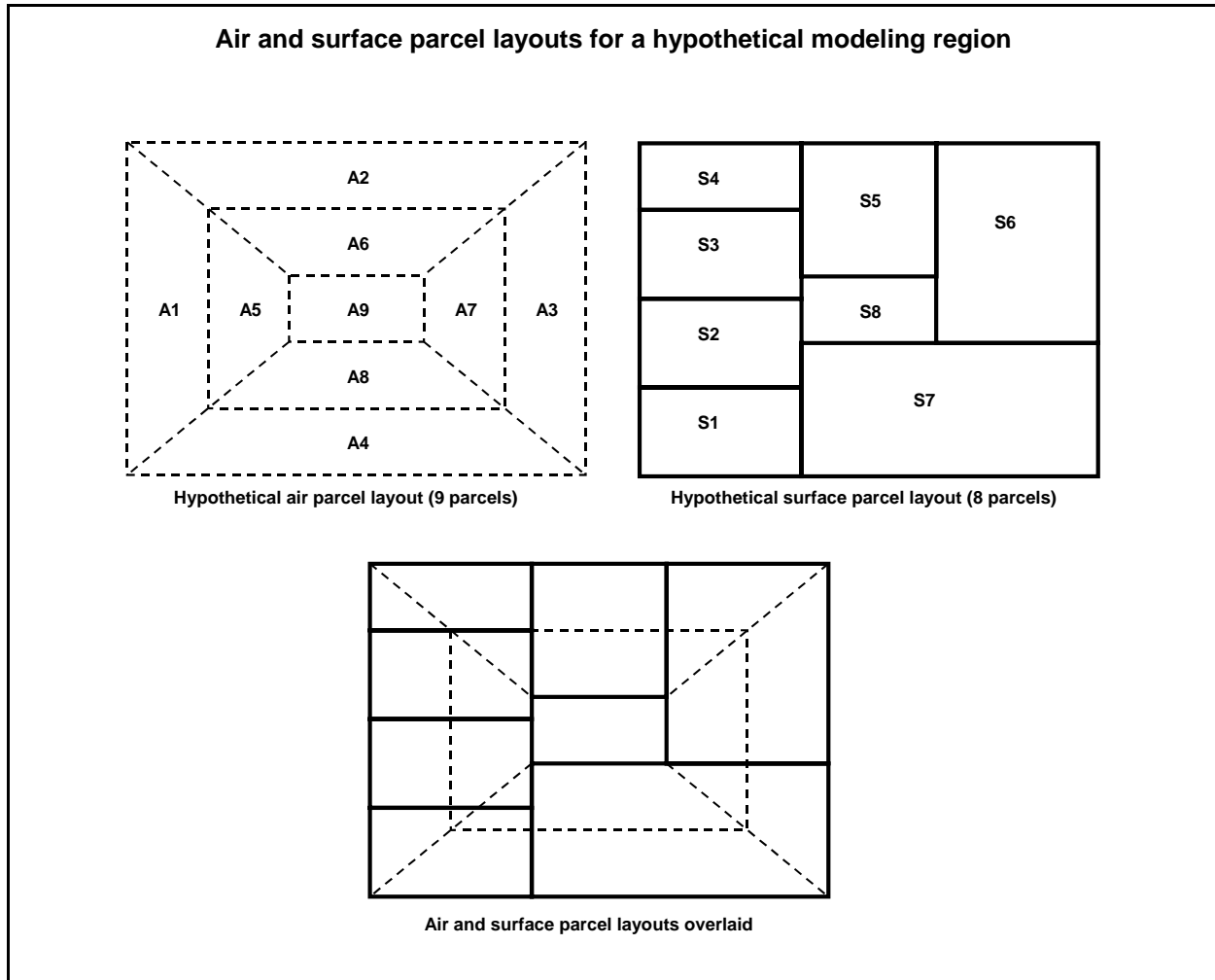
- **Parcels must be contiguous polygons with flat sides.** That is, the parcel cannot contain holes or be comprised of any curves.



- **The spatial layout cannot contain holes between or within parcels or volume elements.** That is, there cannot be spaces between parcels in the horizontal direction or gaps between volume elements in the vertical direction. The entire modeling region must be included in the volume elements (i.e., there can be no space included in the parcel layout that is not accounted for by the assigned volume elements).



- **The parcel layout for surface (soil and water) parcels can differ from that for air parcels.** This flexibility allows the user to design air and surface parcel layouts according to different considerations.



- **Volume elements cannot overlap.** Although volume elements can share surfaces, the three-dimensional space encompassed by a single volume element cannot overlap with the three-dimensional space encompassed by any other volume element. In other words, a point can exist on the surface of more than one volume element, but a point cannot be located *within* more than one volume element.
- **Each horizontal face of the spatial layout must be flat.** In other words, the top and bottom sides of each volume element must have the same elevation over the entire surface (e.g., “ramps” or elements with jagged edges are not allowed).

### 1.1.2 Keywords

Table 1 describes the keywords used in the Volume Element Import File. These keywords are not case-sensitive and should appear in the order indicated in the table (e.g., *start\_volume\_element\_file* should appear first, followed by *version*). In addition, the user cannot use any of these keywords as point, parcel, or volume element names.

**Table 1**  
**Keywords for Volume Element Import File**

<b>Keyword</b>	<b>Description</b>
start_volume_element_file	Indicates the beginning of the Volume Element Import File.
version	Specifies the file format version (currently “1”).
start_points	Indicates the beginning of the section that specifies the points.
end_points	Indicates the end of the section that specifies the points.
start_parcel	Indicates the beginning of the section that specifies the parcels.
end_parcel	Indicates the end of the section that specifies the parcels.
start_volume_elements	Indicates the beginning of the section that specifies the volume elements.
end_volume_elements	Indicates the end of the section that specifies the volume elements.
end_volume_element_file	Indicates the end of the Volume Element File.

### 1.1.3 Adding Comments to File

The user can include comments in the Volume Element Import File in two different ways.

- “//” indicates that all text until the end of the line is a comment and should be ignored by the importer.
- “/\*” indicates that all text until “\*/” is a comment and should be ignored by the importer.

Comments can include any information the user wishes to document in the file (e.g., a general description of the layout for a particular scenario, the rationale for the design of the layout).

## 1.2 Points

The Volume Element Import File uses the “points” section to specify the vertices of the parcels. All vertices (points) used in the parcel layout must be listed, each on a separate line. This section should include the following information (in the specified order) for each point:

- Point name;
- X-coordinate; and
- Y-coordinate.

The user must include at least one space between each data element. The number of spaces between each item is not important as long as there is at least one space between each one. The user may find it convenient to use tabs between each of these items.

The *point name* can be any text string (e.g., Point1, 15, NW\_Corner). If one (or more) spaces is included in the name, the user must enclose the name in double-quotes (e.g., "Point 1"). The format of the *X-* and *Y-coordinates* for each point depends on the map projection selected by the user (see Section 1.5 of this module for more information on map projections). In the current version of TRIM.FaTE, the coordinates can be provided in Lambert meters coordinates, latitude-longitude coordinates, or UTM coordinates. If the user includes more than two decimal places when specifying the coordinates, these coordinates will be rounded to two decimal places when the Volume Element Import File is imported into TRIM.FaTE.

It is possible to determine coordinate locations manually using maps or data sources that include these coordinates. For example, USGS 7.5 minutes series (1:24,000 scale) topographical maps include coordinates for latitude and longitude and UTM. If available, the use of GIS methods is likely to be a more accurate approach for determining point locations.<sup>3</sup>

### 1.3 Parcels

The "parcels" section of the Volume Element Import File uses the previously specified points to define the boundaries of each parcel in the scenario. This section should include the following information (in the specified order) for each parcel, with each parcel listed on a separate line:

- Parcel name;
- Number of points for the parcel; and
- List of point names for the parcel.

The user must include at least one space between each data element. The number of spaces between each item is not important as long as there is at least one space between each one. The user may find it convenient to use tabs between each of these items.

