Response Surface Model – Visualization Analysis Tool (RSM-VAT) User's Manual

Software version 2.3

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Acknowledgements

In cooperation with the U.S. EPA, the Institute for the Environment at the University of North Carolina at Chapel Hill (UNC-IE) along with the Tsinghua University, and the South China University of Technology (SCUT) developed the RSM-VAT software. This project was funded by the U.S. EPA under contract EP-D-12-044 to UNC-IE.

Table of Contents

List of Tables

List of Figures

1 Introduction

RSM-VAT is a tool that takes the CMAQ modeling results as input data, then builds up a "real-time" response between air pollution emission reductions and air pollutant concentrations using statistical techniques (e.g., polynomial fitting method or a maximum likelihood estimation – experimental best linear unbiased predictors). It allows for an instantaneous calculation of the change in ambient concentration resulting from the changes of emissions within a predefined set of sources, locations, and precursor emission types. This response is helpful for policymakers to decide on the best scenario alternative to achieve the attainment of air quality standards.

1.1 Evaluation Process of RSM-VAT

The definition of the CMAQ-based Response Surface Model, its processe is listed as:

(1) A set of control factors are selected based on the decision requirement;

(2) A emission control matrix design is delivered through a Hammersley quasi-random Sequence Sampling (HSS) or a Latin Hypercube Sampling (LHS) method;

(3) A base-year emission inventory is scaled with the emission control matrix, and forming emission control scenarios for CMAQ model runs. These emission inventory factors, together with the identical meteorology and other model input, are applied in CMAQ model to get finally CMAQ simulations.

(4) A great amount of CMAQ simulations are used for non-linear statistics with Polynomial Functions;

(5) The reliability of the created RSM is validated through Cross Validation and Out-of-sample Validation.

1.2 Who Can Use RSM-VAT?

RSM-VAT can be used by a wide range of persons, including scientists, policy analysts, and decision-makers. Less experienced users apply RSM to better understand and analyze the established statistical relationship between air pollution emission reductions and air pollutant concentrations. Most end users (policymakers) would directly use the RSM data analysis module for policy decisions. Advanced users can explore a wide range of advanced options. For example, performing a series of advanced visualization and analysis functions for validating RSM prediction results; Examining the nonlinear interactions among multiple air pollutant precursors and instantly generating the air pollutant concentration surface response to air pollutant emission changes.

In a word, RSM-VAT can be used in the following aspects:

➢**Strategy design and assessment screening tool**

- Comparison of urban vs. regional emission controls
- Comparison across emission controls of different sectors (e.g., industry, transportation and civil sources)
- Comparison across emission controls of different pollutants (e.g., NOx, SO_2, NH_3, VOCs, $PM_{2.5}$)

➢**Optimization**

- Can be used to identity the key emission factors and develop optimal combinations of controls to attain standards at minimum cost

➢**"What If?" Analyses**

- Provide real-time predictions of air quality model responses to emission and inputs
- Quickly provide insights into questions for policy design, e.g. does is it matter whether regional controls are put in place before local controls?
- What emission reduction is more effective for achieving the targeted air quality?
- Which emission source has a greater impact on air quality?
- What is the most effective emission reduction strategy for improving air quality?

➢**Model Sensitivity**

- Can be used to systematically evaluate the relative sensitivity of modeled ozone and PM concentrations to changes in emissions/meteorology inputs

1.3 Computer Requirements

RSM-VAT requires a computer with:

➢ .Net Framework Version 4.0 or higher.

➢ 32-bit or 64-bit Windows 7/Windows 8/Windows 10.

➢ 2 GB RAM or greater.

➢ 10 GB free disk space or greater.

1.4 Installing/Uninstalling RSM-VAT

1.4.1 Installing RSM-VAT

Download RSM-VAT Software Package (e.g., RSM-VAT 2.3.exe) and corresponding example data (e.g., RSM-VAT 2.3 Data.exe) from the ABaCAS website or Google Drive. They are available at the following links:

(1) ABaCAS website:

http://abacas.see.scut.edu.cn/tools.

(2) Google Drive:

https://drive.google.com/open?id=1Xl3VqtlRXeBt_FrfHpuCZYumxjqMR9hL.

➢ Double click the package to start the installation.

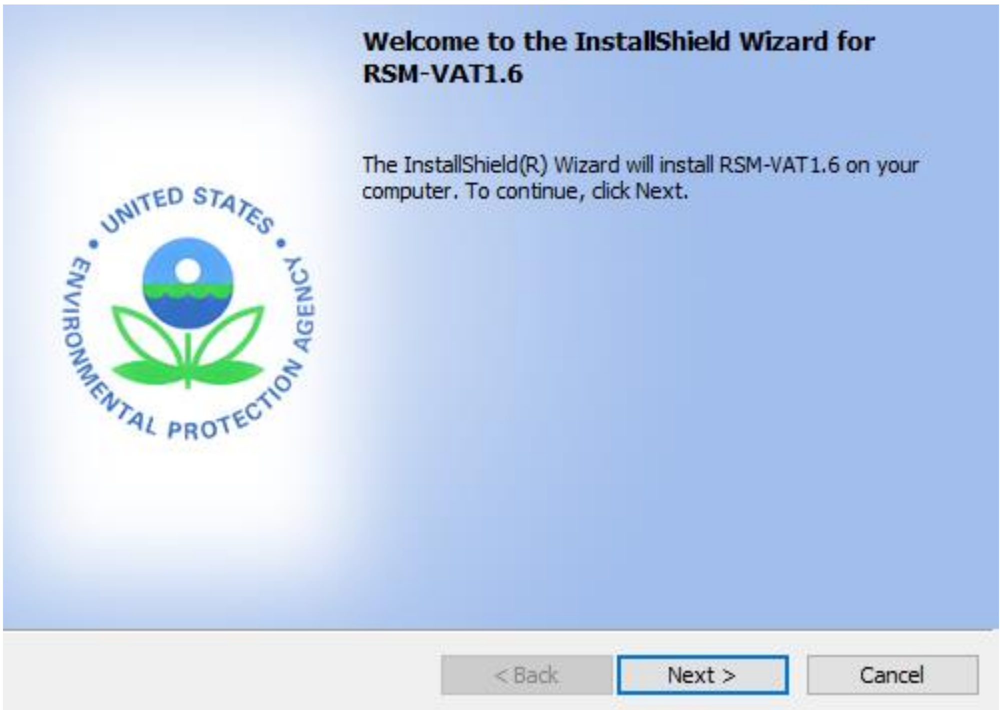


Fig. 1 Setup Window

➢ Click the "**Next**" button, to use the default install location as shown in Fig. 2.

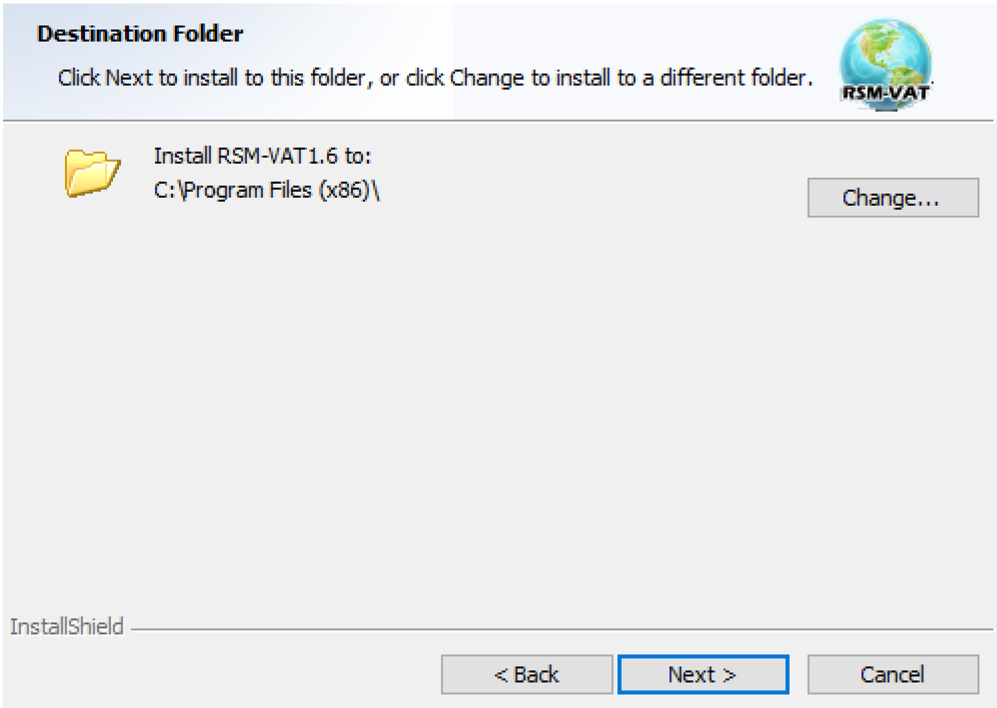


Fig. 2 Choose Install Location

➢ Click the "**Next**" button, it will show the "Ready to Install" window as shown in Fig. 3.

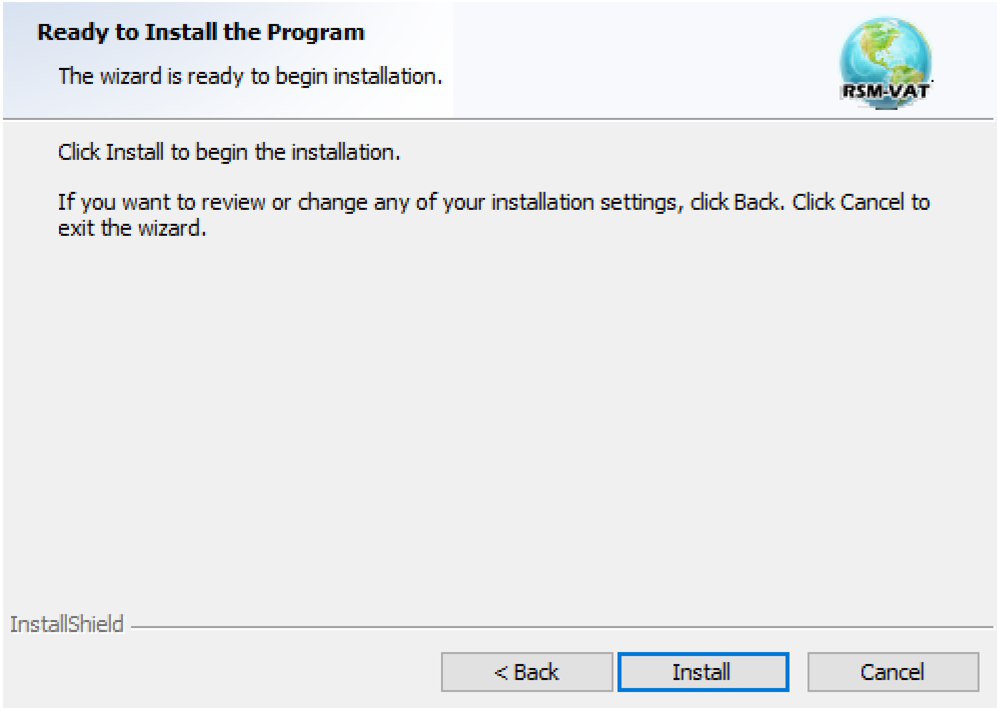


Fig. 3 Ready to Install

➢ Click the "**Install**" button, Fig. 4 shows the installation process of RSM-VAT.

