TRIM.FaTE USER GUIDANCE
MODULE 14: SIMULATION RESULTS AND ANALYSES[1]

This module describes the results that can be obtained from a TRIM.FaTE simulation and the different formats in which they can be produced, as well as utilities for processing and viewing results. This module is divided into the following sections.

1.	**Simulation Output Files**	This section describes the different options for reporting the outputs from a TRIM.FaTE simulation. It is divided into four subsections: compartment results (i.e., moles, mass, and concentrations in individual compartments) (Section 1.1), deposition estimates (Section 1.2), scenario property values and results at a time point (Section 1.3), and scenario configuration and results in MySQL format (Section 1.4).
2.	**Output Processors**	This section describes the available utilities for processing TRIM.FaTE outputs. It is divided into the following three sections, each describing one of the utilities: the Averager (Section 2.1), the Transposer (Section 2.2), and the Aggregator (Section 2.3).
3.	**Graphical Results Viewer**	This section describes the graphical results viewer, a built-in TRIM.FaTE utility that can be used to view and animate changes in compartment moles, mass, or concentration with respect to space and time.
	Appendix A	This appendix contains an example of a compartment results file in semicolon-delimited text format.
	Appendix B	This appendix contains an example of a deposition estimates file in semicolon-delimited text format.
	Appendix C	This appendix describes the configuration of a TRIM.FaTE library required to output deposition estimates.
	Appendix D	This appendix contains several example applications of the Averager utility.
	Appendix E	This appendix contains a sample Format file, which is a file used in running the Aggregator utility.

In addition to the outputs described here, which focus on values generated from a TRIM.FaTE simulation, TRIM.FaTE can facilitate the documentation of a simulation by producing files describing the scenario set-up and settings as well as files of library objects and values. These export files are described fully in Module 3, Library and Scenario Data Files.

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[1]Descriptions of library-specific algorithms and properties presented in this module pertain to the March 2003 versions of the TRIM.FaTE library.

1. SIMULATION OUTPUT FILES

The different types of output data that can be produced by TRIM.FaTE fall into four categories:

- Compartment results (in mass, moles, and/or concentration);
- Deposition estimates for surface soil and surface water compartments;
- Scenario property values and results at a time point (i.e., HTML export); and
- Scenario configuration and results in MySQL format (i.e., MySQL export).

This section describes each of these types of output data and the user options for creating them.

1.1 Compartment Results

As described in Volume I, Section 4.2 of the TRIM.FaTE Technical Support Document (U.S. EPA 2002), output from TRIM.FaTE includes moles, mass, and concentration of the modeled chemicals in each modeled compartment at each user-specified simulation time point. The moles files (in semicolon-delimited text format) are always created automatically during the run. Mass and concentration output files (also in semicolon-delimited text format) can be created by setting the scenario properties *exportMass* and *exportConcentration*, respectively, to "true."

The default moles output file, as well as the mass and concentration files created by setting the appropriate scenario properties, are stored in the directory specified by the scenario property *outputDir*. These files are named using the following format:

<Scenario name>_<Chemical name>_<Output type><Counter>.txt

where:

<Scenario name>	=	name of the scenario
<Chemical name>	=	name of the modeled chemical
<Output type>	=	type of output (i.e., moles, mass, or concentration), and
<Counter>	=	integer assigned by the model (described in more detail below).

Users should note that any spaces in the scenario or chemical names will be converted to underscores (i.e., "_") in the output file names. For example, a scenario named "TestScenario" could have a mass output file for divalent mercury named:

TestScenario_Divalent_Mercury_mass1.txt

To prevent new output files from overwriting previous output files for the same scenario, TRIM.FaTE appends a "counter" to the end of each of the compartment output file names. If users run multiple simulations for a single scenario without shutting down and restarting TRIM.FaTE, the counter appended to the output files will be different for each simulation. For

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example, if a user ran another simulation of the "TestScenario" scenario (as presented in the previous example), the mass output file for divalent mercury could be named:

TestScenario_Divalent_Mercury_mass2.txt

Users should note, however, that if TRIM.FaTE is shut down and restarted, the model can no longer determine if a particular counter has been used and thus previous output files from the scenario may be overwritten. **If TRIM.FaTE has been shut down and restarted prior to performing a simulation of a scenario run previously, users should change the scenario property *outputDir* to ensure the output files from the previous simulation are not overwritten**.

These output files may alternatively be created using the "Results Exporter." The Results Exporter can be used to create moles, mass, and/or concentration results files following the successful completion of a simulation but prior to closing the Scenario window after the simulation. To use the Results Exporter after the completion of a simulation, the user should follow these steps.

1.   Select "Export" from the File menu in the Scenario window.

2.   In the "Choose Exporter" pop-up window, select "Results Exporter" and click "OK."

3.   In the "Results Exporter" pop-up window, specify the directory to which the output file(s) should be written, the types of files to create, and whether rows are to be time points and columns compartments (default) or vice versa. Note that the "Compute summaries using mass" selection does not impact the creation of the results files.
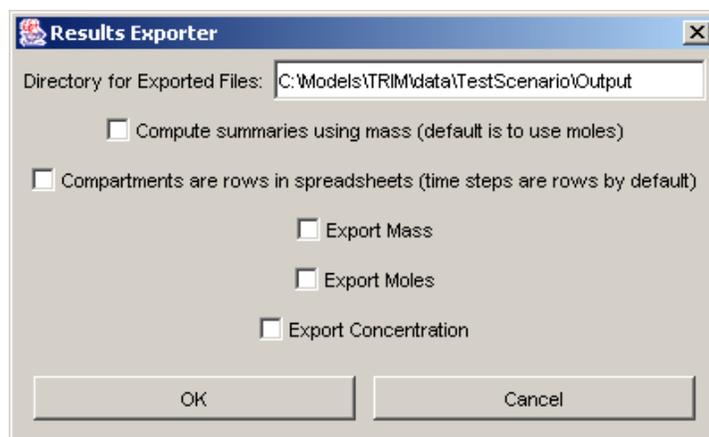
The default units[2] for the mass and concentration files are provided in Table 1, and an example results output file is provided in Appendix A.

Table 1
Default Units[2] for TRIM.FaTE Results

Type of Results	Compartments	Units (chemical[a] per compartment mass or volume)
Mass	All	grams
Concentration	Air	micrograms per cubic meter (: g/m^3)
	Soil - Root Zone	milligrams per kilogram, dry weight (mg/kg, dw)
	Soil - Surface	micrograms per gram, dry weight (: g/g, dw)
	Soil - Vadose Zone	grams per gram, dry weight (g/g, dw)
	Sediment	milligrams per kilogram, wet weight (mk/kg, ww)
	Surface water, Groundwater	milligrams per liter (mg/L)
	All biota	milligrams per kilogram, wet weight (mg/kg, ww)

[a] Mass and concentration outputs are based on a conversion from moles of chemical to mass of chemical using the molecular weight for the chemical. One exception to this occurs in the current library for methyl mercury. For consistency with most applications (e.g., human health and ecological risk analyses), mass and concentration results for methyl mercury are provided in terms of mercury (e.g., methyl mercury in fish is milligrams methyl mercury, as mercury, per kilogram fish, wet weight).

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[2] The units specified in Table 1 are those specified in the current TRIM.FaTE library and those expected by the other TRIM modules. To output results in other units, the user will need to change the values of the *concentrationOutputFactor* and *concentrationOutputUnits* properties in each compartment for which this is desired. It is important to note that if these properties are changed, the outputs from the TRIM.FaTE simulation cannot be used directly as inputs into other TRIM modules.

1.2   Deposition Estimates for Soil Compartments

Deposition outputs can be calculated by TRIM.FaTE for each surface soil and surface water compartment at each output time point of the simulation. When selected by the user, the deposition outputs will be written to semicolon-delimited text files (one for each modeled chemical) and to a MySQL database.[3] A sample text output file of deposition estimates is provided in Appendix B.

When the user chooses to output deposition estimates, the following deposition outputs are created:

- Wet particle deposition (g/m^2-day);
- Dry particle deposition (g/m^2-day);
- Wet vapor deposition (g/m^2-day); and
- Dry vapor deposition (g/m^2-day).

To produce deposition outputs, the user will need to specify values for several scenario properties, as shown below.

1.   Set the scenario property *exportDeposition* to "true."

2.   Set the scenario property *exportDatabase* to "true."

3.   Set the scenario property *outputDatabaseName* to the desired name for the output MySQL database.

4.   Set the scenario property *exportAllResultsToDB* to "true."

The deposition files created by setting the appropriate scenario properties are stored in the directory specified by the scenario property *outputDir*. These files are named using the following format:

<Scenario name>_<Chemical name>_dep<Counter>.txt

where:

<Scenario name>	=	name of the scenario
<Chemical name>	=	name of the modeled chemical
<Counter>	=	integer assigned by the model (described in more detail below).

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[3] The current version of TRIM.FaTE does not allow the user to only export the deposition results in text or MySQL database format. If the user wants deposition outputs, the data will be produced in both formats.

Users should note that any spaces in the scenario or chemical names will be converted to underscores (i.e., "_") in the output file names. For example, a scenario named "TestScenario" could have a deposition output file for divalent mercury named:

TestScenario_Divalent_Mercury_dep1.txt

To prevent new output files from overwriting previous output files for the same scenario, TRIM.FaTE appends a "counter" to the end of each of the deposition output file names. If users run multiple simulations for a single scenario without shutting down and restarting TRIM.FaTE, the counter appended to the output files will be different for each simulation. For example, if a user ran another simulation of the "TestScenario" scenario (as presented in the previous example), the mass output file for divalent mercury could be named:

TestScenario_Divalent_Mercury_dep2.txt

Users should note, however, that if TRIM.FaTE is shut down and restarted, the model can no longer determine if a particular counter has been used and thus previous output files from the scenario may be overwritten. **If TRIM.FaTE has been shut down and restarted prior to performing a simulation of a scenario run previously, users should change the scenario property *outputDir* to ensure the output files from the previous simulation are not overwritten.**

Users should note that if the scenario property *averageResultsFiles* is set to "true," averaged deposition files will also be created and added to the directory specified by the scenario property *outputDir*. These files will include deposition estimates averaged over the number of time points specified by the scenario property *averagingInterval*. These files will be named using the following format:

<Scenario name>_<Chemical name>_dep<Counter>_<Averaging Period>_avg.txt

where:

<Averaging Period> = period over which the deposition estimates are averaged; either a number of hours (e.g., "12hr"), "monthly," or "annual."

