# Software for Model Attainment Test -Community Edition (SMAT-CE) User's Guide

Software version 1.7

December 2019

## Acknowledgements

In Cooperation with the U.S. EPA and the University of North Carolina Institute for the Environment, the South China University of Technology (SCUT) developed the SMAT-CE software. Abt Associates provided much of the content for this User's Guide through the MATS User's Manual (Abt Associates, 2014).

## **SMAT-CE User's Guide Contents**

Acknowledgementsi		
Table of Figuresiv		
1.	Intr	oduction1
2.	Qui	ck Start2
2	2.1.	Install Software 2
2	2.2.	Start SMAT-CE
2	2.3.	Load a Previous Project
2	2.4.	Annual PM Analysis Quick Start
2	2.5.	Daily PM Analysis Quick Start
2	2.6.	Ozone Analysis Quick Start 12
2	2.7.	Visibility Analysis Quick Start15
3.	SM	AT-CE Installation18
4.	SM	AT-CE Start Page20
5.	Rur	nning SMAT-CE23
5	5.1.	Load Previous SMAT-CE Project
5	5.2.	New SMAT-CE Analysis
5	5.3.	Running SMAT-CE in Batch Mode
6.	Ann	ual PM Analysis26
(	5.1.	Choose Desired Output
(	5.2.	Output Choices-Advanced 31
(	5.3.	Data Input
(	5.4.	Species Fraction Options
(	5.5.	PM2.5 Calculation Options 41
7.	Dai	ly PM Analysis47
7	7.1.	Choose Desired Output
7	7.2.	Output Choices-Advanced 52
7	7.3.	Data Input
7	7.4.	Species Fraction Options

7.5.	Model Data Options 64
<b>8.</b> C	Dzone Analysis68
8.1.	Desired Output
8.2.	Data Input74
8.3.	Filtering/Interpolation78
8.4.	RRF/Spatial Gradient
9. V	/isibility Analysis
9.1.	Choose Desired Output
9.2.	Data Input
9.3.	Filtering
10.	The SMAT-CE Data Viewer99
10.1	. Starting the Data Viewer
10.2	2. Starting an Analysis Session100
10.3	8. Creating Data Displays
10.4	4. GIS Window 104
10.5	5. Map Window 107
10.6	5. Data Table Display110
10.7	7. Chart Display112
10.8	8. The SMAT-CE Configuration File115
10.9	0. Exporting Data from SMAT-CE116
11.	Getting Help118
12.	References

# **Table of Figures**

Figure 3-1. SMAT-CE installation window	19
Figure 4-1. SMAT-CE start page window	21
Figure 4-2. SMAT-CE About window	21
Figure 4-3. SMAT-CE development log window	22
Figure 5-1. SMAT-CE batch script	25
Figure 6-1. Annual PM Analysis initial window	27
Figure 6-2. Choose Desired Output for Annual PM <sub>2.5</sub> Analysis	
Figure 6-3. Output Choices-Advanced for Annual PM <sub>2.5</sub> Analysis	31
Figure 6-4. Data Input for Annual PM <sub>2.5</sub> Analysis	34
Figure 6-5. Species Fraction Options for Annual PM <sub>2.5</sub> Analysis	
Figure 6-6. PM2.5 Calculation Options for Annual PM <sub>2.5</sub> Analysis	41
Figure 6-7. Model Data Options for Annual PM <sub>2.5</sub> Analysis	44
Figure 6-8. Annual PM <sub>25</sub> Analysis run status	45
Figure 6-9. Annual PM Analysis Data Viewer	46
Figure 7-1. Daily PM Analysis initial window	48
Figure 7-2. Choose Desired Output for Daily PM <sub>2.5</sub> Analysis	49
Figure 7-3.Output Choices-Advanced for Daily PM <sub>2.5</sub> Analysis	
Figure 7-4. Data Input for Daily PM <sub>2.5</sub> Analysis	54
Figure 7-5. Species Fraction Options for Daily PM <sub>2.5</sub> Analysis	57
Figure 7-6. PM2.5 Calculation Options for Daily PM <sub>2.5</sub> Analysis	62
Figure 7-7. Model Data Options for Daily PM <sub>2.5</sub> Analysis	64
Figure 7-8. Daily PM25 Analysis run status	66
Figure 7-9. Daily PM Analysis Data Viewer	67
Figure 8-1. Ozone Analysis initial window	69
Figure 8-2. Choose Desired Output for Ozone Analysis	70
Figure 8-3. Data Input for Ozone Analysis	74
Figure 8-4. Filtering/Interpolation for Ozone Analysis	78
Figure 8-5. Ozone Analysis run status	84

Figure 8-6.Ozone Analysis data viewer	85
Figure 9-1. Visibility Analysis initial window	87
Figure 9-2. Choose Desired Output for Visibility Analysis	
Figure 9-3. Data Input for Visibility Analysis	92
Figure 9-4. Filtering for Visibility Analysis	95
Figure 9-5. Visibility Analysis run status	97
Figure 9-6. Visibility Analysis data viewer	98
Figure 10-1. SMAT-CE Data Viewer	99
Figure 10-2. Data Viewer window with a completed project	100
Figure 10-3. Log & Msg display window	101
Figure 10-4. Configuration & Batch File display window	102
Figure 10-5. Output files right-click menu	
Figure 10-6. Output files GIS map view	103
Figure 10-7. SMAT-CE GIS window	105
Figure 10-8. GIS map right-click menu	106
Figure 10-9. GIS window with highlighted map controls	107
Figure 10-10. SMAT-CE map window	108
Figure 10-11. Map window with right click menu	109
Figure 10-12. Map window with highlighted map controls	110
Figure 10-13. SMAT-CE Data table window	111
Figure 10-14. Data window with highlighted configuration options	112
Figure 10-15. SMAT-CE chart window	113
Figure 10-16. Chart window with highlighted configuration options	114
Figure 10-17. Viewing a SMAT-CE configuration file	115
Figure 10-18. SMAT-CE Configuration File view	116

## 1. Introduction

The Software of Model Attainment Test – Community Edition (SMAT-CE) is the next generation of Modeled Attainment Test Software (MATS). SMAT-CE implements modeled attainment tests for particulate matter (PM<sub>2.5</sub>) and ozone (O<sub>3</sub>), and performs the uniform rate of progress analysis for regional haze (visibility). The results from SMAT-CE can be used to provide scientific support for air pollution control strategies and decision making. Details of the modeled attainment tests formulated by the U.S. EPA and implemented in SMAT-CE are available in the Draft Modeling Guidance for Attainment of Air Quality Goals for Ozone, PM<sub>2.5</sub>, and Regional Haze (US EPA, 2014). This document provides instructions on how to use SMAT-CE to conduct modeled attainment tests for PM<sub>2.5</sub> and O<sub>3</sub>, and to perform the uniform rate of progress analysis for regional haze (visibility). In addition to a quick start guide, this document includes a description of the SMAT-CE interface, configuration options, and a step-by-step tutorial for using SMAT-CE with sample data from the Eastern U.S.

This manual includes the following sections:

- <u>Chapter 2</u>. Quick Start Guide to quickly get users up and running
- <u>Chapter 3</u>. SMAT-CE installation
- <u>Chapter 4</u>. SMAT-CE User Interface
- <u>Chapter 5</u>. Start new analyses and load previously saved analyses
- <u>Chapter 6</u>. Annual PM<sub>2.5</sub> attainment test details
- <u>Chapter 7</u>. Daily PM<sub>2.5</sub> attainment test details
- <u>Chapter 8</u>. O<sub>3</sub> attainment test details
- <u>Chapter 9</u>. Uniform rate of progress analysis for regional haze details
- <u>Chapter 10</u>. Using the SMAT-CE Data Viewer for analyzing results

1

• <u>Chapter 11</u>. Where to get help for using SMAT-CE

# 2. Quick Start

This chapter provides the steps required to install SMAT-CE and run it for various analyses. The Quick Start will use a pre-loaded Community Multiscale Air Quality (CMAQ) model tutorial data set to demonstrate how to run each of the SMAT-CE analysis modules. These steps will use the default SMAT-CE settings and do not describe the configuration settings for each analysis. For details of the configuration settings for the individual SMET-CE modules, refer to the User's Guide chapter for each module.

## 2.1. Install Software

Details: User's Guide Chapter 3

- Download the SMAT-CE Windows Setup.exe file from ABaCAS website (<u>http://www.abacas-dss.com/abacas/Software.aspx</u>). SMAT-CE runs on 32-bit and 64-bit Windows Operating Systems.
- Uninstall all previous versions of SMAT-CE.
- Install SMAT-CE by double-clicking the Setup.exe file. Follow the instructions to install the program to the default location on your computer.

## 2.2. Start SMAT-CE

Details: User's Guide Chapter 4

- Double click the SMAT-CE desktop icon or SMAT-CE.exe file to start the program.
- The SMAT-CE Start Page window will appear on your screen. There are five main modules available on the Start page: Process Data, Analyze/Visualize Data, Single Source Impact Analysis, BenMAP Benefit Module, and Support & Help.
- The **Process Data** module is on the left-hand panel of the SMAT-CE Start Page. This module allows users to either Load a Previous Project or start a new model attainment test for annual PM<sub>2.5</sub>, daily PM<sub>2.5</sub>, ozone, or visibility.
- The Data Viewer is available through the Analyze/Visualize Data module on

the lower left section of the SMAT-CE Start Page. The **Data Viewer** allows users to load results files (i.e., \*.proj files) from completed in SMAT-CE analyses and view these data in maps, tables, and charts; or export the data.

- The Single Source Impact Analysis is on the top of the right-hand panel of the SMAT-CE Start Page. This module is used to conduct single source PM<sub>2.5</sub> and O<sub>3</sub> air quality impact analyses using output from gridded, dispersion, or fused model data.
- The **BenMAP Benefit Module** is on the middle of the right-hand panel of the SMAT-CE Start Page. This module is used to estimate health and economic benefits that result from changes in modeled concentrations of PM<sub>2.5</sub> and O<sub>3</sub>.
- The **Support & Help** links to this User's Guide and the **About** button displays information about the current version of the software.

## 2.3. Load a Previous Project

Details: User's Guide Chapter 5

• Click Load a Previous Project on the SMAT-CE Start Page to launch a Windows Explorer window. Use this window to navigate to the directory where SMAT-CE project (\*.proj) files are saved to load a previous project.

## 2.4. Annual PM Analysis Quick Start

Details: User's Guide Chapter 6

The steps below describe how to use SMAT-CE to compute monitor RRFs and design values for the NAAQS annual  $PM_{2.5}$  standard.

- **Step 1.** Click **Annual PM Analysis** on the SMAT-CE Start Page to launch the Annual PM Analysis module window.
- <u>Step 2.</u> The Choose Desired Output window display first. This window sets the output that SMAT-CE will generate for the Annual PM Analysis. SMAT-CE can conduct a Standard Analysis (i.e., forecast point estimates at ambient monitors), output quarterly model data, and output a species fractions file.
  - Click on the <u>Choose Desired Output</u> hyperlink to display an electronic version of the User's Manual for this window.

- Type a **Project Name** in the dialog box. For example, type "Annual PM\_Tutorial" in the Project Name box.
- Standard Analysis. Leave the box checked next to "Interpolate monitor data to FRM monitor sites. Temporally-adjust." SMAT-CE will create forecasts for each monitor in the monitor file.
- Quarterly Model Data. Uncheck these options. (If checked, SMAT-CE generates quarterly model files from daily input data). SMAT-CE will run faster if it can skip the step of creating quarterly data from daily data.
- Species Fraction. Check the box next to Output species fractions file.
- Actions on run completion. Check the box next to Automatically extract all selected output files. Upon completing its calculations, SMAT-CE will extract the results into a folder with the name of your scenario.
- Click the **Next** arrow at the bottom right of the Choose Desired Output window to proceed to the next step.
- Step 3. With the advanced options in the Output Choices Advanced window, you can generate spatial fields and a variety of files useful for quality assurance. Simply review these options and then uncheck them all.
  - Click on the <u>Output Choices-Advanced</u> hyperlink to display an electronic version of the User's Manual for this window.
  - Click the **Next** arrow at the bottom right of the Output Choices-Advanced window to proceed to the next step.
- **Step 4.** The **Data Input** window sets the species and PM<sub>2.5</sub> monitor data and the model data to use for the PM attainment test. SMAT-CE calculates the ratio of the base and future year model data to calculate a relative response factor (RRF) for each PM species. SMAT-CE uses the PM<sub>2.5</sub> monitor data and interpolated species monitor data to estimate species values at each FRM site, multiplies the species values from the monitor data with the species-specific RRFs, and then estimates a future-year design value.

Use the default settings in the Data Input window.

- Click on the <u>Data Input</u> hyperlink to display an electronic version of the User's Manual for this window.
- Click the **Next** arrow at the bottom right of the Data Input window to proceed to the next step.
- **Step 5.** The **Species Fraction Options** window has several functions related to the IMPROVE-STN (species) monitor data and the (unofficial) PM<sub>2.5</sub> monitor data. These functions include identifying the years of monitor data to use, deleting any specific data values, and choosing the minimum data requirements of monitors to use in the PM analysis.

Use the default settings in the Species Fraction Options window.

- Click on the <u>Species Fraction Options</u> hyperlink to display an electronic version of the User's Manual for this window.
- Monitor Data Years. Sets the years of monitor data to use for the PM attainment test. The default is to use the three-year period 2010-2012. The default period is based on a modeling year of 2011. The start and end years should be changed to applicable time periods, depending on the base modeling year.
- Delete Specified Data Values. The default is to delete the observations specified by EPA. Valid data are flagged with a value of "0" and observations that should be deleted are flagged with values of "1" to "10". (Leave unchecked the option for the user to flag data.)
- **Minimum Data Requirements**. There are three sets of minimum data requirements for the PM attainment test:
  - 1. *Minimum number of valid days per valid quarter*. This sets the minimum number of site-days per valid quarter. The default is 11 days, which corresponds to >75% completeness for monitors on a 1 in 6-day monitoring schedule. This is the minimum number of samples that is routinely used in calculations of quarterly average concentrations.
  - 2. Minimum number of valid quarters required for valid season.

This sets the number of years of data (within the start year and end year specified) for which valid quarters for a given season are available. The default value is 1 year. If the value is set = 2, then there will need to be 2 years of valid data from quarter1 in order for quarter one to be considered complete (and the same for the other 3 quarters). 3. *Minimum number of valid seasons required for valid monitor*. This sets the number of valid seasons that are needed in order for a particular monitor's data to be considered valid. The default is 1 for IMPROVE-STN monitor data and the range is 1-4. For example, if the value is = 1, then a monitor's data will be used in the species fractions calculations if it has at least one valid season. If the value = 4, then the site must have all 4 seasons of valid data to be used. The default for PM2.5 depends on whether the data are used in point calculations (default = 4) or spatial field calculations (default = 1).

- Species Fraction Options Advanced. Sets additional advanced options for the PM attainment test. Generally speaking, the default options settings are consistent with the EPA modeling guidance. One set of options sets the interpolation weighting to use and whether the interpolation involves a maximum distance or not. The second set of options involves choices regarding ammonium, blank mass, and organic carbon.
- Click the Next arrow at the bottom right of the Species Fraction Options window to proceed to the next step.
- Step 6. The PM<sub>2.5</sub> Calculation Options window sets the particular years of monitor data to use from the input file specified in the Data Input Window Keep the default settings:
  - PM<sub>2.5</sub> Monitor Data Years. Start Year = 2009 and End Year = 2013
  - o Official vs. Custom Values. Set to "Official Design Values"
  - Valid FRM Monitors. Keep the minimum number of design values equal to the default value of 1, and do not specify any particular design

values for inclusion in the calculations.

- **NH4 Future Calculation**. Sets how to forecast NH4 values. Use the default approach, which is to use baseline DON values.
- $\circ$  Click the **Next** arrow at the bottom right of the PM<sub>2.5</sub> Calculation Options window to proceed to the next step.
- **Step 7.** The **Model Data Options** window sets how to perform temporal adjustments on the monitoring data. This option sets how many model grid cells to use in the calculation of RRFs for point estimates and for spatial estimates. Use the default option: 3x3 set of grid cells. Note that for PM analyses, SMAT-CE calculates mean concentrations across the grid cell array (as compared to maximum concentrations used for ozone analyses).

Use the default settings in the Model Data Options window.

- Click on the <u>Model Data Options</u> hyperlink to display an electronic version of the User's Manual for this window.
- Click the Next arrow at the bottom right of the Model Data Options window to complete the Annual PM Analysis configuration and run the attainment test.
- Click Save & Run Project in the pop-up window. Click Save to create a project (\*.proj) file for this tutorial exercise. The Filename should reflect the text entered in the Project Name box from Step 2 above.

The Annual PM Analysis will complete after a few minutes and the SMAT-CE Data Viewer will present the results of the analysis. See <u>Chapter 10</u> for details on how to use the Data Viewer to analyze the results.

## 2.5. Daily PM Analysis Quick Start

Details: User's Guide Chapter 7

The steps below describe how to use SMAT-CE to compute monitor RRFs and design values for the NAAQS daily PM<sub>2.5</sub> standard.

**Step 1.** Click **Daily PM Analysis** on the SMAT-CE Start Page to launch the Daily PM Analysis module window.

- Step 2. The Choose Desired Output window display first. This window sets the output that SMAT-CE will generate for the Daily PM Analysis. SMAT-CE can conduct a Standard Analysis (i.e., forecast point estimates at ambient monitors), output quarterly model data, and output a species fractions file.
  - Click on the <u>Choose Desired Output</u> hyperlink to display an electronic version of the User's Manual for this window.
  - Type a **Project Name** in the dialog box. For example, type "Daily\_PM\_Tutorial" in the Project Name box.
  - Standard Analysis. Leave the box checked next to "Interpolate monitor data to FRM monitor sites. Temporally-adjust." SMAT-CE will create forecasts for each monitor in the monitor file.
  - **Quarterly Peak Model Data**. Check this option. SMAT-CE will generate quarterly model files from daily input data.
  - Species Fraction. Check the box next to Output species fractions file.
  - Actions on run completion. Check the box next to Automatically extract all selected output files. Upon completing its calculations, SMAT-CE will extract the results into a folder with the name of your scenario.
  - Click the **Next** arrow at the bottom right of the Choose Desired Output window to proceed to the next step.
- Step 3. With the advanced options in the Output Choices Advanced window, you can generate spatial fields and a variety of files useful for quality assurance. Simply review these options and then uncheck them all.
  - Click on the <u>Output Choices-Advanced</u> hyperlink to display an electronic version of the User's Manual for this window.
  - Click the **Next** arrow at the bottom right of the Output Choices-Advanced window to proceed to the next step.
- **Step 4.** The **Data Input** window sets the species and PM<sub>2.5</sub> monitor data and the model data to use for the PM attainment test. SMAT-CE calculates the ratio of the base and future year model data to calculate a relative response factor (RRF)

for each PM species. SMAT-CE uses the  $PM_{2.5}$  monitor data and interpolated species monitor data to estimate species values at each FRM site, multiplies the species values from the monitor data with the species-specific RRFs, and then estimates a future-year design value.

Use the default settings in the Data Input window.

- Click on the <u>Data Input</u> hyperlink to display an electronic version of the User's Manual for this window.
- Click the **Next** arrow at the bottom right of the Data Input window to proceed to the next step.
- **Step 5.** The **Species Fraction Options** window has several functions related to the IMPROVE-STN (species) monitor data and the (unofficial) PM<sub>2.5</sub> monitor data. These functions include identifying the years of monitor data to use, deleting any specific data values, and choosing the minimum data requirements of monitors to use in the PM analysis.

Use the default settings in the Species Fraction Options window.

- Click on the <u>Species Fraction Options</u> hyperlink to display an electronic version of the User's Manual for this window.
- Monitor Data Years. Sets the years of monitor data to use for the PM attainment test. The default is to use the three-year period 2010-2012. The default period is based on a modeling year of 2011. The start and end years should be changed to applicable time periods, depending on the base modeling year.
- Delete Specified Data Values. The default is to delete the observations specified by EPA. Valid data are flagged with a value of "0" and observations that should be deleted are flagged with values of "1" to "10". (Leave unchecked the option for the user to flag data.)
- **Minimum Data Requirements**. There are three sets of minimum data requirements for the PM attainment test:

1. *Minimum number of valid days per valid quarter*. This sets the minimum number of site-days per valid quarter. The default is 11

days, which corresponds to >75% completeness for monitors on a 1 in 6-day monitoring schedule. This is the minimum number of samples that is routinely used in calculations of quarterly average concentrations.

Minimum number of valid quarters required for valid season.
 This sets the number of years of data (within the start year and end year specified) for which valid quarters for a given season are available. The default value is 1 year. If the value is set = 2, then there will need to be 2 years of valid data from quarter1 in order for quarter one to be considered complete (and the same for the other 3 quarters).
 Minimum number of valid seasons required for valid monitor.

This sets the number of valid seasons that are needed in order for a particular monitor's data to be considered valid. The default is 1 for IMPROVE-STN monitor data and the range is 1-4. For example, if the value is = 1, then a monitor's data will be used in the species fractions calculations if it has at least one valid season. If the value = 4, then the site must have all 4 seasons of valid data to be used. The default for PM2.5 depends on whether the data are used in point calculations (default = 4) or spatial field calculations (default = 1).