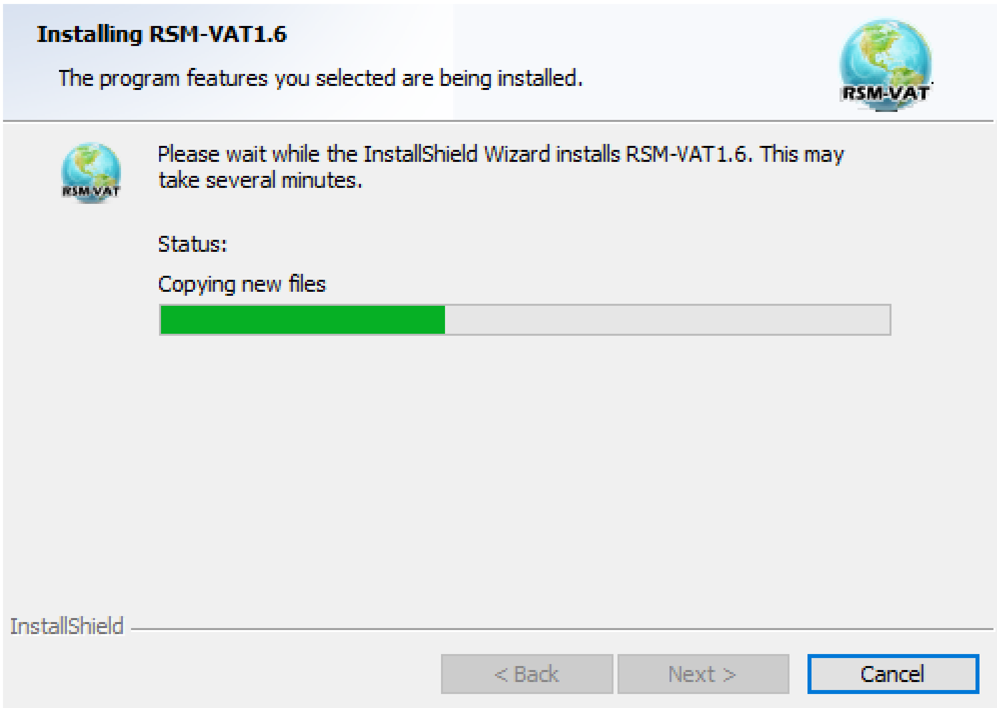


Fig. 4 Installation Process

➢ Click the "**Finish**" button and complete installation.

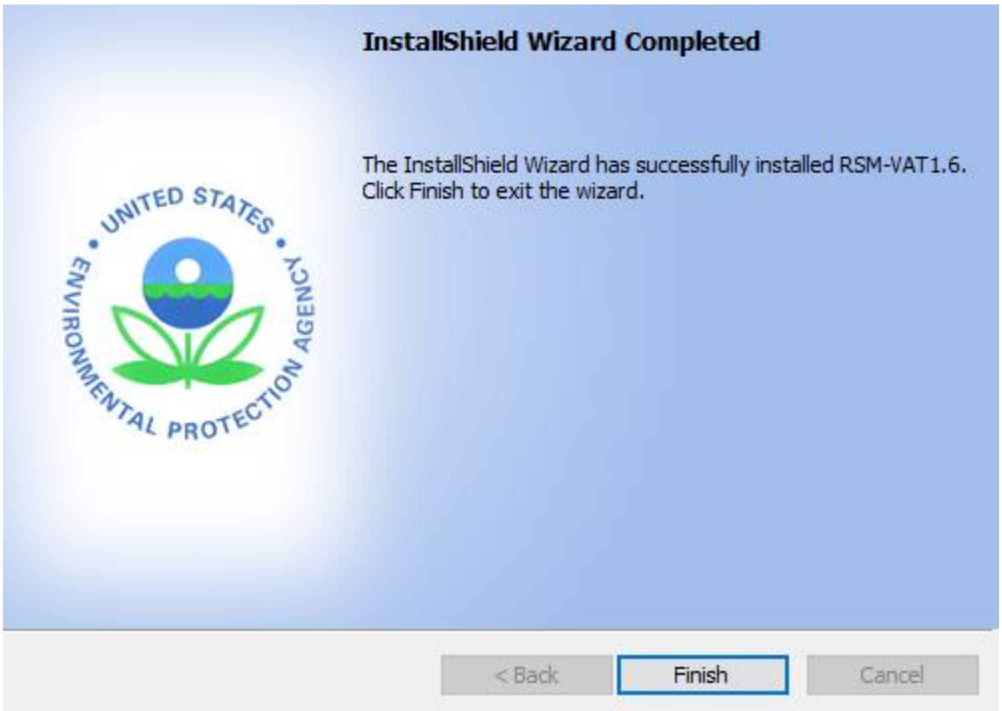


Fig. 5 Complete Installation

1.4.2 RSM-VAT Data Extraction

After finished installation, please extract the RSM-VAT self-extracting example data executable file. Double click self-extracting executable file to unzip it to My Documents directory under \My Documents\My RSM-VAT Files\Data* to replace the old Data folder, as shown in the following figure.

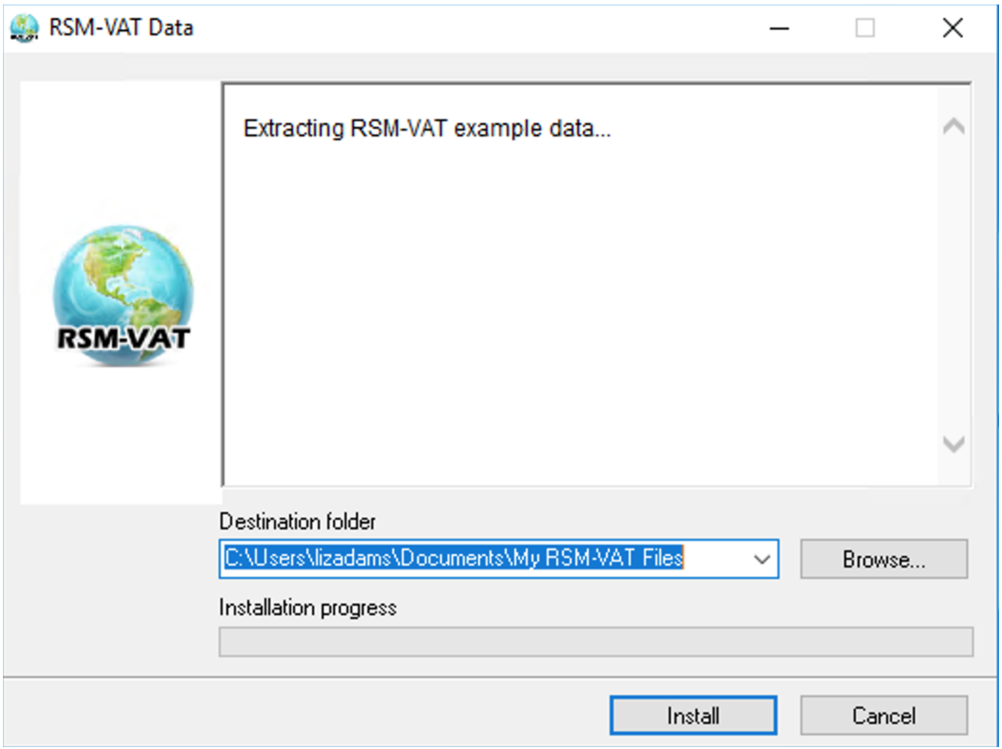


Fig. 6 Ready to Unzip Data Package

➢ Click the "**Install**" button, Fig. 7 shows the unzipping process of the example data.

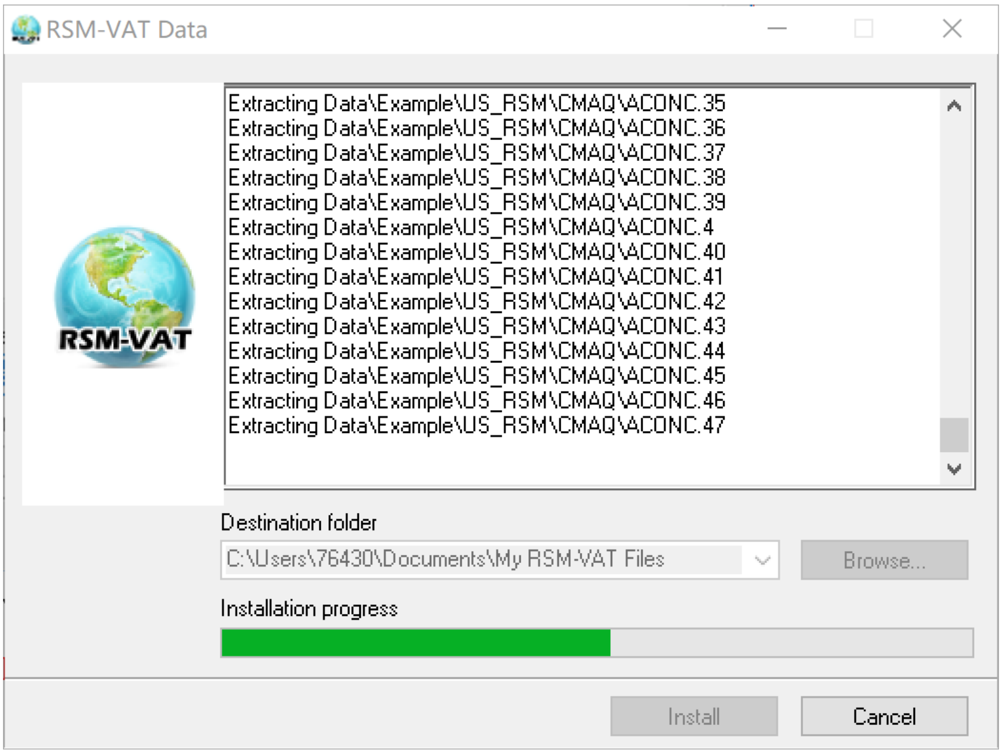


Fig. 7 Unzip Processing

1.4.3 Uninstalling RSM-VAT

➢ Go to Control Panel.

➢ Select RSM-VAT and click Change/Remove, the following figure will appear.

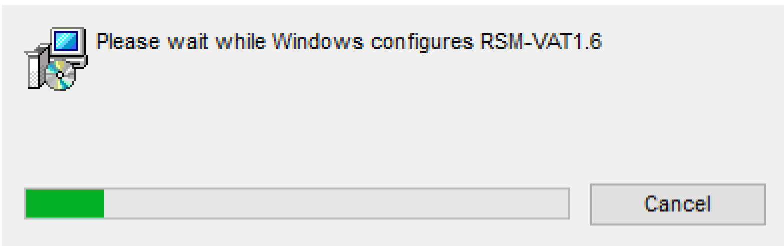


Fig. 8 Uninstallation Processing

➢ After a few seconds, uninstallation will finish.

1.5 Contacts for Comments and Questions

For comments and questions, please contact:

(1) Prof. Yun (Dustin) Zhu at South China University of Technology, Environmental Simulation and Information Laboratory via email at zhuyun@scut.edu.cn;

(2) The Center for Community Modeling and Analyses System (CMAS) at the University of North Carolina at Chapel Hill via email at cmas@unc.edu.

1.6 Sources for More Information

For supplemental information on RSM-VAT, see the following papers:

➢ Jia Xing.(2011) Study on the Nonlinear Responses of Air Quality to Primary Pollutant Emissions (in Chinese)[D], Tsinghua University.

➢ Jia Xing, Shuxiao Wang, Carey J.Jang, Yun Zhu, Jiming Hao.(2011) Nonlinear Response of Ozone to Precursor Emission Changes in China: a Modeling Study using Response Surface Methodology. Atmospheric Chemistry and Physics, 11(10), 5027-5044.

➢ Yunwen Lao, Yu Zhu, Carey J.Jang, et al.(2012) Research and development of regional air pollution control decision support tool based on response surface model (in Chinese)[J]. Acta Scientiae Circumstantiae, 32:1913-1922.

➢ Bin Zhao, ShuXiao Wang, Jia Xing, Joshua S.Fu, Carey J.Jang, Yun Zhu, Xinyi Dong, Yang Gao, Jiandong Wang, Jiming Hao, et al.(2015) Assessing the nonlinear response of fine particles to precursor emissions: development and application of an extended response surface modeling technique v1.0. Geoscientific Model Development, 8(1), 115-128.

➢ Yun Zhu, Yuanwen Lao, Carey J.Jang, Chen-Jen Lin, Jia Xing, Shuxiao Wang, Joshua S.Fu, Shuang Deng, Junping Xie, Shicheng Long.(2015) Development and case study of a science-based software platform to support policy making on air quality. Journal of Environmental Sciences, 27, 97–107.