Important Note About Deposition Outputs

The deposition algorithms in the current library have been formulated to enable the output of deposition estimates. To maintain this capability with the implementation of any new deposition to surface soil or surface water algorithms or revisions to existing algorithms, the user must configure the algorithms as described in Appendix C.

## 1.3   Scenario Property Values and Results at a Time Point

TRIM.FaTE can also create a series of HTML files containing summarized results from a simulation as well as the values of all of the properties in the scenario (e.g., scenario properties, compartment properties, link properties) at an user-specified time point. These files, collectively referred to as the "HTML Export," can be created before or after running a simulation. Note, however, that an HTML Export following a simulation contains a summary of the results (including transfer factors and mass fluxes between linked compartments at the specified time point) that is not contained in an export performed prior to a simulation run. The HTML Export represents a single time point, which is selected by the user; therefore, all time-varying properties and calculated values correspond to that time point. When performed after a simulation, this export can be particularly useful in evaluating model results because the user can see the transfer factors and fluxes between compartments.

The HTML Export can be created before or after a simulation by completing the following steps.

1.   Select "Export" from the File menu of the FaTE Scenario window.

2.   Select "HTML Exporter" in the Choose Exporter window and click "OK."

3.   Specify the directory of exported files and the date and time to evaluate the properties in the HTML Exporter window. Optionally, the user can also have TRIM.FaTE export transfer factors, evaluate algorithm properties for each link, compute simulation summaries using mass instead of moles, and export the results with compartments (instead of time steps) as rows using the check boxes in this window. When all of the options are specified, click "OK."
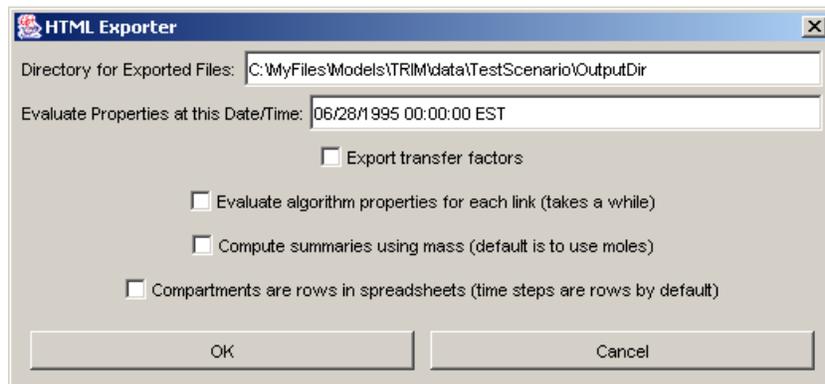
Alternatively, the user can have TRIM.FaTE automatically perform an HTML export at the conclusion of a simulation by completing the following steps.

    1.   Set the scenario property *exportHTML* to "true."

    2.   Set the scenario property *evaluateHTMLPropertiesAtTime* to the date and time at which the property values should be evaluated.

1.4   Scenario Configuration and Results in MySQL Format

The results of a TRIM.FaTE simulation, including the compartment results, deposition estimates, and details about the configuration of the scenario, can also be exported in MySQL database format. This export, referred to as the "MySQL Export," consists of a Property Export, an Outdoor Environment Export, and a Results Export (if simulation has completed successfully) for the simulation written in MySQL database format (these three types of exports are described in detail in Module 3). This export is primarily used for providing the necessary information about a TRIM.FaTE simulation to other TRIM modules (e.g., TRIM.Risk$_{ECO}$), although users familiar with MySQL may find it useful to be able to manipulate the data in a MySQL database. The MySQL Export can be created before or after a simulation by completing the following steps.

    1.   Select "Export" from the file menu of the FaTE Scenario window.

    2.   Select "MySQL Exporter" in the Choose Exporter window and click "OK."

Alternatively, the user can have TRIM.FaTE automatically perform a MySQL Export at the conclusion of a simulation, prior to exiting TRIM.FaTE, by completing the following steps.

    1.   Set the scenario property *exportDatabase* to "true."

    2.   Set one or both of the following scenario properties to "true": *exportAllResultsToDB* or *exportAvgResultsToDB* (this property can only be set to

"true" if *averageResultsFiles* is set to "true" and a value is specified for *averagingInterval*).

3.   Specify a value for the *outputDatabaseName* scenario property.

2.   OUTPUT PROCESSORS

There are three TRIM.FaTE utilities that can be used to process the basic TRIM.FaTE compartment output files (i.e., moles, mass, and concentration semicolon-delimited text files): the Averager, the Transposer, and the Aggregator. The capabilities of these utilities, as well as instructions for using them, are summarized here and described in further details in the sections below.

- The **Averager** allows the user to average data in results files over different time steps and to select particular compartments and time periods for processing. Refer to Section 2.1 for more details.

- The **Transposer** allows the user to take data in results files and transpose the rows into columns and the columns into rows. Refer to Section 2.2 for more details.

- The **Aggregator** allows the user to perform a variety of functions (e.g., average, sum) on selected columns in the results files to create files that summarize the results in different ways. Refer to Section 2.3 for more details.

2.1   The Averager

Large TRIM.FaTE simulations (i.e., simulations with complex spatial layouts, several chemicals, long modeling periods, and/or short output time steps) can produce very large text files that are cumbersome to manipulate and view on most PCs. The Averager allows the user to average data over selected time periods and to select particular compartments and time periods for processing. This tool is particularly useful for reducing the TRIM.FaTE raw output data to a summary file of averaged outputs.

The user can run the Averager in two different ways: (1) configure a scenario to automatically run the Averager at the conclusion of a successful simulation or (2) run it as a command line tool using a DOS batch file. To run the Averager automatically after a simulation, the user should set the scenario property *averageResultsFiles* to "true" and specify a value for the scenario property *averagingInterval*. Using this method, the user does not need to complete any additional steps following the simulation to create averaged files; however, the user can only run the Averager for a single averaging period and must specify this period prior to a simulation. Running the Averager as a command line tool requires additional steps following the simulation, but this method allows the user to average results over multiple averaging periods and does not require the user to select an averaging period prior to performing a simulation. The steps involved in running the Averager as a command line tool are described below.

2.1.1 Configuring the Averager

The Averager can be configured for a user's computer by completing the following steps.

1. Open the file called *Averager.bat* using a text editor. This file is included in the TRIM.FaTE installation and can be found in the main TRIM directory (e.g., C:\models\trim). The first line of this file should resemble:

    set classpath=C:\models\trim\lib\trimv2.7.jar;C:\models\trim\lib\jgl3.1.0.jar

2. Update the two places in the first line of the *Averager.bat* file where "C:\models\trim\lib" appears in order to be consistent with the location of the *trimv2.7.jar* and *jgl3.1.0.jar* files on the user's computer. These files are located in the "lib" directory of the main TRIM directory upon installation of TRIM.FaTE. If the user subsequently changes the directory structure in the main TRIM directory (which is not recommended), these file paths will need to be updated accordingly.

3. Save the *Averager.bat* file with the changes.

2.1.2 Using the Averager

The Averager can be run on a user's computer by completing the following steps.

1. Open the file called *Averager.bat* using a text editor. This file is included in the TRIM.FaTE installation and can be found in the main TRIM directory.

2. Edit the line beginning with "java gov.epa.trim.util.TimeWeightedAverager" to specify the necessary settings. Each of these options are described in Table 2. Make sure to include a space between each flag (e.g., -i, -o) and the value of the setting. At a minimum, the setting specified as "Required" in the table must be specified. The following line provides a template for the required settings for this line of the *Averager.bat* file.

    java gov.epa.trim.util.TimeWeightedAverager -i <Input File> -o <Output file> -a <Ave Period>

To specify settings for any of the optional specifications, simply add the settings to the end of the statement. For example, this following line shows a template where the user would specify the required settings, as well as the delimiter option.

java gov.epa.trim.util.TimeWeightedAverager -i <Input File> -o <Output file> -a <Ave Period> -d <Delimiter>

Several examples of the Averager's "java" statement line are provided in the text box following Table 2.

Table 2
Specifications for "java" Statement in *Averager.bat* File

Required/Optional	Setting	Description
Required	-i \<filename\>	Use this option to specify the TRIM.FaTE results file to be processed.
Required	-o \<filename\>	Use this option to specify a name for the output file.
Required	-a \<ave period\>	Use this option to specify the number of time steps over which to average. The averaging period must be equal to a positive integer, or the text strings "monthly" or "annual." To create monthly averages, set this option to "monthly." To create annual averages, set this option to "annual." For example, if the input file contains hourly data and daily averages were desired, this option would be set to 24.
Optional	-d \<character\>	This option specifies the delimiter between columns and must be placed in double-quotes. The default is a semicolon.
Optional	-s \<MM/dd/yyyy hh:mm:ss z\>	This option specifies the date, time, and associated time zone when averaging should start. If the user only wishes to process part of the TRIM results file, they can ignore the data before this time and only average data after this time.
Optional	-e \<MM/dd/yyyy hh:mm:ss z\>	This option specifies the date, time, and associated time zone when averaging should end. If the user only wishes to process part of the TRIM results file, they can ignore the data after this time and only average data before this time.
Optional (must be used in conjunction with -wsp option)	-wdr \<integer\>	The column number (the first column is column 1) that contains wind direction data. Wind data cannot be averaged as a scalar value; it should be averaged as a vector. To average wind data properly, the user must specify the columns with the wind direction and speed data.
Optional (must be used in conjunction with -wdr option)	-wsp \<integer\>	The column number (the first column is column 1) that contains wind speed data. Wind data cannot be averaged as a scalar value; it should be averaged as a vector. To average wind data properly, the user must specify the columns with the wind direction and speed data.
Optional	-col \<integer-integer\>	This option is used to specify a range of columns to process. For example, to process columns 1 through 200 of a file with 600 columns, this option would be set to "-col 1-200".