- Species Fraction Options Advanced. Sets additional advanced options for the PM attainment test. Generally speaking, the default options settings are consistent with the EPA modeling guidance. One set of options sets the interpolation weighting to use and whether the interpolation involves a maximum distance or not. The second set of options involves choices regarding ammonium, blank mass, and organic carbon.
- Click the Next arrow at the bottom right of the Species Fraction Options window to proceed to the next step.
- <u>Step 6.</u> The PM<sub>2.5</sub> Calculation Options window sets the particular years of monitor data to use from the input file specified in the Data Input Window

Keep the default settings:

- **PM2.5 Monitor Data Years**. Start Year = 2009 and End Year = 2013
- Valid FRM Monitors. Keep the minimum number of design values equal to the default value of 1, and do not specify any particular design values for inclusion in the calculations.
- **NH4 Future Calculation**. Sets how to forecast NH4 values. Use the default approach, which is to use baseline DON values.
- Click the **Next** arrow at the bottom right of the PM<sub>2.5</sub> Calculation Options window to proceed to the next step.
- Step 7. The Model Data Options window sets how to perform temporal adjustments on the monitoring data. This option sets how many model grid cells to use in the calculation of RRFs for point estimates and for spatial estimates. Use the default option: 3x3 set of grid cells. Note that for PM analyses, SMAT-CE calculates mean concentrations across the grid cell array (as compared to maximum concentrations used for ozone analyses).

Use the default settings in the Model Data Options window.

- Click on the <u>Model Data Options</u> hyperlink to display an electronic version of the User's Manual for this window.
- Temporal Adjustment at Monitor. Sets how many model grid cells to use in the calculation of RRFs for point and spatial estimates. Use the default option for both: 1x1 set of grid cells. Note that for PM analyses, SMAT-CE should be set to calculate mean concentrations across the grid cell array.
- Advanced Options: RRF Model Values Used. Sets which monitor data to use to characterize peak values (e.g., top 10 percent of daily model days).
- Click the Next arrow at the bottom right of the Model Data Options window to complete the Daily PM Analysis configuration and run the attainment test.
- o Click Save & Run Project in the pop-up window. Click Save to create

a project (\*.proj) file for this tutorial exercise. The Filename should reflect the text entered in the Project Name box from Step 2 above.

The Daily PM Analysis will complete after a few minutes and the SMAT-CE Data Viewer will present the results of the analysis. See <u>Chapter 10</u> for details on how to use the Data Viewer to analyze the results.

#### 2.6. Ozone Analysis Quick Start

Details: User's Guide Chapter 8

The steps below describe how to use SMAT-CE to compute monitor RRFs and design values for the NAAQS O<sub>3</sub> standard.

- **Step 1.** Click **Ozone Analysis** on the SMAT-CE Start Page to launch the Ozone Analysis module window.
- **Step 2.** The **Desired Output** window displays first. This window sets the ozone analysis output that SMAT-CE will generate. SMAT-CE can output the quarterly model data used in the calculations, use different approaches to interpolate the monitor data, and selectively output data for all of the design value periods.
  - Click on the <u>Desired Output</u> hyperlink to display an electronic version of the User's Manual for this window.
  - Type a Project Name in the dialog box. For example, type "O3\_Tutorial" in the Project Name box.
  - Point Estimates. Leave the box checked next to "Forecast ozone design values at monitors." SMAT-CE will create forecasts for each monitor in the monitor file.
  - **Quarterly Model Data**. Check this option. SMAT-CE will generate quarterly model files from daily input data.
  - **Spatial Field**. Leave unchecked. If checked, SMAT-CE would interpolate from the monitor data to calculate design values for the entire modeling domain.
  - o Actions on run completion. Check the box next to Automatically

extract all selected output files. Upon completing its calculations, SMAT-CE will extract the results into a folder with the name of your scenario.

- Click the **Next** arrow at the bottom right of the Desired Output window to proceed to the next step.
- **Step 3.** The **Data Input** window sets the monitor and model data to use for the O<sub>3</sub> attainment test. SMAT-CE calculates the ratio of the base and future year model data to calculate a relative response factor (RRF) for O<sub>3</sub>. SMAT-CE multiplies the O<sub>3</sub> monitor data by the RRFs, and then estimates a future-year design value.

SMAT-CE includes options to use model data in different ways when calculating forecasts at each monitor. Options include selecting results from the single grid cell that contains the monitor or selecting a grid cell array of 3x3, 5x5, or 7x7 model cells around each monitor. The tutorial dataset contained in SMAT-CE is at 12km resolution and should use a 3x3 grid cell array. The default for ozone analysis is to choose the maximum daily concentration in the array for the RRF calculation

Use the default settings in the Data Input window.

- Click on the <u>Data Input</u> hyperlink to display an electronic version of the User's Manual for this window.
- Click the **Next** arrow at the bottom right of the Data Input window to proceed to the next step.
- **Step 5.** The **Filtering/Interpolation** window has several functions related to interpolating monitoring data. These functions include identifying the years of monitor data to use in the RRF calculations, choosing the particular monitors to use in the analysis, and (when calculating spatial fields) specifying the interpolation method.

Use the default settings in the Filtering/Interpolation window.

Click on the <u>Filtering/Interpolation</u> hyperlink to display an electronic version of the User's Manual for this window.

- Choose Ozone Design Values. Sets the years of monitor data to use for the O<sub>3</sub> attainment test. The default is to use a 5-year period (covering three 3-year design value periods) centered on the modeling year. The default modeling year in SMAT-CE is 2011, so the Start Year is 2009-2011 and the End Year is 2011-2013. The start and end years should be changed to applicable time periods, depending on the base modeling year.
- Valid Ozone Monitors. Identifies the "valid" monitors to include in the analysis. The default settings are to use monitors with at least one valid design value period and that are within 25 kilometers of a model grid cell. SMAT-CE includes a setting to force that a particular design value be available (e.g., 2005-2007) for the data to be valid. The default is to require none in particular.
- Default Interpolation Method. Sets the method to combine the design values from different monitors into a single estimated design value. This option is only used when generating estimates for a Spatial Field. Since we are only generating Point Estimates, this set of options is not active in SMAT-CE.
- Click the Next arrow at the bottom right of the Filtering/Interpolation
   Options window to proceed to the next step.
- Step 6. The RRF/Spatial Gradient window sets the days to be used in the RRF calculation and the model values to use in the calculation of a Spatial Field. Keep the default settings:
  - RRF Setup. Sets the days to be used in the calculation of RRFs. By default, SMAT will select the top 10 highest days for the calculation. Each monitor must meet the minimum allowable threshold value and the minimum number of days at or above minimum allowable threshold value specified in this screen, or it is dropped from the calculation. The default values are 60 and 5, respectively.
  - Spatial Gradient Setup. Sets the model values that will be used in the

calculation of a Spatial Field. Since we are only generating Point Estimates, this set of options is not active in SMAT-CE.

- Click the Next arrow at the bottom right of the RRF/Spatial Gradient
   Options window to complete the Ozone Analysis configuration and run the attainment test.
- Click Save & Run Project in the pop-up window. Click Save to create a project (\*.proj) file for this tutorial exercise. The Filename should reflect the text entered in the Project Name box from Step 2 above.

The Ozone Analysis will complete after a few seconds and the SMAT-CE Data Viewer will present the results of the analysis. See <u>Chapter 10</u> for details on how to use the Data Viewer to analyze the results.

## 2.7. Visibility Analysis Quick Start

Details: User's Guide Chapter 9

The steps below describe how to use SMAT-CE to forecast visibility at U.S. Class I Areas.

- **Step 1.** Click **Visibility Analysis** on the SMAT-CE Start Page to launch the Visibility Analysis module window.
- **Step 2.** The **Choose Desired Output** window displays first. This window sets the visibility analysis output that SMAT-CE will generate.
  - Click on the <u>Choose Desired Output</u> hyperlink to display an electronic version of the User's Manual for this window.
  - Type a **Project Name** in the dialog box. For example, type "Visibility\_Tutorial" in the Project Name box.
  - Forecast. Leave the box checked next to "Temporally adjust visibility levels at Class I Areas" SMAT-CE will create forecasts for each Class I Area in the modeling domain. SMAT-CE includes two IMPROVE equations for calculating visibility from speciated PM<sub>2.5</sub>. Use the new version of the equation.
  - o Use model grid cell at monitor. A single IMPROVE monitor is

associated with each Class I Area. SMAT-CE multiplies the monitor value by an RRF, which is the modeled future-year visibility divided the modeled current-year visibility, to calculate future year visibility in the Class I Area. SMAT-CE provides the option to use either the model values in the grid cell at the IMPROVE monitor or to use the model values in the grid cell at the Class I Area centroid. Select the default option of using model values in the grid cell at the grid cell at the monitor.

- Actions on run completion. Check the box next to Automatically extract all selected output files to direct SMAT-CE to export .CSV files with the results of this analysis.
- Click the **Next** arrow at the bottom right of the Choose Desired Output window to proceed to the next step.
- **Step 3.** The **Data Input** window sets the monitor and model data to use in the visibility forecasts. SMAT-CE calculates the ratio of the future to base year model data to calculate RRFs for the 20% best (B20) and 20% worst (W20) visibility days of the year. SMAT-CE then multiplies the calculated observed visibility at the monitor B20 days by the B20 RRF to calculate a future-year estimate for visibility on the best visibility days. SMAT-CE performs an analogous calculation for the worst visibility days.

SMAT-CE installs with IMPROVE visibility monitor values from 2000 through 2017. It also comes loaded with an example model output dataset for visibility for 2011 and 2017.

SMAT-CE includes options to use model data in different ways when calculating forecasts at each Class I Area monitor. Options include selecting results from the single grid cell that contains the monitor or selecting a grid cell array of 3x3, 5x5, or 7x7 model cells around each monitor. The tutorial dataset contained in SMAT-CE is at 12km resolution and should use a 3x3 grid cell array.

Use the default settings in the Data Input window.

• Click on the **Data Input** hyperlink to display an electronic version of

the User's Manual for this window.

- Click the **Next** arrow at the bottom right of the Data Input window to proceed to the next step.
- **Step 5.** The **Filtering** window has several functions related to interpolating monitoring data. These functions include identifying the years of monitor data to use in the RRF calculations, choosing the particular monitors to use in the analysis, and (when calculating spatial fields) specifying the interpolation method.

Use the default settings in the Filtering window.

- Click on the <u>Filtering</u> hyperlink to display an electronic version of the User's Manual for this window.
- Choose Visibility Data Years. Sets the years of monitor data to use for the visibility forecast. The default is to use a 5-year period (covering three 3-year design value periods) centered on the modeling year. The default modeling year in SMAT-CE is 2011, so the Start Monitor Year is 2009 and the End Monitor Year is 2013. The Base Model Year is 2011.
- Valid Visibility Monitors. Identifies the "valid" monitors to include in the analysis. The default setting, which is consistent with the EPA Modeling Guidance, is to exclude monitors with less than three years of data.
- Click the Next arrow at the bottom right of the Filtering Options window to complete the Visibility Analysis configuration and run the attainment test.
- Click Save & Run Project in the pop-up window. Click Save to create a project (\*.proj) file for this tutorial exercise. The Filename should reflect the text entered in the Project Name box from Step 2 above.

The Visibility Analysis will complete after a few minutes and the SMAT-CE Data Viewer will present the results of the analysis. See <u>Chapter 10</u> for details on how to use the Data Viewer to analyze the results.

# **3. SMAT-CE Installation**

This section of the SMAT-CE User's Manual describes how to install the software on a PC running Windows; SMAT-CE is currently not available for other operating systems. Before installing SMAT-CE, uninstall any previous versions of the software. See Table 3-1 for a description of the recommended PC configuration for running SMAT-CE.

System	Best	Minimum	
Component	Recommendation	Recommendation	
СРИ	Intel, Quad-Core, 3 GHz	Intel, Duo-Core, 1.6 GHz	
Memory (RAM)	6 Gb	2 Gb	
Free Disk Space	10 Gb	10 Gb	
Operating System	64-bit Windows 7	32-Bit Windows XP	
Screen Resolution	1024 x 768 pixels		
Font Size	normal		

 Table 3-1. SMAT-CE computing system recommendations.

After downloading SMAT-CE from ABaCAS website (<u>http://www.abacas-dss.com/abacas/Software.aspx</u>), double click on the SMAT-CE Setup.exe binary file to initiate the SMAT-CE – InstallShield Wizard (Figure 3-1), click the next button, and follow the tips in the window until the installation is finished.



Figure 3-1. SMAT-CE installation window



A successful installation will result in a SMAT-CE desktop icon:

# 4. SMAT-CE Start Page

Double click the SMAT-CE desktop icon to start the program. The SMAT-CE Start Page (Figure 4-1) will appear on your screen. This window provides access to the following SMAT-CE modules:

- The **Process Data** module is the interface for loading air quality data into the software for conducting attainment tests. Users can select data from a project that had been loaded previously, or load new data for conducting PM, ozone, or visibility analysis. The Annual PM, Daily PM, Ozone, and Visibility Analysis options each open new windows to configure and run attainment tests for the applicable pollutant.
- The Analyze/Visualize Data module links to the SMAT-CE Data Viewer. The Data Viewer provides an interface to load previously generated results files (\*.proj files), and view the data as maps, tables and charts; or to export the results as a text file.
- The **Support & Help** module links to the SMAT-CE User's Guide and information about the current version of the software. The About option under this module (Figure 4-2) provides the software version number, a suggested citation for SMAT-CE, and a Development Log (Figure 4-3) listing release notes for current and previous versions of the software.

Additional details about configuring and running the different SMAT-CE processing and analysis modules are included in the following sections.



Figure 4-1. SMAT-CE start page window



Figure 4-2. SMAT-CE About window

	lopment Lo	-	
File	Print Ex	t	
		SMAT-CE Development Log	[
Release	Version	SMAT-CE 0.60	
Release	Date	2016.9.14	
Main Im	proveme	its:	
<ol> <li>Intergrade downscaler method into BenMap Ozone analysis.</li> <li>Change the Spatial field output files names of BenMAP module:</li> </ol>			
	i ""Annı	ial (Quarterly) PM25 spatial field" to "Annual (Quarterly) PM25 spatial f	field (VNA)".
ii ."Grad Adj Annual (Quarterly) PM25 spatial field" to "Annual (Quarterly) PM25 spatial f			5 spatial field
(eVNA)".			
iii . "Downscaler Annual (Quarterly) PM25 spatial field" to "Annual (Quarterly) PM25 spat			
	(Downsc	aler)".	
Release	Version	I SMAT-CE 0.59	
Release Date 2016.9.5			
Main Im	provemer	its:	
3.	Intergra	de downscaler method into BenMap Annual PM analysis.	
4. Add a "select all" check box in the data detail under the chart tab of the data viewer.			ewer.
5. Add a new option to plot the source location on the 2D spatial map window.			
6. Add a new feature to copy the image to the clipboard after right clicking the 2D map.			

Figure 4-3. SMAT-CE development log window

## 5. Running SMAT-CE

Using SMAT-CE to conduct model attainment tests begins with the Process Data module on the Start Page. From this module, users may load a previous project or conduct new model attainment test for Annual PM, Daily PM, Ozone, and Visibility. One of the key features of SMAT-CE is the project (\*.proj) file. This file stores configuration information from a previous SMAT-CE analysis to facilitate recreating or continuing the analysis at a later time. Users may also choose to modify an existing project file to generate a new set of results, avoiding the need to rerun an entire SMAT-CE analysis from the beginning.

To conduct an attainment test with SMAT-CE, either select **Load Previous Project** or one of the pollutant Analysis options in the **Process Data** module on the Start Page.

#### 5.1. Load Previous SMAT-CE Project

SMAT-CE projects that were run previously may be accessed through the **Load Previous Project** menu on the Start Page. When this option is selected a Windows file explorer opens to the default directory (C:/Users/[user ID]/My Documents/My SMAT-CE Files/Result/Project) containing SMAT-CE project files. It is recommended that all project files be saved to this directory. Upon selecting one of the existing projects, SMAT-CE will open to the Analysis module (i.e., Annual PM, Daily PM, Ozone, or Visibility) associated with the project.

Once a previous project is loaded, you will begin from the point where the loaded project was last saved. Refer to the following relevant sections for the details of how to continue the analysis of a previous project.

#### 5.2. New SMAT-CE Analysis

A new SMAT-CE attainment test is initiated by selecting one of the four Analysis options under the Process Data section on the Start Page:

- <u>Annual PM Analysis (Chapter 6)</u>: SMAT-CE will forecast annual PM<sub>2.5</sub> design values at monitor locations. The software will also optionally calculate quarterly model data files and a species fractions file.
- Daily PM Analysis (Chapter 7): SMAT-CE will forecast daily PM<sub>2.5</sub> design

values at monitor locations. The software will also optionally calculate quarterly model data files and a species fractions file.

- Ozone Analysis (Chapter 8): SMAT-CE will forecast ozone design values at explicit (point) monitor locations. Options are also available for a variety of approaches to calculate design values for a spatial field, such as a matrix of model grid cell surrounding each monitor.
- <u>Visibility Analysis (Chapter 9)</u>: SMAT-CE will forecast visibility at specific point locations (centroid) in Class I Areas. Different versions of the IMPROVE light extinction algorithm may be selected along with the option to use either model data at the monitor linked to each Class I Area or model data closest to the Class I Area centroid.
- <u>Analyze/Visualize Data (Chapter 10):</u> The Data Viewer provides a graphical and tabular interface to the input/output data from the attainment test analyses produced by SMAT-CE.

## 5.3. Running SMAT-CE in Batch Mode

<u>SMAT-CE Configuration Files</u> can be concatenated in a Windows batch script to automatically run multiple SMAT-CE analyses in sequence. A SMAT-CE Configuration File stores the configuration options for one SMAT Analysis (i.e., Annual PM, Daily PM, Ozone, or Visibility). Multiple Configuration Files can be used to define a suite of analyses to run at once through a batch script. The Configuration Files are created and saved automatically when setting up an attainment test analysis in SMAT-CE. They can be edited either through the Data Viewer or using a text editor outside of SMAT-Ce.

An example batch script (batsmat.bat) and configuration files (\*.cfg) are included in "Program Files (x86)\SMAT-CE\BatchExample\Batch64". The script "batchsmat.bat" includes a list of configuration files for the four types of analyses supported by SMAT-CE (Figure 5-1). New configuration files can be added to the batch script to run additional analyses.

🕞 batchsmat.txt - Notepad	
File Edit Format View Help	
start /wait SMAT.exe "C:\program files(x86)\SMAT CE\Output\annual analysis.cfg" start /wait SMAT.exe "C:\program files(x86)\SMAT CE\Output\daily analysis.cfg" start /wait SMAT.exe "C:\program files(x86)\SMAT CE\Output\ozone analysis.cfg" start /wait SMAT.exe "C:\program files(x86)\SMAT CE\Output\visibility analysis.cfg	3
	×

#### Figure 5-1. SMAT-CE batch script

After editing the SMAT-CE batch script, save it and double click on the file to run the analyses. A Windows command window will display the status of the different SMAT-CE analysis runs. SMAT-CE will start and run in the background and when the runs are complete, the command window will shut down automatically. The results of the SMAT-CE batch runs are output to the My Documents\My SMAT-CE Files\Result\Batchjob directory. The \*.proj files from these runs can be loaded into the <u>SMAT-CE Data Viewer</u> to probe the results from these runs.

Details of the SMAT-CE Analysis options are provided in the following Chapters. A Continental U.S. (CONUS) example project is used in each of the analysis chapters to demonstrate the options available for each attainment test.

# 6. Annual PM Analysis

SMAT-CE can forecast annual design values at PM<sub>2.5</sub> monitor locations -- these forecasts are referred to as Point Estimates. SMAT-CE can also use a variety of approaches to calculate design values for a Spatial Field. A Spatial Field refers to a set of values comprising calculations for each grid cell in a modeling domain from Eulerian grid models such as CMAQ and CAMx.

The Annual PM Design Value Analysis in SMAT-CE is organized into seven steps. The steps include the input/output and configuration options for computing ozone design values. The following configuration steps correspond to different SMAT-CE windows and are described in detail in this chapter:

- **Output Choice**. Select whether to run the Standard Analysis, and whether to output a species fractions file and/or quarterly model data.
- **Output Choice Advanced**. Configure miscellaneous Point Estimate output files for quality assurance of the PM design value calculations.
- **<u>Data Input</u>**. Specify the species monitoring data, species fractions file, PM<sub>2.5</sub> ambient monitoring data, and the modeling data to use for the design value calculations.
- <u>Species Fractions Calculation Options</u>. Select the years of daily STN-IMPROVE and FRM monitoring data and identify valid monitors. Define data filtering specifications.
- <u>Species Fractions Calculation Options Advanced</u>. Select the method to identify peak monitor values. Choose interpolation options for PM<sub>2.5</sub> and species monitoring data. Choose assumptions for the ammonium calculation, default blank mass, and organic carbon.
- <u>PM2.5 Calculation Options FRM Monitor Data</u>. Select the years of quarterly FRM monitoring data and identify valid monitors. Select the approach for calculating future year ammonium.
- <u>Model Data Options</u>. Specify the maximum distance of monitors from modeling domain. Choose method to identify peak model values. Specify which

File * Analysis * Data Viewer Expand Viewer Single Source Impa	ct Analysis * Start Page
🖗 Annual PM Analysis 🗾 🛃	
Choose Desired Output     Output Choices-Advanced     Data Input     Species Fraction Options	O Log/Msg
PM2.5 Calculation Options Model Data Options	Name Running Messages
Choose Desired Output	
Project Name:	
Standard Analysis	
$\overline{\ensuremath{\mathbb V}}$ Interpolate monitor data to FRM monitor sites. Temporally-adjust.	
Quarterly Model Data	
Output quarterly average model data file.	=
Output used quarterly average model data file.	
Species Fraction	
☑ Output species fractions file.	
Actions on run completion	
☑ Automatically extract all selected output files. Back Next	
Clear Save Project & Run Save Project	

model grid cells will be used when calculating RRFs at monitor locations.