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<sup>3</sup> In the TRIM.FaTE test cases to date, a draft spatial layout was estimated using USGS 7.5 minute topographical maps. The parcel boundaries were then defined using GIS tools by drawing the boundaries on top of geo-referenced electronic versions of the maps and calculating the UTM coordinates of the vertices (an alternative would be to draw the boundaries on a paper map and use a digitizing tool to create an electronic version). Once the coordinates of the parcel boundaries were determined, they were compared to additional GIS data layers representing land use, water, road, and other environmental information that were registered to the same coordinate system. In some cases, adjustments to the parcel boundaries were made based on these data by using computer-based GIS tools capable of automatically measuring distances, areas, and lengths, and snapping to other environmental features, such as lakes and streams.

Like the names of points, the *parcel names* can be any text string (e.g., Parcel1, 23, NW\_Corner\_Air\_Parcel), provided the string has not already been used as a point name. If one (or more) spaces is included in the name, the user must enclose the name in double-quotes (e.g., “Air Parcel 1”). Note that the user may want to distinguish between air and surface parcels in the name for convenience. The *number of points* should be an integer representing the number of points (at least 3) used to create the parcel. Following the number of points, the user should include the *list of points* using the point names. The points **must** be listed in clockwise or counter-clockwise order around the surface of the parcel. That is, the user should be able to connect the points in the order specified in the parcel definition to create a parcel drawn to the correct shape. If a redundant point is included at the end of the list of point names (i.e., the final point in the parcel is identical to the first point), TRIM.FaTE will ignore it without returning a warning or error. However, if the user chooses to include redundant points, the points must be included in the number of points.

## 1.4 Volume Elements

The final step in creating the Volume Element Import File is to complete the “volume element” section. Volume elements are created by assigning an upper and lower bound and abiotic compartment to a previously created parcel. The volume element section includes the following data elements (in the specified order) for each volume element, with each volume element listed on a separate line:

- Volume element name;
- Parcel name;
- Abiotic compartment;
- Upper bound (top) of the volume element; and
- Lower bound (bottom) of the volume element.

The user must include at least one space between each data element. The number of spaces between each item is not important as long as there is at least one space between each one. The user may find it convenient to use tabs between each of these items.

Like the names of points and parcels, the *volume element names* can be any text string (e.g., VolumeElement1, 56, SE\_Corner\_VE), provided the string has not already been used as a point or parcel name. If one (or more) spaces is included in the name, the user must enclose the name in double-quotes (e.g., “Volume Element 1”). The *parcel name* indicates that parcel from which the volume element is derived and should match exactly to the name provided in the parcels section. The *abiotic compartment* indicates the name of the abiotic compartment that defines the primary composition of the volume element. For example, an air volume element will have a abiotic compartment of “Air.” It is important that each of the abiotic compartments included in the Volume Element Import File correspond to a compartment included in one of the referenced libraries. If one (or more) spaces is included in the name of the abiotic compartment, the user must enclose the name in double-quotes (e.g., “Air - Default”).

The *upper* and *lower bounds* indicate the vertical dimensions of each volume element and should be specified in units of meters, with higher values indicating higher elevation. Negative values are permissible and should be indicated using the “-” symbol; however, users should not

use a “+” symbol to indicate positive values as this will result in an error upon importing the file into TRIM.FaTE. Zero is also permissible. TRIM.FaTE test cases to date have been configured with the ground surface equal to zero; this is a logical approach that results in positive dimensions for volume elements above the ground/surface water surface and negative dimensions for subsurface volume elements. Volume elements with zero thickness (i.e., upper boundary equal to lower boundary) will be ignored by TRIM.FaTE, and those with lower boundaries higher than upper boundaries will result in errors.

In some cases, users may wish to specify the upper and/or lower boundaries of volume elements using time-varying data (e.g., by using time-specific mixing height as the top bound of the air volume elements). This can be accomplished by setting that boundary to a valid placeholder value in the Volume Element Import File and then substituting in the time-varying data afterwards. A “valid” placeholder value would be any value that does not lead to an illogical layout (e.g., a layout in which adjacent volume elements are either not contiguous or overlap). It would not be appropriate to set up two air layers (i.e., two sets of volume elements derived from the same air parcel layout but with different vertical dimensions representing an upper and lower atmosphere) with the top of the bottom layer set to 10 and the bottom of the top layer set to 11 (even if both of those values were eventually replaced with site-specific mixing height data). After importing the Volume Element Import File into TRIM.FaTE, the user can change the values of “top” and/or “bottom” properties of the affected volume elements to refer to a file containing the time-varying data. The user should be careful to ensure that the placeholder values are valid. In addition, when the placeholder values are replaced with time-varying values, the shared “top” and “bottom” properties for vertically adjacent volume elements should be set to the same time-varying values. For example, if a scenario included two air layers and the user wanted to set the shared boundary of these layers to be the mixing height, the values of the “top” property for the lower volume elements and the “bottom” property for the upper volume elements would both need to be set to the mixing height to ensure that there are no spatial gaps.<sup>4</sup>

## 1.5 Map Projection Information

The process for importing a completed Volume Element Import File is described in Section 1.2.1 of Module 3, Library and Scenario Data Files. This process is accomplished by selecting the “Import Volume Elements...” command under the *File* pull-down menu on the Scenario window.

When the Volume Element Import File is imported, the user is asked to specify the map projection that is used to define the coordinates of the points comprising the parcel layout and enter in one or more properties related to the selected projection. The projection and properties are specified via the “Map Projections” window that appears the first time the user goes through the process of importing the Volume Elements Import File. An example of this window is portrayed in Figure 1.

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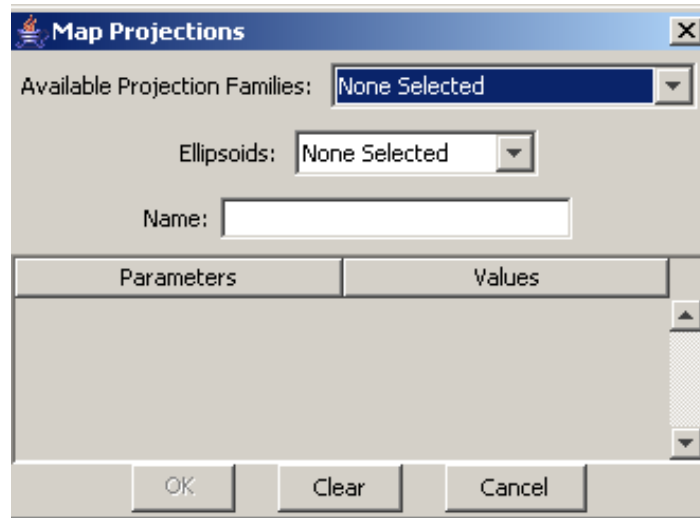
<sup>4</sup> See Volume I of the TRIM.FaTE Evaluation Report (EPA 2002b) for an evaluation of pollutant transport involving a second layer of air volume elements and discussion regarding the limitations of the approach.



The first data point that must be selected is the projection family. A map projection is a way of representing a region of the earth's curved surface onto a flat plane. There are a variety of projection methods available. As noted above, coordinates used by TRIM.FaTE can be specified in one of the following three projection families:

- Lambert meters coordinates;
- Latitude-longitude coordinates; or
- Universal transverse mercator (UTM) coordinates.

**Figure 1**  
**Map Projection Window**



The appropriate projection family can be selected using the pull-down menu at the top of the map projection window. After the projection has been designated, the ellipsoid for that projection must be selected (an ellipsoid is a mathematical representation of the roughly spherical shape of the Earth). Multiple ellipsoid representations can be used by TRIM.FaTE, including:

- Sphere;
- WGS 1984;
- Clarke 1880;
- International 1909;
- SGS 1985;
- GRS (either 1967 or 1980); or
- WGS (either 1960, 1966, or 1972).

In addition, depending on which projection family is selected by the user, there are one or more parameters that must be specified by the user in the table on the lower half of this window.

- If Lambert coordinates are used as the projection, the user must specify four parameters:
  - ▶ Secant latitude south;
  - ▶ Secant latitude north;
  - ▶ Central longitude; and
  - ▶ Central latitude.
- If latitude and longitude coordinates are used, the user must specify the central longitude.
- If UTM coordinates are used, the UTM zone must be specified.