Required/Optional	Setting	Description
Optional	-incl <string>	This option is used to only include columns whose name contains a specified string in the averaging. This is another method for processing only a subset of the columns in the input file.
Optional	-excl <string>	This option is used to exclude columns whose name contains a specified string from the averaging. This is another method for processing only a subset of the columns in the input file.
Optional	-numdec <integer>	This option is used to specify the number of decimal places to display in the output file.

Examples of "java" Statements for the Averager

Example 1.

    java gov.epa.trim.util.TimeWeightedAverager -i input_data.txt -o ave_data.txt -a "annual" -d ";"

Description: This example specifies that the Averager read in the data in the semicolon-delimited file *input_data.txt*, average the data annually, and write the resulting averages to a semicolon-delimited output file named *ave_data.txt*.

Example 2.

    java gov.epa.trim.util.TimeWeightedAverager -i input_data.txt -o ave_data.txt -a 8 -d ";" -incl "Air"

Description: This example specifies that the Averager read in the data in the semicolon-delimited file *input_data.txt*, average the data for the compartments whose name contains the string "Air" over 8 time steps at a time, and write the resulting averages to a semicolon-delimited output file named *ave_data.txt*.

Example 3.

    java gov.epa.trim.util.TimeWeightedAverager -i input_data.txt -o ave_data.txt -a 12 -d ";" -numdec "2"

Description: This example specifies that the Averager read in the data in the semicolon-delimited file *input_data.txt*, average the data over 12 time steps at a time, and write the resulting averages to two decimal places to a semicolon-delimited output file named *ave_data.txt*.

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3. Save the *Averager.bat* file. Users may save this file using a different name as long as the filename ends with ".bat". This may be useful when setting up multiple applications of the Averager.

4. Double-click on the *Averager.bat* (or renamed) file. This should open a DOS window and the Averager should start running. When the window closes, the averaging is complete. If the specified averaged output files are not created,

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review the *Averager.bat* (or renamed) file again to ensure there are no mistakes in it (e.g., input file name that does not exist).

Examples of uses of the *Averager.bat* file for different averaging applications are provided in Appendix D.

Important Notes About the Averager

•   Output files from the Averager cannot be used as input files to the Averager.

•   Users can average multiple results files using a single *Averager.bat* file by including multiple versions of the line beginning with "java gov.epa.trim.util.TimeWeightedAverager" in the *Averager.bat* file.

2.2   The Transposer

The Transposer utility can read in semicolon-delimited text files, transpose the data (i.e., write columns in the input files as rows in the output files and the rows in the input files as columns in the output files), and then write the transposed data to a new file. This can be used to take TRIM.FaTE results text files which list the compartments as columns and create a file with compartments as rows. This utility can be used to process files with many more compartments than time steps into a format that can be easily accommodated in most spreadsheet software. For example, the Transposer can take this file as input:

```
Date;          Time;          Zone;  Comp_1;     Comp_2;     Comp_3;
01/01/1990;    00:00:00;      EST;   1.298E-03;  3.865E-05;  5.670E-07;
01/01/1990;    01:00:00;      EST;   1.409E-03;  3.986E-05;  5.832E-07;
01/01/1990;    02:00:00;      EST;   1.682E-03;  4.279E-05;  5.855E-07;
01/01/1990;    03:00:00;      EST;   1.800E-03;  4.553E-05;  5.878E-07;
```

And turn it into a file like this:

```
Date;          01/01/1990;  01/01/1990;  01/01/1990;  01/01/1990;
Time;          00:00:00;    01:00:00;    02:00:00;    03:00:00;
Zone;          EST;         EST;         EST;         EST;
Comp_1;        1.298E-03;   1.409E-03;   1.682E-03;   1.800E-03;
Comp_2;        3.865E-05;   3.986E-05;   4.279E-05;   4.553E-05;
Comp_3;        5.670E-07;   5.832E-07;   5.855E-07;   5.878E-07;
```

Note that the Transposer is currently limited to handling files that will fit into the user's computer memory (i.e., RAM).

2.2.1 Configuring the Transposer

The Transposer can be configured by following these steps.

1. Open the file called *Transposer.bat* using a text editor. This file is included in the TRIM.FaTE installation and can be found in the main TRIM directory (e.g., C:\models\trim). The first line of this file should resemble:

    set classpath=C:\models\trim\lib\trimv2.7.jar;C:\models\trim\lib\jgl3.1.0.jar

2. Update the two places in the first line of the *Transposer.bat* file where "C:\models\trim\lib" appears in order to be consistent with the location of the *trimv2.7.jar* and *jgl3.1.0.jar* files on the user's computer. These files are located in the "lib" directory of the main TRIM directory upon installation of TRIM.FaTE. If the user subsequently changes the directory structure in the main TRIM directory (which is not recommended), these file paths will need to be updated accordingly.

3. Save the *Transposer.bat* file with the changes.

2.2.2 Using the Transposer

The Transposer can be run on a user's computer by completing the following steps.

1. Open the file called *Transposer.bat* using a text editor. This file is included in the TRIM.FaTE installation and can be found in the main TRIM directory.

2. Edit the line beginning with "java gov.epa.trim.util.Transposer" to specify the necessary options. Each of these options is described in Table 3. Make sure to include a space between each flag (e.g., -i, -o) and the value of the option. At a minimum, the options specified as "Required" in the table must be specified. The following line provides a template for the required settings for this line of the *Transposer.bat* file.

    java gov.epa.trim.util.Transposer -i <Input File> -o <Output file>

To specify a delimiter, simply add the setting to the end of the statement. For example, this following line shows a template where the user would specify the required settings, as well as the delimiter option.

    java gov.epa.trim.util.Transposer -i <Input File> -o <Output file> -d <Delimiter>

Table 3
Specifications for "java" Statement in *Transposer.bat* File

Option	Required/Optional	Description
-i	Required	The name of the input file that you would like to transpose.
-o	Required	The name of the output file to which the results are written.
-d	Optional	The delimiter between columns (default is semicolon).

3.   Save the *Transposer.bat* file. Users may save this file using a different name as long as the filename ends with ".bat". This may be useful when setting up multiple applications of the Transposer.

4.   Double-click on the *Transposer.bat* (or renamed) file in Windows Explorer. This should open a DOS window and the Transposer should start running. When the window closes, the transposition is complete. If the specified transposed output files are not created, review the *Transposer.bat* (or renamed) file again to ensure there are no mistakes in it (e.g., input file name that does not exist).

Important Notes About the Transposer

•   When transposing larger files, the Transposer may run out of available memory and quit before writing the transposed output files. In these cases, the user may need to adjust the amount of memory available to the Transposer and rerun it. This is done by adding the "-Xmx<Memory>m" command in the options line. For example, the option line:

   java -Xmx512m gov.epa.trim.util.Transposer -i input_data.txt -o transposed_data.txt -d ";"

   specifies that 512MB of memory should be made available to the Transposer. Users should specify more available memory than the size of the file to be transposed to allow enough memory for the program to run. Note, however, that users should be careful not to specify more memory than is available on their computer.

•   Users can transpose multiple results files using a single *Transposer.bat* file by including multiple versions of the line beginning with "java gov.epa.trim.util.Transposer" in the *Transposer.bat* file.

An example of the use of the *Transposer.bat* file is provided below.

Example of Transposer Application

set classpath=C:\models\trim\lib\trimv2.7.jar;C:\models\trim\lib\jgl3.1.0.jar

java -Xmx512m gov.epa.trim.util.Transposer -i input_data.txt -o transposed_data.txt -d ";"

Description: This example specifies that 512MB of memory are available to transpose the semicolon-delimited file "input_data.txt" and write the output to a file named "transposed_data.txt."

2.3   The Aggregator

The TRIM Aggregator takes TRIM.FaTE results files (i.e., semicolon-delimited text files of moles, mass, or concentration in each modeled compartment) and aggregates the data in the columns into a smaller number of columns. The aggregation can involve several different operations, such as averaging or summing. An example of where the Aggregator might be useful is in producing a file showing total mass in all biotic compartments and total mass in all abiotic compartments over the output time points in a simulation. The Aggregator can accept input from one or multiple files, thus allowing the user to produce a summary of the results from several files.

2.3.1   Configuring the Aggregator

The Aggregator can be configured by following these steps.

1.   Open the file called *Aggregator.bat* using a text editor. This file is included in the TRIM.FaTE installation and can be found in the main TRIM directory (e.g., C:\models\trim). The first line of this file should resemble:

   set classpath=C:\models\trim\lib\trimv2.7.jar;C:\models\trim\lib\jgl3.1.0.jar

2.   Update the two places in the first line of the *Aggregator.bat* file where "C:\models\trim\lib" appears in order to be consistent with the location of the *trimv2.7.jar* and *jgl3.1.0.jar* files on the user's computer. These files are located in the "lib" directory of the main TRIM directory upon installation of TRIM.FaTE. If the user subsequently changes the directory structure in the main TRIM directory (which is not recommended), these file paths will need to be updated accordingly.

3.   Save the *Aggregator.bat* file with the changes.

2.3.2   Using the Aggregator

After configuring the *Aggregator.bat* file (as described in Section 3.3.1), there are essentially two steps involved in using the Aggregator: (1) creating the Format file and (2) editing the *Aggregator.bat* file. The Format file is used to indicate to the Aggregator the groups

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of columns on which an operation is to be performed and the operations that will be performed. The *Aggregator.bat* file will specify the locations and filenames of the input, output, and Format files. Each of these steps is described below.