➢ Shicheng Long, Yun Zhu, Carey J.Jang, Che-Jen Lin, Shuxiao Wang, Bin Zhao, Jian Gao, Shuang Deng, Junping Xie, Xuezhen Qiu.(2016) A case study of development and application of a streamlined control and response modeling system for PM2.5 attainment assessment in China. Journal of Environmental Sciences, 41, 69-80.

➢Yuzhou Pan, Yun Zhu, Jicheng Jang, Shuxiao Wang, Jia Xing, Pen-Chi Chiang, Xuetao Zhao, Zhiqiang You, and Yingzhi Yuan.(2020) Source and sectoral contribution analysis of PM2.5 based on efficient response surface modeling technique over Pearl River Delta Region of China. Science of The Total Environment 737:139655.

➢Tingting Fang, Yun Zhu, Jicheng Jang, Shuxiao Wang, Jia Xing, Pen-Chi Chiang, Shaojia Fan, Zhiqiang You, and Jinying Li.(2020) Real-time source contribution analysis of ambient ozone using an enhanced meta-modeling approach over the Pearl River Delta Region of China. J Environ Manage 268:110650.

➢Jia Xing, Shuxin Zheng, Dian Ding, James T. Kelly, Shuxiao Wang, Siwei Li, Tao Qin, Mingyuan Ma, Zhaoxin Dong, Carey Jang, Yun Zhu, Haotian Zheng, Lu Ren, Tie-Yan Liu, and Jiming Hao.(2020) Deep learning for prediction of the air quality response to emission changes. Environmental science & technology.

2 Quick Start

This chapter provides the steps required to run RSM-VAT. The Quick Start will use a combined US Case to demonstrate how to run each of the RSM-VAT modules. These steps will use the default RSM-VAT settings and do not describe the configuration settings for each analysis. For details of the configuration settings for the individual RSM-VAT modules, refer to the User's Manual chapter for each module. The steps below describe how to use RSM-VAT to create a RSM for US $PM_{2.5}$.

Step 1. Create an emission control matrix, region control NetCDF file, and Namelist files for the CMAQ model under **Experitmental Design** module.

Step 2. Create a RSM project under **Visualization & Analysis** module.

Step 3. View Results under **Visualization & Analysis** module.

2.1 Experimental Design

Click Experimental Design on the top of RSM-VAT home page to switch to the Experimental Design module. The step below describes how to use RSM-VAT to create an emission control matrix, region control NetCDF file, and Namelist files for the CMAQ model. For more details, please refer to Chapter 7.

2.1.1 Create Emission Control Matrix

Click the **Experimental Design** in the menu bar to enter the **Experimental Design** module. As shown in Fig. 9, the submodule of the **Control Matrix** displays in default.

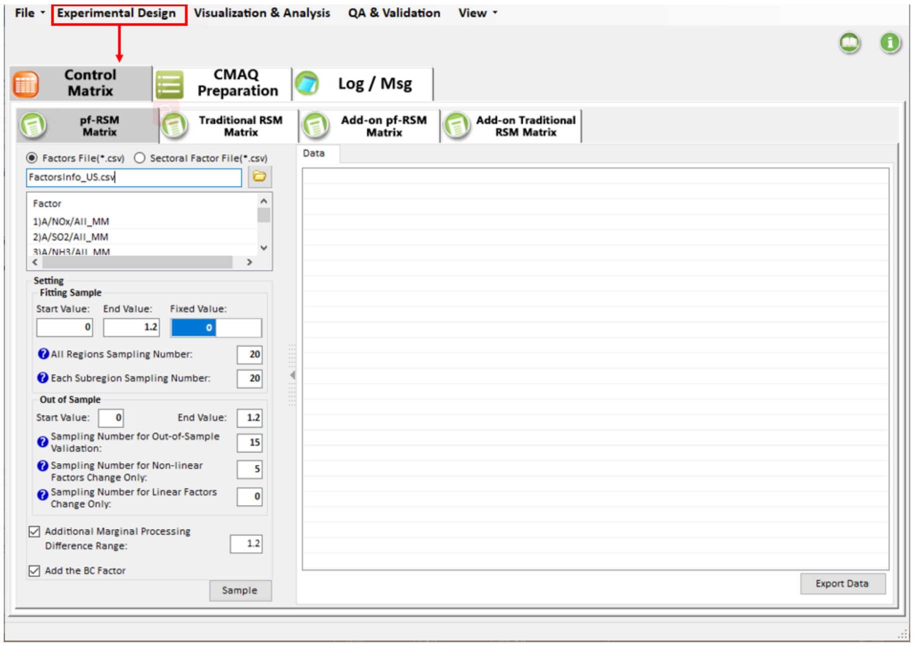


Fig. 9 Enter the Experimental Design Module

Click the **pf-RSM Matrix** and then click the file button to select a **Factors File** and open it. The details of Factors File are shown in Fig. 10, this case has a total of 25 control factors (5 different factors for each single region). The Emission control factors range from 0 to 120%, a zero control factor means that the emission of interest is reduced to zero while a 120% factor indicates that the emission is increased by 20% compared to baseline emission.

Region	Pollutant	Source	Limit	Min	Max
A	NOx	All_MM	1	0	1.2
A	SO2	All_MM	1	0	1.2
A	NH3	All_MM	1	0	1.2
A	VOC	All_MM	1	0	1.2
B	NOx	All_MM	1	0	1.2
B	SO2	All_MM	1	0	1.2
B	NH3	All_MM	1	0	1.2
B	VOC	All_MM	1	0	1.2
C	NOx	All_MM	1	0	1.2
C	SO2	All_MM	1	0	1.2
C	NH3	All_MM	1	0	1.2
C	VOC	All_MM	1	0	1.2
D	NOx	All_MM	1	0	1.2
D	SO2	All_MM	1	0	1.2
D	NH3	All_MM	1	0	1.2
D	VOC	All_MM	1	0	1.2
E	NOx	All_MM	1	0	1.2
E	SO2	All_MM	1	0	1.2
E	NH3	All_MM	1	0	1.2
E	VOC	All_MM	1	0	1.2
A	PM25	All_MM	1	0	1.2
B	PM25	All_MM	1	0	1.2
C	PM25	All_MM	1	0	1.2
D	PM25	All_MM	1	0	1.2
E	PM25	All_MM	1	0	1.2

Fig. 10 Factors File

After setting sampling parameters, click the **Sample** to start sampling. As shown in Fig. 11, it will create a series of emission runs, a row stands for a emission run, a column (except the 1st column) represents the emission control value for current factor. For example, all the result information of case 1 is displayed as 1, which indicates the sampling result without the implementation of control measures.

Click the **Export Data** to export the sampling result to a local path.

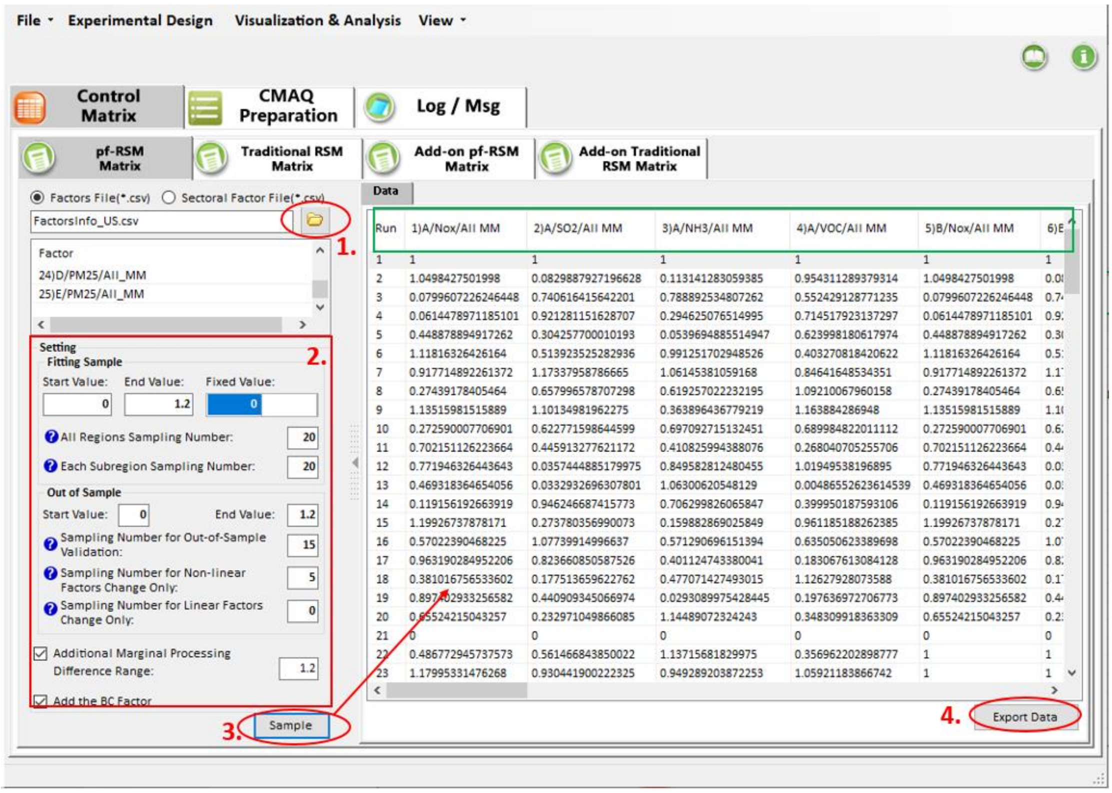


Fig. 11 pf-RSM Matrix Sampling

2.1.2 Create NetCDF File and Namelist Files for CMAQ

Click the **CMAQ Preparation** in the tab bar to enter the **CMAQ Preparation** submodule.

Create a region control NetCDF file based on region control shapefile as shown in Fig. 12.

- Check the **Create Region Control NetCDF File** option to view the setting panel.
- Click the file button to select a grid definition file.
- Click the button to add a region control shapefile.
- Click the **Manage Selected Region** button to select control regions from the loaded region control shapefiles and the list of selected regions below will be

updated.

- Click the **Output** button to generate the NetCDF file, and the result file will then be loaded in the right panel under the NetCDF tab page.

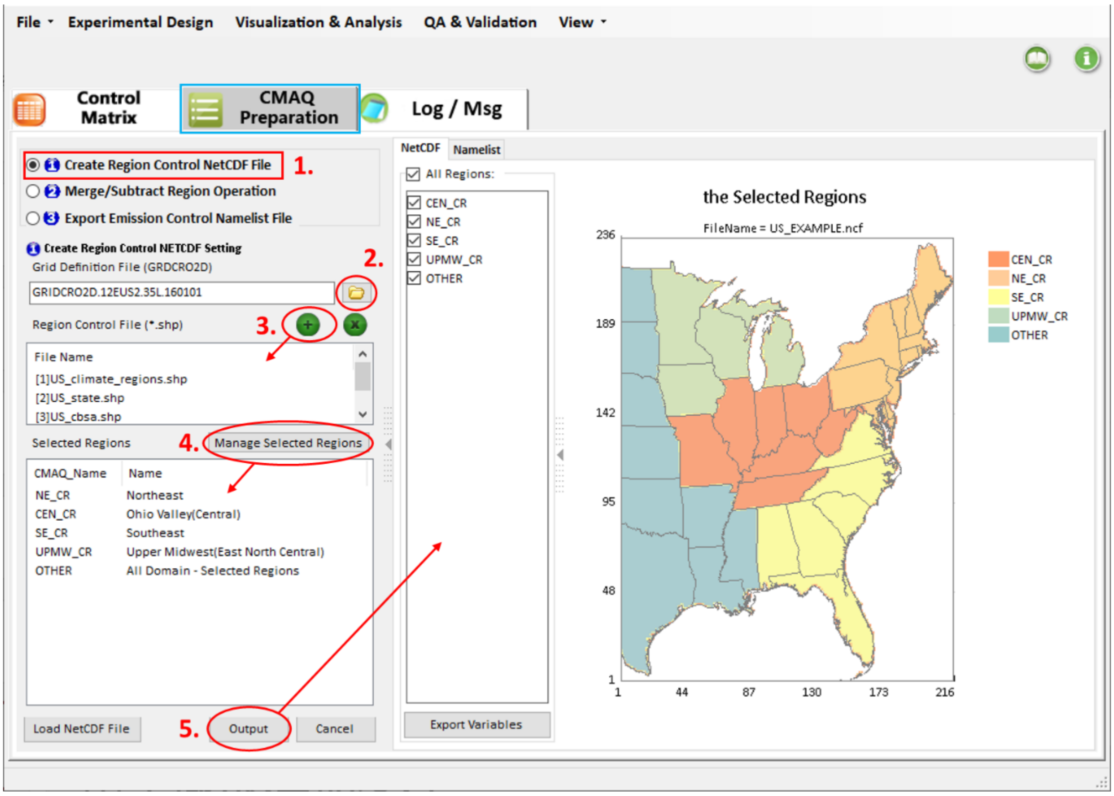


Fig. 12 Create Region Control NetCDF File

Additionally, users can get a new region control NetCDF file through merge operation on the file obtained in the previous step if necessary, as shown in Fig. 13, which is available for a single region case study.