More information regarding map projections is available from the U.S. Geological Survey (for example, see <http://erg.usgs.gov/isb/pubs/MapProjections/projections.html>) and other sources.

Once the projection, ellipsoid, and any required parameters have been set and the “OK” button on the map projection window is clicked, a window entitled “Import Volume Elements” will appear that allows the user to specify their Volume Element Import File. If the projection information needs to be changed at some point in the future, the projections window can be accessed again via the *Edit* menu in the Scenario window (select “Map Projection”).

## 2. DEVELOPING THE SPATIAL LAYOUT

This section outlines a suggested stepwise approach to applying site-specific data in developing the spatial layout for a scenario. For this process, the user completes the following main steps:

- Define the location and geographic extent of the overall modeling region (Section 2.1);
- Define the set of air and surface (e.g., land, water) parcels that make up the two-dimensional subdivisions of the modeled domain (Section 2.2); and
- Define the vertical dimension (i.e., depth or height) of the volume elements within the parcels (Section 2.3).

These three steps, and the substeps contained within each, are described in more detail in the sections that follow. Because there is limited application experience with TRIM.FaTE to date, this section is limited and fairly general.

Because the spatial layout provides the underlying framework for modeling performed in a scenario, it is important to create a layout that is representative of the area being modeled. However, throughout the process of creating the layout, the user should evaluate whether the layout is appropriate in size, shape, and number of subdivisions when compared to other sources of modeling uncertainty. Additional complexity in the spatial layout results in more spatial resolution. At the same time, additional complexity also results in an increase in required data collection and setup resources and, particularly, model run-time. The user will need to balance any benefit perceived from increased resolution (in light of uncertainties and variability in the estimates) with the logistical practicalities associated with the added complexity.

In addition, the approach for defining the spatial layout described in this module should be regarded as a set of suggestions to be used as a starting point, rather than a strict set of rules that the user must follow for each new scenario. TRIM.FaTE is a very flexible model that allows for a variety of approaches to designing the spatial layout of a scenario. The user can take advantage of this flexibility to account for site-specific characteristics and the requirements and goals of a specific assessment. Likewise, it is the responsibility of the user to ensure that the spatial design selected for an assessment is appropriate and reasonable.

### USER TIP: REFINEMENT OF THE MODELING LAYOUT

As described in Section 2.1, the user should be aware that, depending on the complexity of the scenario, making changes to the spatial layout after the TRIM.FaTE scenario has been fully set up (i.e., with all biotic compartments and compartment-specific properties defined) can be resource intensive. Examples of steps that may be necessary in order to use a different spatial layout after the scenario has been fully set up include:

- Revising the Volume Element Import File with the new points, parcels, and volume elements corresponding to the revised spatial layout;
- Recalculating spatially-varying properties, such as population densities and distribution of biotic populations, and erosion and runoff fractions; and
- Creating new scenario input files for compartments, properties, and link properties.

Multiple scenarios designed for the same modeling application, each with different aspects (e.g., different approaches to the spatial layout), can be stored in the same TRIM.FaTE project (see Module 1, Software Overview) and the results from simulations using these scenarios can be compared.

## 2.1 Defining the Overall Modeling Region

The overall modeling region for TRIM.FaTE is defined as the region of space through which the transport and transformation of the modeled chemical(s) is estimated. In other words, in defining this region, the user is establishing the outer bounds of the area to be modeled. Any chemical mass that exits the modeling region over time enters sinks, and its transport and transformation is not modeled further.

This section helps to guide the user through the process of defining the modeling region in location, shape, and size. Although there are no set rules for determining the specific attributes of the modeling region, this section introduces some of the key considerations and concepts associated with developing that region.

### KEYS TO DEFINING THE MODELING REGION

- ▶ Center region on source(s) to be modeled, or use site-specific factors to locate modeling region
- ▶ Consider shape of the modeling region
- ▶ Set the outer boundaries for the overall modeling region, considering receptors and chemical transport

### 2.1.1 Where should the modeling region be located?

The modeling region is often centered approximately on the source or sources of emissions being modeled (e.g., one or more facilities). This approach is appropriate when the site is surrounded by land and there are no site-specific characteristics that need to be considered. An example of a characteristic to consider could be a predominant wind direction that strongly influences the movement of chemical mass in air at a site. Alternatively, if a site is located on the coast and all potential receptors of interest are land-based, then it may be more appropriate to include more land mass in the modeling region than water area.

### 2.1.2 What is an appropriate shape for the modeling region?

The overall shape of the modeling region can be impacted by factors such as spatial variations in wind direction or deposition rate, or physical boundaries that restrict the transport of mass or potentially exposed populations. Because TRIM is not designed to accommodate the use of circular or curved shapes, the overall modeling region and all subdivisions of the region **must** be defined by straight lines (i.e., areas making up the TRIM.FaTE layout are defined by interconnected coordinates). Although TRIM.FaTE can accommodate any polygon, applications to date have focused on using relatively simple shapes (i.e., squares, rectangles, and other simple polygons).

### 2.1.3 How large should the overall modeling region be?

Although there are no preset upper or lower limits on the overall size of the modeling region, the TRIM.FaTE modeling framework is designed to support the modeling of chemical movement on a relatively local or sub-regional scale. Site-specific test applications of TRIM.FaTE to date have typically focused on areas extending out five to seven kilometers from a source, or a total area of approximately 100 to 200 km<sup>2</sup>. Other larger or smaller applications may be appropriate; however, TRIM.FaTE has not been tested for large-scale (e.g., regional) areas or small-scale, fine-resolution modeling applications. If near-source chemical concentrations are expected to be of primary interest, then a more specialized model may be more appropriate.<sup>5</sup> The potential for these circumstances should be considered prior to developing a TRIM.FaTE application.

#### SETTING THE BOUNDARIES OF THE MODELING REGION: Key Characteristics to Consider

- ▶ Major natural attributes (geographical features)
- ▶ Population boundaries (receptor locations)
- ▶ Physicochemical boundaries (chemical transport considerations)

In order to get a sense of the appropriate scale and shape of the modeling region, it may be useful for the user to consider site-specific characteristics that affect site-specific mass transport or the exposure of potential receptors. These characteristics can include (in approximate order, starting with most important): natural, population, or physicochemical boundaries or other attributes. These three characteristics are described in more detail in the subsections below.

#### *Natural Boundaries and Attributes*

Natural boundaries and attributes that affect the transport of mass or the presence of potential receptors include physical or geographic characteristics such as airsheds, watersheds, water bodies, topography, and regions of homogeneous land-use or land cover.

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<sup>5</sup>Note that the focus of TRIM.FaTE is on the distribution of multimedia pollutants into non-air media. For applications where concentrations in air are the primary interest, specialized air models are recommended.

- **Airshed boundaries** are useful in providing information about the size of the overall modeled region and external boundaries of the system by providing information about the limitations of chemical transport in air. An airshed can include large valleys such as the Sacramento Valley in California, where, due to inversion layers and diurnal wind patterns, the air mass is confined and well mixed throughout the area for an extended period. Airshed boundaries might also include smaller valleys when meteorological conditions produce long residence time for the air mass in the bounded region.
- **Watersheds and water bodies** can also be useful in determining the scale of the system as well as the size and location of parcels within the system (discussed in a subsequent section). For example, if a specific water body is of interest, (such as a reservoir that is used as a source for drinking water), it may be appropriate to design the overall modeling region to include that water body and the surrounding watershed. Watershed boundaries can be identified or approximated from topographical maps by tracing ridge lines and noting the origin and direction of flow for streams and rivers.
- **Land-use or land cover characteristics** should be considered to take into account the presence of receptors. For example, sensitive ecological habitat located near a source can be of interest in assessing potential ecological risks. For bioaccumulative chemicals, the potential for food chain exposures may lead to the inclusion of nearby farmland regions and fishable water bodies.

These characteristics should also be considered by the user when defining specific parcels within the modeling region (see discussion in Section 2.2).