Creating Format Files

The Format file is a text file consisting of a header line (which must contain "version; 1") followed by groups of commands, with each group providing the necessary formatting instructions for a single column in the output file. There is no limit on the number of groups that can be included in a single Format file. Each group must contain (in order):

- an output column name;
- an operation; and
- a list of input columns.

The "output" and "operation" lines occur only once per output column, while there will typically be multiple input lines per group of commands for an output column. A simple example of a Format file is provided in the text box below.

```
                    Example Format File


            version;1
            output;All Abiotic Comps.
            operation; sum
            input; in1; {include}Air in
            input; in1; {include}Surface water in
            input; in2; {include}Air in
            input; in2; {include}Surface water in
            input; in3; {include}Air in
            input; in3; {include}Surface water in
```

The **"output" line** has the following format:

output;<Name of Output Column>

where the user defines the name of the output column as it should appear in the output file.

The **"operation" line** has the following format:

operation;<Type of operation>

where the user selects the type of operation to perform on the input columns from those described in Table 4.

Table 4
Types of Operations for Format File

Operation	Description	Function	Number of Input Columns
sum	Sums all of the inputs	col1+col2...col[n]	unlimited
average	Averages all of the inputs	(col1+col2+...col[n])/n	unlimited
diff	Calculates the difference between 2 inputs	col1 - col2	2
mult	Multiplies 2 inputs	col1 * col2	2
ratio	Calculates the ratio of 2 inputs	col1 / col2	2
percent	Calculates the percent of the sum of the 2 inputs comprised of in1	[col1 / (col1+col2)] x 100%	2
percentdiff	Calculates the percent different between 2 inputs	[(col1 - col2) / (col1+col2)] x 100%	2
copy	Copies an input column into the output column	col1	1

Following the "output" and "operation" lines must be the input column or columns on which the selected operation will be performed. The number of input columns may be limited by the selected operation. The "sum" and "average" operations can process an unlimited number of columns, whereas the remaining operations require a specific number of input columns. The number of columns associated with each operation is provided in Table 4.

Each of the **input lines** should have the following format:

input;<Input ID>;<Column selector>

where the "Input ID" is either an input file ID (i.e., the first listed input file in the *Aggregator.bat* file is "in1", the second is "in2", and so forth) or the word "out".

When an input file ID is provided, the Aggregator searches for the "Column selector" in the specified input file and selects those columns that match. When "out" is provided, the Aggregator searches for the "Column selector" in the previously created output columns and selects those columns that match. The "Column selector" can be the complete name of a compartment, or a combination of a column keyword and a string. The different column selector keywords are described in Table 5.

Table 5
Column Selector Keywords

Keyword	Description
{all}	This keyword will select all of the columns in a file and will use them to compute the output.
{include}	This keyword will select all of the columns in a file containing the text following the keyword and will use them to compute the output.
{exclude}	This keyword will exclude columns containing the text following the keyword and will use the remaining columns to compute the output. This keyword requires that some columns have already been selected using the {all} and/or {include} keywords, or using the exact column name.

After completing the Format file, the user can save the file in any convenient location on their computer. In configuring the *Aggregator.bat* file, the user will indicate the path and filename of the Format file. An example of a Format file, including a description of what this format file would create, can be found in Appendix E.

Editing and Running the Aggregator.bat File

After creating a Format file, the user must edit the *Aggregator.bat* file. The steps involved in this are described below.

1.   Open the file called *Aggregator.bat* using a text editor. This file is included in the TRIM.FaTE installation and can be found in the main TRIM directory.

2.   Edit the line beginning with "java gov.epa.trim.util.TRIMResultsFileAggregator" to specify the necessary options. Each of these options is described in Table 6. Make sure to include a space between each flag (e.g., -i, -o) and the value of the option. At a minimum, the options specified as "Required" in the table must be specified. The following line provides a template for the required settings for this line of the *Aggregator.bat* file.

> java gov.epa.trim.util.Transposer -i <Input File> -o <Output file> -f <Format file>

To specify a delimiter and/or header, simply add the setting(s) to the end of the statement. For example, this following line shows a template where the user would specify the required settings, as well as the header option.

java gov.epa.trim.util.TRIMResultsFileAggregator -i <Input File> -o <Output file> -f <Format file>-h <Header>

Table 6
Specifications for "java" Statement in *Aggregator.bat* File

Option	Required/Optional	Can it be repeated?	Description
-i	Required	Y	This option is used to specify the input file(s) the user wants to aggregate. Multiple input files can be specified by using this option repeatedly (this is useful when comparing or merging data from multiple files).
-o	Required	Y	This option specifies the output file(s) to be produced. The Aggregator allows the user to produce output files in three different formats: text file with the same delimiter used by input file(s) (indicated by an output file name ending with .txt), comma-delimited text (indicated by an output file name ending with .csv), and HTML (indicated by an output file name ending with .html). The user can select multiple output formats by using this option multiple times. Note, however, that each output file will contain the same data.
-f	Required	N	This option specifies the Format file that will be used. See "Creating Format Files" section for more details.
-d	Optional	N	This option indicates the data delimiter used in the input file(s). The default is semicolon delimited (";").
-h	Optional	N	This option provides a header/title that will be used at the top of each of the output files.

3.   Save the *Aggregator.bat* file. Users may save this file using a different name as long as the filename ends with ".bat". This may be useful when setting up multiple applications of the Aggregator.

4.   Double-click on the *Aggregator.bat* (or renamed) file in Windows Explorer. This should open a DOS window and the Aggregator should start running. When the window closes, the specified operation is complete. If the specified aggregated output files are not created, review the *Aggregator.bat* (or renamed) file again to ensure there are no mistakes in it (e.g., input file name that does not exist).

Important Note About the Aggregator

Users can perform Aggregator functions on multiple results files using a single *Aggregator.bat* file by including multiple versions of the line beginning with "java gov.epa.trim.util.TRIMResultsFileAggregator" in the *Aggregator.bat* file.

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3.   GRAPHICAL RESULTS VIEWER

After completing a simulation, the results can be viewed in the context of the air or soil/water parcel layout using the Graphical Results Viewer. This tool provides the user with the ability to view how the results change over space (from a "bird's eye view") and time. The Graphical Results Viewer can be accessed from the Scenario window by selecting "Graphical Results" from the "View" menu. This will bring up a file browser. Using this file browser, the user should select the results file to be viewed and then click "Open." **Note: only simulation results for the currently open FaTE Scenario can be viewed in the Graphical Results Viewer.**

Figure 1 displays the main screen of the Graphical Results Viewer. To view the results, the user must first select the type of volume element that contains the compartment of interest from the "Volume Element Types" pull-down menu above the legend. The list of compartments contained in the selected volume element type will appear in the "Compartments" column. When a compartment is selected from this list, the results for that compartment will appear in the box on the left of the window. When a compartment has been selected, the legend of concentrations appears on the right and the time step is displayed below the plot. The units of the results for the currently displayed compartment are provided above the legend.

The user can use the magnifying glasses icon to zoom in and out. In addition, the user can view the Lat/Long and X/Y coordinates of certain points in the plot by checking the "Location" check box and moving the mouse to a point on the plot. The Lat/Long or X/Y coordinates will be displayed next to the check box.

When a new compartment is selected, TRIM.FaTE will automatically rescale the legend based on the minimum and maximum values for the compartment being viewed. The legend's scale can be set to linear or logarithmic by selecting the Linear or Log radio buttons below the list of values. At the top is a drop down box where you can select the number of legend colors to use. This can range from 2 to 20. To change the colors, the user can click on the color and select a new color from the pop-up window. After changing the color(s), the user should click the "Redraw" button to redraw the plot with the new colors. The user can also manually change the values and use the Redraw button to reflect these changes. In addition, the user can enter a minimum value in the lowest text field and a maximum value in the uppermost text field and then click the Redistribute button to redistribute the between the selected minimum and maximum value.

Figure 1
Graphical Results Viewer: Main Screen
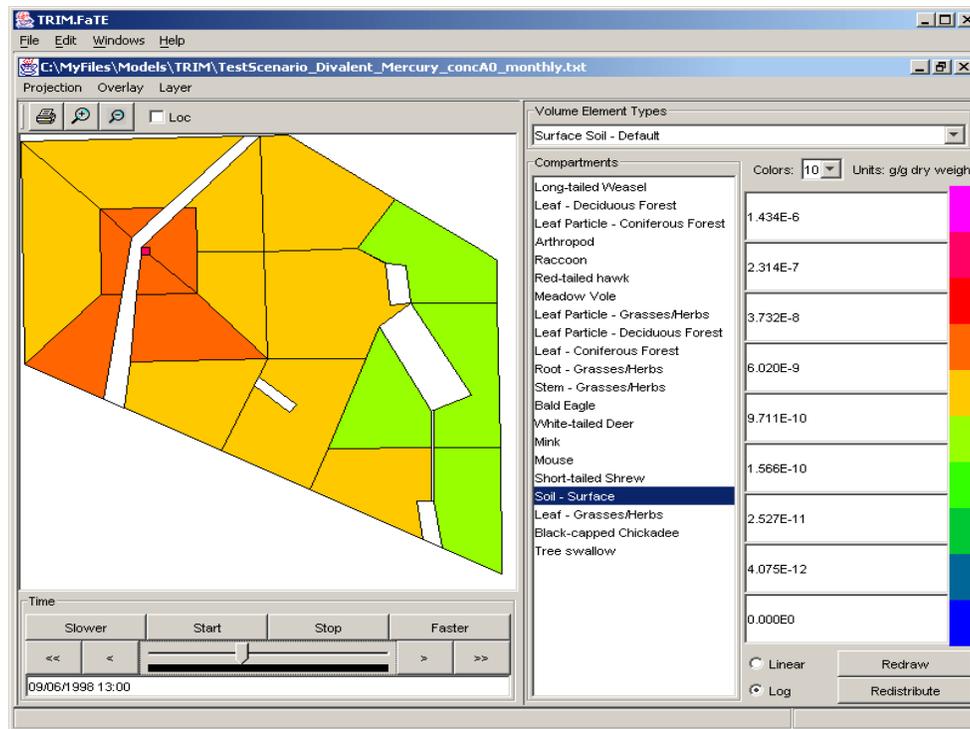
The time step that is being displayed can be controlled from the Time panel beneath the plot. To advance the time step forward one time step, click the ">" button. To move the time step backward one time step, click the "<" button. The "<<" button will set the plot to the first time step and the ">>" will set it to the last time step. The user can also move the slider to change the time step. Note that for very large files, there may be a delay between when the slider is moved and when the plot refreshes. The user can also animate the plot with respect to time. This is done by clicking the "Start" button to begin the animation and the "Stop" button to stop at the current time step. The "Faster" and "Slower" buttons will speed up or slow down the animation.