- Check the ❷ **Merge/Subtract Region Operation** option to view the setting panel.
- Click the file button [folder icon] to load the region control NetCDF file attained in the previous step.
- Check the **Create Region with Formula** option, then click the **Add/Remove** button to add an expression to merge regions.
- Click the **Output** button to generate a new region control NetCDF file by the merge operation, and the result file will then be loaded in the right panel under the NetCDF tab page.

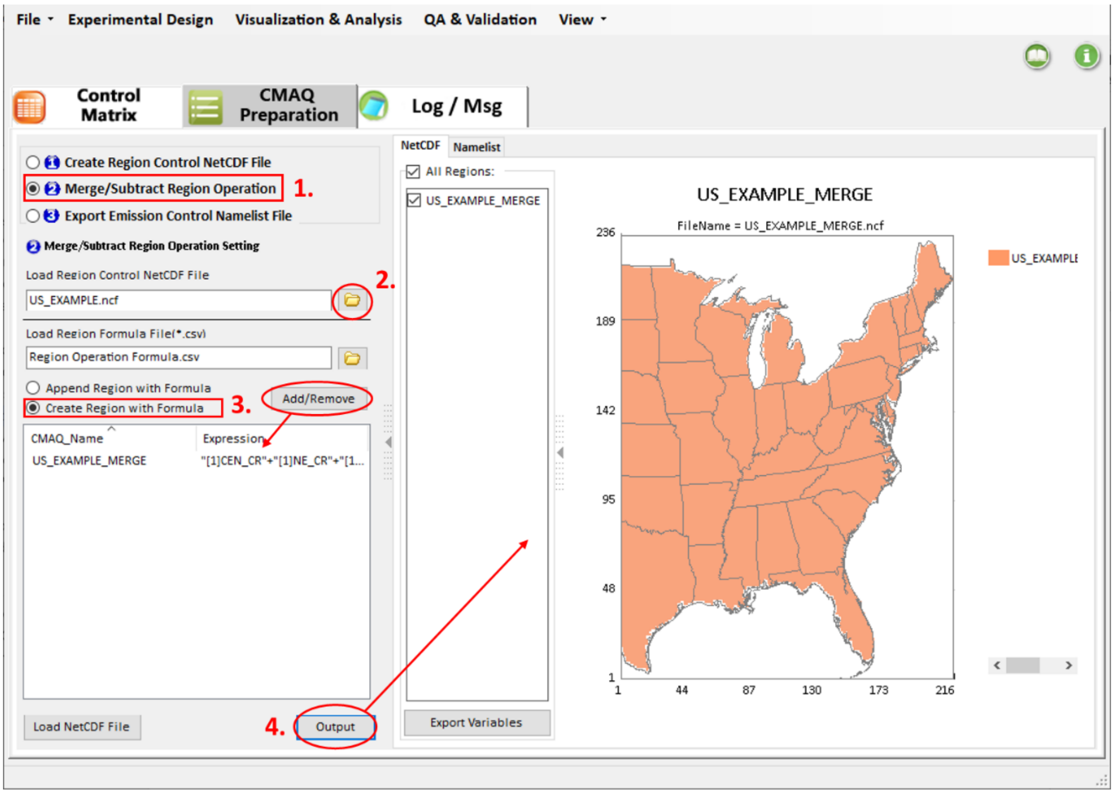


Fig. 13 Merge/Subtract Region Operation

Export emission control namelist files for CMAQ based on the control matrix and NetCDF file obtained in previous steps, as shown in Fig. 14.

- Check the ❸ **Export Emission Control Namelist File** option to view the setting panel.
- Click the file button to select a namelist template file.
- Click the file button to select the region control NetCDF file generated in previous steps.
- Click the file button to select the control matrix file generated in the **Control Matrix** submodule.
- Click the file button to select the mapping file corresponding to the input NetCDF file and control matrix file.
- Click the **Output** button to generate the namelist files for CMAQ, and the result files will then be loaded in the right panel under the Namelist tab page.

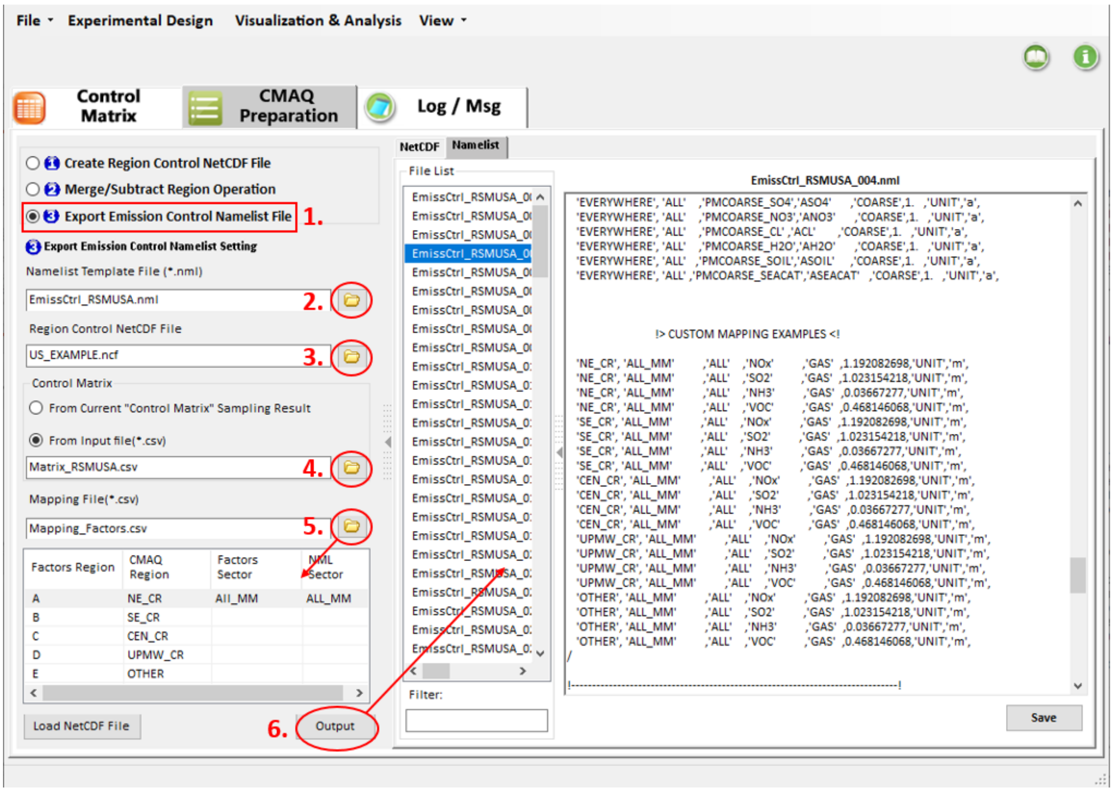


Fig. 14 Export Emission Control Namelist File

2.2 Create a New RSM Project

The steps below describe how to create and run a new RSM project.

2.2.1 Run a New RSM Project

Click the **Visualization & Analysis** in the menu bar to enter the module. As shown in Fig. 15, the interface of Create/Input RSM Option displays on the left.

Click the **File** button, and choose the **New Project** option to create a new RSM project.

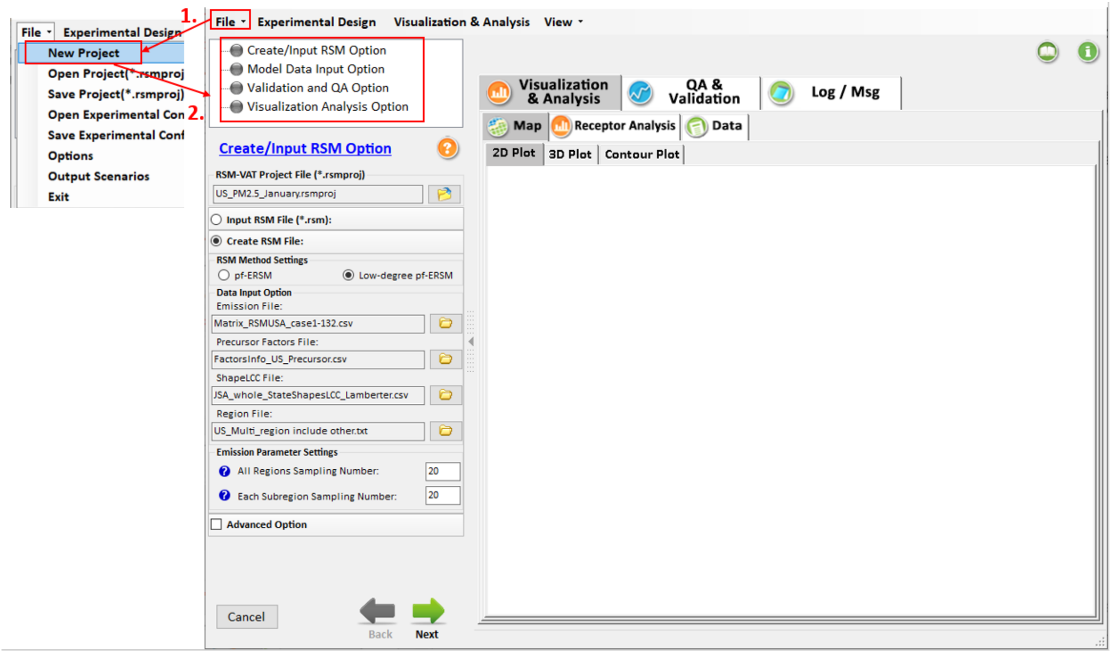


Fig. 15 Create a New Project

2.2.2 Set Input Parameters

The parameter setting for **Create/Input RSM Option** is shown in Fig. 16.

- Choose the **Create RSM File** option and then click the file button  to select the input files for creating RSM, including the **Emission File, Precursor Factors File, ShapeLCC File, Region File**. After selecting the input files, the **All Regions Sampling Number** and **Each Subregion Sampling Number** are needed to set based on the Emission File.
- Click the **Next** button to proceed to the configuration of the **Model Data Input Option**.