### ***Population Boundaries***

Population boundaries are geographic delineations based on the presence of human or ecological groups. These boundaries can be considered when exposure to a specific population is of interest. The characteristics, distribution, and density of the population can influence the layout of the modeling region. For example, if the user wants to assess exposure to a particular wildlife population whose range is within a large area, then the modeled region's boundaries might be extended farther from the source. If only exposures to nearby populations are of interest, a smaller region might be appropriate. Note that population boundaries can sometimes be correlated with certain land-use or land cover characteristics.

### ***Physicochemical Boundaries and Attributes***

Physicochemical boundaries are limits on chemical mass transport that result from physical and chemical processes. Physicochemical boundaries are difficult to define precisely without extensive modeling and analysis; however, general information related to these boundaries (e.g., relative trends of dispersion or deposition) can be useful for defining the modeling region. Because TRIM.FaTE is designed to model the fate of emissions to air, processes that affect transport in air and remove chemical mass from the air (i.e., transformation/degradation processes and wet and dry deposition) may be of interest to the user

when setting up the overall modeling region. Generally, chemical transport in multiple directions should be considered to account for variations in weather patterns and other site-specific characteristics. Chemical- and site-specific information on the range over which the modeled chemical is likely to spread in air can be useful for determining the modeling system boundaries. For chemicals that degrade quickly or rapidly deposit from the air, it may be possible to model the majority of this range. However, many chemicals are relatively mobile and/or persistent and will be transported beyond the ranges of local-scale TRIM.FaTE model layouts. In local-scale (e.g., measuring 10 km from source to modeling region boundary) modeling of persistent chemicals such as mercury and PAHs, most (e.g., 90 to 99 percent) of the emitted chemical mass can be blown out of the modeling region before deposition. A potentially useful metric for defining the extent of a layout is the distance over which a certain percent of the chemical has been removed from the air by reactions and deposition (or, the amount of chemical removed within a certain distance).

Air dispersion and deposition modeling (e.g., ISCST3) or calculations of the characteristic travel distance can be used to obtain information on the distance that a chemical will travel from the source and possible physicochemical boundaries.

*Air Dispersion Models.* Air dispersion models such as ISCST3 can provide the user with information related to air transport and deposition patterns that can be useful in assigning TRIM.FaTE modeling system boundaries. By plotting spatial coordinates along with air concentration or deposition, a map or map-overlay of concentration or deposition isopleths can be generated and used in the same way that a topographical map is used for identifying natural boundaries. Alternatively, deposition rates (which will drive chemical concentrations in most non-air media in a TRIM.FaTE scenario) can be plotted versus distance for multiple directions. If deposition is modeled with depletion (i.e., accounting for mass deposited as distance from the source increases), the total mass deposited within a given distance can be estimated by multiplying deposition rates by the modeled area. When applying dispersion modeling, the user should be aware that chemical processes such as degradation may not always be included in the model.

One approach that has been used for previous TRIM.FaTE test runs is to extend the modeled region out to capture the highest deposition rates according to site-specific ISC modeling (e.g., the highest two orders of magnitude of deposition rate relative to directional maximum deposition rates). For test runs completed on sources emitting mercury and PAHs, a radius (i.e., distance from the source) of 5,000 to 10,000 meters captured this deposition rate gradient. In general, it will be difficult to set up a model layout to capture a specific, predetermined amount of deposited mass or fraction of mass emitted (e.g., it would be complicated to set up a TRIM.FaTE scenario where 25 percent of the emitted chemical is deposited rather than blown out of the system). ISC or other dispersion models could inform and support the TRIM.FaTE modeling region determination but should not be expected to provide specific information for calculating the exact modeling region boundaries.

*Characteristic Travel Distance.* A simpler alternative to dispersion modeling is the calculation and application of the characteristic travel distance (CTD). The CTD is the distance at which the ambient concentration of an emitted chemical has decreased to 37

percent (i.e.,  $1/e$ ) of the initial concentration due to removal processes, including wet and dry deposition and reaction/degradation processes that transform the chemical (Bennett et al. 1998). This distance is approximated through a series of relatively simple calculations and assumptions that account for advection, dispersion, and physical loss of chemical in the atmosphere. Using the results of these calculations, the length over which a certain percent of the mass of the chemical species is lost is estimated, providing information that may inform the decision on size of the modeling region.

The CTD is calculated based on the chemical's estimated removal rate from the atmosphere and the speed of the moving phase (Bennett et al. 1998). Although the CTD does not take into account certain site-specific variables that refined dispersion modeling includes (e.g., wind direction), the CTD can account for chemical-specific removal processes. In addition, calculation of a CTD is much less resource-intensive than site-specific dispersion modeling (i.e., calculations can be completed quickly via simple hand calculations). Refer to Appendix B of this guidance module for details on CTD calculation.

## 2.2 Designing the Parcel Layout

A parcel is defined as a planar (i.e., two-dimensional) geographic subdivision of the modeling region. For a specific TRIM.FaTE scenario, the overall modeling region is divided into parcels of various sizes, shapes, and locations, which are correlated with air, land, or surface water. This section describes a suggested approach to determining the spatial layout of the individual parcels within the modeling region.

### 2.2.1 What are the general rules of thumb for defining the parcels?

As with the modeling region, parcel boundaries must be comprised of straight lines because they are defined by specific coordinates within a TRIM.FaTE scenario. Curved shapes used to inform the parcel designations (e.g., geographic features) should be converted to polygons with flat sides while conserving the area and approximate location relative to the source.

The following three general guidance tips are suggested based on the test applications of TRIM.FaTE to date:

- (1) The outer boundaries of the air parcel layout should be at least as large as the underlying surface parcel layout;<sup>6</sup>

#### SUGGESTIONS FOR DEFINING THE PARCEL LAYOUT

- ▶ Consider the three general guidance tips (Section 2.2.1)
- ▶ Set up air parcels first using a regular pattern (Section 2.2.2)
- ▶ Set up surface parcels second based on site-specific characteristics and assessment goals (Section 2.2.3)

---

<sup>6</sup> Additional air compartments around the edge of the modeled region can capture some additional mass that would be lost via advective transport otherwise (i.e., the "blowback" of mass into the system is modeled). Refer to the TRIM.FaTE Evaluation Report (EPA 2002b) for a discussion of this phenomenon.

- (2) The individual air and surface parcel layouts do *not* need to coincide (i.e., the number and shape of parcels within each parcel layout can be different).
- (3) A greater number of parcels can increase the spatial resolution but also increases complexity and run-time requirements. Note that run-time is actually dependent on the number of *compartments* (and the associated links and transfer/transformation processes). Additional air parcels will generally result in no more than an equivalent number of air compartments, but one additional surface parcel can result in numerous additional compartments and links once biota are added to a scenario. Consequently, additional surface parcel resolution can have a magnified affect on model complexity and run-time requirements.

#### **USER TIP: A NOTE ABOUT RESOLUTION**

In general, the parcel layout need not be highly resolved in areas where media concentrations are of lesser interest to the modeler and decreased resolution will not greatly affect the overall fate and transport of a chemical. As a pollutant moves away from the source through adjacent air parcels in TRIM.FaTE, it may be appropriate to increase the distance across each parcel (i.e., resolution should be reduced with increased distance from source). This characteristic is intuitive in that at some distance from the source, the pollutant will become a regional or global pollutant, and one will no longer be able to directly link the pollutant back to the original source. In addition, decreasing the resolution where it is unnecessary will help to conserve resources required for computer run-time and user set-up, as stated at the beginning of Section 2.

Separate sections are presented below with suggestions for the modeler to consider when designing the layout of air and surface parcels. In general, it is easiest to begin by defining the air parcels. Air parcels are generally more uniform in shape, with a pattern centered around the source. The surface parcels can be less uniform, as they are defined based on various natural and population boundary types or are focused on specific receptors.

#### **2.2.2 How should the air parcel boundaries be defined?**

TRIM.FaTE allows for significant flexibility when setting up the air parcel layout. However, one suggested step-wise approach based on applications to date is as follows:

- (1) Define the air parcel that includes the source(s) to be modeled.
- (2) Determine the parcel shapes and the general pattern to be used for the overall layout.
- (3) Define the resolution of the layout, incorporating increased resolution in areas of interest if desired.