> **TIP**: Always try to "rewind" to the beginning of the time period before changing compartment types. This simple step will greatly decrease the time it takes to bring up the data for the newly selected compartment type.

The user can also add GIS layers on top of the TRIM data results by going to the "Layer" menu and selecting "Edit Layers." Figure 2 shows the "Edit Layers" window. This window contains information about the layers in the plot. The first layer is the parcel layer. This is the outline of the parcels in your Scenario. The next layer is the data layer (e.g., concentration estimates). This contains the colored polygons that represent the data being displayed.

Figure 2
Layer Control Window
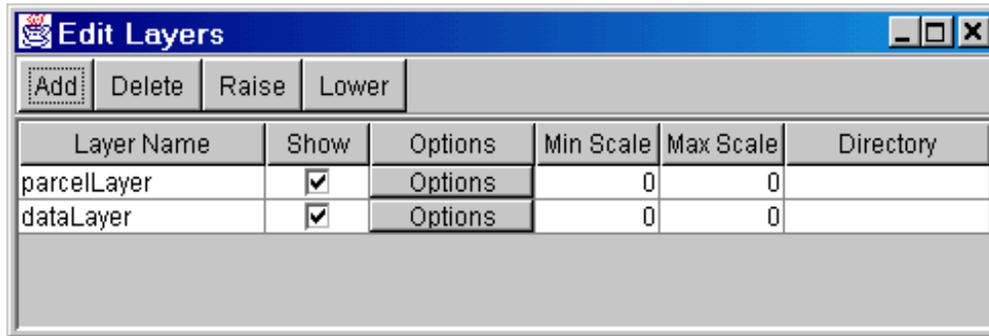
New layers can be added by clicking the "Add" button. This will bring up an "Open File" dialog which allows the user to choose a file to add. Currently, TRIM.FaTE can only read ESRI shape files (i.e., *.shp files). Layers can be turned on and off by checking or unchecking, respectively, the Show check box next to the name of the layer. The user can also raise and lower layers by selecting them and using the "Raise" and "Lower" buttons. A layer can be deleted from the plot by selecting it and clicking the "Delete" button.

The options for a layer, such as polygon and line colors, can be set by clicking the "Options" button on the same row as the layer name. Figure 3 shows the "Layer Options" pop-up window for a parcel layer. This window allows the user to change attributes of the polygons, line, and points in the layers.

- **Polygons**. The user can specify whether it is filled or open by using the "Filled" and "Outline" radio buttons on the right. If "Outline" is selected then only the Outline color will be used to draw the outline of the polygon. If "Filled" is selected then the Fill color will be used to fill the polygon and the Outline color will be used to draw outline of the polygon. The user can change the color of a polygon by clicking on the "Fill Color" box. Note that the transparency of the color can be set to allow lower layers to bleed through higher layers. The line thickness of the outline in pixels can be set using the Thickness box.

- **Lines**. The user can specify color of the lines by clicking on the "Color" button. In addition, the line style can be selected from the "Line Style" pull-down menu. The line thickness of the outline in pixels can be set using the Thickness box.

- **Points**. If there are points in the shape file, the type, color and size can be set in the Points area. The available types are circle, square, triangle, diamond, cross and star.

Figure 3
Layer Options Window
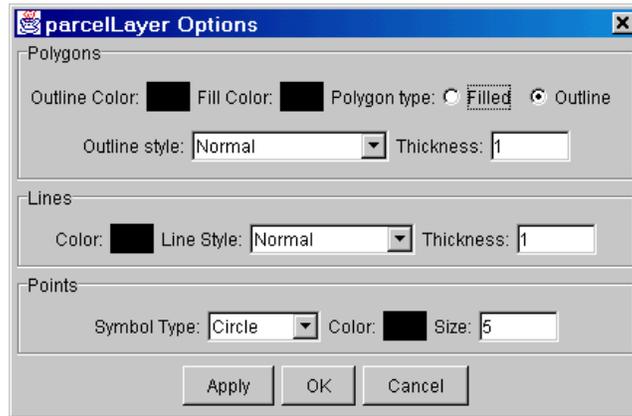
The user can preview the changes before closing the window, by clicking "Apply" to apply the changes. When finished editing the layer, the user can click "OK" to close and apply the changes.

Figure 4 contains an example of GIS layers displayed with TRIM data. Some of the streams and ponds in the area have been loaded and their color has been set to a transparent blue to allow the data colors to be seen with the water boundaries.

Figure 4
GIS Layers on Top of TRIM.FaTE Data
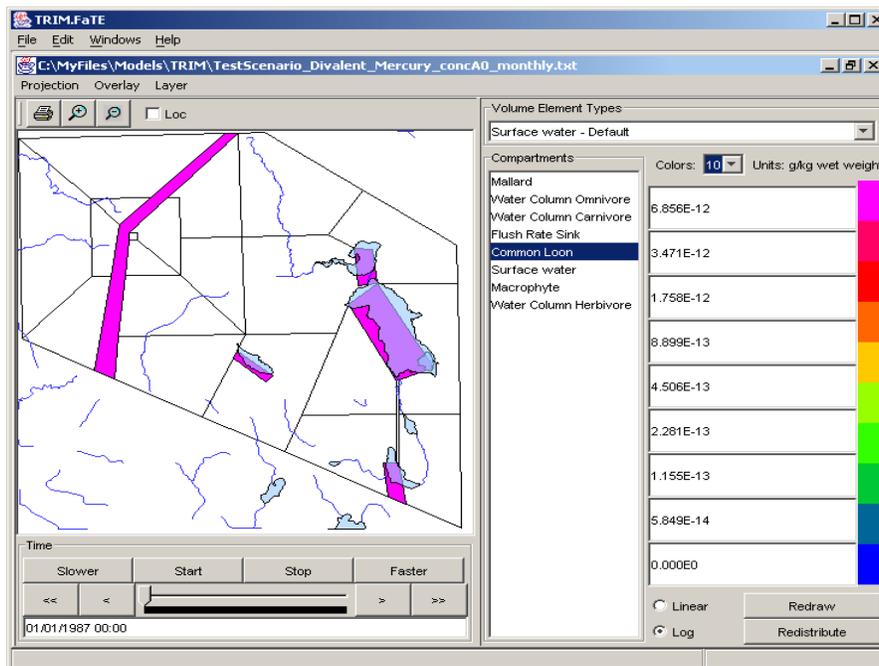
Users can also add custom overlays to the map with points, lines and polygons. These are specified in a text file format which is detailed in Section 2.1 of Module 3. The overlay files can be imported into the Graphical Results Viewer by completing the following steps.

1.   Select "Load Overlay" from the "Overlay" pull-down menu.

2.   Select the desired overlay file using the File Browser and click "OK."

APPENDIX A
EXAMPLE OF COMPARTMENT RESULTS TEXT FILE

Note that the actual text file generated by TRIM.FaTE contains all of the results for a single time point on a single line. To indicate where the line breaks occur in the actual results file, "**<HR>**" has been inserted at the end of each line.

Date;Time;TimeZone;Air in Air_Source;Air in Air_NNE1;Air in Air_ENE1;Surface water in SW_Lake;Water Column Carnivore in SW_Lake;Water Column Herbivore in SW_Lake;Water Column Omnivore in SW_Lake;Sediment in Sed_Lake;Benthic Invertebrate in Sed_Lake;Benthic Omnivore in Sed_Lake;Soil - Surface in SurfSoil_Source;Soil - Surface in SurfSoil_N1;Leaf - Grasses/Herbs in Grasses/Herbs in SurfSoil_N1;Leaf Particle - Grasses/Herbs in Grasses/Herbs in SurfSoil_N1;Root - Grasses/Herbs in Grasses/Herbs in SurfSoil_N1;Stem - Grasses/Herbs in Grasses/Herbs in SurfSoil_N1;Meadow Vole in SurfSoil_N1;Mouse in SurfSoil_N1;Short-tailed Shrew in SurfSoil_N1;White-tailed Deer in SurfSoil_N1;American Robin in SurfSoil_N1;Red-tailed hawk in SurfSoil_N1;Arthropod in SurfSoil_N1;Soil - Surface in SurfSoil_E1;Leaf - Grasses/Herbs in Grasses/Herbs in SurfSoil_E1;Leaf Particle - Grasses/Herbs in Grasses/Herbs in SurfSoil_E1;Root - Grasses/Herbs in Grasses/Herbs in SurfSoil_E1;Stem - Grasses/Herbs in Grasses/Herbs in SurfSoil_E1;Meadow Vole in SurfSoil_E1;Mouse in SurfSoil_E1;Short-tailed Shrew in SurfSoil_E1;White-tailed Deer in SurfSoil_E1;Raccoon in SurfSoil_E1;Mink in SurfSoil_E1;Tree swallow in SurfSoil_E1;American Robin in SurfSoil_E1;American Woodcock in SurfSoil_E1;Red-tailed hawk in SurfSoil_E1;Bobwhite Quail in SurfSoil_E1;Arthropod in SurfSoil_E1;Soil - Root Zone in RootSoil_Source;Soil - Root Zone in RootSoil_N1;Worm in RootSoil_N1;Soil - Root Zone in RootSoil_E1;Worm in RootSoil_E1;Soil - Vadose Zone in VadoseSoil_Source;Soil - Vadose Zone in VadoseSoil_N1;Soil - Vadose Zone in VadoseSoil_E1;Groundwater in GW_Source;Groundwater in GW_N1;Groundwater in GW_E1**<HR>**