Figure 6-1. Annual PM Analysis initial window

To conduct an attainment test for the annual  $PM_{2.5}$  NAAQS, select **Annual PM Analysis** from the Process Data module on the SMAT-CE Start Page. Figure 6-1 shows the initial window that is displayed when Annual PM Analysis is selected. The box in the upper left of the window (highlighted in red in Figure 6-1) lists the configuration steps of the Annual PM Analysis. Each step listed in this box has a different set of configuration options that are displayed in the Annual PM Analysis window. Once each step is successfully configured, the yellow buttons in the box will change from yellow to green. In general, the configuration steps must be followed in order, from top to bottom, as they are listed in the box. Previously completed steps may be accessed and modified by double clicking on the step name in the box. Once the configuration for a step is complete, you may move to the next step by either clicking on it or by selecting the Next button (shown in the blue box in Figure 6-1).

A previous project may be loaded or a new project may be initiated at any time in the Annual PM Analysis window by selecting one of the icons to the right of the "Annual PM Analysis" text above the red box in Figure 6-1. Each of the Annual PM Analysis configuration steps are described in the following sections.

File * Analysis * Data Viewer Expand Viewer Single Source Impact A	Analysis * Start Page				
🕞 Annual PM Analysis 🗾 🛃					
Choose Desired Output     Output Choices-Advanced     Output Choices-Advanced     Spacies Fraction Options     PM2.5 Calculation Options	Log/Msg Name Running Messages				
Hodel Data Options	Name Running Messages				
Choose Desired Output  Project Name:					
Standard Analysis					
☑ Interpolate monitor data to FRM monitor sites. Temporally-adjust.					
Quarterly Model Data					
☑ Output quarterly average model data file.					
☑ Output used quarterly average model data file.					
Species Fraction					
☑ Output species fractions file.					
Actions on run completion					
☑ Automatically extract all selected output files.					
Back Next Clear Save Project & Run Save Project	۲				

#### 6.1. Choose Desired Output

Figure 6-2. Choose Desired Output for Annual PM2.5 Analysis

**Choose Desired Output** is the first configuration step that is displayed when the Annual PM Analysis module is selected (Figure 6-2). The blue hyperlinked text in this window brings up the documentation for this configuration step. The settings in this step include:

#### **Project Name**

Text string to identify this analysis and set the name of the project file

#### **Standard Analysis**

Since most Federal Reference Method (FRM) PM<sub>2.5</sub> monitoring sites do not have collocated chemical speciation monitors, spatial interpolation is used to estimate species data at FRM PM<sub>2.5</sub> monitor locations. SMAT-CE provides options to use different methods for spatially interpolating chemical speciation information to the FRM monitors. These options are available from the **Output Choices-Advanced** configuration window. Complete details of the Standard Analysis approach, including

the formula used to calculate species concentrations, are available in the U.S. EPA Draft Modeling Guidance for Attainment of Air Quality Goals for Ozone, PM<sub>2.5</sub>, and Regional Haze (U.S. EPA, 2014) and in Section 5.1.2 of the MATS User's Manual (Abt, 2014).

Most SMAT-CE users will run the standard analysis and it is checked by default.

#### **Quarterly Model Data**

Directs SMAT-CE to calculate and output quarterly averaged modeled PM<sub>2.5</sub> data from daily model data input to the system. SMAT-CE requires two types of data input: ambient monitor data and gridded model output data. For the annual PM<sub>2.5</sub> calculations, SMAT-CE will accept either SMAT-CE formatted daily average gridded model files or quarterly average files. If daily average model files are used as inputs, SMAT-CE will calculate quarterly averages from the daily averages and optionally output the quarterly average concentrations into text files (CSV files). The quarterly average text files can then be re-used in subsequent SMAT-CE analyses. Quarterly average input files are smaller and run faster than daily average files.

There are two options to output quarterly average model concentration CSV files:

- Selecting the **Output quarterly average model data file** box creates quarterly average CSV for all grid cells in the modeling domain. SMAT-CE will create one baseline year file and one future year file. This will create relatively large files, but they will still be ~90 times smaller than daily average files (assuming a full year of model data).
- Selecting the **Output used quarterly average model data file** causes SMAT-CE to output only the grid cells that are subsequently used in the particular SMAT-CE configuration. For example, if SMAT-CE calculates future year design values at 20 FRM sites using a 1 X 1 grid array, then SMAT-CE will output base and future model values for only 20 grid cells (assuming each monitor is in a unique grid cell). The advantage of these files is that they are extremely small. But if subsequent SMAT-CE runs use a different set of monitors or grid arrays, then the files may not contain all of the necessary data to complete the analysis. This option is recommended as a QA tool to examine

the grid cells and the model concentrations that SMAT-CE is using in the analysis.

Additional details of the Quarterly Model Data option are available in Section 5.1.3 of the SMAT-CE User's Manual (Abt, 2014).

#### **Species Fractions**

After calculating the ambient level of SO<sub>4</sub>, NO<sub>3</sub>, OC, EC, PBW, NH<sub>4</sub>, and crustal, SMAT-CE then divides these ambient levels by the non-blank mass of PM<sub>2.5</sub> to calculate species fractions. Select this box to output a text file of species fractions at each FRM monitor. This species fraction file can be re-used in MATS as an input file. The species fraction file can be useful for several reasons. One, using a species fraction file saves time because MATS won't have to interpolate species data and calculate fractions each time it is run. Two, it can provide consistency between MATS runs by ensuring that the same species fractions are used each time. And for the same reason, the species fraction file can be used interchangeably between different users to ensure that multiple groups are using the same species fractions (if that is a goal). And finally, the fractions file can serve as a template for creating a custom species fractions file using whatever data and techniques (e.g. alternative interpolation techniques) are desired by any particular user. Additional details of the Species Fractions calculation are available in Section 5.1.4 of the MATS User's Manual (Abt, 2014).

#### Actions on run completion

Checking the "Automatically extract all selected output files" box will export CSV files of all selected output to a separate folder named with the Project Name in the SMAT "\Result\Output" folder. The results may also be exported later from the **Data Viewer**.

#### 6.1.1. Run the Eastern U.S. Example

The default settings for these options, and the configuration to use for the Eastern U.S. example project, is to check all of the boxes in the SMAT-CE **Choose Desired Output** window. After setting a Project Name and selecting all of the boxes in the window either click Next or double-click the **Output Choices-Advanced** button in the upper left-hand panel of **Annual PM Analysis** window. The icon next to **Choose Desired Output** will turn from yellow to green, indicating that this step is complete.
# 6.2. Output Choices-Advanced



## Figure 6-3. Output Choices-Advanced for Annual PM2.5 Analysis

The **Output Choices – Advanced** configuration step provides detailed control over the calculations, output, and quality assurance fields used by SMAT-CE (Figure 6-3). The blue hyperlinked text in this window brings up the documentation for this configuration step. The settings in this step include the following.

## **Spatial Field Estimates**

This option provides PM<sub>2.5</sub> forecasts for each grid cell in the modeling domain (e.g., CMAQ 36 km). **The Interpolate FRM & speciation monitor data to spatial field. Temporally-adjust (VNA)** option calculates interpolated spatial fields that are temporally adjusted using the Voronoi Neighbor Averaging (VNA) technique. This option creates gridded spatial fields of future year PM<sub>2.5</sub> data. To create PM<sub>2.5</sub> spatial fields, SMAT-CE interpolates both speciation data and PM<sub>2.5</sub> data (FRM and IMPROVE).

The Interpolate gradient-adjusted FRM & speciation monitor data to spatial field. Temporally-adjust (eVNA) option calculates interpolated spatial fields that are temporally adjusted and gradient adjusted. Check this option to create gridded spatial fields of gradient adjusted future year  $PM_{2.5}$  data. To create  $PM_{2.5}$  spatial fields, SMAT-CE interpolates both gradient adjusted speciation data and  $PM_{2.5}$  data (FRM and IMPROVE). This option creates the recommended spatial fields for the "Unmonitored Area Analysis" from the  $PM_{2.5}$  modeling guidance.

The configuration options in this step provide a variety of output files that can be used in the quality assurance of the SMAT-CE calculations. The options are organized under the "Miscellaneous Outputs" heading and include the following.

#### **Quarterly Average Files**

Augments the SMAT-CE default of outputting annual average results for all analyses (point, spatial fields). Checking any one of these boxes will direct SMAT-CE to output more detailed quarterly average data, which are the basis of all of the SMAT-CE annual PM<sub>2.5</sub> calculations.

#### High County Sites

Augments the SMAT-CE default of outputting the point results for all FRM sites. Checking this box will also produce a file that contains the single highest monitor in each county, based on the highest future year value. This dataset is a subset of the all sites file.

#### **Species Fractions Spatial Field**

Produces the same result as the species fraction file created from the **Standard Analysis** except it outputs the species fractions file created from a spatial field. The file will contain species fraction data for each quarter for each grid cell.

### **Quarterly Average Speciated Monitors**

Directs SMAT-CE to produce a file with the raw quarterly average speciated data that were used to interpolate species fractions to the FRM monitors. These data are derived from the "species for fractions" input file.

#### **Design Value Periods**

Directs SMAT-CE to produce a file with the standard SMAT-CE output for each design period within the period covered by the analysis. By default, SMAT-CE outputs one set of files covering the entire analysis period specified by the user. The outputs represent the averages of the values for each 3-year design value period. If the "Output design value periods" option is checked, SMAT-CE will produce discrete outputs for each design value period. The output files will be the same as a standard analysis, but with "Period 1", "Period 2", etc., attached at the end of the name. Selecting this option will increase the SMAT-CE run time.

# Neighbor files

Directs SMAT-CE to produce files of "nearest neighbor" data for the VNA interpolation scheme. The data include the distance to neighbor monitors and weights used to do the interpolations. There is information for each FRM monitor (for point analyses) or each grid cell (for spatial fields) for each quarter and for each species.

Additional details of the Output Choices – Advanced options, including the formats of the output files from this step, are available in Section 5.2 of the MATS User's Manual (Abt, 2014).

# 6.2.1. Run the Eastern U.S. Example

Use the default settings for these options for the Eastern U.S. example project. Either click Next or double-click the **Data Input** button in the upper left-hand panel of **Annual PM Analysis** window. The button next to **Output Choices-Advanced** will turn from yellow to green, indicating that this step is complete.

# 6.3. Data Input

File * Analysis * Data Viewer Expand Viewer	Single Source Impact A	Analysis 🔹 Start Pag	je	
Annual PM Analysis				0
Choose Desired Output     Output Choices-Advanced     Data Input     Species Fraction Options		Cog/Msg		
PM2.5 Calculation Options Model Data Options		Name	Running Messages	
Data Input	0			
Species Data	<u>^</u>			
Species Monitor Data File				
Species-for-fractions-02-10-v3.csv	E			
Species Fractions File				
point +				
spatial fiel 👻	1			
PM2.5 Monitor Data				
Unofficial Daily Average PM2.5 Data File (for All Species Fraction PM2.5 Spatial Field)				
PM25-for-fractions-02-10-v3.csv	- 12			
	Back Next			
Clear Save Project & Run	Save Project	•	m	•

#### Figure 6-4. Data Input for Annual PM2.5 Analysis

The **Data Input** configuration step sets the ambient  $PM_{2.5}$  species data,  $PM_{2.5}$  monitor data (FRM and IMPROVE), and the gridded model output data to use for the SMAT-CE project (Figure 6-4).

There is specific terminology that is used on the Data Input page. "Official" data refers to PM<sub>2.5</sub> FRM data that can be used to determine official design values for compliance purposes (comparison to the NAAQS). Other datasets which may not have rigid regulatory significance are sometimes referred to as "unofficial" data. The blue hyperlinked text in this window brings up the documentation for this configuration step. The settings in this step include:

#### **Species Data**

SMAT-CE uses ambient PM<sub>2.5</sub> species data to calculate species concentrations at FRM monitoring sites and spatial fields. Users have a choice of supplying a "Species Monitor Data File" or a "Species Fractions File".

• Species Monitor Data File. This is the SMAT-CE default of daily average species data from STN and IMPROVE sites across the country. Users can also

provide their own ambient data file. MATS uses the daily average species data to calculate species fractions at each FRM monitor (or at each grid cell, in the case of spatial fields). The species fraction data is combined with the "unofficial daily average PM2.5 data" to calculate species concentrations. The default SMAT-CE species data file contains all available data. However, there is a data flag to indicate site days that are recommended to be removed from the species fractions calculations. SMAT-CE has incorporated flagging routines that remove data that are considered to be outliers and/or incomplete data. Section 5.4.2 of the MATS User's Manual (Abt, 2014) describes the flags used in the species fractions calculations.

Species Fraction File. An alternative to the Species Monitor Data File. This file contains pre-calculated species fractions with quarterly species information for the FRM monitors of interest. SMAT-CE can use a species fractions file (either "point" or "spatial fields") generated by a previous project. To use an existing fractions file, enter the correct path to the file in the Data Input window. When using spatial fields for existing species fractions files, select either "spatial field" or gradient adjusted spatial fields" from the drop-down box.

#### PM2.5 Monitor Data

SMAT-CE uses both "official" and "unofficial" data in its calculations.

Unofficial Daily Average PM2.5 Data File. PM<sub>2.5</sub> data that are needed to calculate species fractions. These data are used in combination with the Species Monitor Data File. This file is not needed if the user supplies a pre-calculated species fractions file.

Similar to the **Species Monitor Data File**, the **Unofficial Daily Average PM<sub>2.5</sub> Data File** contains a data flag to indicate site days that are recommended to be removed from the species fractions calculations. The flagged data is matched between the species file and the PM<sub>2.5</sub> file so that the same site days are removed. The PM<sub>2.5</sub> data file contains additional data (sites that don't contain speciation measurements) and therefore has additional flagged site days. These are not the same data flags that have been identified by State agencies. SMAT-CE has incorporated flagging routines that remove data that are considered to be outliers and/or incomplete data. SMAT-CE users are free to alter the flags as needed for their applications.

• Official Quarterly Average FRM Data File. The EPA-approved quarterly average FRM data that have been used to calculate PM<sub>2.5</sub> design values. These data are used to calculate design values and 5 year weighted average design values as part of the attainment test.

The default data file in SMAT-CE was created by EPA OAQPS. In most cases, the data should not be altered, however in some cases (e.g. sensitivity analyses) there may be a need to add or remove data.

A detailed description of the formats of the input data files used in this step, are available in Section 5.3.2 of the MATS User's Manual (Abt, 2014).

# Model Data

These are gridded model output from models such as CMAQ or CAMx. The user can choose either daily model data input or quarterly model data input (which is just a quarterly average of the daily model data). Either will work for the Annual PM<sub>2.5</sub> Analysis. The default setting is daily average data. Model data must be selected for all SMAT-CE projects. The size of the modeling grid defines the outputs for point estimates and for spatial fields. For point estimates, SMAT-CE will output the results for all specified monitors within the domain. For spatial fields, SMAT-CE will create spatial fields that match the size of the gridded model domain.

SMAT-CE requires both a Baseline File and a Forecast File. The baseline file should be consistent with the historical monitor data used for the project, and the forecast year is the future-year of interest.

# 6.3.1. Run the Eastern U.S. Example

Use the default settings for the Data Input options for the Eastern U.S. example project. Either click Next or double-click the **Species Fraction Options** button in the upper left-hand panel of **Annual PM Analysis** window. The button next to **Data Input** will turn from yellow to green, indicating that this step is complete.

# 6.4. Species Fraction Options

File • Analysis • Data Viewer Expand Viewer DataError-Checking	Start Page
🕞 Annual PM Analysis 📃 🌉	
Choose Desired Output	
Data Input     Species Fraction Options	C Log/Msg
Openes fraction options     Options     Model Data Options	Name Running Messages
Species Fraction Options	
IMPROVE-CSN Monitor Data	
Monitor Data Years	
Start Year 2010 ~ End Year 2012 ~	
Delete Specified Data Values	
☑ EPA-specified deletions from monitor data	
User-specified deletions from monitor data	
Minimum Data Requirements	
Minimum number of valid days per valid quarter	
Minimum number of valid years required for valid 1	
Minimum number of valid seasons required for valid monitor	
Back Next	
Clear Save Project & Run Save Project	<>

Figure 6-5. Species Fraction Options for Annual PM2.5 Analysis

The **Species Fraction Calculation Options** configuration step shown in Figure 6-5 has several options related to the speciated monitor data (IMPROVE and STN) monitor data and the total PM<sub>2.5</sub> monitor data (FRM and IMPROVE). These functions include identifying the years of monitor data to use in the attainment test, deleting any specific data values, and choosing the minimum data requirements of monitors to use in the analysis. These options are listed below.

*IMPROVE-STN Monitor Data*. The speciation data from STN and IMPROVE monitors are interpolated by SMAT-CE in order to provide species data for any point in a modeling domain. The interpolated species data is used to calculate species fractions at FRM monitors (point estimates) and/or species fractions at all grid cells (spatial fields). Note that you do not need to have values for all species for a monitor to be considered valid, as each species is considered individually. However, the "EPA\_Flag" variable in the default "species for fractions" file has been set so that all monitor days that do not have complete species data are not used in the calculations (flag = 1). If the user wants to use

the incomplete species data, the flag should be set to "0".

• *PM2.5 Monitor Data.* The total PM<sub>2.5</sub> data from FRM are used by SMAT-CE to calculate species fractions for point estimates (in conjunction with the interpolated speciation data from STN and IMPROVE monitors). The interpolated species data is used to calculate species fractions at FRM monitors (point estimates) and/or species fractions at all grid cells (spatial fields).

#### Monitor Data Years

Use the drop-down menus to choose the three years of monitor data for the Annual  $PM_{2.5}$  Analysis. The SMAT-CE default is to use the three-year period 2010 to 2012. (That is, for both IMPROVE-STN and  $PM_{2.5}$  monitor data, the **Start Year** is *2010* and the **End Year** is *2012*.) The default period is based on a modeling year of 2011. The start and end years should be changed to applicable time periods, depending on the base modeling year.

SMAT-CE handles multiple years of data by calculating averages for each species by quarter and year. SMAT-CE then averages the quarterly values across the years (e.g., average quarter 1 values of SO<sub>4</sub> across two years to get a single "quarter 1" estimate). After completing this step, SMAT-CE will have four quarterly estimates for each species at each monitor. These quarterly values are then ready to be interpolated to FRM sites or to grid cell centroids in spatial fields.

Delete Specified Data Values

The default is to delete the observations specified by EPA. Valid data are given a value of "0" and observations that should be deleted are given a value of "1" to "10". There is also an option for the user to flag data, using the same convention of "0" for valid data and "1" to "10" for data marked for deletion. If both the **EPA-specified** and **User-specified** flags are checked, then SMAT-CE deletes any observations that are marked for deletion by either the EPA or the user. These settings make it easy for the user to flag additional data for removal from the calculations (without deleting the actual record from the ambient data file). See Section 5.4.2 of the MATS User's Manual (Abt, 2014) for a description of the observational data flags.

Minimum Data Requirements

There are three sets of minimum data requirements for calculating design values:

- Minimum number of valid days per valid quarter. This is the minimum number of site-days per valid quarter. The default is 11 days, which corresponds to > 75% completeness for monitors on a 1-in-6 day monitoring schedule. This is the minimum number of samples that is routinely used in calculations of quarterly average concentrations.
- *Minimum number of valid quarters required for valid season*. This is the number of years of data (within the start year and end year specified) for which there are valid quarters for a given season. The default value is 1 year. If the value is set = 2, then there will need to be 2 years of valid data from quarter 1 in order for quarter one to be considered complete (and the same for the other 3 quarters).
- Minimum number of valid seasons required for valid monitor (point and spatial fields calculation). This is the number of valid seasons that are needed in order for a particular monitor's data to be considered valid. The default is 1 for IMPROVE-STN monitor data and the range is 1-4. For example, if the value is = 1, then a monitor's data will be used in the species fractions calculations if it has at least one valid season. If the value = 4, then the site must have all 4 seasons of valid data to be used. The default for PM<sub>2.5</sub> depends on whether the data are used in point calculations (default = 4) or spatial field calculations (default = 1).

Section 5.4.3 of the MATS User's Manual (Abt, 2014) shows an example of how the minimum data requirements are used in calculating averages for monitoring data.

Clicking the Advanced box displays additional Species Fractions Calculations Options. The Species Fractions Calculation Options - Advanced screen allows you to make relatively advanced choices for your analysis. Generally speaking, the default options settings are consistent with the EPA modeling guidance document. One set of options allows you to specify the interpolation weighting that you want to use and whether the interpolation involves a maximum distance or not. The second set of options involves choices regarding ammonium, blank mass, and organic carbon. These options are described below.

#### Interpolation Options

The selections in this section set how SMAT-CE will interpolate, or combine, the values from different monitors. One approach is to use Inverse Distance Weights, which assigns a weight to any particular monitor that is inversely proportional to its distance from the point of interest. A second approach is Inverse Distance Squared Weights, which means that the weights are inversely proportional to the square of the distance. And the third approach is Equal Weighting of Monitors. The default approach for PM is Inverse Distance Squared Weights.

When interpolating monitor values, SMAT-CE identifies monitors based on their distance away from the point of interest (*e.g.*, the center of a grid cell). The first step in the interpolation process is to identify the monitors that are nearby, or neighbors, for each point of interest. The next step is to determine the distance (in kilometers) from the nearby monitors to the point of interest. The default approach is to include all valid monitors (*i.e.*, those that satisfy the three criteria in the Species Fractions Calculation Options panel), regardless of distance. To limit the use of monitors based on distance, type in the distance in km (e.g., 100) next to the pollutant of interest. Note that a distance of one hundred (100) kilometers means that any monitors further than 100 kilometers can no longer be used in the interpolation. If a point of interest has no monitors within the specified distance, then no value is calculated.