In general, the size and shape of the air parcel containing the modeled source should match up with the approximate dimensions of the modeled facility. Consequently, the air parcel containing the source will likely mirror the land surface parcel for the facility. In general, it is suggested that these both be a square or other regular polygon and match up exactly. The user

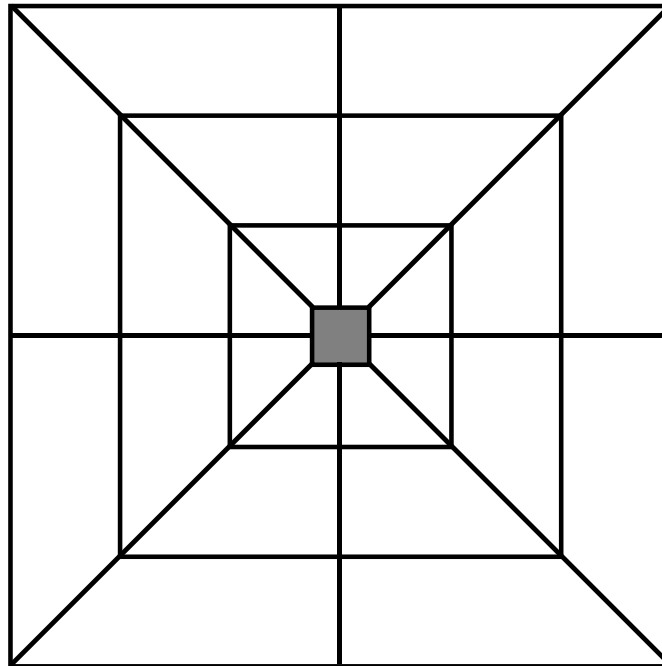


should take caution when interpreting air or surface soil media concentrations for the source parcel. Because TRIM.FaTE operates on the assumption that chemicals are instantaneously and homogeneously dispersed throughout compartments, predicted chemical concentrations in compartments located at the source parcel may not be reliable. As with all TRIM.FaTE spatial entities, the air parcels must be constructed as contiguous polygons. In other words, flat-sided shapes must be used (i.e., no curves), with no enclosed shapes (e.g., concentric, “donut-like” shapes are not allowed).

Any configuration of air parcels is theoretically possible in the TRIM.FaTE framework. However, based on TRIM.FaTE test applications and evaluations, the following suggestions are provided for setting up the air parcels.

- **Use a regular pattern.** Unless there are site-specific characteristics that significantly affect air movement at a site (such as airshed boundaries), a regular pattern (i.e., same basic shape for all parcels) is appropriate. Because of the assumption of instantaneous, homogeneous mass distribution within compartments, the user should be very cautious about using irregular shapes (e.g., L-shaped parcels) for individual air parcels due to the added complexity that these shapes might introduce. Generally speaking, simpler is considered better with respect to air parcel shapes.
- **A radial pattern is a reasonable default layout.** Based on previous applications of TRIM.FaTE, an “approximated radial grid” is recommended as the default air parcel layout. This pattern is formed by trapezoids that radiate from a central source parcel (see Figure 2). The parcel area increases with distance from the source in order to reduce grid complexity and model calculations where the rate of change in air concentration and deposition rate decreases. Note that a square grid (i.e., a “checkerboard” pattern) can also be applied, but the user should be aware of limitations associated with this layout (see the User Tip in the text box below).
- **Select a resolution scale that is appropriate to the assessment.** A balance should be maintained between higher resolution (more parcels) and the increased resource requirements associated with a resolution scale. Refer to the user tip presented above (see text box).
- **If appropriate, apply information on physicochemical boundaries.** The results of dispersion modeling or CTD calculations can be used to inform the air parcel divisions. For example, parcel widths could be set at increments that gradually increase to match up with concentration gradient steps (i.e., each parcel ring could be set up to roughly represent the same concentration/deposition gradient). Note that estimated concentration gradients may vary in different directions according to site-specific wind speed and direction.

**Figure 2**  
**Example of Approximated Radial Grid Layout**  
(shaded square designates source parcel)



**USER TIP: WHY A SQUARE GRID MIGHT NOT BE APPROPRIATE**

When a square grid (i.e., a “checkerboard” pattern) is used with a compartment-based air model like TRIM.FaTE that does not consider lateral dispersion, too much mass can accumulate in the compartments along the four primary axes of the grid. This over-accumulation occurs when the winds blow directly toward or close to the directions perpendicular to the grid sides (i.e., usually north, south, east or west). This effect, referred to as “pipeline flow” in the TRIM.FaTE Evaluation Report (EPA 2002b), is a result of the alignment of the x-y vectors used to model wind direction with the square grid pattern and is an inherent limitation of a square layout. This effect is reduced in the approximated radial grid layout (although that layout may produce too much “artificial dispersion” in some cases). For a comparison of different shapes that have been used for air parcels, refer to the TRIM.FaTE Evaluation Report, where several structural evaluation activities were performed to assess the response to changes in the size, shape, and location of air compartments.

As discussed in the TRIM.FaTE Evaluation Report (EPA 2002b), the amount of grid resolution for a given region does not significantly affect the total mass retained in the system but can have a substantial impact on the spatial distribution of mass in the system. More grid resolution reduces “artificial” dispersion (i.e., the apparent “spreading out” of mass throughout a compartment based on the assumption of homogeneous mixing).

### 2.2.3 How should the surface parcels be defined?

Because TRIM.FaTE surface parcels are designed to capture some of the heterogeneity of the modeling region, it is easier to recommend a general stepwise approach for defining the surface parcel layout. At the same time, this heterogeneity introduces complexity that makes it difficult to include specific details in this guidance. A recommended approach for developing the layout follows, with suggestions on how to develop the layout based on TRIM.FaTE evaluations performed to date. Note that surface parcels typically will be somewhat irregular in shape and size.

(1) **Define the source parcel.** As a starting point, the source parcel should be identified. A square or other regular polygon that is centered on the primary emission point or the centroid of a facility is usually a good shape for this parcel. The size of the source parcel should approximate the area of the facility and its associated emissions, including the point sources and fugitive emission sources. As mentioned previously, it is suggested that the source parcel correspond to the air parcel overlying the source.

(2) **Define the parcels for the water bodies that will be modeled in the scenario.** Water bodies within the modeling domain should be included if they (1) are of particular interest according to the objectives of the analysis or (2) significantly influence the movement of chemicals to other parcels via advection. These can include either still or flowing water bodies.

▶ **For lakes and ponds,** a square or other polygon that approximates the shape and location of the lake is recommended. It is more important to preserve the surface area of the water body parcel than its exact shape and location, as many processes (e.g., deposition, volatilization) are tied to the surface area.

▶ **For rivers and streams,** a parcel can be designed to approximate the actual location and straightened out into thin rectangular shapes. It is also important for rivers and streams that the surface area is preserved. The path of the flowing water body can be approximated by straight line segments. Separate parcels can be created for rivers and streams if desired, or all connected segments can be considered a single parcel.

#### USER TIP: STREAMS AND SOIL PARCELS

Stream (or river) segments that bisect a soil parcel will create additional parcels. Therefore, the user might want to “move” the stream to line up with the soil parcel edges (and thereby reduce the number of soil parcels to be modeled). Because this adjustment will increase the length of the stream, the user may need to reduce the stream width to preserve the surface area of the stream segment.

Note that the design can include water bodies connected by rivers or streams (i.e., via a flowing surface water compartment) if desired and the

necessary data (e.g., flow rates, stream dimensions) are available to model the connecting stream. In addition, the user has the option of linking two surface water compartments (in volume elements of separate parcels) without including a parcel for a connecting stream. Chemical mass can be transported via a hypothetical “pipeline” between water bodies where advective water flow is modeled but other processes are not modeled (e.g., dispersion, volatilization). This simplification option may be useful for relatively small streams and short distances.