n/a;n/a;n/a;ug/m3;ug/m3;ug/m3;mg/L;g/kg wet weight;g/kg wet weight;g/kg wet weight;mg/kg wet weight;g/kg wet weight;g/kg wet weight;ug/g dry weight;ug/g dry weight;g/kg wet weight;g/kg wet weight;g/kg wet weight;g/kg wet weight;mg/kg wet weight;mg/kg wet weight;mg/kg wet weight;mg/kg wet weight;mg/kg wet weight;mg/kg wet weight;g/kg wet weight;ug/g dry weight;g/kg wet weight;g/kg wet weight;g/kg wet weight;g/kg wet weight;mg/kg wet weight;mg/kg wet weight;mg/kg wet weight;mg/kg wet weight;mg/kg wet weight;mg/kg wet weight;mg/kg wet weight;mg/kg wet weight;mg/kg wet weight;mg/kg wet weight;mg/kg wet weight;g/kg wet weight;g/kg wet weight;mg/kg wet weight;mg/kg wet weight;g/kg wet weight;mg/kg wet weight;g/kg wet weight;g/g dry weight;g/g dry weight;g/g dry weight;g/L;g/L;g/L**<HR>**

12/29/2009;0:00:00;EST;0.00E+00;0.00E+00;0.00E+00;0.00E+00;0.00E+00;0.00E+00;0.00E+00;0.00E+00;0.00E+00;0.00E+00;0.00E+00;-1.00E+06;-1.00E+06;0.00E+00;0.00E+00;0.00E+00;0.00E+00;0.00E+00;0.00E+00;0.00E+00;0.00E+00;0.00E+00;0.00E+00;-1.00E+06;-1.00E+06;0.00E+00**<HR>**

12/29/2009;2:00:00;EST;9.70E-07;4.71E-09;4.46E-22;1.02E-12;4.02E-25;4.60E-20;9.17E-24;7.92E-13;3.74E-19;1.73E-23;5.79E-09;1.02E-10;-1.00E+06;-1.00E+06;0.00E+00;0.00E+00;5.12E-13;6.33E-13;7.00E-13;1.18E-13;7.22E-13;2.01E-13;5.02E-26;1.79E-14;-1.00E+06;-1.00E+06;0.00E+00;0.00E+00;2.23E-17;3.01E-17;4.38E-17;1.06E-17;4.49E-17;1.61E-17;3.41E-17;4.51E-17;9.68E-17;3.51E-17;3.01E-20;8.86E-30;2.85E-18;4.87E-20;7.58E-27;8.57E-24;1.34E-30;5.52E-36;9.14E-38;1.62E-41;3.26E-46;5.23E-48;9.29E-52**<HR>**

12/29/2009;4:00:00;EST;5.36E-07;1.05E-08;6.16E-21;1.56E-12;3.16E-24;1.65E-19;1.44E-22;2.86E-12;2.93E-18;2.85E-22;9.01E-09;2.21E-10;-1.00E+06;-1.00E+06;0.00E+00;0.00E+00;1.90E-12;2.36E-12;2.65E-12;4.38E-13;2.74E-12;7.53E-13;4.27E-25;2.55E-14;-1.00E+06;-1.00E+06;0.00E+00;0.00E+00;1.46E-16;1.78E-16;2.25E-16;6.93E-17;1.97E-16;1.07E-16;2.27E-16;2.24E-16;3.83E-16;3.93E-16;1.57E-19;6.80E-29;1.01E-17;2.08E-19;6.45E-26;2.99E-23;1.03E-29;4.17E-35;7.80E-37;1.25E-40;5.27E-45;9.33E-47;1.57E-50**<HR>**

12/29/2009;6:00:00;EST;5.90E-07;1.54E-08;1.51E-20;2.00E-12;9.78E-24;3.28E-19;6.75E-22;5.70E-12;9.03E-18;1.36E-21;1.25E-08;3.77E-10;-1.00E+06;-1.00E+06;0.00E+00;0.00E+00;4.27E-12;5.33E-12;6.03E-12;9.84E-13;6.24E-12;1.71E-12;1.51E-24;3.22E-14;-1.00E+06;-1.00E+06;0.00E+00;0.00E+00;3.83E-16;4.54E-16;5.41E-16;1.82E-16;4.40E-16;2.84E-16;5.99E-16;5.32E-16;8.10E-16;1.70E-15;3.80E-19;2.05E-28;2.07E-17;5.01E-19;2.28E-25;5.82E-23;3.11E-29;1.30E-34;2.77E-36;3.77E-40;2.59E-44;5.09E-46;7.68E-50**<HR>**

APPENDIX B
EXAMPLE OF DEPOSITION ESTIMATES TEXT FILE

Note that the actual text file generated by TRIM.FaTE contains all of the results for a single time point on a single line. To indicate where the line breaks occur in the actual results file, "**<HR>**" has been inserted at the end of each line.

```
Date;Time;Timezone;Wet Particle Deposition to Soil - Surface in SurfSoil_Source; Dry Particle Deposition to Soil - Surface in SurfSoil_Source; Wet Vapor Deposition to Soil - Surface
in SurfSoil_Source; Dry Vapor Deposition to Soil - Surface in SurfSoil_Source; Wet Particle Deposition to Soil - Surface in SurfSoil_N1; Dry Particle Deposition to Soil - Surface in
SurfSoil_N1; Wet Vapor Deposition to Soil - Surface in SurfSoil_N1; Dry Vapor Deposition to Soil - Surface in SurfSoil_N1; Wet Particle Deposition to Soil - Surface in SurfSoil_E1;
Dry Particle Deposition to Soil - Surface in SurfSoil_E1; Wet Vapor Deposition to Soil - Surface in SurfSoil_E1; Dry Vapor Deposition to Soil - Surface in SurfSoil_E1; Wet Particle
Deposition to Surface water in SW_Lake; Dry Particle Deposition to Surface water in SW_Lake; Wet Vapor Deposition to Surface water in SW_Lake; Dry Vapor Deposition to Surface
water in SW_Lake
n/a;n/a;n/a;g/day/m2;g/day/m2;g/day/m2;g/day/m2;g/day/m2;g/day/m2;g/day/m2;g/day/m2;g/day/m2;g/day/m2;g/day/m2;g/day/m2;g/day/m2;g/day/m2;g/day/m2;g/day/m2<HR>
6/28/1995; 00:00:00; EST;0.00E+00;0.00E+00;0.00E+00;0.00E+00;0.00E+00;0.00E+00;0.00E+00;0.00E+00;0.00E+00;0.00E+00;0.00E+00;0.00E+00;
0.00E+00;0.00E+00;0.00E+00;0.00E+00<HR>
6/28/1995; 02:00:00; EST;0.00E+00;1.24E-11;0.00E+00;1.26E-08;0.00E+00;3.72E-13;0.00E+00;3.76E-10;0.00E+00;3.18E-17;0.00E+00;3.22E-14;0.00E+00;
5.84E-13;0.00E+00;5.91E-10<HR>
6/28/1995; 04:00:00; EST;0.00E+00;2.82E-11;0.00E+00;2.86E-08;0.00E+00;6.87E-13;0.00E+00;6.98E-10;0.00E+00;8.03E-17;0.00E+00;8.15E-14;0.00E+00;
1.32E-12;0.00E+00;1.34E-09<HR>
6/28/1995; 06:00:00; EST;0.00E+00;5.52E-10;0.00E+00;5.65E-07;0.00E+00;9.72E-12;0.00E+00;9.95E-09;0.00E+00;2.26E-13;0.00E+00;2.32E-10;0.00E+00;
2.52E-11;0.00E+00;2.58E-08<HR>
6/28/1995; 08:00:00; EST;0.00E+00;1.72E-10;0.00E+00;1.74E-07;0.00E+00;2.17E-12;0.00E+00;2.19E-09;0.00E+00;1.04E-12;0.00E+00;1.05E-09;0.00E+00;
8.54E-12;0.00E+00;8.64E-09<HR>
6/28/1995; 10:00:00; EST;0.00E+00;7.95E-11;0.00E+00;7.93E-08;0.00E+00;1.78E-12;0.00E+00;1.78E-09;0.00E+00;7.77E-13;0.00E+00;7.76E-10;0.00E+00;
3.81E-12;0.00E+00;3.80E-09<HR>
6/28/1995; 12:00:00; EST;0.00E+00;3.12E-11;0.00E+00;3.08E-08;0.00E+00;9.69E-13;0.00E+00;9.57E-10;0.00E+00;1.71E-14;0.00E+00;1.68E-11;0.00E+00;
9.82E-13;0.00E+00;9.70E-10<HR>
6/28/1995; 14:00:00; EST;0.00E+00;2.06E-11;0.00E+00;2.02E-08;0.00E+00;2.68E-13;0.00E+00;2.63E-10;0.00E+00;4.74E-14;0.00E+00;4.65E-11;0.00E+00;
1.03E-12;0.00E+00;1.01E-09<HR>
6/28/1995; 16:00:00; EST;0.00E+00;1.58E-11;0.00E+00;1.55E-08;0.00E+00;2.19E-13;0.00E+00;2.14E-10;0.00E+00;8.63E-14;0.00E+00;8.44E-11;0.00E+00;
8.83E-13;0.00E+00;8.64E-10<HR>
6/28/1995; 18:00:00; EST;0.00E+00;1.25E-11;0.00E+00;1.23E-08;0.00E+00;1.79E-13;0.00E+00;1.75E-10;0.00E+00;9.60E-14;0.00E+00;9.41E-11;0.00E+00;
7.42E-13;0.00E+00;7.27E-10<HR>
6/28/1995; 20:00:00; EST;0.00E+00;1.22E-11;0.00E+00;1.20E-08;0.00E+00;1.74E-13;0.00E+00;1.72E-10;0.00E+00;1.09E-13;0.00E+00;1.08E-10;0.00E+00;
7.30E-13;0.00E+00;7.21E-10<HR>
6/28/1995; 22:00:00; EST;0.00E+00;1.92E-11;0.00E+00;1.91E-08;0.00E+00;2.74E-13;0.00E+00;2.73E-10;0.00E+00;1.92E-13;0.00E+00;1.91E-10;0.00E+00;
1.16E-12;0.00E+00;1.15E-09<HR>
6/29/1995; 00:00:00; EST;0.00E+00;3.27E-11;0.00E+00;3.27E-08;0.00E+00;4.46E-13;0.00E+00;4.46E-10;0.00E+00;1.87E-13;0.00E+00;1.87E-10;0.00E+00;
1.80E-12;0.00E+00;1.80E-09<HR>
```