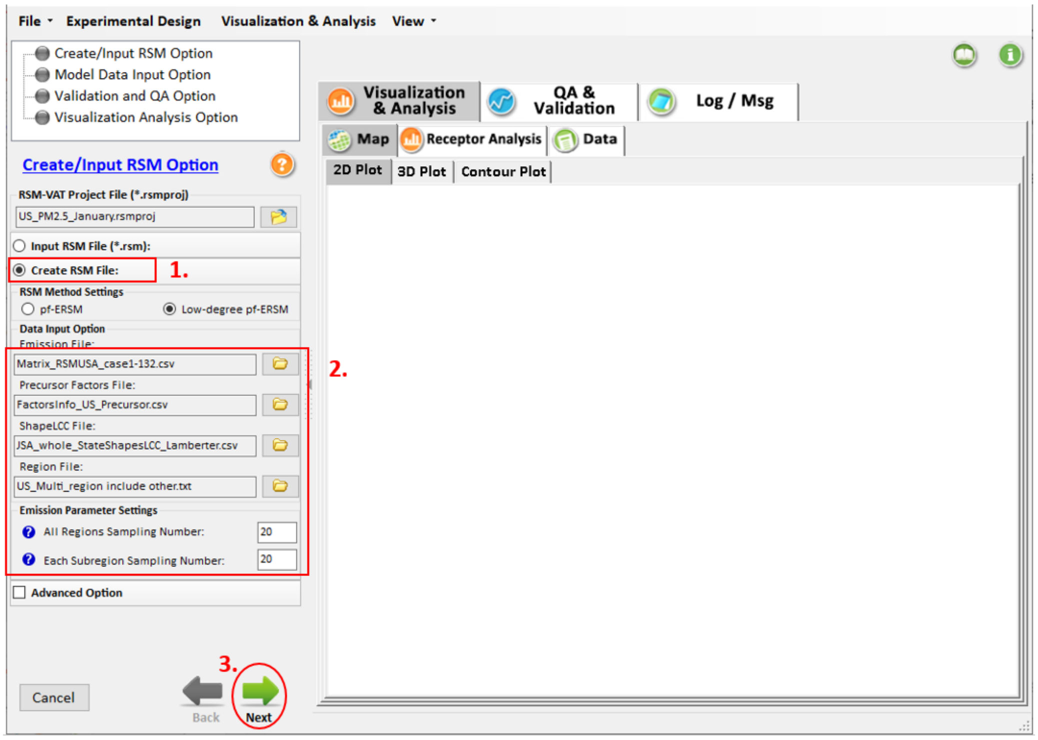


Fig. 16 Create/ Input RSM Option

The parameter setting for **Model Data Input Option** is shown in Fig. 17.

- Click the file button  which is in the upper-right of the main interface to select a **Base Case CMAQ File** and open it.
- Check the **Scenario Plot** and then select cases, this operation is optional.
- Click the **Next** button to proceed to the configuration of the **Validation and QA Option,** as shown in Fig. 17.

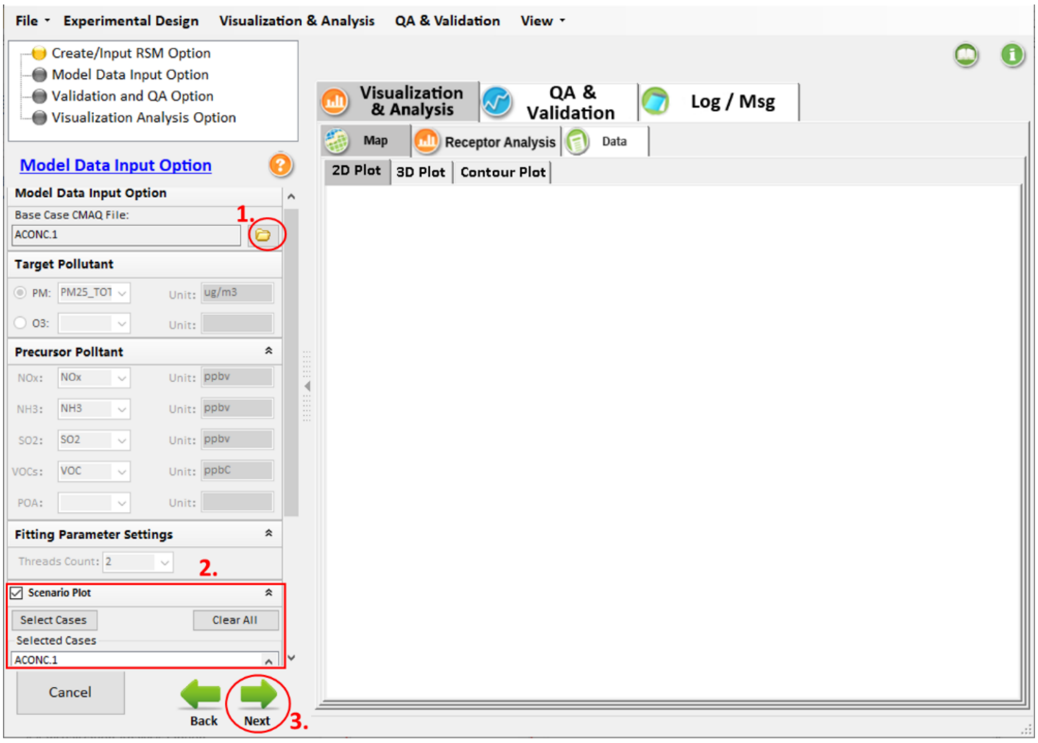


Fig. 17 Model Data Input Option

The parameter setting for **Validation and QA Option** is shown in Fig. 18.

- Click the file button  to select an **Emission File for Out of Sample,** as shown in Fig. 18.
- Click the **Next** button to proceed to the configuration of the **Validation and QA Option**.

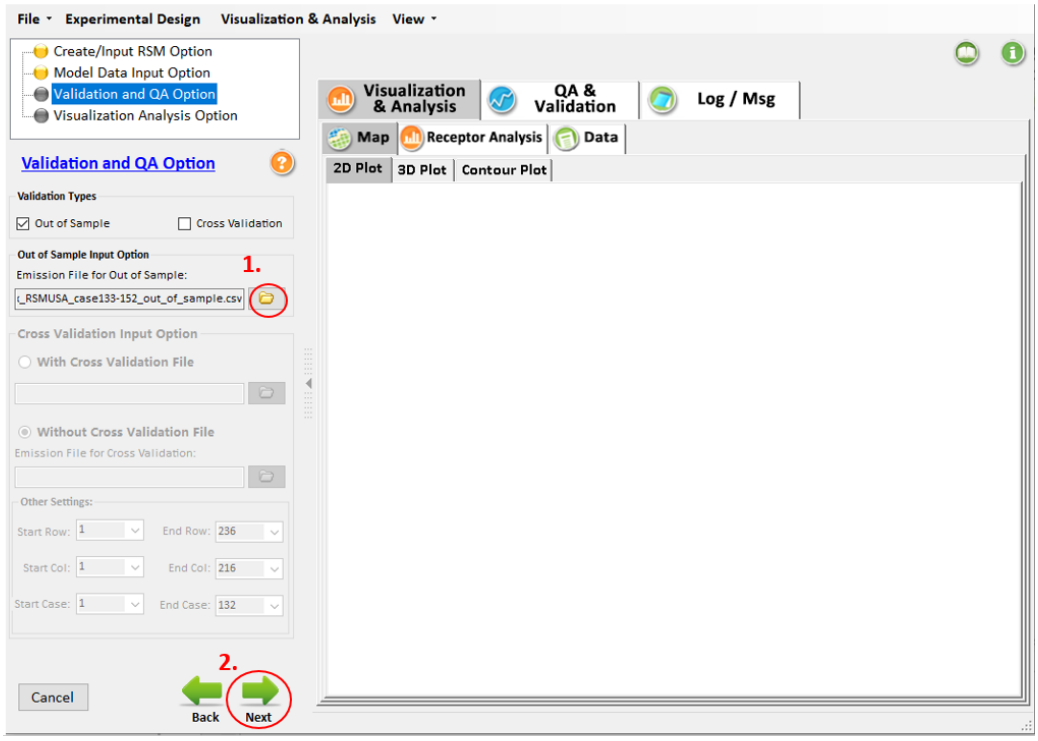


Fig. 18 Validation and QA Option

The parameter setting for **Validation and QA Option** is shown in Fig. 19.

- Click the file button  to select a **Receptor Region File** and the details of the Receptor Region File are shown in Fig. 20.

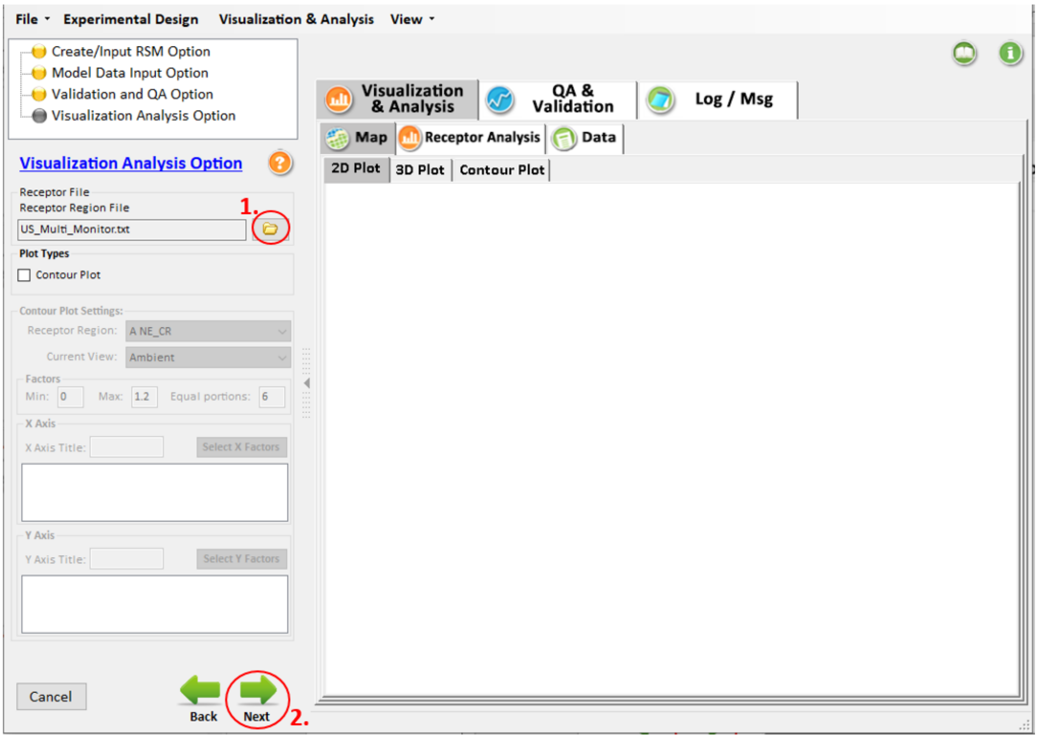


Fig. 19 Visualization Analysis Option

```
1 144 173 100 A NE_CR
1 145 173 100 A NE_CR
1 151 172 100 A NE_CR
............
2 51 94 100 B SE_CR
2 78 107 100 B SE_CR
2 90 92 100 B SE_CR
............
3 150 103 100 C CEN_CR
3 124 102 100 C CEN_CR
3 125 103 100 C CEN_CR
............
4 154 68 100 D UPMW_CR
4 151 59 100 D UPMW_CR
4 140 60 100 D UPMW_CR
............
5 86 62 100 E OTHER
5 73 60 100 E OTHER
5 93 72 100 E OTHER
............
```

Fig. 20 Receptor Region File

- Click the **Next** button and Fig. 21 will appear, choose **yes** to run the program.

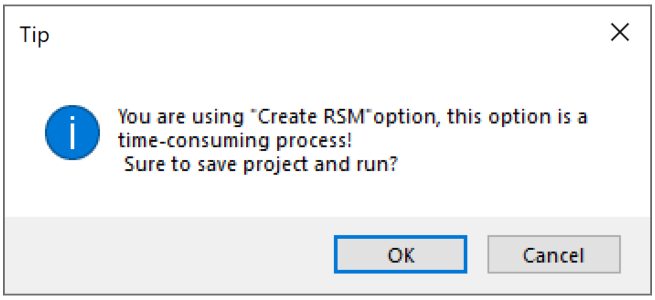


Fig. 21 Save Project and Run

2.3 View Results

The steps below describe how to view the result of an RSM project. More details refer to Chapter 7.

2.3.1 QA & Validation

2.3.1.1 Out of Smaple Validation

As shown in Fig. 22, it shows the **Out of Sample Validation** results of RSM, in which the predicted values derived from the RSM are compared with the actual CMAQ simulations of a set of model runs that are not included creating RSM, and the comparison results are displayed in **Error & Bias Plot, Comparison Plot, RSM .vs CMAQ and Error & Bias Table**.