(3) **Define the remaining land surface parcels according to site-specific characteristics.**

The land area of a TRIM.FaTE scenario can be subdivided into parcels according to several different types of site-specific information. The user should consider the overall objectives of the analysis and take into account the most appropriate information. For example, if ecological risks are of concern, then the user may wish to divide the land parcels according to habitat area or the location of a specific ecological population. In general, the user should consider the topics outlined in the bullets that follow. Note that these data can be related to and overlap with the information used to define the overall modeling region but may include a higher level of resolution (i.e., subdivisions of the whole). In addition, note that these characteristics and boundaries are often correlated (e.g., the boundaries of an ecological population may be aligned with land use or natural boundaries). Thus, it may be difficult to designate one specific characteristic that should drive the determination of parcel divisions; a “holistic” approach taking into account multiple factors may be appropriate.

- ▶ **Natural or geographic boundaries** are defined by natural features or other geographic areas, such as water bodies, watersheds, and land cover patterns. Dividing the surface parcels according to this information can be especially useful if the concentration in a particular lake or wetland is of interest. Locations and sizes of other features such as mountain ranges or agricultural areas can also indicate important boundaries in the system. If the analysis objective includes estimating the impact of a source on a particular water body, agricultural area, or forest, these boundaries can be incorporated into the scenario setup for surface parcels.

If watershed boundaries are used as a primary criterion for determining surface parcels, then the calculation of runoff/erosion fractions (which are

**USER TIP: DEFINING WATERSHEDS**

Recall that a surface soil parcel cannot fully “contain” a surface water parcel, nor can surface soil and surface water parcels overlap. Therefore:

- ▶ All surface water parcels defined in Step 2 must be considered boundaries for the land parcels.
- ▶ A stream parcel cannot flow through and “bisect” a single soil parcel.
- ▶ A “donut” shape, where a single surface parcel entirely surrounds a water body is not allowed.

required input parameters) will be simplified and compartment mass calculations will better represent the watershed. The user should make sure that the resolution of the watershed data that are obtained corresponds with the desired TRIM.FaTE parcel size. In addition, the presence of one or more source parcels located in the middle of a watershed will likely necessitate subdivision of a watershed. Off-line calculation of runoff/erosion fractions can accommodate these irregularities.

- ▶ **Land use or type characteristics** can provide a basis for defining the surface parcels in order to maximize the homogeneity within parcels with respect to various land use categories, such as industrial/mixed use areas, forests, or grasslands. In order to capture differences in landscape regions, the land can be split into multiple parcels. Likewise, if there is a large forest area that covers much of the modeling region, then it might be helpful to designate more than one parcel for that area, even though it is all the same land use, as there are likely to be some variations if the area is large enough and it increases the resolution of the scenario. It may be logical in some cases to use land-use characteristics as the driving force for dividing surface parcels; note that the current library algorithms would need to be refined to accurately model multiple vegetation types within a single volume element.
  
- ▶ **Population boundaries** can be used to take into account information about the habitat of ecological receptors of interest or and the different locations in which the target is likely to be during an exposure event. Population boundaries can be used to justify increased complexity of a landscape parcel within a natural boundary or within the range of a bounded target. For example, an antelope may spend most of its life foraging in the high desert sage around a munitions storage facility. No natural boundaries exist and physicochemical boundaries may provide more resolution than is appropriate. If the seasonal foraging area of the antelope can be identified, this information can be used to construct parcels that encompass the animal's range for each season. If that range is large, physicochemical boundaries can be used to increase resolution (more parcels) within the boundaries as necessary.

A consideration of lesser importance that should be factored into the parcel layout design process where possible is matching up surface boundaries exactly with air boundaries. By designing a surface parcel that matches up with an air parcel, there will be fewer points and boundaries in the modeled system, which can make it simpler to display the layout and results. In addition, correlating these layers can reduce complications related to spatial “averaging” of deposition rates and ambient concentrations. However, it is not necessary to match up surface and air parcel boundaries, and in many applications it may be more appropriate to design boundaries so that they are not correlated.

## 2.3 Defining the Vertical Dimensions of Volume Elements

Vertical dimensions must be defined for all volume elements based on the abiotic compartments (e.g., air, soil, surface water, groundwater) contained by the volume element. The vertical dimensions should be representative of site-specific geography and the environmental setting of the modeled region; however, the spatial measurements can be entered relative to other volume elements in the scenario (i.e., they do not have to be actual topographic values). This section provides general assistance on defining the vertical dimensions of volume elements based on TRIM.FaTE test cases. Detailed information on obtaining site-specific information (e.g., data sources, suggested default values) is not included in this section.

### *Air Volume Elements*

For a single layer of air volume elements, the bottom dimension should be set equal to the ground level and the top dimension set equal to the atmospheric mixing height for the region. The mixing height changes with time and can be entered as a time-varying property according to the values in the meteorologic input file (see Module 10).

### *Soil Volume Elements*

In the TRIM.FaTE test cases, there have been three contiguous soil volume elements for which vertical dimensions were defined: surface, root zone, and vadose zone. The top of the surface soil is considered ground level, and typically has been set to zero. Site-specific data should be used, if available, to determine the depths of the each soil layer in the scenario. Note that if the ground level (i.e., the top dimension of the surface soil volume element) is set equal to zero, the soil layers will have negative values for their vertical dimensions. In addition, as a requirement of the algorithms used to model vertical advection of chemical mass through the soil, the depths of the soil layers must **increase** from the surface to the root zone to the vadose zone (with the surface soil layer being the most shallow).

### *Surface Water and Groundwater Volume Elements*

Both surface water and groundwater vertical dimensions should be determined using site-specific information, if available. For instance, the average measured depth of a lake or river should be used to define the bottom of the surface water volume element for that water body. The top of the surface water layer has typically been set to zero (i.e., level with the top of the surface soil volume element).

## 3. REFERENCES

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## APPENDIX A EXAMPLE OF VOLUME ELEMENT IMPORT FILE

Text of a sample volume element import file follows. The air and surface parcel layouts corresponding to these data are displayed in Figure A-1 following the example file.

```
/*
Example Volume Element Import File
*/

start_volume_element_file
version 1
start_points
// PointID UTMx UTMy

1      548472.17    4595052.17
2      553472.16    4595052.17
3      558472.17    4595052.17
4      558472.17    4590052.17
5      558472.17    4585052.17
6      553472.16    4585052.17
7      548472.17    4585052.17
8      548472.17    4590052.16
9      550972.16    4592552.17
10     553472.16    4592552.16
11     555972.16    4592552.16
12     555972.16    4590052.16
13     555972.16    4587552.18
14     553472.16    4587552.16
15     550972.16    4587552.16
16     550972.16    4590052.17
17     553347.16    4590177.16
18     553472.16    4590177.16
19     553597.16    4590177.16
20     553597.16    4590052.16
21     553597.16    4589927.16
22     553472.16    4589927.16
23     553347.16    4589927.16
24     553347.16    4590052.17
102    554351.28    4595052.17
104    558472.17    4589920.88
105    558472.13    4589884.40
107    551897.19    4585052.16
108    551859.12    4585052.17
1010   548472.17    4591522.61
1011   553138.31    4592556.55
1013   555970.00    4589076.90
1014   552922.43    4588048.95
1015   552953.91    4588018.51
1016   552638.19    4587270.15
1017   551373.33    4586973.70
1018   549265.99    4588753.70
1019   550248.06    4590349.56
1020   550863.17    4590224.88
1021   551347.61    4590224.88
1022   551348.60    4589745.49
1023   550863.17    4589745.75
1024   552283.46    4590797.75
1025   551893.85    4589888.65
1026   552624.30    4589205.83
1031   558472.49    4587999.59
1032   555971.73    4587999.67
1033   555970.03    4589038.79
1034   552641.00    4587279.00
2001   548472.17    4595052.17
2002   553472.16    4595052.17
2003   558472.17    4595052.17
2004   558472.17    4590052.17
2005   558472.17    4585052.17
2006   553472.16    4585052.17
```



```

2007 548472.17 4585052.17
2008 548472.17 4590052.16