The Miscellaneous Options panel sets the following options for SMAT-CE:

#### <u>Ammonium</u>

Specify whether to use degree of neutralization (DON) values to calculate ammonium (NH4) or to use measured ammonium in conjunction with an assumption about the percentage of NH4 that evaporates. The default option is to use DON values. To use measured ammonium, click the button and choose a NH4 percentage evaporating (e.g., 50). The default is "0", which assumes that no ammonium evaporates from the FRM filters.

#### Default Blank Mass

The Default Blank Mass option sets default blank mass to the desired level. The default is 0.5. Either type in or use the arrows to increase or decrease the value.

## Organic Carbon

Set the "floor" and the "ceiling" for the mass balance calculation for organic carbon.

### Run the Eastern U.S. Example

Use the default settings for the Species Fraction Options for the Eastern U.S. example project. Either click Next or double-click the **PM<sub>2.5</sub> Calculation Options** button in the upper left-hand panel of **Annual PM Analysis** window. The button next to **Species Fraction Options** will turn from yellow to green, indicating that this step is complete.

# 6.5. PM2.5 Calculation Options

File - Analysis - Data Viewer Expand Viewer DataError-Checking S	itart Page
🖗 Annual PM Analysis 📃 関	
Choose Desired Output Output Choices-Advanced Data Input Species Fraction Options HM2.5 Calculation Options	Log/Msg Name Running Messages
└── Model Data Options	
PM2.5 Calculation Options	
PM2.5 Monitor Data Years	
Start Year 2009 v End Year 2013 v	
Official Design Values	
○ Custom Design Values	
Valid FRM Quarters	
Minimum days for valid quarter	
Valid FRM Design Values	
Minimum valid quarters in design value period	
Valid FRM Monitors	
Minimum number of Design Values	
🗰 🌩	
Back         Next           Clear         Save Project & Run         Save Project	٤

Figure 6-6. PM2.5 Calculation Options for Annual PM2.5 Analysis

The **PM2.5 Calculation Options** window shown in Figure 6-6 sets the particular years of monitor data to use from the input file specified in the **Data Input** window. The following options are available in this window.

PM2.5 Monitor Data Years

The Start Year and End Year drop-down menu options list the years of available official PM monitor data to use in the calculation of future  $PM_{2.5}$  design values. The default approach in SMAT-CE is to use five years of data.

SMAT-CE provides the option to use "official" design values, which are generally

recommended, or to choose "custom" design values. The custom design values option requires the specification of the minimum number of observation days in each quarter and the minimum number of quarters to produce valid design values.

#### Valid FRM Quarters

Set the minimum number of site-days per valid quarter. The default is 11 days, which corresponds to > 75% completeness for monitors on a 1-in-6 day monitoring schedule. This is a minimum number of samples that is routinely used in calculations of quarterly average concentrations.

#### Valid FRM Design Values

Set the minimum number of quarters for which there are data within three consecutive design value periods. The default value is 12 quarters. If the value is set to 11, then there will need to be at least 11 valid quarters (i.e., two years must have 4 valid quarters and one year must have at least 3 valid quarters.)

#### Completion Code

Use this variable from the official quarterly PM<sub>2.5</sub> monitor database to identify valid data. As noted above in Section 6.4, the completion code has values of: 1, 2, 3, 4, or 5; and the codes are valid for the end year of each three-year design value period. SMAT-CE uses the completion code variable somewhat differently when using official design values and when using custom design values:

- When using official data, SMAT-CE will only use completion codes: 1 and 2.
- When using custom data, SMAT-CE will potentially use completion codes: 1, 2, 3, and 4 (if the user specified completion criteria are met).

The following is an explanation of the official EPA completion codes:

- Code "1"- complete data and violates the NAAQS
- Code "2"- complete data that is below the NAAQS
- Code "3"- incomplete data and violates the NAAQS
- Code "4" incomplete data that is below the NAAQS
- Code "5" data that is not comparable to the NAAQS and should not be used.
   For example, FRM data collected at a micro-scale site cannot be compared to the annual PM2.5 NAAQS.

# Valid FRM Monitors

By default, SMAT-CE assumes that there only needs to be one design value for a monitor to be considered valid. In addition, SMAT-CE assumes that no particular design value is required, so different monitors with different years of data could be used. For example, a start year and end year as 2005 and 2009 gives potential 3-year design values of 2005-2007, 2006-2008, and 2007-2009. When the Minimum Number of Design Values is set to 1, one monitor could have data for, say, 2005-2007 and another monitor data for 2006-2008, and both monitors would be used. A Minimum Number of Design Values setting of 2 would only use monitors that have design values for two of the three design value periods, ignoring monitors that only have design values for a single period.

# NH4 Future Calculation

SMAT-CE can forecast NH<sub>4</sub> in two different ways. The default approach uses base year DON values. See Section 5.1.2.3 of the MATS User's Manual for details on the forms of the two equations that are available to forecast NH<sub>4</sub>.

# Run the Eastern U.S. Example

Use the default settings for the PM<sub>2.5</sub> Calculation Options for the Eastern U.S. example project. Either click Next or double-click the **Model Data Options** button in the upper left-hand panel of **Annual PM Analysis** window. The button next to **PM<sub>2.5</sub> Calculation Options** will turn from yellow to green, indicating that this step is complete.

# 6.5.1.1. Model Data Options

File * Analysis * Data Viewer Expand Viewer Single Source Impact A	Analysis - Start Page
Annual PM Analysis	Co ()
PM2.5 Calculation Options     Model Data Options	Name Running Messages
Model Data Options  Comporel adjustment at monitor	
Grid for Point Forecast Grid for Spatial Forecast	
Back Next	
Clear Save Project & Run Save Project	۰ ( الله الله الله الله الله الله الله ال

Figure 6-7. Model Data Options for Annual PM2.5 Analysis

The **Model Data Options** window shown in Figure 6-7. This window sets the temporal adjustments for each monitor:

#### Temporal Adjustment at Monitor

This option specifies how many model grid cells to use in the calculation of RRFs for point estimates and for spatial estimates. A drop down menu provides options to use 1x1, 3x3, 5x5, and 7x7 arrays of model grid cells. The default for a 12 kilometer by 12 kilometer grid is to use a 3x3 array of grid cells. The U.S. EPA Draft Modeling Guidance for Attainment of Air Quality Goals for Ozone, PM<sub>2.5</sub>, and Regional Haze (U.S. EPA, 2014) includes discussion on selecting the appropriate grid call array size for different model resolutions.

Note that for PM analyses, SMAT-CE calculates **mean** concentrations across the grid cell array (as compared to maximum concentrations used for ozone analyses).

## Run the Eastern U.S. Example

Use the default settings for the Model Data Options for the Eastern U.S. example project. Either click **Next**, which will bring up a window prompting to "Save & Run

Project" or click the **Save Project & Run** button at the bottom of the SMAT-CE window. The Annual PM<sub>2.5</sub> Analysis project may also be saved without running SMAT-CE by clicking the **Save Project** button. A file explorer window will request a filename to which the project settings will be saved to a \*.proj file. This file can be loaded later to restart the analysis.

For the Eastern U.S. example, select save and run for the Annual PM<sub>2.5</sub> Analysis project. A file explorer window will request a filename (\*.proj) to which to save the project settings. While the Analysis is running, the icon next to **Model Data Options** will turn to a running status and status messages will be displayed in the **Log & Msg** tab on the right panel of the SMAT-CE main window (Figure 6-8).



Figure 6-8. Annual PM25 Analysis run status

When the Annual PM<sub>2.5</sub> Analysis is completed, the Data Viewer will automatically display in the SMAT-CE main window (Figure 6-9). The Output Files section of the Data Viewer left panel will display all of output files selected in the **Choose Desired Output** and **Output Choices-Advanced** Annual PM<sub>2.5</sub> Analysis windows.

The Data Viewer provides options to display the Annual  $PM_{2.5}$  Analysis results as maps, bar charts, and tables. <u>Chapter 10</u> describes how to load and analyze data using the

## SMAT-CE Data Viewer.

Data Viewer	Annual PM Analysis
Name	(double-click/right-click files in left panel to view data & map)         Image: Gis       Image: Gis
Load         Extract All         Extract Selected           VNA              eVNA         Send to BenMAP-CE	۲

## Figure 6-9. Annual PM Analysis Data Viewer

This concludes the chapter on the SMAT-CE Annual PM<sub>2.5</sub> Analysis. As described in this section, details of the calculations and settings used in this analysis are available in the U.S. EPA Draft Modeling Guidance for Attainment of Air Quality Goals for Ozone, PM<sub>2.5</sub>, and Regional Haze (U.S. EPA, 2014) and in Chapter 5 of the MATS User's Manual (Abt, 2014).

# 7. Daily PM Analysis

SMAT-CE can forecast daily (24-hour) design values at PM<sub>2.5</sub> monitor locations -- these forecasts are referred to as Point Estimates. SMAT-CE can also use a variety of approaches to calculate design values for a Spatial Field. A Spatial Field refers to a set of values comprising calculations for each grid cell in a modeling domain from Eulerian grid models such as CMAQ and CAMx.

The Daily PM Design Value Analysis in SMAT-CE is organized into seven steps. The steps include the input/output and configuration options for computing ozone design values. The following configuration steps correspond to different SMAT-CE windows and are described in detail in this chapter:

- **Output Choice**. Select whether to run the Standard Analysis, and whether to output a species fractions file and/or quarterly model data.
- **Output Choice Advanced**. Configure miscellaneous Point Estimate output files for quality assurance of the PM design value calculations.
- **Data Input**. Specify the species monitoring data, species fractions file, PM<sub>2.5</sub> ambient monitoring data, and the modeling data to use for the design value calculations.
- <u>Species Fractions Calculation Options</u>. Select the years of daily STN-IMPROVE and FRM monitoring data and identify valid monitors. Define data filtering specifications.
- <u>Species Fractions Calculation Options Advanced</u>. Select the method to identify peak monitor values. Choose interpolation options for PM<sub>2.5</sub> and species monitoring data. Choose assumptions for the ammonium calculation, default blank mass, and organic carbon.
- <u>PM2.5 Calculation Options FRM Monitor Data</u>. Select the years of quarterly FRM monitoring data and identify valid monitors. Select the approach for calculating future year ammonium.
- <u>Model Data Options</u>. Specify the maximum distance of monitors from modeling domain. Choose method to identify peak model values. Specify which

File - Analysis - Data Viewer Expand Viewer Single Source Impact A	nalysis * Start Page
💮 Daily PM Analysis 📃 📃	
Choose Desired Output     Output Choices-Advanced     Data Input     Species Fraction Options	C Log/Msg
PM2.5 Calculation Options  Model Data Options	Name Running Messages
Choose Desired Output	
Project Name:	
Standard Analysis	
☑ Interpolate monitor data to FRM monitor sites. Temporally-adjust.	
Quarterly Peak Model Data	
✓ Output quarterly peak model data file.	
Species Fraction	
Output species fractions file.	
Actions on run completion	
Automatically extract all selected output files.	
Back Next	
Clear Save Project & Run Save Project	۰ m

model grid cells will be used when calculating RRFs at monitor locations.

#### Figure 7-1. Daily PM Analysis initial window

To conduct an attainment test for the daily PM<sub>2.5</sub> NAAQS, select **Daily PM Analysis** from the Process Data module on the SMAT-CE Start Page. Figure 7-1 shows the initial window that is displayed when Daily PM Analysis is selected. The box in the upper left of the window (highlighted in red in Figure 7-1) lists the configuration steps of the Daily PM Analysis. Each step listed in this box has a different set of configuration options that are displayed in the Daily PM Analysis window. Once each step is successfully configured, the icons next to each step in the box will change from yellow to green. In general, the configuration steps must be followed in order, from top to bottom, as they are listed in the box. Previously completed steps may be accessed and modified by double clicking on the step name in the box. Once the configuration for a step is complete, you may move to the next step by either clicking on it or by selecting the Next button (shown in the blue box in Figure 7-1).

A previous project may be loaded or a new project may be initiated at any time in the Daily PM Analysis window by selecting one of the icons to the right of the "Daily PM Analysis" text above the red box in Figure 7-1.

Each of the Daily PM Analysis configuration steps are described in the following sections.

File - Analysis - Data Viewer Expand Viewer DataEr	ror-Checking	BenMAP *	Single Source	Impact Analysis	• USA • Sta	art Page
Daily PM Analysis					Ç	
Output Choices-Advanced     Data Input     Species Fraction Options			/Msg			
<ul> <li>PM2.5 Calculation Options</li> <li>Model Data Options</li> </ul>		Name		Running Message	25	
Choose Desired Output	0					
Project Name:						
Standard Analysis						
$\overline{\mathbb{V}}$ Interpolate monitor data to FRM monitor sites. Tempo	rally-adjust.					
Quarterly Peak Model Data						
$\overline{\mathbb{V}}$ Output quarterly peak model data file.						
Species Fraction						
$\overline{\mathbb{V}}$ Output species fractions file.						
Actions on run completion						
$\blacksquare$ Automatically extract all selected output files.						
	-					
Clear Save Project & Run S	ck Next ave Project	•				4

# 7.1. Choose Desired Output

Figure 7-2. Choose Desired Output for Daily PM2.5 Analysis

**Choose Desired Output** is the first configuration step that is displayed when the Daily PM Analysis module is selected (Figure 7-2). The blue hyperlinked text in this window brings up the documentation for this configuration step. The settings in this step include:

## **Project Name**

Text string to identify this analysis and set the name of the project file.

#### **Standard Analysis**

Since most Federal Reference Method (FRM) PM<sub>2.5</sub> monitoring sites do not have collocated chemical speciation monitors, spatial interpolation is used to estimate species data at FRM PM<sub>2.5</sub> monitor locations. SMAT-CE provides options to use different methods for spatially interpolating chemical speciation information to the FRM monitors. These options are available from the **PM2.5 Calculation Options** configuration window. Complete details of the Standard Analysis approach, including the formula used to calculate species concentrations, are available in the U.S. EPA Draft

Modeling Guidance for Attainment of Air Quality Goals for Ozone, PM<sub>2.5</sub>, and Regional Haze (U.S. EPA, 2014) and in Section 7.1.2 of the MATS User's Manual (Abt, 2014).

Most SMAT-CE users will run the standard analysis and it is checked by default.

#### **Quarterly Peak Model Data**

SMAT-CE requires two types of data input: ambient monitor data and gridded model output data. For the daily PM<sub>2.5</sub> calculations, SMAT-CE will accept either SMAT-CE formatted daily average gridded model files or quarterly peak average files.

If daily average model files are used as inputs, SMAT-CE will calculate quarterly peak averages from the daily averages and optionally output the quarterly peak average concentrations into text files (CSV files). The quarterly average text files can then be re-used in subsequent SMAT-CE analyses. Quarterly average input files are smaller and run faster than daily average files. Choosing this option will direct SMAT-CE to generate two types of quarterly peak average model concentration CSV files:

- *All Data.* SMAT-CE outputs quarterly peak data for all grid cells in the modeling domain. MATS will create one baseline year file and one future year file. This will create relatively large files, but they will still be much smaller than daily average files.
- Used Data. SMAT-CE outputs quarterly peak data for the grid cells that are subsequently used in the particular SMAT-CE configuration. For example, if SMAT-CE calculates future year design values at 20 FRM sites using a 1 X 1 grid array, then SMAT-CE will output base and future model values for only 20 grid cells (assuming each monitor is in a unique grid cell). The advantage of these files is that they are extremely small. But if subsequent SMAT-CE runs use a different set of monitors or grid arrays, then the files may not contain all of the necessary data to complete the analysis. This option is recommended as a QA tool to examine the grid cells and the model concentrations that MATS is using in the analysis.

Additional details of the Quarterly Peak Model Data option are available in Section 7.1.3 of the MATS User's Manual (Abt, 2014).

#### **Species Fraction**

Checking the "Output species fraction file" box will create an output file containing the calculated PM<sub>2.5</sub> species fractions at each FRM site used by SMAT-CE. Species fractions are simply the fraction of quarterly average PM<sub>2.5</sub> at a given monitor attributable to seven (and potentially eight) species: nitrate (NO<sub>3</sub>), sulfate (SO<sub>4</sub>), organic carbon (OC), crustal, elemental carbon (EC), ammonium (NH<sub>4</sub>), and particle-bound water (PBW). And pending data availability, sea salt can be included as well. While the default SMAT-CE species files include sea salt data, it is an optional species in the model files. If base and future year modeled sea salt data are available, a sea salt RRF will be calculated by SMAT-CE. If the salt data are not available in the model files, then the sea salt RRF will be set to 1.

This species fraction file can be re-used in SMAT-CE as an input file. The species fraction file can be useful for several reasons. Using a species fraction file saves time because SMAT-CE won't have to interpolate species data and calculate fractions each time it is run. This file can provide consistency between SMAT-CE runs by ensuring that the same species fractions are used each time. And for the same reason, the species fraction file can be used interchangeably between different users to ensure that multiple groups are using the same species fractions (if that is a goal). And finally, the fractions file can serve as a template for creating a custom species fractions file using whatever data and techniques (e.g. alternative interpolation techniques) are desired by any particular user.

Additional details of the Species Fractions calculation are available in Section 7.1.4 of the MATS User's Manual (Abt, 2014).

#### Actions on Run Completion

Checking the "Automatically extract all selected output files" box will export CSV files of all selected output to a separate folder named with the Project Name in the SMAT "\Result\Output" folder. The results may also be exported later from the **Data Viewer**.

#### 7.1.1. Run the Eastern U.S. Example

The default settings for these options, and the configuration to use for the Eastern U.S. example project, is to check all of the boxes in the SMAT-CE **Choose Desired Output** 

window. After setting a Project Name and selecting all of the boxes in the window either click Next or double-click the **Output Choices-Advanced** button in the upper left-hand panel of **Daily PM Analysis** window. The icon next to **Choose Desired Output** will turn from yellow to green, indicating that this step is complete.

# 7.2. Output Choices-Advanced

File * Analysis * Data Viewer Expand Viewer	Single Source Impact A	Analysis 🔹 Start Page		
Daily PM Analysis				01
Choose Desired Output     Output Choices-Advanced     Data Input     Species Fraction Options		Cog/Msg		
		Name	Running Messages	
Output Choices-Advanced Miscellaneous Outputs	<b>0</b>			
Quarterly average files				
✓ Point				
High county sites				
V Yes	E			
Quarterly average speciated monitors				
V Yes				
Design Value Periods				
🔲 Output Design Value Periods				
Neighbor files	-			
	Back Next			
Clear Save Project & Run	Save Project	•	Ш	×

Figure 7-3. Output Choices-Advanced for Daily PM2.5 Analysis

The **Output Choices – Advanced** configuration step provides detailed control over the calculations, output, and quality assurance fields used by SMAT-CE (Figure 7-3). The blue hyperlinked text in this window brings up the documentation for this configuration step. All of the settings in this step are organized under the "Miscellaneous Outputs" heading and include the following.

# **Quarterly Average Files**

SMAT-CE outputs by default the 98th percentile design values, which are based on a weighted average of five years of data. Checking the **Point** box under **Quarterly average files** will direct SMAT-CE to output detailed parameters from the peak calculations that are the basis of all of the PM design value calculations. Two additional files are output by SMAT-CE when this option is selected:

- *Daily All Years All Days PM*<sub>2.5</sub> *Point*. This file has baseline and future values for the Top 32 ranked PM<sub>2.5</sub> values and constituent species. In addition, it gives the speciated RRFs.
- *Daily All Years High Days PM*<sub>2.5</sub> *Point*. This file identifies the 98th percentile PM<sub>2.5</sub> value in the baseline and future for each year at each monitor. Note that the baseline and future quarters and days may differ.

# **High County Sites**

Augments the SMAT-CE default of outputting the point results for all FRM sites. Checking this box will also produce a file that contains the single highest monitor in each county, based on the highest future year value. This dataset is a subset of the all sites file.

## **Quarterly Average Speciated Monitors**

Directs SMAT-CE to produce a file with the raw quarterly average speciated data that were used to interpolate species fractions to the FRM monitors. These data are derived from the "species for fractions" input file.

## **Design Values Periods**

Directs SMAT-CE to produce a file with the standard SMAT-CE output for each design period within the period covered by the analysis. By default, SMAT-CE outputs one set of files covering the entire analysis period specified by the user. The outputs represent the averages of the values for each 3-year design value period. If the "Output design value periods" option is checked, SMAT-CE will produce discrete outputs for each design value period. The output files will be the same as a standard analysis, but with "Period 1", "Period 2", etc., attached at the end of the name. Selecting this option will increase the SMAT-CE run time.

# <u>Neighbor Files</u>

Directs SMAT-CE to produce files of "nearest neighbor" data for the VNA interpolation scheme. The data include the distance to neighbor monitors and weights used to do the interpolations. This option will generate information for each FRM monitor (for point analyses) or each grid cell (for spatial fields) for each quarter and for each species.

Additional details of the Output Choices – Advanced options, including the formats of the output files from this step, are available in Section 7.2 of the MATS User's Manual (Abt, 2014).

# 7.2.1. Run the Eastern U.S. Example

Use the default settings for these options for the Eastern U.S. example project. Either click Next or double-click the **Data Input** button in the upper left-hand panel of the **Daily PM Analysis** window. The button next to **Output Choices-Advanced** will turn from yellow to green, indicating that this step is complete.

# 7.3. Data Input

File * Analysis * Data Viewer Expand Viewer	Single Source Impact A	Analysis + Start Page	1	
Choose Desired Output Choose Desired Output Output Choices-Advanced Data Input Species Fraction Options	88	Log/Msg		0
- HORD PM2.5 Calculation Options - HORD PHI Data Options		Name	Running Messages	
Data Input Species Data	0			
• Species Monitor Data File				
Species-for-fractions-02-10-v3.csv	E			
Species Fractions File				
point -				
spatial fiel 💌	1			
PM2.5 Monitor Data				
Unofficial Daily Average PM2.5 Data File (for All Species Fractions)				
PM25-for-fractions-02-10-v3.csv	-			
Clear Save Project & Run	Back Next	•	III.	•

Figure 7-4. Data Input for Daily PM<sub>2.5</sub> Analysis

The **Data Input** configuration step sets the ambient PM<sub>2.5</sub> species data, PM<sub>2.5</sub> monitor data (FRM and IMPROVE), and the gridded model output data to use for the SMAT-CE project (Figure 7-4).