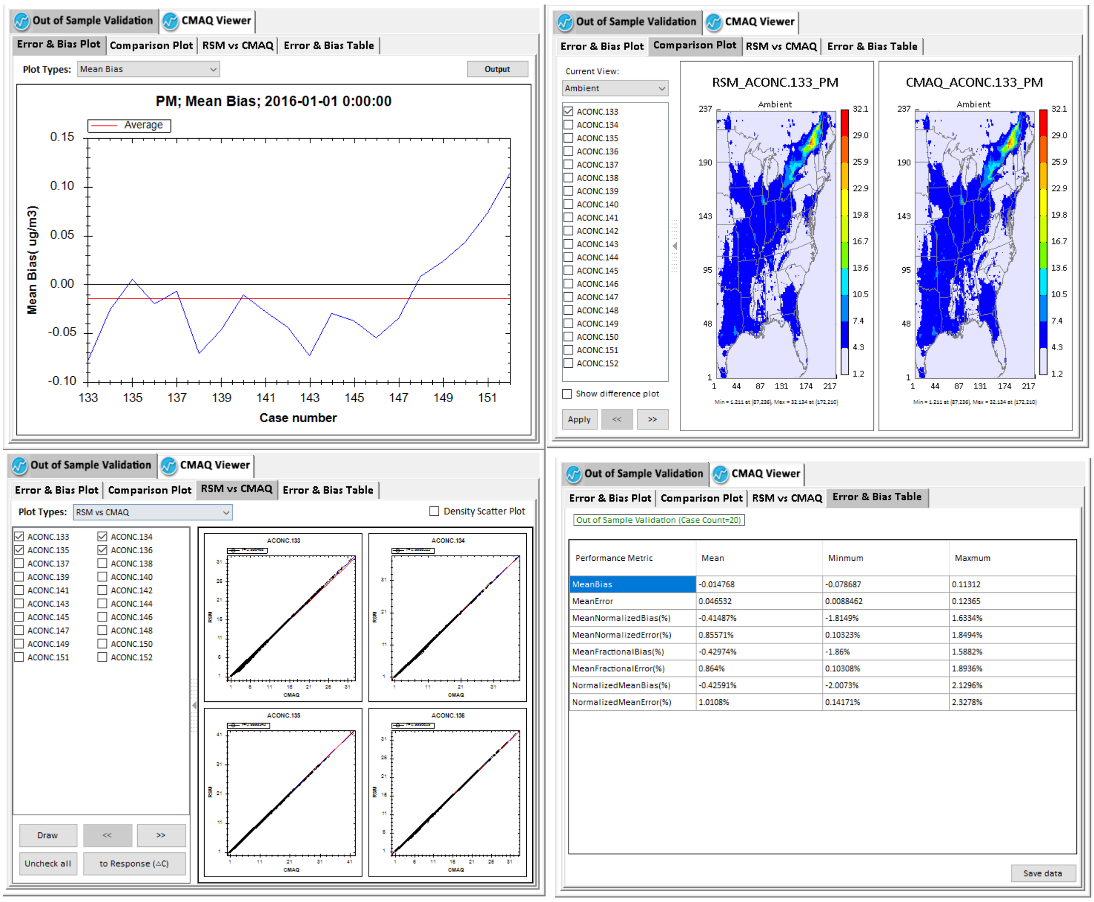


Fig. 22 Out of Sample Validation Results

2.3.1.2 CMAQ Viewer

Fig. 23 shows the distribution of the $PM_{2.5}$ concentration under different emission runs from emission control matrix file.This module can help users check the results of CMAQ simulations under different emission runs.

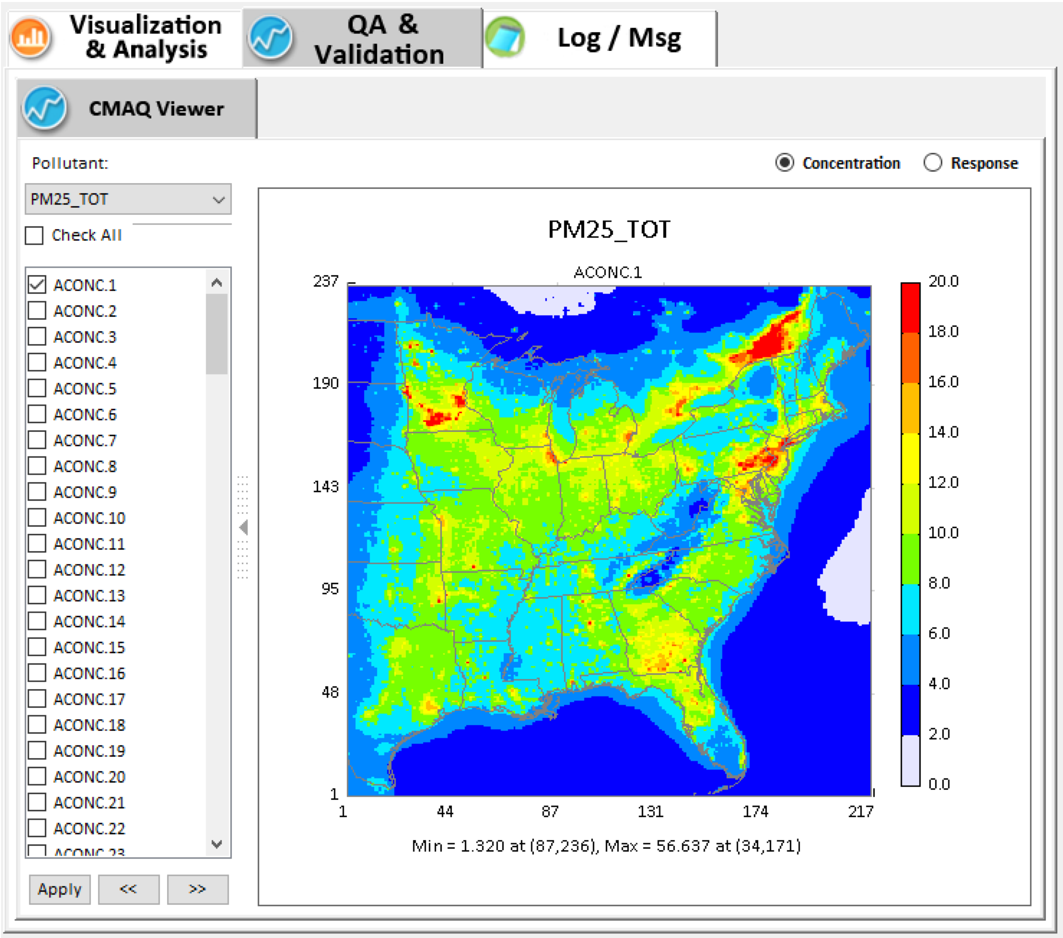


Fig. 23 Results of CMAQ simulations

2.3.2 Visualization & Analysis

2.3.2.1 Map Results

As shown in Fig. 24, the maps show the ambient levels of $PM_{2.5}$ simulated by RSM through 2D&3D Plot. The values of 1 in Fig. 24 represent the $PM_{2.5}$ **concentration** without the implementation of control measures compared to baseline, users can change the value of the control factors and check the **Response** to view air quality changes compared to baseline.

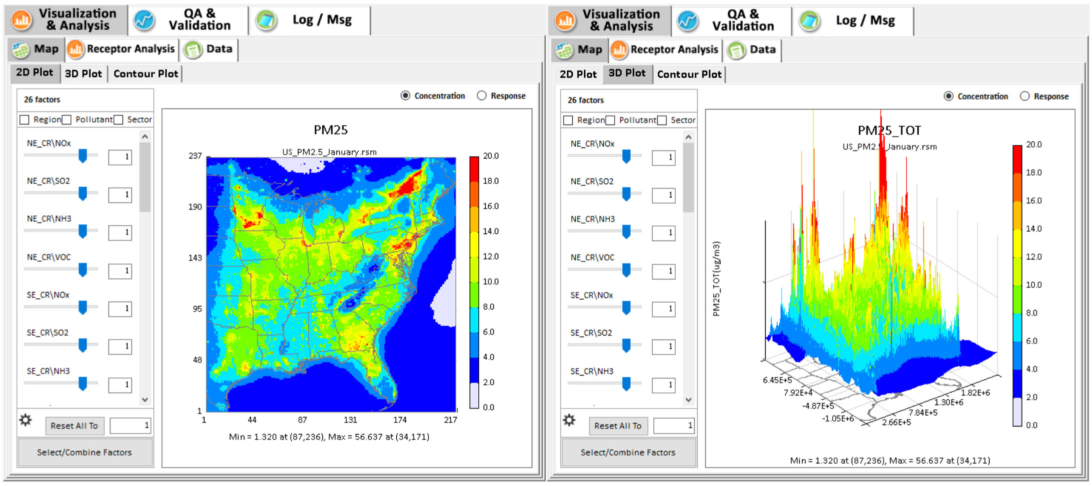


Fig. 24 Map Results

2.3.2.2 Chart Results

Fig. 25 shows source contributions for air quality ($PM_{2.5}$) in each receptor region under different emission control by various charts.For more details, refer to Chapter 7.

Fig. 25 Chart Results

2.3.2.3 Data Results

Fig. 26 shows the $PM_{2.5}$ concentration of each grid in the simulation domain.Users can output it for further study, e.g., as input for SMAT-CE.

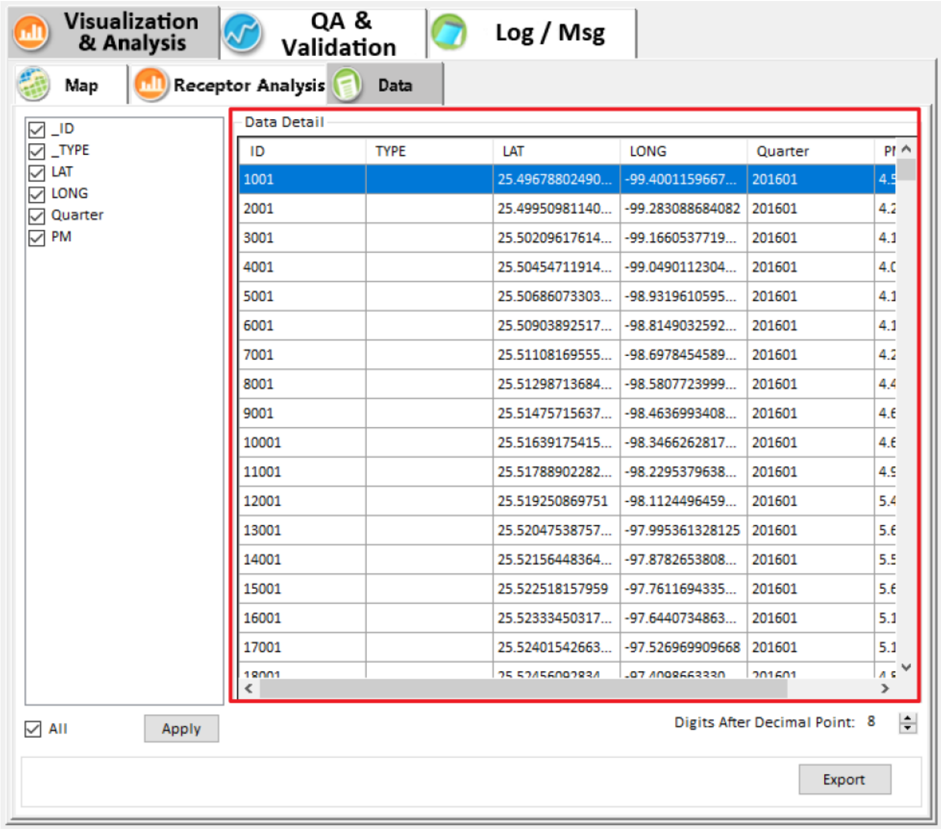


Fig. 26 Data Results

3 Terminology and File Types

The first section of this chapter explains common terms used in this user manual, and references to other sections in this manual to find more detailed information. Section 3.2 describes the necessary format for externally-generated model and monitor data files that can be read into RAM-VAT in detail.

3.1 Common Terms

➢ **CMAQ (Community Multi-Scale Air Quality).** A state-of-the-art air quality model able to model secondary ambient particulate levels, as well as other pollutants, including ozone.