```

```
end_points
```

```
start_parcel
// Parcel name, #points, pointIDs
```

```

AirNNE1      4      10      11      19      18
AirENE1      4      19      11      12      20
AirESE1      4      20      12      13      21
AirSSE1      4      22      21      13      14
AirSSW1      4      23      22      14      15
AirWSW1      4      16      24      23      15
AirWNW1      4      9       17      24      16
AirNNW1      4      9       10      18      17
AirNNE2      4      2       3       11      10
AirENE2      4      11      3       4       12
AirESE2      4      12      4       5       13
AirSSE2      4      14      13      5       6
AirSSW2      4      15      14      6       7
AirWSW2      4      8       16      15      7
AirWNW2      4      1       9       16      8
AirNNW2      4      2       10      9       1
AirSource    8      17      18      19      20      21      22      23      24
AirLayer2   8      2001   2002   2003   2004   2005   2006   2007   2008
SurfaceSource 4      17      19      21      23
SurfaceN1    8      19      17      23      1026   1025   1024   1011   11
SurfaceE1    8      21      19      11      1013   1014   1034   1026   23
SurfaceSW2   12     1016   1017   1018   1019   1020   1023   1022   1021
            1024   1025   1026   1034
SurfaceNNE2  4      102     3       11      1011
SurfaceENE2  4      3       104     1013   11
SurfaceSE2   6      1031   5       107     1015   1033   1032
SurfaceSW3   7      108     7       1010   1019   1018   1017   1016
SurfaceNW2   8      1010   1       102     1011   1024   1021   1020   1019
SurfaceESE2  4      105     1031   1032   1033
WaterSilver  4      1020   1021   1022   1023
WaterWallkill 10     104     105     1033   1015   107     108     1016   1034
            1014   1013

```

```
end_parcel
```

```
start_volume_elements
```

```
// name, Parcel name, abiotic compartment, z_lower, z_upper
```

Air_Source	AirSource	Air	0	100
Air_NNE1	AirNNE1	Air	0	100
Air_ENE1	AirENE1	Air	0	100
Air_ESE1	AirESE1	Air	0	100
Air_SSE1	AirSSE1	Air	0	100
Air_SSW1	AirSSW1	Air	0	100
Air_WSW1	AirWSW1	Air	0	100
Air_WNW1	AirWNW1	Air	0	100
Air_NNW1	AirNNW1	Air	0	100
Air_NNE2	AirNNE2	Air	0	100
Air_ENE2	AirENE2	Air	0	100
Air_ESE2	AirESE2	Air	0	100
Air_SSE2	AirSSE2	Air	0	100
Air_SSW2	AirSSW2	Air	0	100
Air_WSW2	AirWSW2	Air	0	100
Air_WNW2	AirWNW2	Air	0	100
Air_NNW2	AirNNW2	Air	0	100
Air_Layer2	AirLayer2	Air	100	200
SW_Silver	WaterSilver	"Surface water"	-3.0	0
SW_Wallkill	WaterWallkill	"Surface water"	-0.75	0
Sed_Silver	WaterSilver	Sediment	-3.05	-3.0
Sed_Wallkill	WaterWallkill	Sediment	-0.80	-0.75
SurfSoil_Source	SurfaceSource	"Soil - Surface"	-0.01	0
SurfSoil_N1	SurfaceN1	"Soil - Surface"	-0.01	0
SurfSoil_E1	SurfaceE1	"Soil - Surface"	-0.01	0
SurfSoil_SW2	SurfaceSW2	"Soil - Surface"	-0.01	0
SurfSoil_NNE2	SurfaceNNE2	"Soil - Surface"	-0.01	0
SurfSoil_ENE2	SurfaceENE2	"Soil - Surface"	-0.01	0

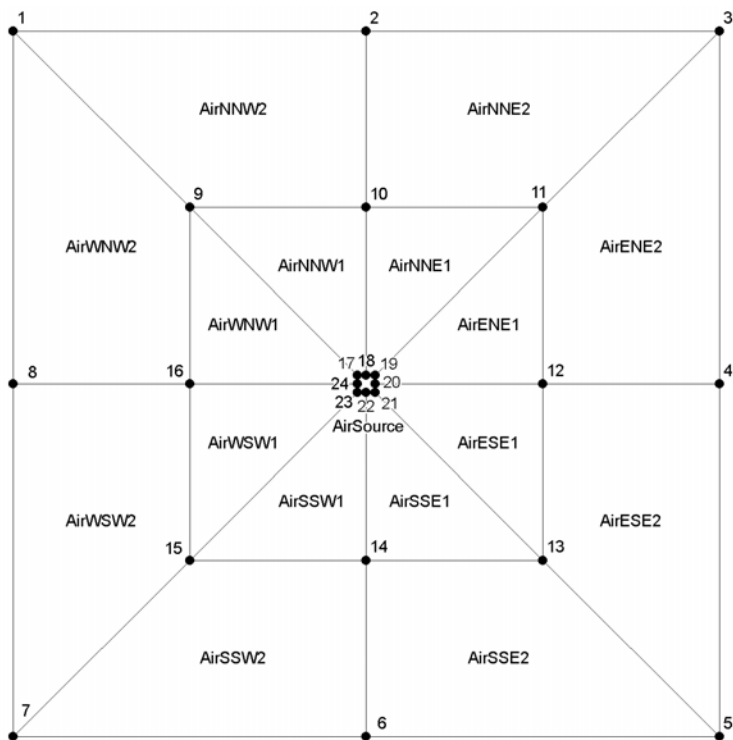
Note that the upper dimensions for the air layer (i.e., 100 m) are inserted as "placeholder" values in the volume element import file. The user can replace these values within TRIM.FaTE with time-varying values (e.g., mixing height data from the meteorological data set) once the scenario has been set up.

SurfSoil_SE2	SurfaceSE2	"Soil - Surface"	-0.01	0
SurfSoil_SW3	SurfaceSW3	"Soil - Surface"	-0.01	0
SurfSoil_NW2	SurfaceNW2	"Soil - Surface"	-0.01	0
SurfSoil_ESE2	SurfaceESE2	"Soil - Surface"	-0.01	0
RootSoil_Source	SurfaceSource	"Soil - Root Zone"	-0.56	-0.01
RootSoil_N1	SurfaceN1	"Soil - Root Zone"	-0.56	-0.01
RootSoil_E1	SurfaceE1	"Soil - Root Zone"	-0.56	-0.01
RootSoil_SW2	SurfaceSW2	"Soil - Root Zone"	-0.56	-0.01
RootSoil_NNE2	SurfaceNNE2	"Soil - Root Zone"	-0.56	-0.01
RootSoil_ENE2	SurfaceENE2	"Soil - Root Zone"	-0.56	-0.01
RootSoil_SE2	SurfaceSE2	"Soil - Root Zone"	-0.56	-0.01
RootSoil_SW3	SurfaceSW3	"Soil - Root Zone"	-0.56	-0.01
RootSoil_NW2	SurfaceNW2	"Soil - Root Zone"	-0.56	-0.01
RootSoil_ESE2	SurfaceESE2	"Soil - Root Zone"	-0.56	-0.01
VadoseSoil_Source	SurfaceSource	"Soil - Vadose Zone"	-1.31	-0.56
VadoseSoil_N1	SurfaceN1	"Soil - Vadose Zone"	-1.31	-0.56
VadoseSoil_E1	SurfaceE1	"Soil - Vadose Zone"	-1.31	-0.56
VadoseSoil_SW2	SurfaceSW2	"Soil - Vadose Zone"	-1.31	-0.56
VadoseSoil_NNE2	SurfaceNNE2	"Soil - Vadose Zone"	-1.31	-0.56
VadoseSoil_ENE2	SurfaceENE2	"Soil - Vadose Zone"	-1.31	-0.56
VadoseSoil_SE2	SurfaceSE2	"Soil - Vadose Zone"	-1.31	-0.56
VadoseSoil_SW3	SurfaceSW3	"Soil - Vadose Zone"	-1.31	-0.56
VadoseSoil_NW2	SurfaceNW2	"Soil - Vadose Zone"	-1.31	-0.56
VadoseSoil_ESE2	SurfaceESE2	"Soil - Vadose Zone"	-1.31	-0.56
GW_Source	SurfaceSource	Groundwater	-4.31	-1.31
GW_N1	SurfaceN1	Groundwater	-4.31	-1.31
GW_E1	SurfaceE1	Groundwater	-4.31	-1.31
GW_SW2	SurfaceSW2	Groundwater	-4.31	-1.31
GW_NNE2	SurfaceNNE2	Groundwater	-4.31	-1.31
GW_ENE2	SurfaceENE2	Groundwater	-4.31	-1.31
GW_SE2	SurfaceSE2	Groundwater	-4.31	-1.31
GW_SW3	SurfaceSW3	Groundwater	-4.31	-1.31
GW_NW2	SurfaceNW2	Groundwater	-4.31	-1.31
GW_ESE2	SurfaceESE2	Groundwater	-4.31	-1.31