There is specific terminology that is used on the Data Input page. "Official" data refers to  $PM_{2.5}$  FRM data that can be used to determine official design values for compliance purposes (comparison to the NAAQS). Other datasets which may not have rigid regulatory significance are sometimes referred to as "unofficial" data. The blue

hyperlinked text in this window brings up the documentation for this configuration step. The settings in this step include:

#### **Species Data**

SMAT-CE uses ambient  $PM_{2.5}$  species data to calculate species concentrations at FRM monitoring sites and spatial fields. Users have a choice of supplying a "Species Monitor Data File" or a "Species Fractions File".

- *Species Monitor Data File.* This is the SMAT-CE default of daily average species data from STN and IMPROVE sites across the country. Users can also provide their own ambient data file. MATS uses the daily average species data to calculate species fractions at each FRM monitor (or at each grid cell, in the case of spatial fields). The species fraction data is combined with the "unofficial daily average PM2.5 data" to calculate species concentrations. However, there is a data flag to indicate site days that are recommended to be removed from the species fractions calculations. SMAT-CE has incorporated flagging routines that remove data that are considered to be outliers and/or incomplete data. Section 7.4.2 of the MATS User's Manual (Abt, 2014) describes the flags used in the species fractions calculations.
- Species Fraction File. Alternative to the Species Monitor Data File. This file contains pre-calculated species fractions with quarterly species information for the FRM monitors of interest. SMAT-CE can use a species fractions file (either "point" or "spatial fields") generated by a previous project. To use an existing fractions file, enter the correct path to the file in the Data Input window. When using spatial fields for existing species fractions files, select either "spatial field" or gradient adjusted spatial fields" from the drop-down box.

#### PM2.5 Monitor Data

SMAT-CE requires model data in the form of a text file. SMAT-CE uses both "official" and "unofficial" data in its calculations.

Unofficial Daily Average PM2.5 Data File. PM<sub>2.5</sub> data that are needed to calculate species fractions. These data are used in combination with the Species Monitor Data File. This file is not needed if the user supplies a pre-calculated

species fractions file.

Similar to the **Species Monitor Data File**, the **Unofficial Daily Average PM<sub>2.5</sub> Data File** contains a data flag to indicate site days that are recommended to be removed from the species fractions calculations. The flagged data is matched between the species file and the PM<sub>2.5</sub> file so that the same site days are removed. The PM<sub>2.5</sub> data file contains additional data (sites that don't contain speciation measurements) and therefore has additional flagged site days. These are not the same data flags that have been identified by State agencies. SMAT-CE has incorporated flagging routines that remove data that are considered to be outliers and/or incomplete data. SMAT-CE users are free to alter the flags as needed for their applications.

• Official Quarterly Average FRM Data File. The EPA-approved quarterly average FRM data that have been used to calculate PM<sub>2.5</sub> design values. These data are used to calculate design values and 5 year weighted average design values as part of the attainment test.

The default data file in SMAT-CE was created by EPA OAQPS. In most cases, the data should not be altered, however in some cases (e.g. sensitivity analyses) there may be a need to add or remove data.

A detailed description of the formats of the input data files used in this step, are available in Section 7.3.2 of the MATS User's Manual (Abt, 2014).

#### <u>Model Data</u>

These are gridded model output from models such as CMAQ or CAMx. The user can choose either daily model data input or quarterly model data input (which is just a quarterly average of the daily model data). Either will work for the Daily PM<sub>2.5</sub> Analysis. The default setting is daily average data. Model data must be selected for all SMAT-CE projects. The size of the modeling grid defines the outputs for point estimates and for spatial fields. For point estimates, SMAT-CE will output the results for all specified monitors within the domain. For spatial fields, SMAT-CE will create spatial fields that match the size of the gridded model domain.

Subsequent versions of SMAT-CE will support reading directly from CMAQ data files.

This option is currently greyed out in SMAT-CE.

SMAT-CE requires both a Baseline File and a Forecast File. The baseline file should be consistent with the historical monitor data used for the project, and the forecast year is the future-year of interest.

# 7.3.1. Run the Eastern U.S. Example

Use the default settings for the Data Input options for the Eastern U.S. example project. Either click Next or double-click the **Species Fraction Options** button in the upper left-hand panel of **Daily PM Analysis** window. The button next to **Data Input** will turn from yellow to green, indicating that this step is complete.

# 7.4. Species Fraction Options

File * Analysis * Data Viewer Expand Viewer DataError-Checking	Start Page
🕞 Daily PM Analysis 📃 📙	
Choose Desired Output Choices-Advanced Data Input Species Fraction Options	Log/Msg
PM2.5 Calculation Options Hodel Data Options	Name Running Messages
Species Fraction Options  IMPROVE-CSN Monitor Data	
Monitor Data Years       Start Year       2010       Year       2012	
Delete Specifed Data Values	
EPA-specified deletions from monitor data	
□ User-specified deletions from monitor data	
Minimum Data Requirements	
Minimum number of valid days per quarter	
Minimum number of valid quarters per valid year	
Minimum number of valid years required for valid mnitor 1 Back Next	
Clear Save Project & Run Save Project	< >>

Figure 7-5. Species Fraction Options for Daily PM2.5 Analysis

The **Species Fraction Calculation Options** configuration step shown in Figure 7-5 has several options related to the speciated monitor data (IMPROVE and STN) monitor data and the total PM<sub>2.5</sub> monitor data (FRM and IMPROVE). These functions include identifying the years of monitor data to use in the attainment test, deleting any specific data values, and choosing the minimum data requirements of monitors to use in the analysis. These options are listed below.

- *IMPROVE-STN Monitor Data*. The speciation data from STN and IMPROVE monitors are interpolated by SMAT-CE in order to provide species data for any point in a modeling domain. The interpolated species data is used to calculate species fractions at FRM monitors (point estimates) and/or species fractions at all grid cells (spatial fields). Note that you do not need to have values for all species for a monitor to be considered valid, as each species is considered individually. However, the "EPA\_Flag" variable in the default "species for fractions" file has been set so that all monitor days that do not have complete species data are not used in the calculations (flag = 1). If the user wants to use the incomplete species data, the flag should be set to "0".
- *PM2.5 Monitor Data.* The total PM<sub>2.5</sub> data from FRM are used by SMAT-CE to calculate species fractions for point estimates (in conjunction with the interpolated speciation data from STN and IMPROVE monitors). The interpolated species data is used to calculate species fractions at FRM monitors (point estimates) and/or species fractions at all grid cells (spatial fields).

#### Monitor Data Years

Use the drop down menus to choose the three years of monitor data for the Annual  $PM_{2.5}$  Analysis. The SMAT-CE default is to use the three-year period 2010 to 2012. (That is, for both IMPROVE-STN and  $PM_{2.5}$  monitor data, the **Start Year** is *2010* and the **End Year** is *2012*.) The default period is based on a modeling year of 2011. The start and end years should be changed to applicable time periods, depending on the base modeling year.

SMAT-CE handles multiple years of data by calculating averages for each species by quarter and year. SMAT-CE then averages the quarterly values across the years (e.g., average quarter 1 values of SO<sub>4</sub> across two years to get a single "quarter 1" estimate). After completing this step, SMAT-CE will have four quarterly estimates for each species at each monitor. These quarterly values are then ready to be interpolated to FRM sites or to grid cell centroids in spatial fields.

#### Delete Specified Data Values

The default is to delete the observations specified by EPA. Valid data are given a value

of "0" and observations that should be deleted are given a value of "1" to "10". There is also an option for the user to flag data, using the same convention of "0" for valid data and "1" to "10" for data marked for deletion. If both the **EPA-specified** and **User-specified** flags are checked, then SMAT-CE deletes any observations that are marked for deletion by either the EPA or the user. These settings make it easy for the user to flag additional data for removal from the calculations (without deleting the actual record from the ambient data file). See Section 7.4.2 of the MATS User's Manual (Abt, 2014) for a description of the observational data flags.

#### Minimum Data Requirements

There are three sets of minimum data requirements for calculating design values:

- Minimum number of valid days per valid quarter. This is the minimum number of site-days per valid quarter. The default is 11 days, which corresponds to > 75% completeness for monitors on a 1-in-6 day monitoring schedule. This is the minimum number of samples that is routinely used in calculations of quarterly average concentrations.
- *Minimum number of valid quarters required for valid season*. This is the number of years of data (within the start year and end year specified) for which there are valid quarters for a given season. The default value is 1 year. If the value is set = 2, then there will need to be 2 years of valid data from quarter 1 in order for quarter one to be considered complete (and the same for the other 3 quarters).
- *Minimum number of valid seasons required for valid monitor (point and spatial fields calculation).* This is the number of valid seasons that are needed in order for a particular monitor's data to be considered valid. The default is 1 for IMPROVE-STN monitor data and the range is 1-4. For example, if the value is = 1, then a monitor's data will be used in the species fractions calculations if it has at least one valid season. If the value = 4, then the site must have all 4 seasons of valid data to be used. The default for PM<sub>2.5</sub> depends on whether the data are used in point calculations (default = 4) or spatial field calculations (default = 1).

Section 7.4.3 of the MATS User's Manual (Abt, 2014) shows an example of how the

minimum data requirements are used in calculating averages for monitoring data.

Clicking the Advanced box displays additional Species Fractions Calculations Options. The Species Fractions Calculation Options - Advanced screen allows you to make relatively advanced choices for your analysis. Generally speaking, the default options settings are consistent with the EPA modeling guidance document. One set of options allows you to specify the interpolation weighting that you want to use and whether the interpolation involves a maximum distance or not. The second set of options involves choices regarding ammonium, blank mass, and organic carbon. These options are described below.

Using Monitor Data to Calculate Species Fractions

The Using Monitor Data to Calculate Species Fractions panel sets how IMPROVE and STN speciated monitor data and ("unofficial") PM<sub>2.5</sub> monitor data will be used to calculate quarterly peak values. Three data filtering options are available to apply to the averaging calculations:

- Use Top X Percent of Daily Monitor Days. SMAT-CE uses the top "X" percent of days per quarter to calculate the quarterly peak values. Set the percent cutoff to use for this option.
- Use All Daily Monitor Values Greater than Fixed Amount (ug/m3). SMAT-CE averages all monitor values greater than or equal to a concentration cutoff. Set the concentration cutoff and the minimum number of days greater than or equal to the cutoff concentration. If there is an insufficient number of days, SMAT-CE will drop the data for that particular quarter.
- Use Top X Number of Daily Monitor Days. SMAT-CE averages the concentrations for the top "X" number of days per quarter. Set the number of days to use for this option.

These three filtering options work in essentially the same way for IMPROVE and STN speciated monitor data and for ("unofficial")  $PM_{2.5}$  monitor data. Section 7.5.1 of the MATS User's Manual (Abt, 2014) shows examples of how the data filters are used in calculating averages for monitoring data.

Note that the IMPROVE and STN speciated monitor data uses the "measured\_FM"

variable to identify peak days. Note also that it is possible that the option used to identify peak days (e.g., Use Top X Percent of Daily Monitor Days) does not give a unique set of days because a number of days may have the same value.

### Interpolation Options

The selections in this section set how SMAT-CE will interpolate, or combine, the values from different monitors. One approach is to use Inverse Distance Weights, which assigns a weight to any particular monitor that is inversely proportional to its distance from the point of interest. A second approach is Inverse Distance Squared Weights, which means that the weights are inversely proportional to the square of the distance. And the third approach is Equal Weighting of Monitors. The default approach for PM is Inverse Distance Squared Weights.

When interpolating monitor values, SMAT-CE identifies monitors based on their distance away from the point of interest (*e.g.*, the center of a grid cell). The first step in the interpolation process is to identify the monitors that are nearby, or neighbors, for each point of interest. The next step is to determine the distance (in kilometers) from the nearby monitors to the point of interest. The default approach is to include all valid monitors (*i.e.*, those that satisfy the three criteria in the Species Fractions Calculation Options panel), regardless of distance. To limit the use of monitors based on distance, type in the distance in km (e.g., 100) next to the pollutant of interest. Note that a distance of one hundred (100) kilometers means that any monitors further than 100 kilometers can no longer be used in the interpolation. If a point of interest has no monitors within the specified distance, then no value is calculated.

The Miscellaneous Options panel sets the following options for SMAT-CE:

## Ammonium

Specify whether to use degree of neutralization (DON) values to calculate ammonium (NH4) or to use measured ammonium in conjunction with an assumption about the percentage of NH4 that evaporates. The default option is to use DON values. To use measured ammonium, click the button and choose a NH4 percentage evaporating (e.g., 50). The default is "0", which assumes that no ammonium evaporates from the FRM filters.

### Default Blank Mass

The Default Blank Mass option sets default blank mass to the desired level. The default

is 0.5. Either type in or use the arrows to increase or decrease the value.

## Organic Carbon

Set the "floor" and the "ceiling" for the mass balance calculation for organic carbon.

# Run the Eastern U.S. Example

Use the default settings for the Species Fraction Options for the Eastern U.S. example project. Either click Next or double-click the PM2.5 Calculation Options button in the upper left-hand panel of Daily PM Analysis window. The button next to Species Fraction Options will turn from yellow to green, indicating that this step is complete.

# 7.4.1. PM2.5 Calculation Options

File • Analysis • Data Viewer Expand Viewer DataError-Checking S	Start Page
Daily PM Analysis	
Choose Desired Output     Output Choices-Advanced     Data Input     Species Fraction Options	
PM2.5 Calculation Options     Model Data Options	Name Running Messages
PM2.5 Calculation Options	
PM2.5 Monitor Data Years	
Start Year 2009 ~ End Year 2013 ~	
Valid FRM Monitors	
Minimum Number of Design Value Periods 1	
Required Design Value Periods	
None selected Select	
NH4 Future Calculation	
<ul> <li>Calculate future year NH4 using base year (constant) DON values</li> </ul>	
- Calculate future year NH4 using base yearNH4 and the	
Clear Save Project & Run Save Project	< >>

Figure 7-6. PM2.5 Calculation Options for Daily PM2.5 Analysis

The **PM2.5 Calculation Options** window shown in Figure 7-6 sets the particular years of monitor data to use from the input file specified in the **Data Input** window. The following options are available in this window.

## PM2.5 Monitor Data Years

The Start Year and End Year drop-down menu options list the years of available official

PM monitor data to use in the calculation of future  $PM_{2.5}$  design values. The default approach in SMAT-CE is to use five years of data.

SMAT-CE provides the option to use "official" design values, which are generally recommended, or to choose "custom" design values. The custom design values option requires the specification of the minimum number of observation days in each quarter and the minimum number of quarters to produce valid design values.

## Valid FRM Monitors

By default, SMAT-CE assumes that there only needs to be one design value for a monitor to be considered valid. In addition, SMAT-CE assumes that no particular design value is required, so different monitors with different years of data could be used.

For example, a start year and end year as 2005 and 2009 gives potential 3-year design values of 2005-2007, 2006-2008, and 2007-2009. When the Minimum Number of Design Values is set to 1, one monitor could have data for, say, 2005-2007 and another monitor data for 2006-2008, and both monitors would be used. A Minimum Number of Design Values setting of 2 would only use monitors that have design values for two of the three design value periods, ignoring monitors that only have design values for a single period.

## NH4 Future Calculation

SMAT-CE can forecast NH<sub>4</sub> in two different ways. The default approach uses base year DON values. See Section 7.1.2.4 of the MATS User's Manual for details on the forms of the two equations that are available to forecast NH<sub>4</sub>.

# Run the Eastern U.S. Example

Use the default settings for the PM<sub>2.5</sub> Calculation Options for the Eastern U.S. example project. Either click Next or double-click the **Model Data Options** button in the upper left-hand panel of **Daily PM Analysis** window. The button next to **PM<sub>2.5</sub> Calculation Options** will turn from yellow to green, indicating that this step is complete.

# 7.5. Model Data Options

File * Analysis * Data Viewer Expand Viewer S	ingle Source Impa	ict Analysis 🔹 Start Pag	e
Daily PM Analysis     Choose Desired Output     Output Choices-Advanced     Data Input	<b>B B</b>		
Species Fraction Options     PM2.5 Calculation Options     Model Data Options		Name	Running Messages
Model Data Options	0		
Temporal Adjustment at Monitor		<b>^</b>	
Grid for Point Forecast 1x1 👻			
Grid for Spatial Forecast 1x1 -			
Statistic Mean 👻			
Advanced Options: RRF Model Values Used			
RRF-model values used			
• Use top X percent of daily model days	10		
<ul> <li>Use all daily model values greater than fixed amount(ug/m3)</li> </ul>	0		
Minimum number of days required above	1	-	
	<b>* *</b>		
Clear Save Project & Run	Back Next Save Project		4

Figure 7-7. Model Data Options for Daily PM2.5 Analysis

The **Model Data Options** window shown in Figure 7-7. This window sets the temporal adjustments for each monitor:

#### Temporal Adjustment at Monitor

This option specifies how many model grid cells to use in the calculation of RRFs for point estimates and for spatial estimates. A drop down menu provides options to use 1x1, 3x3, 5x5, and 7x7 arrays of model grid cells. The default for a 12 kilometer by 12 kilometer grid is to use a 3x3 array of grid cells. The U.S. EPA Draft Modeling Guidance for Attainment of Air Quality Goals for Ozone, PM<sub>2.5</sub>, and Regional Haze (U.S. EPA, 2014) includes discussion on selecting the appropriate grid call array size for different model resolutions.

Note that for PM analyses, SMAT-CE calculates **mean** concentrations across the grid cell array (as compared to maximum concentrations used for ozone analyses).

#### Advanced Options: RRF Model Values Used

This option allows presents three different ways to calculate quarterly peak modeled values: (1) the top X percent of daily model days, (2) all daily model values greater than

or equal to a specified amount, and (3) the top X number of model days. The three options are described in Section 7.4: Species Fractions Calculation Options - Advanced. SMAT-CE determines the peak modeled days by sorting the PM<sub>2.5</sub> concentrations in the baseline model data input file.

# Run the Eastern U.S. Example

Use the default settings for the Model Data Options for the Eastern U.S. example project. Either click **Next**, which will bring up a window prompting to "Save & Run Project" or click the **Save Project & Run** button at the bottom of the SMAT-CE window. The Daily PM<sub>2.5</sub> Analysis project may also be saved without running SMAT-CE by clicking the **Save Project** button. A file explorer window will request a filename to which the project settings will be saved to a \*.proj file. This file can be loaded later to restart the analysis.

For the Eastern U.S. example, choosing to save and run the Daily PM<sub>2.5</sub> Analysis project. A file explorer window will request a filename (\*.proj) to which to save the project settings. While the Analysis is running, the icon next to **Model Data Options** will turn to a running status and status messages will be displayed in the **Log & Msg** tab on the right panel of the SMAT-CE main window (Figure 7-8).

File • Analysis • Data Viewer Expand Viewer	Single Source Impact	Analysis 🔹 Start Page	
Daily PM Analysis			
Choose Desired Output     Output Choices-Advanced     Data Input     Species Fraction Options		C Log/Msg	
PM2.5 Calculation Options		Name	Running Messages
		Daily PM	Start SMAT-CE 0.29 run 2013/11/26 11:5 Set up model data: D:\Program Files (x86)\SMA
Model Data Options	•		
Temporal Adjustment at Monitor	Tip		
Grid for Point Forecast 1x1	Bunn	ing project	
Grid for Spatial Forecast 1x1		e wait!	
Statistic Mean			
Advanced Options: RRF Model Values Used	E		
RRF-model values used			
Output Sector Content of Conte	10		
<ul> <li>Use all daily model values greater than fixed amount(ug/m3)</li> </ul>	d O	J	
Minimum number of days required above	1		
	Back Next		
Clear Save Project & Run	Save Project	•	

Figure 7-8. Daily PM25 Analysis run status

When the Daily PM2.5 Analysis is completed, the Data Viewer will automatically display in the SMAT-CE main window (Figure 7-9). The Output Files section of the Data Viewer left panel will display all of output files selected in the **Choose Desired Output** and **Output Choices-Advanced** Daily PM<sub>2.5</sub> Analysis windows.

The Data Viewer provides options to display the Daily  $PM_{2.5}$  Analysis results as maps, bar charts, and tables. <u>Chapter 10</u> describes how to load and analyze data using the SMAT-CE Data Viewer.


Figure 7-9. Daily PM Analysis Data Viewer

This concludes the chapter on the SMAT-CE Daily PM<sub>2.5</sub> Analysis. As described in this section, details of the calculations and settings used in this analysis are available in the U.S. EPA Draft Modeling Guidance for Attainment of Air Quality Goals for Ozone, PM<sub>2.5</sub>, and Regional Haze (U.S. EPA, 2014) and in Section 7 of the MATS User's Manual (Abt, 2014).

# 8. Ozone Analysis

SMAT-CE can forecast design values at ozone monitor locations -- these forecasts are referred to as Point Estimates. SMAT-CE can also use a variety of approaches to calculate design values for a Spatial Field. A Spatial Field refers to a set of values comprising calculations for each grid cell in a modeling domain from Eulerian grid models such as CMAQ and CAMx.