APPENDIX C
REQUIRED ALGORITHM CONFIGURATION FOR PRODUCING DEPOSITION OUTPUTS

When adding new deposition to surface soil or surface water algorithms or revising existing algorithms, users must ensure that the algorithms are properly configured for producing deposition estimates. The configuration requirements for these algorithms are described below.

(1)   All deposition to surface soil and surface water algorithms must specify the value for the "category" property based on the type of deposition represented by the algorithm. The rules for specifying values for the "category" property are provided in the table below.

Type of Deposition Algorithm	Category
Dry Deposition of Particles	Deposition | Dry | Particle
Dry Deposition of Vapor	Deposition | Dry | Vapor
Wet Deposition of Particles	Deposition | Wet | Particle
Wet Deposition of Vapor	Deposition | Wet | Vapor

(2)   All deposition to surface soil algorithms must include the *FractionDepositionToSoil* property. This property is not required for deposition to surface water algorithms. The value of this property depends on the type of deposition represented by the algorithm. The rules for specifying values for the *FractionDepositionToSoil* property are provided in the table below.

Type of Deposition Algorithm	Formula
Dry Deposition of Particles	1 - receivingVolumeElementSumOf[Plant | Leaf].DryDepInterceptionFraction
Dry Deposition of Vapor	1 - receivingVolumeElementSumOf[Plant | Leaf].DryDepInterceptionFraction
Wet Deposition of Particles	1 - receivingVolumeElementSumOf[Plant | Leaf].WetDepInterceptionFraction
Wet Deposition of Vapor	1 - receivingVolumeElementSumOf[Plant | Leaf].WetDepInterceptionFraction

APPENDIX D
EXAMPLES OF USES OF THE AVERAGER

This appendix presents several example applications of the Averager, a utility that allows the user to average TRIM.FaTE compartment results files over selected time periods and to select particular compartments and time periods for processing. For a description of the syntax used to run the Averager, refer to Section 2.1 of this module. The following text box contains an example TRIM.FaTE compartment results file that will be used in the examples provided in this appendix.

Example TRIM.FaTE Compartment Results File: *Input_file.txt*

```
Date;Time;TimeZone;Air in Air_Source;Air in Air_NNE1;Air in Air_ENE1;Air in Air_ESE1;Air in Air_SSE1
n/a;n/a;n/a;ug/m3;ug/m3;ug/m3;ug/m3;ug/m3
12/29/2009;0:00:00;EST;0.00E+00;0.00E+00;0.00E+00;0.00E+00;0.00E+00
12/29/2009;2:00:00;EST;9.70E-07;4.71E-09;4.46E-22;4.20E-21;6.48E-21
12/29/2009;4:00:00;EST;5.36E-07;1.05E-08;6.16E-21;1.40E-20;1.49E-20
12/29/2009;6:00:00;EST;5.90E-07;1.54E-08;1.51E-20;2.59E-20;1.56E-20
12/29/2009;8:00:00;EST;7.99E-07;1.84E-08;1.66E-20;3.21E-20;2.70E-20
12/29/2009;10:00:00;EST;5.45E-07;1.21E-08;1.94E-20;3.88E-20;3.51E-20
12/29/2009;12:00:00;EST;4.17E-07;1.02E-08;2.55E-20;4.64E-20;3.36E-20
12/29/2009;14:00:00;EST;3.44E-07;1.00E-08;3.20E-20;4.89E-20;2.75E-20
12/29/2009;16:00:00;EST;3.91E-07;1.36E-08;3.79E-20;4.87E-20;2.57E-20
12/29/2009;18:00:00;EST;3.71E-07;1.15E-08;3.80E-20;5.46E-20;2.98E-20
12/29/2009;20:00:00;EST;5.27E-07;2.05E-08;4.70E-20;5.43E-20;2.82E-20
12/29/2009;22:00:00;EST;5.34E-07;1.91E-08;4.80E-20;5.98E-20;3.13E-20
```

Example 1

This example illustrates how the *Averager.bat* file would be configured to:

(1)   Average the data in the semicolon-delimited input file *Input_file.txt*
(2)   Over 2 time steps at a time and
(3)   Write the resulting averages to a semicolon-delimited output file named *Output_file1.txt*, the contents of which are provided in the text box below.

Example 1 *Averager.bat* File

```
set classpath=c:\models\trim\lib\trimv2.7.jar;c:\models\trim\lib\jgl3.1.0.jar

java gov.epa.trim.util.TimeWeightedAverager -i Input_file.txt -o Output_file1.txt -a 2 -d ";"
```

Example 1 Averaged Output: *Output_file1.txt*

```
Averaged data from file 'Input_file.txt': each line averaged over 2 time steps.
Date;Time;TimeZone;Air in Air_Source;Air in Air_NNE1;Air in Air_ENE1;Air in Air_ESE1;Air in Air_SSE1;
n/a;n/a;n/a;ug/m3;ug/m3;ug/m3;ug/m3;ug/m3;
12/29/2009;00:00:00;EST;0.00000000E00;0.00000000E00;0.00000000E00;0.00000000E00;0.00000000E00;
12/29/2009;04:00:00;EST;7.53000000E-07;7.60500000E-09;3.30300000E-21;9.10000000E-21;1.06900000E-20
12/29/2009;08:00:00;EST;6.94500000E-07;1.69000000E-08;1.58500000E-20;2.90000000E-20;2.13000000E-20
12/29/2009;12:00:00;EST;4.81000000E-07;1.11500000E-08;2.24500000E-20;4.26000000E-20;3.43500000E-20
12/29/2009;16:00:00;EST;3.67500000E-07;1.18000000E-08;3.49500000E-20;4.88000000E-20;2.66000000E-20
12/29/2009;20:00:00;EST;4.49000000E-07;1.60000000E-08;4.25000000E-20;5.44500000E-20;2.90000000E-20
12/29/2009;22:00:00;EST;5.34000000E-07;1.91000000E-08;4.80000000E-20;5.98000000E-20;3.13000000E-20
```

Example 2

This example illustrates how the *Averager.bat* file would be configured to:

(1)   Average the data in the semicolon-delimited input file *Input_file.txt* beginning on December 29, 2009 at 00:00:00 EST and ending on December 29, 2009 at 12:00:00 EST
(2)   Over 4 time steps at a time and
(3)   Write the resulting averages to a semicolon-delimited output file named *Output_file2.txt*, the contents of which are provided in the text box below.

Note that the last time step in the output file only included two time steps. In cases where there are not enough time steps in the file (or selected date range in this case), the Averager simply averages the remaining time steps.

Example 2 *Averager.bat* File

```
set classpath=c:\models\trim\lib\trimv2.7.jar;c:\models\trim\lib\jgl3.1.0.jar

java gov.epa.trim.util.TimeWeightedAverager -i Input_file.txt -o Output_file2.txt -a 4 -d ";" -s 12/29/2009 00:00:00 EST -e 12/29/2009 12:00:00 EST
```

Example 2 Averaged Output: *Output_file2.txt*

```
Averaged data from file 'Input_file.txt': each line averaged over 4 time steps.
Date;Time;TimeZone;Air in Air_Source;Air in Air_NNE1;Air in Air_ENE1;Air in Air_ESE1;Air in Air_SSE1;
n/a;n/a;n/a;ug/m3;ug/m3;ug/m3;ug/m3;ug/m3;
12/29/2009;00:00:00;EST;0.00000000E00;0.00000000E00;0.00000000E00;0.00000000E00;0.00000000E00;
12/29/2009;08:00:00;EST;7.23750000E-07;1.22525000E-08;9.57650000E-21;1.90500000E-20;1.59950000E-20
12/29/2009;12:00:00;EST;4.81000000E-07;1.11500000E-08;2.24500000E-20;4.26000000E-20;3.43500000E-20
```

Example 3

This example illustrates how the *Averager.bat* file would be configured to:

(1)   Average the data in columns 5 through 7 of the semicolon-delimited input file *Input_file.txt*
(2)   Over 6 time steps at a time and
(3)   Write the resulting averages to a semicolon-delimited output file named *Output_file.txt*, the contents of which are provided in the text box below.

Note that the last time step in the output file only included five time steps. In cases where there are not enough time steps in the file, the Averager simply averages the remaining time steps.