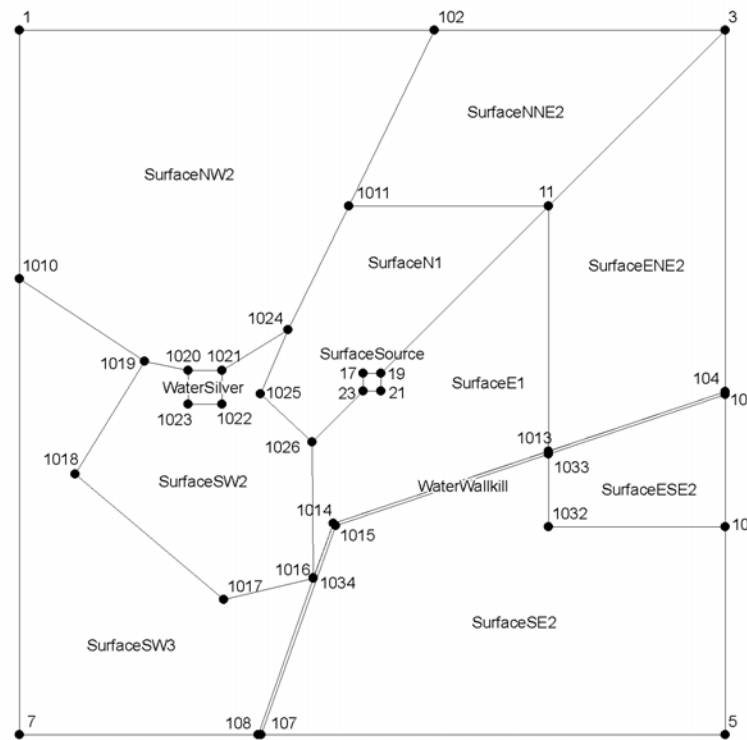
end\_volume\_elements  
end\_volume\_element\_file

**Figure A-1: Example Air and Surface Parcel Layouts**

The two figures and the point labels (e.g., 1, 2, 3, 102, 1011) and parcel names (e.g., “AirNNW2,” “SurfaceN1,”) shown below correspond to the location point labels and parcel names included in the example Volume Element Import File presented above.

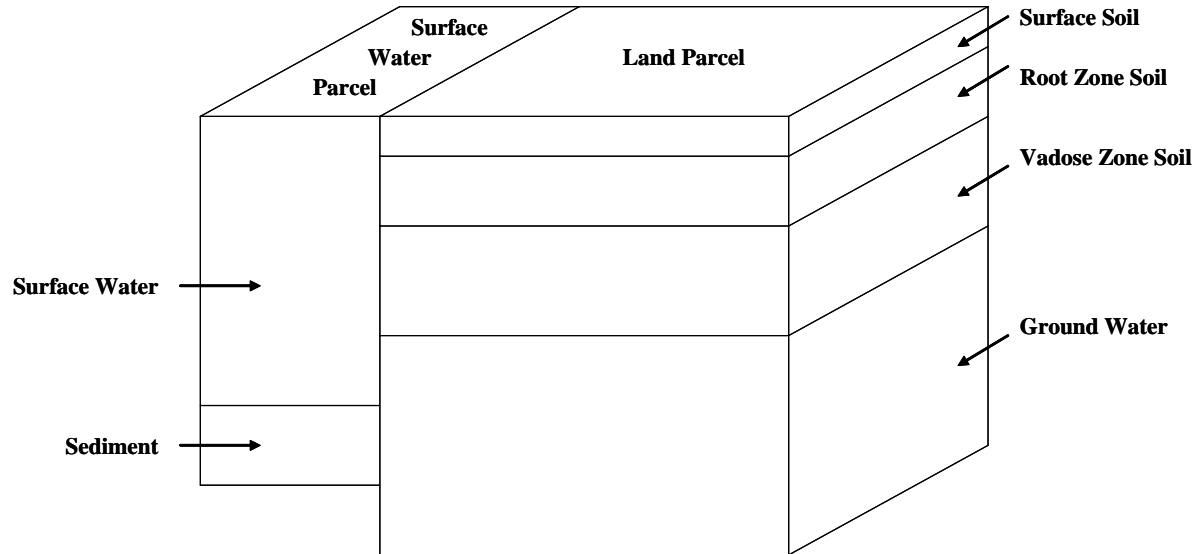


**Air Parcel Layout**



**Surface Parcel Layout**

**Figure A-2:  
Schematic of Volume Element Layering: Two Hypothetical Surface Parcels**



This figure (not drawn to scale) illustrates two sample surface parcels and the volume elements assigned to the parcels. On the left is a surface water parcel, with surface water and sediment volume elements assigned; on the right is a land parcel, with three layered soil volume elements and an underlying ground water volume element. A corresponding compartment (surface water, root zone soil, etc.) would be assigned to each of the volume elements. Although the shape of the parcels depicted here do not correspond exactly to the shapes in the sample parcel layout presented in this Appendix, the types of volume elements and number of layers do correspond to those presented in the sample file above.

## APPENDIX B CALCULATION OF THE CHARACTERISTIC TRAVEL DISTANCE (CTD)

The CTD can be calculated based on a chemical's estimated removal rate from the atmosphere and the speed of the moving phase (Bennett et al. 1998):

$$\text{CTD} = 0.23 * \frac{\text{Wind Velocity}}{\text{Loss Rate}}$$

where:

CTD = distance at which 63 percent of the chemical mass in the air has been removed (i.e., reduced to 1/e of original concentration, assuming a constant mixing volume)

Wind velocity = average wind velocity (m/day)

Loss rate = loss rate from the atmosphere from combined transformation and deposition processes (1/day)

The 0.23 term approximates the effects of atmospheric dispersion. Gifford and Hanna (1973) have shown that the yearly average concentration in a simple box model is proportional to the source strength in mass per unit area divided by the wind speed. McKone (1993a, 1993b, 1993c) has used the Gifford and Hanna work with Benarie (1980) to derive the proportionality constant in this relationship. Multiplying the average unidirectional wind velocity by 0.23 accounts for multiple wind directions (i.e., the average wind speed in any one direction is about 23 percent of the absolute wind speed at a given time). This factor may underestimate the characteristic travel distance in locations with persistent wind flow in a single direction.

The loss rate for transformation (involving the half-life of the chemical, if appropriate) and deposition (involving the rate of deposition and mixing height) can be estimated using the following equation for first order reactions:

$$\text{Loss rate} = \left( \frac{0.693}{\text{Half - life}} + \frac{\text{Deposition Rate}}{\text{Mixing Height}} \right)$$

where:

Half-life = reaction half-life of the chemical in the atmosphere (day)

Deposition fate = total deposition rate including wet and dry deposition to soil, water, and vegetation (m/day)

Mixing height = average mixing height of the atmosphere (i.e., the height over which pollutants are assumed to be evenly mixed) (m)

The atmospheric mixing height is a function of climatic conditions and can be calculated from meteorological data. When determining the characteristic travel distance for a chemical,

individual calculations for each season may be appropriate because the meteorological characteristics such as mixing height, precipitation, and wind speed may vary significantly. The reaction half-life and deposition rates are chemical-specific.

The following equation applies the CTD calculated above to approximate the distance (L) for a specified reduction in chemical mass:

$$L = - \ln\left(\frac{100 - [\% \text{ Reduction}]}{100}\right) * \text{Characteristic Travel Distance}$$

where [% Reduction] refers to the fractional reduction in chemical mass. This information can be used in a similar manner as ISC dispersion modeling results to guide and inform the layout of the overall modeling region.

### **References for Appendix B**

Benarie, M.M. 1980. Urban Air Pollution Modeling. Cambridge, MA: MIT Press.

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