The Ozone Design Value Analysis in SMAT-CE is organized into four steps. The steps include the input/output and configuration options for computing ozone design values. The following four configuration steps correspond to different SMAT-CE windows and are described in detail in this chapter:

- <u>Choose Desired Output</u>. Select point estimates, spatial field estimates, or both.
- <u>Data Input</u>. Specify the air quality modeling and ambient monitoring data to use for the design value calculations. Specify which model grid cells will be used when calculating RRFs at monitor locations.
- <u>Filtering Interpolation</u>. Select the monitoring data years, identify valid monitors, and define the interpolation approach to use when calculating a Spatial Field.
- **<u>RRF and Spatial Gradient</u>**. Specify the daily ozone values to use in the calculation of RRFs and Spatial Gradients.

File * Analysis * Data Viewer Expand Viewer Single Source Impact A	nalysis + Start Page
Ozone Analysis       Desired Output       Data Input       Filtering/Interpolation       RRF/Spatial Gradient	Log/Msg
	Name Running Messages
Choose Desired Output	
Project Name:	
Point Estimates	
Forecast	
Temporally-adjust ozone levels at monitors	
Quarterly model data	
Output quarterly average model data file.	
Spatial Field	
Interpolate monitor data to spatial field. Temporally adjust. (VNA)	
□ Interpolate gradient-adjusted monitor data to spatial field. Temporally adjust. (eVNA)	
Back Next	
Clear Save Project & Run Save Project	۲ <u></u>

Figure 8-1. Ozone Analysis initial window

To conduct an attainment test for the ozone  $(O_3)$  NAAQS, select **Ozone Analysis** from the Process Data module on the SMAT-CE Start Page. Figure 8-1 shows the initial window that is displayed when Ozone Analysis is selected. The box in the upper left of the window (highlighted in red in Figure 8-1) lists the configuration steps of the Ozone Analysis. Each step listed in this box has a different set of configuration options that are displayed in the Ozone Analysis window. Once each step is successfully configured, the yellow icons next to each step in the box will change from yellow to green. In general, the configuration steps must be followed in order, from top to bottom, as they are listed in the box. Previously completed steps may be accessed and modified by double clicking on the step name in the box. Once the configuration for a step is complete, you may move to the next step by either clicking on it or by selecting the Next button (shown in the blue box in Figure 8-1).

A previous project may be loaded or a new project may be initiated at any time in the Ozone Analysis window by selecting one of the icons to the right of the "Ozone Analysis" text above the red box in Figure 8-1.

Each of the Ozone Analysis configuration steps are described in the following sections.

## 8.1. Desired Output

File * Analysis * Data Viewer Expand Viewer DataError-Checking	g BenMAP 🔹 Single Source Impact Analysis 👻 USA 👻 Start Page
👩 Ozone Analysis 📃 関	0
Desired Output	
Data Input     Filtering/Interpolation	
RRF/Spatial Gradient	
	Running Messages
Desired Output 2	
Project Name:	
Point Estimates	
Forecast	E
Forecast ozone design values at monitors	
Quarterly model data	
Output used model data file	
Spatial Field	
Interpolate monitor data to spatial field. Base year and Future year (VNA)	
Interpolate gradient-adjusted monitor data to spatial field. Base year and Future year (eVNA)	
•••••	
Clear Save Project & Run Save Project	۲

Figure 8-2. Choose Desired Output for Ozone Analysis

**Choose Desired Output** is the first configuration step that is displayed when the Ozone Analysis module is selected (Figure 8-2). The blue hyperlinked text in this window brings up the documentation for this configuration step. SMAT-CE supports design value calculations as Point Estimates, which refer to forecasts made at fixed locations, such as monitors. SMAT-CE can also generate Spatial Fields, which refer to air pollution estimates made at the center of each grid cell in a specified model domain. The Spatial Field estimates can be baseline estimates or forecasts, generated with or without a gradient adjustment.

The settings in this step include:

## **Project Name**

Text string to identify this analysis and set the name of the project file.

## **Point Estimates**

The calculation of Point Estimates, or future-year ozone levels at monitors, has several steps. The first step is to calculate the baseline value as a function of up to three design

values. The second step is to use model data to temporally adjust the baseline value. For details of these calculations see the U.S. EPA Draft Modeling Guidance for Attainment of Air Quality Goals for Ozone, PM<sub>2.5</sub>, and Regional Haze (U.S. EPA, 2014).

• *Baseline Ozone*. The baseline ozone design value is the simple average of design values, where the average carries one significant figure to the right of the decimal point. Generally, design value years should match the modeling data being used. The EPA modeling guidance recommends using an average of the 3 design values periods which straddle the emissions base year. For example, if the modeled emissions base year is 2007, then design values from 2005-2007, 2006-2008, and 2007-2009 should be used to compute the baseline ozone. An average of design values is, in effect, a weighted average of annual averages -- 2007 is "weighted" three times, 2006 and 2008 are weighted twice, and 2005 and 2009 are weighted once. This creates a 5-year weighted average design value which is used to project future air quality levels.

The default design value years in SMAT-CE are the periods 2009-2013, which assumes a model base year of 2011.

• *Temporally Adjusted Ozone*. The first step in temporally adjusting baseline ozone involves identifying the model grid cells near the monitor site. Next, SMAT-CE calculates the average of daily 8-hour average maximum model values for both the baseline and future-year model runs, and then takes the ratio of the two to calculate the RRF. Finally, SMAT-CE calculates the future-year design value by multiplying the RRF with the baseline design value measured at the monitor.

The equation for temporally adjusting baseline ozone is as follows:

$$Monitor_{i,future} = Monitor_i * RRF_i$$

where:

*Monitor*<sub>*i*, *future*</sub> = future-year ozone design value at monitor site i, measured in parts per billion (ppb)

 $Monitor_i$  = baseline ozone design value at monitor site i, measured in ppb  $RRF_i$  = relative response factor at monitor site i. The RRF is the ratio of the future 8-hour daily maximum concentration predicted near a monitor (averaged over multiple days) to the baseline 8-hour daily maximum concentration predicted near the monitor (averaged over the same days).

Selecting **Forecast ozone design values at monitors** configures SMAT-CE to generate future year design values at each monitor in the modeling domain.

#### **Quarterly Model Data**

Directs SMAT-CE to calculate and output quarterly averaged modeled Ozone data from daily model data input to the system. SMAT-CE requires two types of data input: ambient monitor data and gridded model output data. For the annual Ozone calculations, SMAT-CE will accept either SMAT-CE formatted daily average gridded model files or quarterly average files. If daily average model files are used as inputs, SMAT-CE will calculate quarterly averages from the daily averages and optionally output the quarterly average concentrations into text files (CSV files). The quarterly average text files can then be re-used in subsequent SMAT-CE analyses. Quarterly average input files are smaller and run faster than daily average files.

#### **Spatial Field**

A Spatial Field refers to air pollution estimates made at the center of each grid cell in a specified model domain. For example, SMAT-CE may be configured to calculate ozone design values for each grid cell in a modeling domain.

SMAT-CE calculates two types of ozone-related Spatial Fields:

• Interpolate monitor data to spatial field. Base year and Future year (VNA). This is an interpolation of baseline monitor values at each grid cell, including temporal adjustments to a specified future year. SMAT-CE identifies the "neighbor" monitors for each grid cell and then calculates an inverse-distance-weighted average of the monitor values at each grid cell. The future year forecasts are derived by multiplying the baseline spatial fields with RRFs at each monitor.

Checking this option will interpolate the data for both the base and future years. Upon selecting this option, additional selections become available to interpolate the monitor values for either the "Base only" or "Future only". • Interpolate gradient-adjusted monitor data to spatial field. Base year and *Future year (eVNA)*. This is an interpolation of model-adjusted baseline monitor values at each grid cell, including temporal adjustments to a specified future year. SMAT-CE identifies the "neighbor" monitors for each grid cell, it adjusts the monitor values to account for the modeled spatial gradient, and then calculates an inverse-distance weighted average of the monitor values. The future year forecasts are derived by multiplying the gradient-adjusted baseline spatial fields with RRFs at each monitor.

Checking this option will interpolate the data for both the base and future years. Upon selecting this option, additional selections become available to interpolate the monitor values for either the "Base only" or "Future only".

Selecting each of the interpolation options produce additional configure

Details of the interpolation calculations are available in Section 9.1.3 of the SMAT-CE User's Manual (Abt, 2014).

#### <u>Neighbor File</u>

Selecting "Spatial Field" directs SMAT-CE to produce files of "nearest neighbor" data for the VNA interpolation scheme. The data include the distance to neighbor monitors and weights used to do the interpolations. This option will generate information for each monitor (for point analyses) or each grid cell (for spatial fields) for each quarter and for each species.

#### Actions on Run Completion

Checking the "Automatically extract all selected output files" box will export CSV files of all selected output to a separate folder named with the Project Name in the SMAT "\Result\Output" folder. The results may also be exported later from the **Data Viewer**.

#### **Design Value Periods**

Normally, SMAT-CE will output one set of files covering the entire analysis period specified by the user. The outputs represent the averages of the values for each 3-year design value period. If the "Output all design value periods" option is checked, SMAT-CE will produce discrete outputs for each design value period. The output files will include a period identifier (e.g., "Period 1", "Period 2") inserted into the file name.

Checking this option will increase the SMAT-CE run time by up to four times.

## **Base & Future Design Values**

The maximum design values are based on the highest future year value from the three design value periods. These values can be output by checking the "Output Max Design Values" option. The output file will include "maximum forecast" inserted into the file name.

## 8.1.1. Run the Eastern U.S. Example

Use the default settings for these options for the Eastern U.S. example project. Either click Next or double-click the **Data Input** button in the upper left-hand panel of the **Ozone Analysis** window. The button next to **Desired Output** will turn from yellow to green, indicating that this step is complete.

## 8.2. Data Input

File • Analysis • Data Viewer Expand Viewer DataError-Checking E	SenMAP 🔹 Single Source Impact Analysis 🔹 USA 👻 Start Page
Ozone Analysis     Image: Constraint of the second se	Log/Msg
	Running Messages
Data Input	
Monitor Data	
Ozone Data MATS_OZONE_DV_2012_V2_off.csv	
Model Data	
Input From CMAQ	
Baseline File O3_small_USA_12km_2011.csv	
Forecast File O3_small_USA_12km_2018.csv	
Using Model Data	
Temporal adjustment at monitor	
3x3   Maximum-paired in space	
Back         Next           Clear         Save Project & Run         Save Project	<

## Figure 8-3. Data Input for Ozone Analysis

The **Data Input** configuration step sets the ambient O<sub>3</sub> monitor data and the gridded model output data to use for the SMAT-CE project (Figure 8-3). This step also sets the model grid cells to use for calculating RRFs at the monitor locations.

SMAT-CE is pre-loaded with ozone design values at U.S. monitors for the period from

2002-2017. It is also distributed with example ozone model data for 2001 and 2018.

The blue hyperlinked text in this window brings up the documentation for this configuration step. The settings in this step include:

## **Monitor Data**

Monitor data should be in the form of a simple text file. The first row specifies the nature or frequency of the data (e.g., Design Value or Day). The second row presents comma-separated variable names. The third row begins the data values. **Error! Reference source not found.** shows the format of the ozone monitor data for input to SMAT-CE.

Variable	Description
_ID	The ID is a unique name for each monitor in a
	particular location. The default value is the AIRS ID.
	(This is a character variable.)
_TYPE	Leave this blank.
LAT	Latitude in decimal degrees. Values in the northern
	hemisphere are positive, and those in the southern
	hemisphere are negative
LONG	Longitude in decimal degrees. Values in the eastern
	hemisphere are positive, and those in the western
	hemisphere (e.g., United States) are negative.
DATE	The time period of the monitor observation. As a
	convention, the date represents the last year of the
	three-year design value period (e.g., 2001 represents
	the 1999-2001 design value).
O3	Observed monitor value. Note that missing values are
	represented by a minus nine (-9).
_STATE_NAME	State name. (This is a character variable.)
_COUNTY_NAME	County name. (This is a character variable.)

 Table 8-1. Ozone monitor data format

## <u>Model Data</u>

SMAT-CE requires model data in the form of a text file. A forthcoming feature will support reading CMAQ output files directly; the **Input from CMAQ** option is currently greyed out in SMAT-CE. To compute RRFs and future year design values, SMAT-CE requires text files of Baseline and Forecast (future) ozone concentrations. The first row of these text files specifies the frequency of the data (e.g., Day or Hour). The second row presents comma-separated variable names. The third row begins the data values. For design value calculations, the ozone model data must be daily 8-hour average maximum concentrations in each grid cell. lists the file format and descriptions of the variables in the ozone model data file.

Variable	Description
_ID	The ID is a unique number for each model grid cell in
	the air quality model domain. It is generally based on
	the column and row identifiers from the air quality
	modeling domain. The default convention is to
	calculate the ID by multiplying the column identifier by
	one thousand (1000) and adding the row identifier.
	(This is a character variable.)
_TYPE	Leave this blank.
LAT	Latitude in decimal degrees. Values in the northern
	hemisphere are positive, and those in the southern
	hemisphere are negative.
LONG	Longitude in decimal degrees. Values in the eastern
	hemisphere are positive, and those in the western
	hemisphere (e.g., United States) are negative.
DATE	The time period of the monitor observation. As a
	convention, the date represents the last year of the

Table 8-2. Ozone modeling data format

	three-year design value period (e.g., 2001 represents
	the 1999-2001 design value).
O3	Modeled ozone concentration in the form of an 8-hour
	average daily maximum. Note that missing values are
	represented by a minus nine (-9).

## **Using Model Data**

The RRF for a monitor is calculated from "nearby" model grid cells. For purposes of this calculation, a monitor is assumed to be at the center of the cell in which it is located, and this cell is at the center of an array of "nearby" cells. The number of cells considered "nearby" a monitor is a function of the size of the grid cells used in the modeling. In the example case of a 12 km grid, EPA uses as a default 3x3 array of grid cells. See the U.S. EPA Draft Modeling Guidance for Attainment of Air Quality Goals for Ozone, PM<sub>2.5</sub>, and Regional Haze (U.S. EPA, 2014) for details on how model data arrays are used in the design value calculation.

With the array size determined, SMAT-CE provides three options for how the modeling data are extracted from array:

- *Maximum*. For each day of modeling data, SMAT-CE will identify the highest 8-hour daily maximum among the grid cells in the chosen array. In the case of a 3x3 array, SMAT-CE will identify the highest daily 8-hour average maximum from among the nine "nearby" grid cells for each day and for each monitor site.
- Mean. For each day of modeling data, SMAT-CE will average the 8-hour daily values for the grid cells in the chosen array. In the case of a 3x3 array, SMAT-CE will average nine values.
- *Maximum-paired in space*. For each day of modeling data, SMAT-CE will identify the grid cell with the highest 8-hour daily maximum in the chosen array in the baseline file, and calculate the RRF using the same grid cell in the control file.

The default choice for the ozone analysis in SMAT-CE is to use the maximum-paired

in space option to calculate temporally-adjusted ozone concentrations at each monitor. For monitors located on the border of a modeling domain where it may not be possible to have a full array of grid cells, SMAT-CE uses as much available modeling data as possible to fill the array.

See section 9.2.3.1 of the SMAT-CE User's Manual (Abt, 2014) for examples of how the matrix of grid cells are used to compute RRFs and ozone design values.

## Run the Eastern U.S. Example

Use the default settings for these options for the Eastern U.S. example project. Either click Next or double-click the **Filtering/Interpolation** button in the upper left-hand panel of the **Ozone Analysis** window. The button next to **Data Input** will turn from yellow to green, indicating that this step is complete.

## 8.3. Filtering/Interpolation

File - Analysis - Data Viewer Expand Viewer DataError-Checking S	tart Page
🔂 Ozone Analysis 📃 📙	
Desired Output	
Data Input     Filtering/Interpolation	
RRF/Spatial Gradient	
	Name Running Messages
Filtering/Interpolation 0	
Choose Ozone Design Values	
Start Year 2009-2011 V End Year 2011-2013 V	
Valid Ozone Monitors	
Minimum Number of Design Values 1	
Required Design Values	
None selected Select	
Default Interpolation Method	
Inverse Distance Weights	
check to set a maximum interpolation distance[km]	
Back Next	
Clear Save Project & Run Save Project	< >>

## Figure 8-4. Filtering/Interpolation for Ozone Analysis

The **Filtering and Interpolation** window (Figure 8-4) identifies the years of monitor data to use for calculating RRFs, sets the monitors to use in the analysis, and specifies the interpolation method to use when calculating spatial fields.

The blue hyperlinked text in this window brings up the documentation for this

configuration step. The settings in this step include:

#### **Choose Ozone Design Values**

Setting the Start Year and the End Year defines the range of the ozone design values that will be used in the calculation of the baseline ozone level. You can vary the number of design values used in this calculation. The default in SMAT-CE is to use a 5-year design value period (three design values) centered on the 2011 base year. A base year of 2011 uses the following design value periods: 2009-2011, 2010-2012, and 2011-2013. The Start Year is set to 2009-2011 and the End Year is set to 2011-2013.

#### Valid Ozone Monitors

MATS provides two choices for identifying monitors that are "valid" and thus included in your analysis:

- *Minimum Number of Design Values*. Specifies the minimum number of design value periods that need to be included in the calculation of the baseline ozone design value (1, 2, or 3). The default option is to require the one design value be available in the specified range of dates.
- *Required Design Values*. Specifies whether a particular design value period needs to be valid for the calculations to be performed at that monitor. The default option is *None Selected*.

#### **Default Interpolation Method**

The Default Interpolation Method sets the interpolation method to use for combining the values from different monitors. One approach is to use *Inverse Distance Weights* such that the weight given to any particular monitor is inversely proportional to its distance from the point of interest. A second approach is *Inverse Distance Squared Weights*, in which the weights are inversely proportional to the square of the distance. And the third approach is *Equal Weighting of Monitors*. The default approach for ozone is Inverse Distance Weights.

The first step in the interpolation process is to identify the monitors that are nearby, or neighbors, for each point of interest. The next step is to determine the distance from the nearby monitors to the point of interest. The default approach in SMAT-CE is to include all valid monitors (i.e., those that satisfy the two criteria under **Valid Ozone Monitors**),

regardless of distance. If you want to limit the use of monitors based on distance, select *check to set a maximum interpolation distance*, and then specify a distance (in kilometers). A distance of one hundred (100) kilometers means that any monitors more than 100 kilometers from the point of interest can no longer be used in the interpolation. If a point of interest has no monitors within the specified distance, then no value is calculated. The default is to leave this box unchecked.

The interpolation method option is only used when generating estimates for Spatial Field. Since the ozone analysis only uses point estimates, the interpolation method is not active.

## 8.4. RRF/Spatial Gradient

In calculating an ozone RRF or a Spatial Gradient not all of the model data are typically used. In the case of RRFs, daily values falling below specified thresholds can be excluded from the calculation. In the case of a spatial gradient, SMAT-CE may be setup to follow the same thresholds as used for point estimates. If a valid result is needed in all grid cells a Backstop minimum threshold can be used. A sub-range of days to be included in the RRF calculation may also be specified along with whether to pair the days by high concentration rather than by date. SMAT-CE can also average a user-specified range of values to calculate gradient adjustments.

The blue hyperlinked text in this window brings up the documentation for this configuration step. The settings in this step include:

#### <u>RRF Setup</u>

The RRF Setup involves four variables that specify the thresholds and the numbers of days above the thresholds -- *Initial threshold value*; *Minimum number of days in baseline at or above threshold*; *Minimum allowable threshold value*; and *Min number of days at or above minimum allowable threshold*.

The first step in calculating the RRF is to determine the days to use in the RRF calculation. Select to either use the highest concentration days (i.e., a specified number of highest ozone days) or the number of days above a concentration threshold. If the number of days is above the Minimum number of days in baseline at or above threshold,

then SMAT-CE averages the 8-hour values for those grid cells with at least this concentration.

SMAT-CE performs the following steps in calculating RRFs:

 In the case of a 3x3 array, SMAT-CE identifies the highest daily 8-hour average maximum from among the nine "nearby" grid cells for each day and for each monitor site. In the case where there are 90 days of model outputs, SMAT-CE generates 90 daily values.

SMAT-CE can do this calculation separately for the baseline and future-year scenarios. If you chose an option other than "Maximum – paired in space" under the **Data Input** menu, two different grid cells in the baseline and future-year might be used to represent a given day.

- If the *Top X modeled ozone days* option is selected, SMAT-CE will select the specified number of days based on their ranking by value and date. If there are fewer days above the minimum allowable threshold than specified, then the monitor site will be dropped. Otherwise the selected days will be used in computing the RRF.
- If the *Initial threshold value* option is selected, SMAT-CE will find the days with concentrations above the specified threshold and average the concentrations across all of the selected days. The *Minimum number of days in baseline at or above threshold* setting is used to set the minimum number days required for a valid calculation. If SMAT-CE does not find the minimum number of days above the specified threshold, it will lower the threshold concentration by 1 ppb to try to meet the minimum number of days is met.
- The default *Minimum allowable threshold value* in SMAT-CE is 60 ppb. If there are fewer days with concentrations above this threshold value than is set by the *Min number of days at or above minimum allowable threshold*, then the monitor site will be dropped from the RRF calculations. The SMAT-CE default setting for the Min number of days at or above minimum allowable threshold is 5.

SMAT-CE checks the daily 8-hour maxima calculated for the baseline scenario, and sets to missing any daily value falling below the minimum allowable concentration threshold. For all days set to missing in the baseline scenario, SMAT-CE also sets the corresponding day in the future-year scenario to missing.