Example 3 *Averager.bat* File

```
set classpath=c:\models\trim\lib\trimv2.7.jar;c:\models\trim\lib\jgl3.1.0.jar

java gov.epa.trim.util.TimeWeightedAverager -i Input_file.txt -o Output_file3.txt -a 6 -d ";" -col 5-7
```

Example 3 Averaged Output: *Output_file3.txt*

```
Averaged data from file 'Input_file.txt': each line averaged over 6 time steps.
Date;Time;TimeZone;Air in Air_NNE1;Air in Air_ENE1;Air in Air_ESE1;
n/a;n/a;n/a;ug/m3;ug/m3;ug/m3;
12/29/2009;00:00:00;EST;0.00000000E00;0.00000000E00;0.00000000E00;
12/29/2009;12:00:00;EST;1.18850000E-08;1.38676667E-20;2.69000000E-20;
12/29/2009;22:00:00;EST;1.49400000E-08;4.05800000E-20;5.32600000E-20;
```

Example 4

This example illustrates how the *Averager.bat* file would be configured to:

(1)   Average the data in the semicolon-delimited input file *Input_file.txt* for columns with compartment names that include the string "NE"
(2)   Over 2 time steps at a time and
(3)   Write the resulting averages to a semicolon-delimited output file named *Output_file4.txt*, the contents of which are provided in the text box below.

Example 4 *Averager.bat* File

```
set classpath=c:\models\trim\lib\trimv2.7.jar;c:\models\trim\lib\jgl3.1.0.jar

java gov.epa.trim.util.TimeWeightedAverager -i Input_file.txt -o Output_file4.txt -a 2 -d ";" -incl "NE"
```

Example 4 Averaged Output: *Output_file4.txt*

Averaged data from file 'Input_file.txt': each line averaged over 2 time steps.
Date;Time;TimeZone;Air in Air_NNE1;Air in Air_ENE1;
n/a;n/a;n/a;ug/m3;ug/m3;
12/29/2009;00:00:00;EST;0.00000000E00;0.00000000E00;
12/29/2009;04:00:00;EST;7.60500000E-09;3.30300000E-21;
12/29/2009;08:00:00;EST;1.69000000E-08;1.58500000E-20;
12/29/2009;12:00:00;EST;1.11500000E-08;2.24500000E-20;
12/29/2009;16:00:00;EST;1.18000000E-08;3.49500000E-20;
12/29/2009;20:00:00;EST;1.60000000E-08;4.25000000E-20;
12/29/2009;22:00:00;EST;1.91000000E-08;4.80000000E-20;

Example 5

This example illustrates how the *Averager.bat* file would be configured to:

(1)   Average the data in the semicolon-delimited input file *Input_file.txt* for columns with compartment names that do not include the string "NE"

(2)   Over 2 time steps at a time and

(3)   Write the resulting averages out to two decimal places to a semicolon-delimited output file named *Output_file5.txt*, the contents of which are provided in the text box below.

Example 5 *Averager.bat* File

```
set classpath=c:\models\trim\lib\trimv2.7.jar;c:\models\trim\lib\jgl3.1.0.jar

java gov.epa.trim.util.TimeWeightedAverager -i Input_file.txt -o Output_file5.txt -a 2 -d ";" -excl "NE" -numdec 2
```

Example 5 Averaged Output: *Output_file5.txt*

```
Averaged data from file 'Input_file.txt': each line averaged over 2 time steps.
Date;Time;TimeZone;Air in Air_Source;Air in Air_ESE1;Air in Air_SSE1;
n/a;n/a;n/a;ug/m3;ug/m3;ug/m3;
12/29/2009;00:00:00;EST;0.00E00;0.00E00;0.00E00;
12/29/2009;04:00:00;EST;7.53E-07;9.10E-21;1.07E-20
12/29/2009;08:00:00;EST;6.94E-07;2.90E-20;2.13E-20
12/29/2009;12:00:00;EST;4.81E-07;4.26E-20;3.43E-20
12/29/2009;16:00:00;EST;3.68E-07;4.88E-20;2.66E-20
12/29/2009;20:00:00;EST;4.49E-07;5.45E-20;2.90E-20
12/29/2009;22:00:00;EST;5.34E-07;5.98E-20;3.13E-20
```

Example 6

This example illustrates how the *Averager.bat* file would be configured to:

(1)   Average the data in the semicolon-delimited input file *Input_file.txt* for columns with compartment names that include the string "NE"
(2)   Over 2 time steps at a time and
(3)   Write the resulting averages out to two decimal places to a semicolon-delimited output file named *Output_file6_NE.txt*, the contents of which are provided below;
(4)   Average the data in the semicolon-delimited input file *Input_file.txt* for columns with compartment names that do not include the string "NE"
(5)   Over 2 time steps at a time and
(6)   Write the resulting averages out to two decimal places to a semicolon-delimited output file named *Output_file6_noNE.txt*, the contents of which are provided below

Example 6 *Averager.bat* File

```
set classpath=c:\models\trim\lib\trimv2.7.jar;c:\models\trim\lib\jgl3.1.0.jar

java gov.epa.trim.util.TimeWeightedAverager -i Input_file.txt -o Output_file6_NE.txt -a 2 -d ";" -incl "NE"
java gov.epa.trim.util.TimeWeightedAverager -i Input_file.txt -o output_file6_noNE.txt -a 2 -d ";" -excl "NE"
```

Example 6 Averaged Output: *Output_file6_NE.txt*

```
Averaged data from file 'Input_file.txt': each line averaged over 2 time steps.
Date;Time;TimeZone;Air in Air_NNE1;Air in Air_ENE1;
n/a;n/a;n/a;ug/m3;ug/m3;
12/29/2009;00:00:00;EST;0.00000000E00;0.00000000E00;
12/29/2009;04:00:00;EST;7.60500000E-09;3.30300000E-21;
12/29/2009;08:00:00;EST;1.69000000E-08;1.58500000E-20;
12/29/2009;12:00:00;EST;1.11500000E-08;2.24500000E-20;
12/29/2009;16:00:00;EST;1.18000000E-08;3.49500000E-20;
12/29/2009;20:00:00;EST;1.60000000E-08;4.25000000E-20;
12/29/2009;22:00:00;EST;1.91000000E-08;4.80000000E-20;
```

Example 6 Averaged Output: *Output_file6_noNE.txt*

```
Averaged data from file 'Input_file.txt': each line averaged over 2 time steps.
Date;Time;TimeZone;Air in Air_Source;Air in Air_ESE1;Air in Air_SSE1;
n/a;n/a;n/a;ug/m3;ug/m3;ug/m3;
12/29/2009;00:00:00;EST;0.00000000E00;0.00000000E00;0.00000000E00;
12/29/2009;04:00:00;EST;7.53000000E-07;9.10000000E-21;1.06900000E-20
12/29/2009;08:00:00;EST;6.94500000E-07;2.90000000E-20;2.13000000E-20
12/29/2009;12:00:00;EST;4.81000000E-07;4.26000000E-20;3.43500000E-20
12/29/2009;16:00:00;EST;3.67500000E-07;4.88000000E-20;2.66000000E-20
12/29/2009;20:00:00;EST;4.49000000E-07;5.44500000E-20;2.90000000E-20
12/29/2009;22:00:00;EST;5.34000000E-07;5.98000000E-20;3.13000000E-20
```

APPENDIX E
EXAMPLE OF AGGREGATOR FORMAT FILE

```
version;1
output;All Abiotic Comps.
operation; sum
input; in1; {include}Air in
input; in1; {include}Surface water in
input; in2; {include}Air in
input; in2; {include}Surface water in
input; in3; {include}Air in
input; in3; {include}Surface water in

output;All Biotic Comps.
operation; sum
input; in1; {all}
input; in1; {exclude}Air in
input; in1; {exclude}Surface water in
input; in1; {exclude}Sink
input; in2; {all}
input; in2; {exclude}Air in
input; in2; {exclude}Surface water in
input; in2; {exclude}Sink
input; in3; {all}
input; in3; {exclude}Air in
input; in3; {exclude}Surface water in
input; in3; {exclude}Sink

output;Air Sinks
operation; sum
input; in1; {include}for Air
input; in2; {include}for Air
input; in3; {include}for Air

output;Flush Rate Sinks
operation; sum
input; in1; {include}Flush Rate Sink
input; in2; {include}Flush Rate Sink
input; in3; {include}Flush Rate Sink

output;Total in Sinks
operation; sum
input; out; Air Sinks
input; out; Flush Rate Sinks

output;Total in Modeling Region and Sinks
operation; sum
input; out; Total in Sinks
input; out; All Abiotic Comps.
input; out; All Biotic Comps.

output; Fraction in Sinks
operation; percent
input; out; Total in Sinks
input; out; Total in Modeled System
```

Description: This example was designed to create an aggregated file containing total mercury mass in different groups of compartments. Data from three different inputs files (each containing mercury mass data for a different type of mercury for an identical set of compartments) was aggregated using this format file to create the following columns in the output file:

- All Abiotic Comps.
- All Biotic Comps.
- Air Sinks
- Flush Rate Sinks
- Total in Sinks
- Total in Modeling Region and Sinks
- Fraction in Sinks

Each of these columns are described below.

All Abiotic Comps. - This column will consist of the sum of all of the compartments in input files 1 through 3 containing the strings "Air in" and "Surface water in."

All Biotic Comps. - This column will consist of the sum of all of the compartments in input files 1 through 3 that do not include the string "Air in," "Surface water in," and "Sink."

Air Sinks. - This column will consist of the sum of all of the compartments in input files 1 through 3 that contain the string "for Air."

Flush Rate Sinks. - This column will consist of the sum of all of the compartments in input files 1 through 3 that contain the string "Flush Rate Sink."

Total in Sinks. - This column will consist of the sum of the "Air Sinks" and "Flush Rate Sinks" columns.

Total in Modeling Region and Sinks. - This column will consist of the sum of the "Total in Sinks," "All Abiotic Comps.," and "All Biotic Comps." columns.

Fraction in Sinks. - This column will be calculated by dividing the "Total in Sinks" column by the "Total in Modeling Region and Sinks" column, and then multiplying the result by 100%.

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