➢ **Response Surface Model (RSM).** RSM is a "reduced form" model of a complex air quality model (e.g. CMAQ) – "meta-model", based on a systematically selected set of model runs. Statistical techniques are used to represent the relationship between model inputs and outputs (e.g. emissions control and concentrations of PM & ozone). Once the "response surface" has been generated, it can be used to simulate the functions of the more computationally expensive photochemical air quality model. It can also be used to derive analytical representations of model sensitivities to changes in the model inputs.

➢ **Latin Hypercube Sampling (LHS).** LHS is often applied to generate the experimental design for a Kriging model. It is a statistical method for generating a sample of plausible collections of parameter values from a multidimensional distribution which is more efficient than random sampling from a large number of factors.

➢ **Hammersley quasi-random Sequence Sampling (HSS).** HSS uses low-discrepancy sequences (quasi-random points) which have the better uniformity or evenness in their domain of definition. This sampling technique provides a generalized approach for increasing simulation efficiency by systematically replacing the pseudo-random numbers used in Monte Carlo (MC) simulations with quasi-random numbers.

➢ **Control Factor:** it means the emission of a specified precursor pollutant from particular source and location.

➢ **Control Matrix.** An experimental design that specifies the type of emission control factors used in a matrix as inputs to the CMAQ air quality model. The matrix is created by sampling the control factors in the design space (e.g., from 0.00 to 1.50) using Latin Hypercube Sampling(LHS) or Hammersley quasi-random Sequence Sampling (HSS).

➢ **High-dimensional Kriging Interpolation.** Kriging is a geostatistical method based on an exponentially weighted sum of the sample run results. A high-dimensional Kriging approach is applied for the response surface regression of the CMAQ simulation results. RSM adopted and recoded the Parametric Empirical Kriging algorithm and accelerated the calculation efficiency using multi-threading technology.

➢ **Add-on Sampling.** A sampling method that generates additional runs for CMAQ simulations if the RSM prediction bias does not meet the desired tolerance.

➢ **Out of Sample Validation (OOS).** OOS is a validation metnod to evaluate the RSM performance. It compares RSM-predicted values to those of CMAQf or a set ofmodel runs not used in created the RSM.

➢ **Cross Validation(CV).** CV is another validation metnod to evaluate the RSM performance.During each CV routine, one of the experimental runs is left out for creating the RSM. The RSM predicted data are then verified against the CMAQ results that are left out.

3.2 File Types

➢ **RSM-VAT Project File:** An pre-run RSM project file, which contains those inputs data and RSM fitting paramters.

➢ **RSM File**: A *.rsm file created by RSM-VAT, which contains RSM fitting paramters.

➢ **Emission File**: A *.csv file that contains a series of emission runs created by Control Matrix module, it is an essential input for RSM creation (Config Files/ Matrix_RSMUSA_case1-132.csv),

➢ **ShapeLCC File**: A *.csv file defines a sequence of points for each state or county, or any other contour, in terms of X, Y coordinates, this file can be created by Model-VAT or ArcGIS (Config Files/USA_whole_StateShapesLCClamberter.csv).

➢ **Region File**: A separate *.txt file that defines the grids information of the each region of insterest, and it can be created by ArcGIS(Config Files/ US_Multi_region include other.txt).

➢ **CMAQ File:** These files are CMAQ simulation result files (ACONC) which are NetCDF format, containing the grid data at a single layer and single period. Each emission run in **Emission File** has a corresponding simulation result file. The filename can be customized, but the filename extension must correspond to the sample serial number of experimental scenes. Therefore, the file can be named using the convention: (CMAQ/Jan/ACONC1, ACONC2, ACONC3, …).

➢ **Receptor Region File**: A separate *.txt file that defines the grids information of each region of insterest. Generally, this file defines those grids information that contains monitor sites in selected regions. The format of this file is the same as **Region File** (Config Files/US_Multi_Monitor.txt).

➢ **Experimental Configuration File:** A *.expproj file that records the settings in Experimental Design module.

➢ **Factors File**: A *.csv file for emission factor information. It contains each factor's region, pollutant, source, minium/maxium emission reduction (Config Files/FactorsInfo_US_Precursor.csv).

➢ **Grid Definition File**: A GRDCRO2D file that defines the model domain when generating NetCDF files. It usually comes from the CMAQ model (Config Files/RegCtrlNCFfiles/GRIDCRO2D.12EUS2.35L.160101).

➢ **Region Control File**: A *.shp that contains shape, location and other related properties of regions (Config Files/RegCtrlNCFfiles/Shapefiles/USA.shp).

➢ **Region Control NetCDF File:** It is a NetCDF file that contains the grids information of selected regions, which is created by CMAQ Preparasion module.

➢ **Namelist Template File**: A *.nml file that contains information about how to scale emissions to model species (Config Files/RegCtrlNCFfiles/ EmissCtrl_RSMUSA.nml).

➢ **Control Matrix File**: It is the same as the above Emission File that created by Control Matrix module (Config Files/RegCtrlNCFfiles/ Matrix_RSMUSA.csv).

➢ **Mapping File**: An *.csv file that matches the regions and sectors in the emission control matrix and NetCDF file with the namelist template file (Config Files/RegCtrlNCFfiles/Mapping_Factors.csv).

Table 1 and Table 2 presents the above the different file types, their name, and their file extension.

Table 1 Types of RSM Input files

Module	Filename	File Extension
Visualization & Analysis	RSM-VAT Project File	*.rsmproj
	RSM File	*.rsm
	Emission File	*.csv
	Precursor Factors File	*.csv
	ShapeLCC File	*.csv
	Region File	*.txt
	CMAQ File	NetCDF
	Receptor Region File	*.txt
Experimental Design	Experimental Configuration File	*.expproj
	Factors File	*.csv
	Grid Definition File	NetCDF file
	Region Control File	*.shp
	Namelist Template File	*.nml
	Region Control NetCDF File	*.ncf
	Control Matrix File	*.csv
	Mapping File	*.csv

Table 2 File Types Generated by RSM

Module	Filename	File Extension
Visualization & Analysis	RSM-VAT Project File	*.rsmproj
	RSM File	*.rsm
Experimental Design	Experimental Configuration File	*.expproj
	Control Matrix File	*.csv
	Region Control NetCDF File	*.ncf

	Namelist File	*.nml

4 Main Interface

The main interface of RSM-VAT can be shown in Fig. 27.

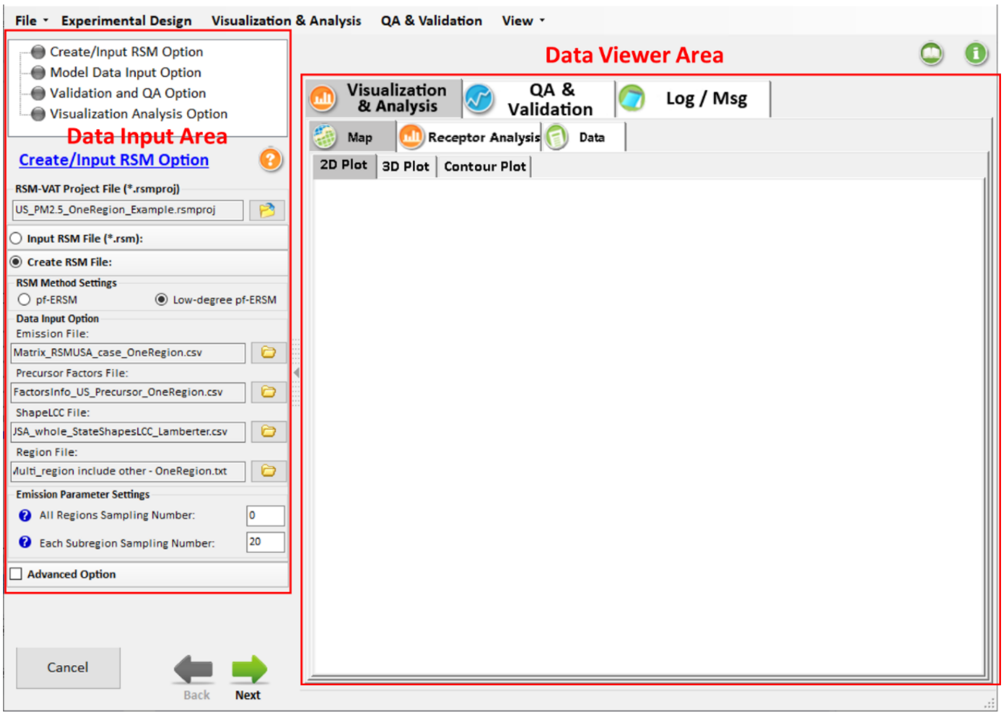


Fig. 27 Main Interface of RSM-VAT

Click **File** button on the top of RSM-VAT main page, there are five options that users can choose.

- Go to File, click **Open Project** button, locate the *.rsmproj file and open it.
- Click the **New Project** button to create a new project.
- Click the **Save Project** button to save a created project.
- Click the **Options** button to set the default configuration, show language menu, and show start page menu.
- Click the **Exit** button to exit the RSM-VAT.

Click the **Experimental Design** button on the top of RSM-VAT main page to switch to **Experimental Design** module.

Click the **Visualization & Analysis** button on the top of RSM-VAT main page to switch to **Visualization & Analysis** module.

Click the **View** button on the top of RSM-VAT main page, there are two options that users can choose.

- Click the **Setting Viewer** button to show the setting panel.

- Click the **Data Viewer** button to collapse the Setting Viewer panel and show the Visualization & Analysis panel.

5 Experimental Design

Under "Experimental Design" module, it includes two submodules: (1) Control Matrix and (2) CMAQ Preparation; Control matrix module is used to create emission control matrix based on the selected control factors, while CMAQ preparation module provides region control NetCDF file and Namelist files for CMAQ model.

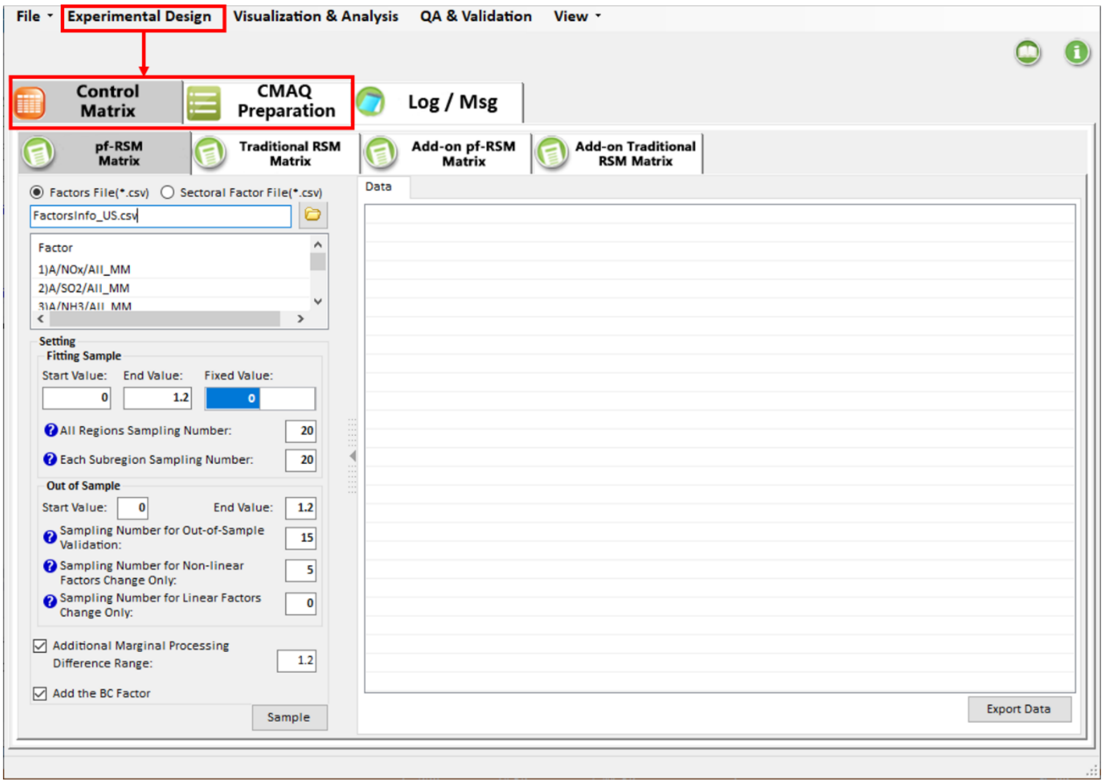


Fig. 28 GUI of Experimental Design Module

5.1 Control Matrix

5.1.1 pf-RSM Matrix

In the pf-RSM Matrix sampling module, users are allowed to create an emission control matrix for the pf-RSM model based on various pollutants in different regions/cities using the HSS method. Users can also export data for further study, as shown in Fig. 29.