- By enabling the *Backstop minimum threshold for spatial fields*, a lower bound concentration is set for the iterative lowering of the minimum concentration when SMAT-CE is trying to meet the minimum number of days criteria in the RRF calculation. The backstop threshold is only used for grid cells which do not have enough days above the minimum allowable threshold concentration to meet the minimum number of days criteria. The backstop threshold does not change the calculation for grid cells that already meet the minimum number of days.
- SMAT-CE also supports using date ranges to define an ozone season to use for RRF calculations. The *Subrange first day of ozone season used in RRF* and *Subrange last day of ozone season used in RRF* set the start day and end day of the subrange based on a count of the number of days from the first day in the modeled ozone concentration file. For example, if the model files contained data for June 1 through August 30, a subrange start and end day of "31" and "61" respectively would specify the period for July 1 through July 31.
- The *Pair days based on high concentration instead of date* option is available for simulations in which the future year meteorology is different than the base year (such as climate modeling). SMAT-CE will pair the future year highest concentrations with the highest concentrations in the base year file, regardless of date. The number of days in the RRF will continue to be based on the threshold variables. For example, if eleven days are greater than the selected threshold in the base year, then the RRF will be calculated based on the eleven highest base and future year concentration days.
- For each monitor site, SMAT-CE averages the non-missing daily values for the baseline and future-year scenarios, and then calculates the RRF as the ratio of the future-year average concentration to the baseline average concentration.

#### **Spatial Gradient Setup**

In using a spatial gradient to estimate ozone levels, SMAT-CE estimates ozone levels in unmonitored locations by using the values of nearby monitored data scaled by a ratio of model values. The ratio, or spatial gradient, is a mean of model values at the unmonitored location over the mean of the model values at a monitor.

Note that several "nearby" monitors (and their associated model values) are used in the calculation of ozone values at an unmonitored location. SMAT-CE uses a process called Voronoi Neighbor Averaging (VNA) to identify these neighbors, and then takes an inverse distance-weighted average of these monitors.

SMAT-CE sorts the daily 8-hour maximum ozone values from high to low, averages a certain number of these values (by default the top five), and then uses these averages in the calculation of the spatial gradient. Note that the highest days for Cell A and Cell E are determined independently of each other.

To select a different set of days for the gradient adjustment, set the Start Value and End Value. SMAT-CE assigns an index value of 1 to the highest daily 8-hour maximum ozone value in each grid cell, the second-highest an index value of 2, etc. Use the Start Value and the End Value to identify the values to average by using these indices.

Since point estimates are currently only available for ozone design values in SMAT-CE, the Spatial Gradient Setup option is not active.

Detailed examples of the RRF calculations are available in Section 9.4.1 of the MATS User's Manual (Abt, 2014).

#### Run the Eastern U.S. Example

Use the default settings for the RRF/Spatial Gradient options for the Eastern U.S. example project. Either click **Next**, which will bring up a window prompting to "Save & Run Project" or click the **Save Project & Run** button at the bottom of the SMAT-CE window.

The Ozone Analysis project may also be saved without running SMAT-CE by clicking the **Save Project** button. A file explorer window will request a filename to which the project settings will be saved to a \*.proj file. This file can be loaded later to restart the analysis. For the Eastern U.S. example, select save and run for the Ozone Analysis project. A file explorer window will request a filename (\*.proj) to which to save the project settings. While the Analysis is running, the icon next to **Model Data Options** will turn to a running status and status messages will be displayed in the **Log & Msg** tab on the right panel of the SMAT-CE main window (Figure 8-5).

File * Analysis * Data Viewer Expand Viewer	· Single Source Impact	Analysis * Start Page	
Ozone Analysis Contemporation Contem		Log/Msg Name Ozone	Running Messages Start SMAT-CE 0.29 run 2013/11/25 17:1
	0		Setting up run structure
RRF/Spatial Gradient RRF Setup		6	Finish reading monitor data: 0 s.
Initial threshold value (ppb) Minimum number of days in baseline at or abov threshold	Plea	ning project se wait!	
Minimum allowable threshold value Min number of days at or above minimum allow threshold	vable 5		
🔲 Enable backstop minimum threshold for sp	atial fields		
Backstop minimum threshold for spatial fields Subrange first day of ozone season used in RRF	60		
Subrange last day of ozone season used in RRF		-	
Clear Save Project & Run	Back Next	•	m •

Figure 8-5. Ozone Analysis run status

When the Ozone Analysis is completed, the Data Viewer will automatically display in the SMAT-CE main window (Figure 8-6). The Output Files section of the Data Viewer left panel will display all of output files selected in the **Desired Output** Ozone Analysis window.

The Data Viewer provides options to display the Ozone Analysis results as maps, bar charts, and tables. <u>Chapter 10</u> describes how to load and analyze data using the SMAT-CE Data Viewer.

Data Viewer	Ozone (double-click/right-click files in left panel to view data & map)
<ul> <li>Project Name</li> <li>Ozone</li> <li>Output Files</li> <li>Monitors monitor data, temporally adj</li> <li>Baseline Quarterly Avg Model Data</li> <li>Future Quarterly Avg Model Data</li> <li>Monitors county high monitoring sites,</li> <li>Log &amp; Msg</li> <li>Log &amp; Msg</li> <li>Configuration &amp; Batch File</li> <li>Configuration &amp; Batch File</li> </ul>	Ozone Start SMAT-CE 0.29 run 2013/11/26 12:02:42     Setting up run structure     Finish reading monitor data: 0 s
Load Extract All Extract Selected Output for BenMAP Link to BenMAP	۲ ۳

## Figure 8-6.Ozone Analysis data viewer

This concludes the chapter on the SMAT-CE Ozone Analysis. As described in this section, details of the calculations and settings used in this analysis are available in the U.S. EPA Draft Modeling Guidance for Attainment of Air Quality Goals for Ozone, PM<sub>2.5</sub>, and Regional Haze (U.S. EPA, 2014) and in Chapter 9 of the MATS User's Manual (Abt, 2014).

# 9. Visibility Analysis

SMAT-CE can calculate baseline and future-year visibility levels for the best and worst days for Class I Areas -- these estimates are referred to as Point Estimates, as they refer to particular locations.

The Visibility Analysis in SMAT-CE is organized into three steps. The steps include the input/output and configuration options for conducting visibility analysis. The following configuration steps correspond to different SMAT-CE windows and are described in detail in this chapter:

- <u>Choose Desired Output</u>. Select whether to calculate Point Estimates at IMPROVE monitors or at Class I Area centroids and whether to use the old or new version of the IMPROVE visibility equation.
- **Data Input**. Specify the species monitoring data, species fractions file, PM<sub>2.5</sub> ambient monitoring data, and the modeling data to use for the design value calculations.
- <u>Filtering</u>.

Refer to the EPA Visibility and Regional Haze<sup>1</sup> webpage for the latest guidance and data related to Visibility Analysis.

<sup>&</sup>lt;sup>1</sup> https://www.epa.gov/visibility

File • Analysis • Data Viewer Expand Viewer Single Source Impact A	analysis * Start Page
Choose Desired Output Data Input Filtering	Log/Msg
	Name Running Messages
Choose Desired Output	
Point Estimates	
Project Name:	
Forecast	
Temporally-adjust visibility levels at Class I Areas	
IMPROVE Algorithm	
○ Use old version	
<ul> <li>Use model grid cells at monitor</li> </ul>	
<ul> <li>Ose model grid cells at Class 1 area centroid</li> </ul>	
Actions on run completion	
Automatically avtract all calacted autout files	
Clear Save Project & Run Save Project	K

Figure 9-1. Visibility Analysis initial window

To conduct a visibility analysis, select **Visibility Analysis** from the Process Data module on the SMAT-CE Start Page. Figure 9-1 shows the initial window that is displayed when Visibility Analysis is selected. The box in the upper left of the window lists the configuration steps of the Visibility Analysis. Each step listed in this box has a different set of configuration options that are displayed in the Visibility Analysis window. Once each step is successfully configured, the icons next to each step in the box will change from yellow to green. In general, the configuration steps must be followed in order, from top to bottom, as they are listed in the box. Previously completed steps may be accessed and modified by double clicking on the step name in the box. Once the configuration for a step is complete, you may move to the next step by either clicking on it or by selecting the Next button.

A previous project may be loaded or a new project may be initiated at any time in the Visibility Analysis window by selecting one of the icons to the right of the "Visibility Analysis" text shown in Figure 9-1.

Each of the Visibility Analysis configuration steps are described in the following sections.

## 9.1. Choose Desired Output



Figure 9-2. Choose Desired Output for Visibility Analysis

**Choose Desired Output** is the first configuration step that is displayed when the Visibility Analysis module is selected (Figure 9-2). The blue hyperlinked text in this window brings up the documentation for this configuration step. The settings in this step include:

## **Project Name**

Text string to identify this analysis and set the name of the project file.

## **Forecast**

SMAT-CE produces a forecast of visibility in Class I Areas through the following steps:

Identify best & worst visibility monitor days in Base Model Year. Use monitored total extinction data from a user-specified year to identify the 20% best (B20) and 20% worst (W20) visibility days at each Class I area. At this stage SMAT-CE is using extinction values (measured in Mm<sup>-1</sup>). By the end of this series of calculations, SMAT-CE will convert these extinction visibility measures to deciviews.

Note that you specify the particular year, the Base Model Year, from the

available monitoring data in the Filtering window. SMAT-CE labels the year of monitoring data as the Base Model Year, because this particular year of monitor data matches the baseline model data, specified in the Data Input window.

- Average best & worst baseline model days. Using baseline speciated model data (specified in the Data Input window), average the B20 visibility days and then average the W20 visibility days at each Class I areas (matched with the ambient data). The model data comes into SMAT-CE as speciated values with units in ug/m<sup>3</sup>. These data are averaged to produce speciated baseline concentrations for the B20 and W20 days with units of ug/m<sup>3</sup>.
- Average best & worst forecast model days. Calculate these same averages for the forecast model data (specified in the Data Input window). Identify the same B20 and W20 days from the model results and then average the speciated model data (reported in ug/m<sup>3</sup>). These data are averaged to produce speciated forecast (future) concentrations for the B20 and W20 days with units of ug/m<sup>3</sup>.
- *Calculate RRFs.* Use the speciated B20 and W20 averages from the baseline and forecast model data to calculate B20 and W20 RRFs for each species at each Class I area. The B20 RRF is simply the ratio of the baseline B20 average to the forecast B20 average. The result of this step will be two unitless RRFs for each species at each Class I area.
- Identify best & worst visibility days in other monitored years. Using the monitored total extinction, identify the B20 visibility days and the W20 visibility days from the other available years of monitoring data. The default in SMAT-CE is that there should be at least three valid years and one of those years should be the base modeling year (the base meteorological year). (Monitor validity is discussed further in the section on the Visibility Analysis Filtering window.)

Note that the B20 days will occur on a different set of days for each year; similarly, the W20 days will occur on a different set of days for each year.

• Multiply RRFs with speciated monitor data from each year. Multiply the species specific B20 RRF (unitless) with the B20 daily speciated monitor

values (measured in  $ug/m^3$ ) from each of the available years. Do analogous calculations for the W20 days.

Note that the RRF is based on best/worst days identified from the base model year. This same "Base Model Year" RRF is used with all of the valid monitor years. For example, if the Base Model Year is 2001, then the RRF developed from 2001 modeling data will be applied to all valid monitoring data in the five year period surrounding the model year.

- *Convert ug/m<sup>3</sup> values to daily extinction values and sum to get total extinction.* For each day in each valid monitor year (for both the baseline and forecast), use either the new or old IMPROVE equation to estimate daily total extinction (measured in Mm<sup>-1</sup>). After this calculation, there will be a set of total extinction values for B20 and W20 days in each valid year for both the baseline and the forecast.
- Convert extinction to deciviews. For each valid year in both the baseline and forecast, convert the B20 and W20 daily averages from Mm<sup>-1</sup> to deciviews. The formula for this conversion is as follows:

Deciviews =  $10*\ln(\text{extinction}/10)$ 

- Average daily B20 days and W20 days. For each valid year, average the daily deciview values from the B20 visibility days and calculate the same average for the W20 visibility days. There will be up to five "best" averages and "worst" total visibility measures (measured in deciviews) for both the baseline and the forecast.
- *Calculate final average*. Average the valid B20 and W20 yearly visibility measures. The final result will be a single "best" value and a single "worst" deciview estimate at each Class I Area for both the baseline and forecast.

Additional details of the visibility forecasting approach using by SMAT-CE, including the forms of the new and old IMPROVE equations, are available in the U.S. EPA Draft Modeling Guidance for Attainment of Air Quality Goals for Ozone, PM<sub>2.5</sub>, and Regional Haze (U.S. EPA, 2014) and in Section 11.1.2 of the MATS User's Manual (Abt, 2014).

SMAT-CE includes two options for how model data are selected for the visibility RRF calculation. When forecasting visibility, SMAT-CE can calculate RRFs from model data at either the grid cell containing the monitor or at the centroid of the Class I Area. Monitors assigned to represent a Class I Area are generally close to the Class I Area. However, in some cases, this distance can be substantial. For example, the YELL2 monitor in Wyoming (44.5653 latitude, -110.4002 longitude) is located more than a degree longitude away from the Red Rocks Lake Class I Area (44.64 latitude, -111.78 longitude). By default, SMAT-CE uses model data at the monitor.

#### Actions on Run Completion

By checking Automatically extract all selected output files SMAT-CE will generate the following five output files:

- Visibility forecast (average of design values). (Up to) five year average of forecasted and base-year average visibility. When Use model grid cells at monitor is selected, the name of this output file is "Forecasted Visibility Data.csv" with the Scenario Name appended at the beginning. When Use model grid cells at Class 1 area centroid is selected the name of this output file is "Forecasted Visibility Data for Class 1 Areas.csv" plus the Scenario Name.
- Visibility forecast (all design values). Forecasted and base-year values for individual years. The name of this file is "Forecasted Visibility – all design values.csv" plus the Scenario Name.
- Class I areas and the monitors. The list of all of the Class I areas and the monitors assigned to each. The name of this file is "Class 1 Area and IMPROVE Monitor Identifiers and Locations.csv" plus the Scenario Name.
- Base-year model data. The base year model values for PM species for the grid cells and days used in the RRF calculations. The name of this file is: "Used Model Grid Cells Base Data.csv" plus the Scenario Name.
- Future-year model data. This future year model values for PM species for the grid cells and days used in the RRF calculations. The name of this file is: "Used Model Grid Cells - Future Data.csv" plus the Scenario Name.

The formats of these output files are detailed in Section 11.1.3. of the MATS User's

## Manual (Abt, 2014).

## Run the Eastern U.S. Example

Use the default settings for these options for the Eastern U.S. example project. Either click Next or double-click the **Data Input** button in the upper left-hand panel of the **Visibility Analysis** window. The button next to **Choose Desired Output** will turn from yellow to green, indicating that this step is complete.

## 9.2. Data Input



Figure 9-3. Data Input for Visibility Analysis

The **Data Input** window (Figure 9-3) sets the monitor and model data files to use for the SMAT-CE visibility forecasts. It also includes a specification for how SMAT-CE will average the model data for the RRF calculation. The blue hyperlinked text in this window brings up the documentation for this configuration step. The settings in this step include:

## **Monitor Data**

Daily monitor data of speciated aerosol concentrations (ug/m<sup>3</sup>) and visibility (Mm<sup>-1</sup>) measures are available from the Federal Land Manager Environmental Database

website<sup>2</sup>. These monitor data are used to: (1) identify the B20 and W20 visibility days for a given year; and (2) calculate the 5-year baseline conditions.

Note that one IMPROVE monitor is associated with each Class I site, and the calculated visibility for the IMPROVE site is assumed to representative of the Class I site. SMAT-CE comes with a default cross-walk that it uses for IMPROVE monitors and Class I Areas.

SMAT-CE is distributed with monitored species concentrations (ug/m<sup>3</sup>) along with extinction (Mm<sup>-1</sup>) and deciview estimates for the period 2000 to 2012. SMAT-CE uses these data to project concentrations and extinctions for the observed species AMM\_SO4, AMM\_NO3, OMC, EC, CRUSTAL, and CM. The monitored data files include the variable GOOD\_YEAR, which indicates whether a particular monitor should be used for a given year. A value of "1" means the monitor can be used, and a value of "0" means that the monitor should be dropped for the year.

The monitor data variable GROUP identifies the percentile for the overall visibility level for a particular day. A value of "90" means that the particular day is among the 20 percent worst days for the year. A value of "10" means that the particular day is among the 20 percent best days for that year. (Days with other GROUP values are not needed) There are a number of extra variables in the ambient data input file that are not directly used by SMAT-CE (such as extinction values). These additional data can be used to QA the SMAT-CE output or for additional data analysis.

SMAT-CE can use two different types of IMPROVE monitor data:

- IMPROVE Monitor Data Old Algorithm. Monitor data needed for calculating extinction with the old IMPROVE algorithm. Section 11.2.1.1 of the MATS User's Manual (Abt, 2014) includes a description of the file format.
- IMPROVE Monitor Data New Algorithm. Monitor data needed for calculating extinction with the new IMPROVE algorithm. Section 11.2.1.2 of the MATS User's Manual (Abt, 2014) includes a description of the file format.

<sup>&</sup>lt;sup>2</sup> http://views.cira.colostate.edu/fed/

#### Model Data

Model data for the B20 and W20 visibility days are used to calculate RRFs, which provide an estimate of the relative change in visibility from the baseline conditions to a future year. The monitor data are used to identify the B20 and W20 days. SMAT-CE will match the best and worst measured days to the correct modeled days, by date. The model data input to SMAT-CE are PM species concentrations (ug/m<sup>3</sup>).

See Section 11.2.2 of the MATS User's Manual (Abt, 2014) for a description of the required modeled data file format.

#### **Using Model Data**

For the *Temporal adjustment at monitor* setting select the matrix of model grid cells to use in the RRF calculation (1x1 matrix, 3x3 matrix, etc). SMAT-CE will average the concentrations in the selected matrix to use for the RRF calculation.

RRFs are then calculated for the species sulfate, nitrate, EC, OMC, Crustal, and Coarse Matter (CM) by taking the ratio of the average of the B20 or W20 days in the future to the average corresponding B20 or W20 days in the baseline. For example, when calculating the sulfate RRF for the B20 days, SMAT-CE does the following calculation:

$$RRF_{Sulfate,j} = \frac{\frac{1}{n}\sum_{i=1}^{n}Sulfate_{future,j,i}}{\frac{1}{n}\sum_{i=1}^{n}Sulfate_{baseline,j,i}}$$

where,

$$j = \text{Class I area}$$

i = day

n = number of B20 days

Sulfate = modeled sulfate concentration  $(ug/m^3)$  on B20 days

When identifying the model data for this calculation, SMAT-CE first selects the model values located at either the monitor or at the centroid of the Class I Area, based on the setting in the Choose Desired Output window.

#### Run the Eastern U.S. Example

Use the default settings for these options for the Eastern U.S. example project. Either click Next or double-click the **Filtering** button in the upper left-hand panel of the

**Visibility Analysis** window. The button next to **Data Input** will turn from yellow to green, indicating that this step is complete.

## 9.3. Filtering

File • Analysis • Da	ta Viewer Expand Viewer	Single Source Impact /	Analysis 🔹 Start Pag	e	
Gaze Visibility	y Analysis				
Choose Desired	d Output		Cog/Msg		
			Name	Running Messages	1
Filtering		0			
Choose Visibility Dat	ta Years				
Start Monitor Year	2005 •				
End Monitor Year	2009 •				
Base Model Year	2007 •				
Valid Visibility Moni	tors				
Minimum years req	uired for a valid monitor 3				
		Back Next			
Clear	Save Project & Run	Save Project	•	Ш	4

Figure 9-4. Filtering for Visibility Analysis

The **Filtering** window (Figure 9-4) sets the years of monitor and model data to use in the visibility forecasts. It also sets criteria for a monitor to be included in the analysis. The blue hyperlinked text in this window brings up the documentation for this configuration step. The settings in this step include:

## **Choose Visibility Data Years**

SMAT-CE presents as a series of drop down menus the available years of monitor data that were loaded through the Data Input window. The *Start Monitor Year* and *End Monitor Year* drop-down menus set the range of years to use for the visibility calculations.

The *Base Model Year* drop-down menu sets the year to use in determining the B20 and W20 monitor days. The Base Model Year should correspond to the year of the model data and must fall within the range specified by the Start Monitor Year and End Monitor Year. After setting the Base Model Year, SMAT-CE identifies and saves for each

monitor the particular dates during this year that registered the best and worst visibility days. These dates are then used to identify the model values used in the calculation of RRFs for the temporal adjustment.

## Valid Visibility Monitors

The *Minimum years required for a valid monitor* sets the minimum number of years of data that a monitor must have to be included in the visibility analysis. SMAT-CE excludes from the analysis any monitors with fewer than the minimum years set here. The SMAT-CE default value is 3 years.

## Run the Eastern U.S. Example

Use the default settings for the Filtering options for the Eastern U.S. example project. Either click **Next**, which will bring up a window prompting to "Save & Run Project" or click the **Save Project & Run** button at the bottom of the SMAT-CE window.

The Visibility Analysis project may also be saved without running SMAT-CE by clicking the **Save Project** button. A file explorer window will request a filename to which the project settings will be saved to a \*.proj file. This file can be loaded later to restart the analysis.

For the Eastern U.S. example, select save and run for the Visibility Analysis project. A file explorer window will request a filename (\*.proj) to which to save the project settings. While the Analysis is running, the icon next to **Filtering** will turn to a running status and status messages will be displayed in the **Log & Msg** tab on the right panel of the SMAT-CE main window (Figure 9-5).

File * Analysis * Da	ta Viewer Expand Viewe 7 Analysis	r Single Source Impact	Analysis - Start Page	(	0
Choose Desired	l Output		C Log/Msg		
			Name	Running Messages	
			Visibility	Start SMAT-CE 0.29 run Starting Visibility Analysis	2013/11/25 19:1
Filtering		0		starting visionity vitalysis	
Choose Visibility Dat	ta Years	Tip			
Start Monitor Year	2005		ing project		
End Monitor Year	2009		se wait!		
Base Model Year	2007	1,		5	
Valid Visibility Moni	tors				
Minimum years req	uired for a valid monitor	3			
Clear	Save Project & Run	Back Next Save Project	10000 p.		
Cieai	Save Project & Run	Jave Project	•		•

Figure 9-5. Visibility Analysis run status

When the Visibility Analysis is completed, the Data Viewer will automatically display in the SMAT-CE main window (Figure 9-6). The Output Files section of the Data Viewer left panel will display all of output files selected in the **Choose Desired Output** Visibility Analysis window.

The Data Viewer provides options to display the Visibility Analysis results as maps, bar charts, and tables. <u>Chapter 10</u> describes how to load and analyze data using the SMAT-CE Data Viewer.

Data Viewer	Visibility (double-click/right-click files in left panel to view data & map)
	Map       GIS       Data       Chart       Log/Msg       Config/Bate         Name       Log Messages         Visibility       Starting Visibility Analysis         Starting Visibility Analysis         Finish reading monitor data: 2 s.         Finish computing geometry: 0 s.         Finish loading model data: 11 s.         Finish generating RRFs and computing forecast: 0 s.         Total SMAT-CE run time: 19 s.         Finish SMAT-CE run       2013/11/25 19:11:56
Output for BenMAP Link to BenMAP	4

Figure 9-6. Visibility Analysis data viewer

This concludes the chapter on the SMAT-CE Visibility Analysis. As described in this section, details of the calculations and settings used in this analysis are available in the U.S. EPA Draft Modeling Guidance for Attainment of Air Quality Goals for Ozone, PM<sub>2.5</sub>, and Regional Haze (U.S. EPA, 2014) and in Chapter 11 of the MATS User's Manual (Abt, 2014).

# **10.The SMAT-CE Data Viewer**

The SMAT-CE Data Viewer displays the results from completed attainment test analyses. The results may be displayed as maps, tables, and charts; or they may be exported to text files for use in external data processing programs. This section describes how to use and configure the Data Viewer for the different analyses supported by SMAT-CE.

## **10.1.** Starting the Data Viewer

The SMAT-CE Data Viewer (Figure 10-1) can be started in the following ways.

- From the SMAT-CE Start Page, click on **Data Viewer** in the Analyze/Visualize Data section of the window
- From any of the SMET-CE analysis windows, click on **Data Viewer** in the menu bar along the top of the window
- When a SMAT-CE analysis finishes, the Data Viewer window displays automatically



Figure 10-1. SMAT-CE Data Viewer

## 10.2. Starting an Analysis Session

To load results from a saved project, click on the **Load** button on the bottom left of the Data Viewer window and select a SMAT-CE project (\*.proj) file to load. The Data Viewer will then display the following selections in the left-hand filename window pane (Figure 10-2).



Figure 10-2. Data Viewer window with a completed project

**Project Name**. The name of the currently loaded project. Clicking on the project name will open the completed analysis window for the project. For example, if the loaded project is for an ozone attainment test, the Ozone Analysis window for that project will open upon clicking the project name in the Data Viewer filename menu.

<u>**Output Files**</u>. The list of the output files specified during configuration of the SMAT-CE analysis. The types of Output Files available depend on the type of analysis (PM, Ozone, or Visibility) and the output choices set in the Configuration File. Clicking on any of the output files will load the data into the Data Viewer graphical and tabular analysis modules.

Log & Msg. The SMAT-CE logging information generated during the currently loaded

project. Clicking on the Log & Msg menu item displays the steps used to create the SMAT-CE results and the time that the run completed (Figure 10-3).

File • Analysis • Data Viewer Expand Viewer	DataError-Checking BenMAP - Single Source Impact Analysis - USA - Start Page
Data Viewer	Annual PM Analysis
Name	(double-click/right-click files in left panel to view data & map)
Project Name     Annual PM     Output Files	GIS 👩 Map 🕞 Data 🧭 Chart 💽 Log/Msg 💽 Config/Batch
Annual PM25 Point Baseline Quarterly Avg Model Data Future Quarterly Avg Model Data Delta Quarterly Avg Model Data Quarterly Avg PM2.5 Monitors Quarterly Avg Speciated Monitors Quarterly Avg NH4_DON Monitors Quarterly Avg Spec Frac Point Quarterly PM25 Point Used Baseline Quarterly Avg Model Data Used Future Quarterly Avg Model Data Used Delta Quarterly Avg Model Data Used Seture Quarterly Avg Model Data Used Delta Quarterly Avg Model Data	Name       Log Messages         Annual PM       Start SMAT-CE 0.47 run       2015/6/10 18:16:57         Starting Annual PM Analysis       Read model data "PM_small_USA_12km_2011.csv".         Finish reading model data: 38 s.       Read model data "PM_small_USA_12km_2011.csv".         Finish reading model data: 38 s.       Read model data "PM_small_USA_12km_2018.csv".         Finish reading model data: 44 s.       Read official PM monitor data "official_annual-PM25_allFRM 121013.c         Finish reading official PM monitor data: 0 s.       Read unofficial PM monitor data: 0 s.         Read unofficial PM monitor data "PM25ForFractions2002to2012.csv".       Finish reading unofficial PM monitor data: 12 s.         Read species monitor data "SpeciesForFractions2002to2012.csv".       Finish reading species monitor data: 3 s.         Finish reading species monitor data: 3 s.       Finish interpolating FRM sites: 13 s.         Finish interpolating SJ,FRM data to grid. 0 s.       Finish interpolating Spatial Field: 0 s.         Finish interpolating Spatial Field: 0 s.       Total SMAT-CE run time: 143 s.         Finish SMAT-CE run time: 143 s.       Finish SMAT-CE run time: 143 s.
Load Extract All Extract Selected	C Fillish SWAPCE full 2013/0/10 10:15:20
○ VNA ⊚ eVNA Send to BenMAP-CE	۲

Figure 10-3. Log & Msg display window

<u>Configuration & Batch File</u>. The SMAT-CE batch script commands used to generate the results for the current project. Clicking on the Configuration & Batch File menu item displays the configuration settings for the project (Figure 10-4).



Figure 10-4. Configuration & Batch File display window.

## 10.3. Creating Data Displays

To examine the results from a completed SMAT-CE analysis, select one of the project Output Files in the left-hand pane of the Data Viewer window. Either double-click or right-click on one of the filenames to select for analysis. Different types of output files are displayed in the Data Viewer file list. The attainment test results will be named according to the form of the test: Annual PM25 Point, Daily PM25 Point, etc. The model data used in the attainment test will be have file names that end in "Model Data". The monitoring data used in the attainment test will have file names that end in "Monitors".

A right-click on a file name will display a pop-up menu with different analysis choices. For everything but model data, the menu will show: Add to GIS, View, and Extract (Figure 10-5). For the model data results, the right-click pop-up menu will show: Add to Map, Add to GIS, View, and Extract. Double-clicking on any data file will display the file data on the SMAT-CE GIS map and data table viewer (Figure 10-6).
🕖 Data Viewer	Annual PM Analysis
Annual PM Output Files Annual PM Output Files Annual PM25 Point Baseline Quarter Future Quarterly Uiew Delta Quarterly Extract Quarterly Avg PM2.5 Monitors Quarterly Avg Speciated Monitors Quarterly Avg Speciated Monitors Quarterly Avg Spec Frac Point Quarterly PM25 Point Used Baseline Quarterly Avg Model Data Used Future Quarterly Avg Model Data Used Future Quarterly Avg Model Data Used Delta Quarterly Avg Model Data Configuration & Batch File Configuration & Batch File	(double-click/right-click files in left panel to view data & map)
Load Extract All Extract Selected	Double-click legend to reset scale/color





Figure 10-6. Output files GIS map view

The Data Viewer window right-hand analysis pane includes the following six tabs that display different analysis and configuration settings for the current SMAT-CE project:

**<u>GIS</u>**. Open-source geographic information system (GIS) graphical interface for displaying SMAT-CE point analysis results at monitor locations. Multiple data layers may be added to the map and different attributes within each layer can be plotting in the GIS tab.

Map. Spatial tile plots of model output data used for estimating relative response factors.

Data. Tabulated display of the SMAT-CE input and output data.

Chart. Bar chart display of the SMAT-CE input and output data.

Log/Msg. Logging information generated during the currently loaded project

Config/Batch. Batch script commands used to generate the results for the current project

Details of how to display data in the analysis tabs and how to configure the plots in each tab are included in the following sections.

#### 10.4. GIS Window

The SMAT-CE GIS window displays the results of point analyses at monitor locations in the selected modeling domain. Example results available to view in the GIS window include base and future year design values, RRFs, and input monitor data.

To plot results in the GIS window either right-click on an output file name in the Data Viewer file list and select **Add to GIS** (Figure 10-5); or click on the GIS tab of the Data Viewer right-hand panel and then double click an output file on the file list. Alternatively, click on the  $\overrightarrow{P}$  on the GIS and Map Controls toolbar to load a saved data file into the GIS viewer. The GIS view will display the analysis results or input monitor data as a thematic map with a colored legend that uses a legend and color scale that are set according the minimum and maximum values of the loaded dataset (Figure 10-7).



Figure 10-7. SMAT-CE GIS window

The GIS map can be saved quickly by right-clicking anywhere in the map window and selecting one of the three options (Figure 10-8).



Figure 10-8. GIS map right-click menu

The configuration options available in the GIS window include:

<u>Zoom and Map Controls</u>. Shown in the red box in Figure 10-9, these options control zooming in/out and panning the map display, probing monitor values, exporting the map image, saving a shapefile of the results, and adding external shapefile data to the GIS map.

Laver Controls. Shown in the yellow box in Figure 10-9, these options control the SMAT-CE result layer attributes to display on the map, quick zooms to selected subregions (Zoom To), and boundary layer attributes to display on the map (Domain Selections). The Map Layers section of this area displays the different GIS layers shown on them. Right-clicking on any of the layers provides advanced configuration controls for the layer.

**Legend Controls.** Shown in the blue box in Figure 10-9, this option provides a quick adjustment of the GIS map legend levels. Double click the color bar to display the legend controls. The legend controls set the minimum and maximum values of the

legend and the individual colors on the scale. More detailed customization of the map display legend is available by double clicking a map layer in the Layer Controls section of the GIS window.



Figure 10-9. GIS window with highlighted map controls

#### 10.5. Map Window

The SMAT-CE Map window displays the results of model results at monitor locations in the modeling domain. Example results available to view in the Map window include base and future year model result used in the calculation of RRFs.

To plot results in the Map window either right-click on a *model data* output file name in the Data Viewer file list and select **Add to Map** (Figure 10-5); or click on the Map tab of the Data Viewer right-hand panel and then double click a *model data* output file on the file list. Note that if there is no option to view the data on the map (i.e., only Add to GIS is displayed) then the selected data are not compatible with the Map view. The Map view will display the analysis results as a tile plot map with a colored legend that uses a legend and color scale that are set according the minimum and maximum values of the loaded dataset (Figure 10-10).



Figure 10-10. SMAT-CE map window

The Map display can be saved quickly by right-clicking anywhere in the map and selecting one of the three options (Figure 10-11).



Figure 10-11. Map window with right click menu

The configuration options available in the GIS window include:

**Zoom and Map Controls**. Shown in the red box in Figure 10-12, these options control zooming in/out, adding county lines, exporting the map image, and overlaying monitor data on the map image.

**Legend Controls.** Shown in the blue box in Figure 10-12, this option adjusts the map legend levels. Double click the color bar to display the legend controls. The legend controls set the minimum and maximum values of the legend and the individual colors on the scale.



Figure 10-12. Map window with highlighted map controls

### **10.6.** Data Table Display

The SMAT-CE Data Table window displays the SMAT-CE input and output data in a tabulated format.

To plot results in the Data Table window either right-click on a file name in the Data Viewer file list and select **View** (Figure 10-5); or click on the Data tab of the Data Viewer right-hand panel and then double click a file on the file list. The Data view will display the analysis results as a table on the right-hand panel of the Data Viewer window (Figure 10-13).

🕖 Data Viewer	Annual PM An Annual PM	alysis			C	
Name  Project Name Annual PM  Output Files  Annual PM25 Point Baseline Quarterly Avg Model Data	(double-click/right-	Map Point	Data	Chart	ap)	Config/Bate
<ul> <li>Future Quarterly Avg Model Data</li> <li>Delta Quarterly Avg Model Data</li> <li>Quarterly Avg PM2.5 Monitors</li> <li>Quarterly Avg Speciated Monitors</li> <li>Quarterly Avg NH4_DON Monitors</li> <li>Quarterly Avg Spec Frac Point</li> <li>Quarterly PM25 Point</li> <li>Used Baseline Quarterly Avg Model Data</li> <li>Used Future Quarterly Avg Model Data</li> <li>Used Delta Quarterly Avg Model Data</li> <li>High County Sites</li> <li>Log &amp; Msg</li> <li>Qog &amp; Msg</li> <li>Configuration &amp; Batch File</li> <li>Configuration &amp; Batch File</li> </ul>	<ul> <li>b_pm25_ann_DV</li> <li>f_pm25_ann_DV</li> <li>b_blank_mass</li> <li>b_crustal_mass</li> <li>b_EC_mass</li> <li>b_NH4_mass</li> <li>b_Ocmb_mass</li> <li>b_SO4_mass</li> <li>b_N03_mass</li> <li>b_water_mass</li> <li>f_blank_mass</li> <li>f_crustal_mass</li> <li>f_EC_mass</li> <li>f_NH4_mass</li> </ul>		id 010030010 010270001 010331002 010491003 010550010 010690003 010730023 010731005 010731010 010732003 010890014 < □m	type FRM FRM FRM FRM FRM FRM FRM FRM FRM FRM	STATE_NAME Alabama Alabama Alabama Alabama Alabama Alabama Alabama Alabama Alabama Alabama Digits After Decima	
Load Extract All Extract Selected		Apply	Distand	ce from source t	Threshold (% of N to exclude recepto Show All	

Figure 10-13. SMAT-CE Data table window

The configuration and viewing options available in the Data window include:

<u>Variable Filtering</u>. Shown in the red box in Figure 10-14, the list shows the variables in the data table. Checking the boxes next to the variables and clicking "Apply" will filter out rows in the table where the values of the selected variable(s) are null (-9).

**Data Table.** Shown in the yellow box in Figure 10-14, the data table shows the tabulated results from the selected SMAT-CE data file. The table can be sorted by any of the columns by left-clicking on the column header.

**Data Precision and Export.** Shown in the blue box in Figure 10-14, this section of the data window sets the precision of the values in the table, exports the data to a CSV file, and removes the filtering selections.

💮 GIS 💮 Map	Data	Chart	Cog/Msg	Config/Batch		
Baseline Quarterly Peak Quantifiers that must be >= 0						
🔲 crustal	id	type	lat	long ^		
🔲 nh4	130139		39.946411	-107.14183		
so4	77165		41.840206	-115.23772		
ec	130140		40.054249	-107.15761		
no3	76165		41.818516	-115.38026		
oc	77164		41.733971	-115.20876		
✓ pm25 ☐ cm	76164		41.712311	-115.35108		
in cm	130138		39.838566	-107.12609		
	129139		39.934242	-107.28247		
	129138		39.826412	-107.26651		
	129121		37.992939	-107.00264		
	75165		41.796654	-115.52271 *		
	<			•		
		Dig	its After Decim	al Point: 4 🍦		
		Т	hreshold (% of I	NAAQS): 1		
Apply	Distance from source to exclude receptors (km): 100					
			Show All	Export		

Figure 10-14. Data window with highlighted configuration options

#### **10.7.** Chart Display

The SMAT-CE Chart window displays the SMAT-CE input and output data as bar charts. This type of display is useful for comparing data values, such as design values or observations, between monitors.

To plot results in the Chart window or click on the Chart tab of the Data Viewer righthand panel and then double click a file on the file list on the left-hand panel. The Chart view will display the analysis results as bars on the right-hand panel of the Data Viewer window (Figure 10-15).



Figure 10-15. SMAT-CE chart window

The configuration and viewing options available in the Chart window include:

**Type and Filter Selection.** Shown in the red box in Figure 10-16, two drop boxes include data variables and regions to include in the chart. Selecting from the **Type** menu will both display the selected variable in the Chart and filter the Data Detail list by the selected variable. Selecting from the **Filter** menu will display the selected region in the Chart and filter the Data Detail list by the selected region. One or both of the variables may be selected to filter the chart data. Note that the Filter (region) selection is not available for model data.

**Data Detail.** Shown in the yellow box in Figure 10-16, the Data Detail shows the tabulated results from the selected SMAT-CE data file. The table can be sorted by any of the columns by left-clicking on the column header. The check boxes in the first column may be used to select individual data rows to include in the Chart. After checking the rows to be plotted, use the "Apply" button to plot the selected rows in the Chart. The "Select All" box can be used to select/unselect all of the rows with one click. Use the Type menu (described above) to select the variable (column) to include in the Chart.

**<u>Chart.</u>** Shown in the blue box in Figure 10-16, this section of the Chart window displays the bar chart and includes options to configure the chart. The "Setting" button displays a window for configuring the chart title and axes, including axis titles and min/max ranges. Right-clicking on the chart will display a selection box with options to **Copy** the chart to the clipboard, export (**Save Image As**) an image of the chart, **Print** the chart, and zoom out (**Un-Zoom**) from the chart. The **Show Point Values** right-click option enables the values of a bar to be displayed when the mouse hovers over the bar. The **Change Title and Legend** right-click option enables customization of the variable names, title, and axes.

Zoom into sections of the chart by left-clicking and dragging a box over the chart region to highlight. Use the right-click menu to un-zoom.



Figure 10-16. Chart window with highlighted configuration options

114

#### **10.8.** The SMAT-CE Configuration File

Windows batch scripts can be used to run several SMAT-CE analyses in sequence. The batch script can string together a list of SMET-CE Configuration Files to define the settings for each analysis. The SMAT-CE Configuration File stores the configuration options for a completed SMAT Analysis. A Configuration File can be used to duplicate (re-run) a previously completed analysis or in a batch script to run in sequence with other analyses. The SMAT-CE Configuration Files (\*.cfg) files are saved in the \My SMAT-CE Files\Result\CFG directory.

An existing Configuration File can also be edited to generate a new set of results, without having to explicitly set each of the choices made in the previous Configuration. Stored Configuration Files can be used to run SMAT-CE in batch mode, for example to run several attainment test analyses using a single batch script.

To view a Configuration file from the Data Viewer, either double-click/right-click on the Configuration & Batch File name in the left-hand window pane (Figure 10-17) or left-click on the Config/Batch tab in the right-hand window pane.



Figure 10-17. Viewing a SMAT-CE configuration file

The Configuration file contents will be displayed in the Config/Batch window (Figure

10-18). Clicking the **Edit** button in the lower-right corner of this window enables editing of the configuration file contents. Click three times on the configuration line to make some changes to the file. After editing the Configuration File, click the **Export** button to save it as a new configuration file. The \*.cfg file can also be edited outside of SMAT-CE using a text editor.

<u>Section 5.3</u> describes how to use Configuration Files in a batch script to run several SMAT-CE analyses in sequence.

Data Viewer	Annual PM Analysis
Annual PM  Annual PM  Annual PM  Annual PM  Annual PM  Annual PM  Annual PM25 Point  Baseline Quarterly Avg Model Data  Future Quarterly Avg Model Data  Quarterly Avg PM2.5 Monitors  Quarterly Avg PM2.5 Monitors  Quarterly Avg Speciated Monitors  Quarterly Avg Spec Frac Point  Quarterly PM25 Point  Used Baseline Quarterly Avg Model Data Used Future Quarterly Avg Model Data Used Future Quarterly Avg Model Data Used Delta Quarterly Avg Model Data Used Delta Quarterly Avg Model Data Used Delta Quarterly Avg Model Data Used Future Quarterly Avg Model Data Used Delta Quarterly Avg Model Data Used Msg  Log & Msg  Configuration & Batch File Configuration & Batch File  Muture Configuration & Batch File  Muture Configuration & Batch File Configuration & Sento BenMAP-CE	(double-click/right-click files in left panel to view data & map)

Figure 10-18. SMAT-CE Configuration File view

#### 10.9. Exporting Data from SMAT-CE

Output data from the SMAT-CE analyses can be exported to text files. Data export is most relevant to the Output Files (as opposed to the Configuration & Batch/Log & Msg Files), which can be viewed and manipulated in external data analysis programs such as Excel. SMAT-CE generates .CSV files that import cleanly into spreadsheets and database programs.

The easiest way to export data from SMAT-CE is in the analysis windows. By checking the box "Automatically Extract All Selected Output Files" on the initial window of a

SMAT-CE analysis (the same window where the Project Name is set), SMAT-CE will automatically output the result to .CSV files. Alternatively, the Data Viewer includes options to export the SMAT-CE results.

The **Extract All** button at the bottom of the left-hand window pane in the Data Viewer will initiate an export of the SMAT-CE results. A pop-up window will display for setting a root output filename and directory path.

To export an individual file, right click on the filename, and choose the *Extract* option, or click the **Extract Selected** button on the bottom left panel of the main window. A pop-up window will display for setting the output filename and directory path.

# **11.Getting Help**

Support for SMAT-CE is available from the <u>CMAS Center</u>.

## **12.References**

- Abt, Associates, Inc. 2014. "Modeled Attainment Test Software: User's Manual". Prepared for Office of Air Quality Planning and Standards, U.S. EPA. Research Triangle Park, NC.
- U.S. EPA. 2014. "Memorandum: Draft Modeling Guidance for Demonstrating Attainment of Air Quality Goals for Ozone, PM<sub>2.5</sub>, and Regional Haze". From Richard Wayland, Division Director – Air Quality Assessment Division, U.S. EPA. Research Triangle Park, NC.