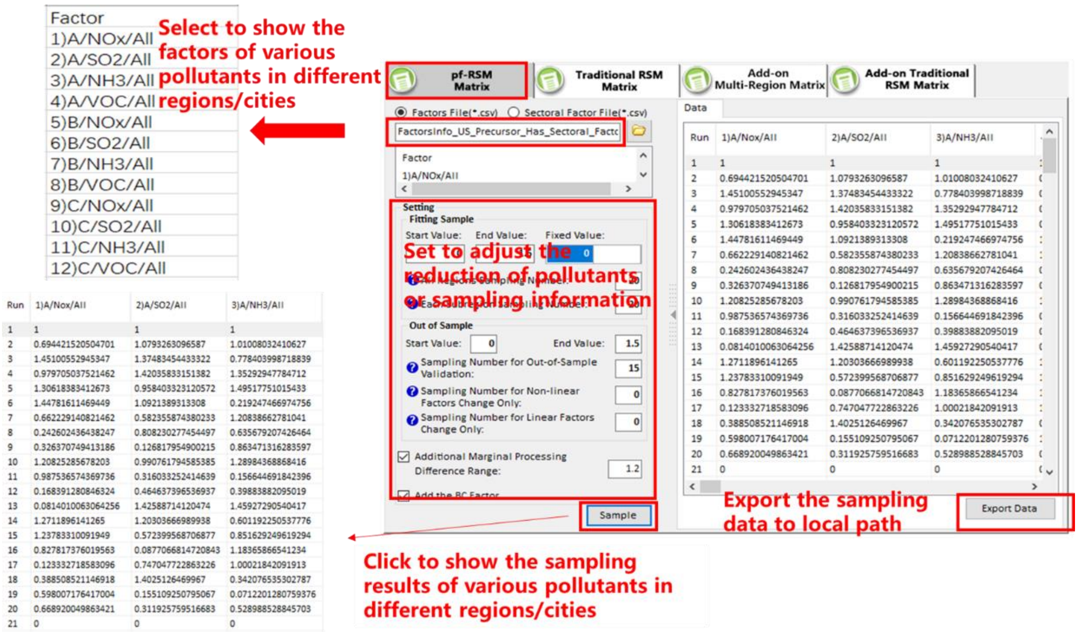


Fig. 29 pf-RSM Sampling Module

5.1.2 Traditional RSM Matrix

In the traditional RSM sampling matrix module, users are allowed to create the emission control matrix for traditional RSM (e.g., RSM using High-dimensional Kriging interpolation technique) based on selected pollutants in different regions/cities using LHS method. Users can also export data for further study, as shown in Fig. 30.

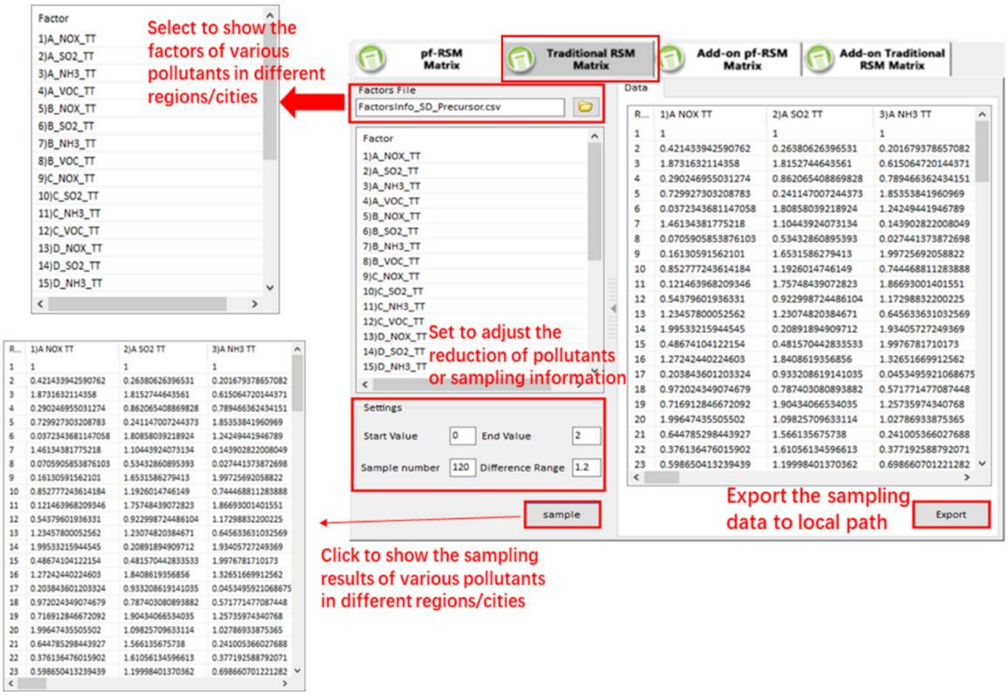


Fig. 30 Traditional RSM Matrix Sampling

5.1.3 Add-on pf-RSM Matrix Sampling

In the Add-on pf-RSM matrix sampling module, it is also for appending a certain amount of samples when the pf-RSM prediction error or bias exceeds acceptable ranges, as shown in Fig. 31. Increasing the sampling density will further improve the RSM prediction accuracy (Xing et al., 2011). The add-on sampling function allows users to choose the factors, and to set the number of samples and the factor range. The module uses HSS methods to generate a sub-matrix supplementing the existing-matrix for additional sampling runs. For example, to further reduce the difference between RSM and CMAQ results, one can use the function of this module to generate additional 20 experiment runs. The CMAQ simulation results of the 20 additional runs together are then used to recreate the RSM.

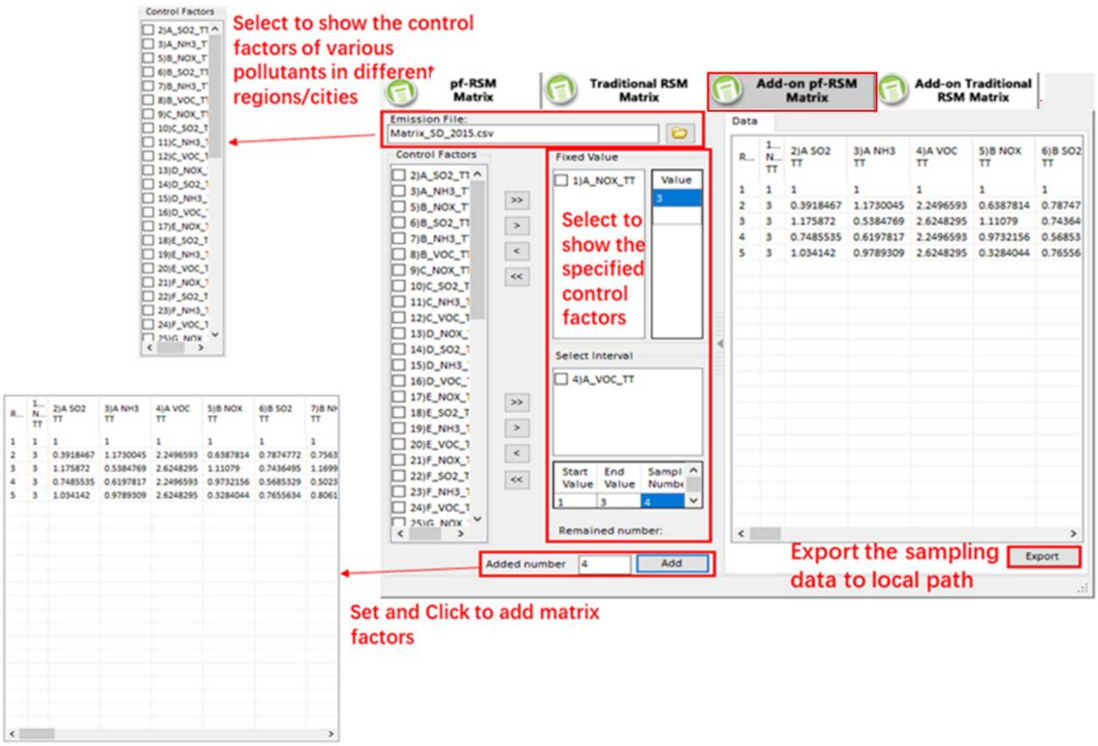


Fig. 31 Add-on pf-RSM Matrix Sampling

5.1.4 Add-on Traditional RSM Matrix Sampling

In Add-on traditional RSM matrix sampling module, it is for appending a certain amount of samples when the traditional RSM prediction error or bias exceeds acceptable ranges, as shown in Fig. 32.

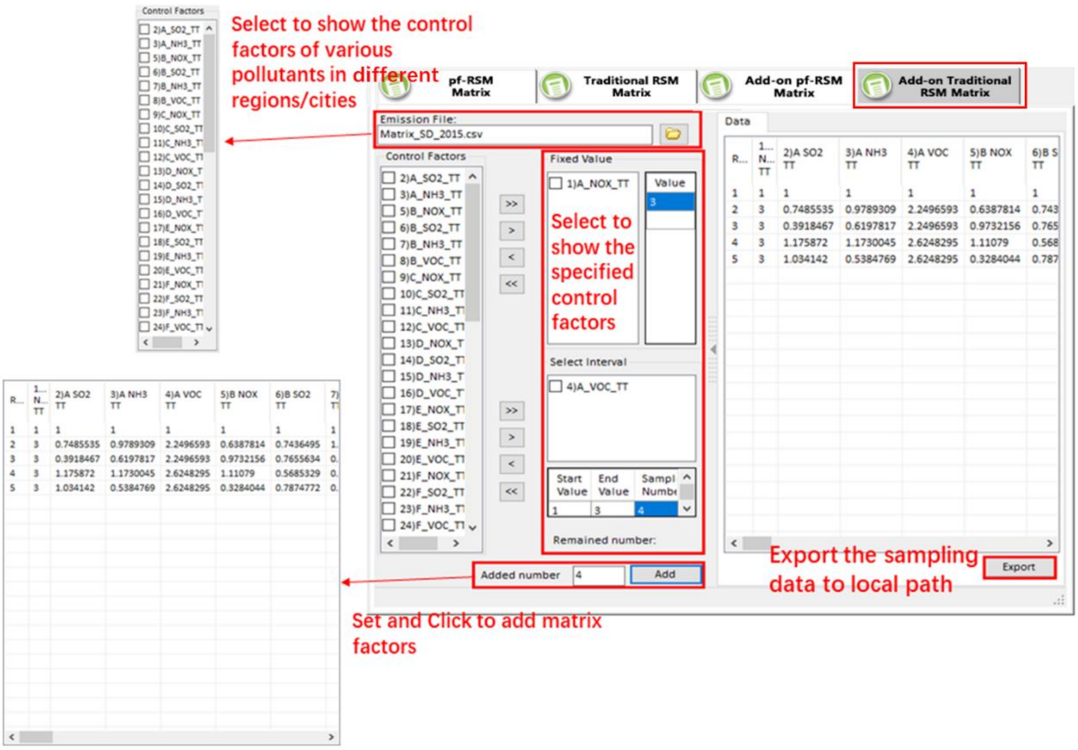


Fig. 32 Add-on Traditional RSM Matrix Sampling

5.2 CMAQ Preparation

Under the CMAQ preparation modules, it provides three kinds of functions for users to create region control NetCDF file and export emission control Namelist files that are needed in CMAQ 5.3 or later. There are (1) Create Region Control NetCDF File (2) Merge/Subtract Region Operation (3) Export Emission Control Namelist File.

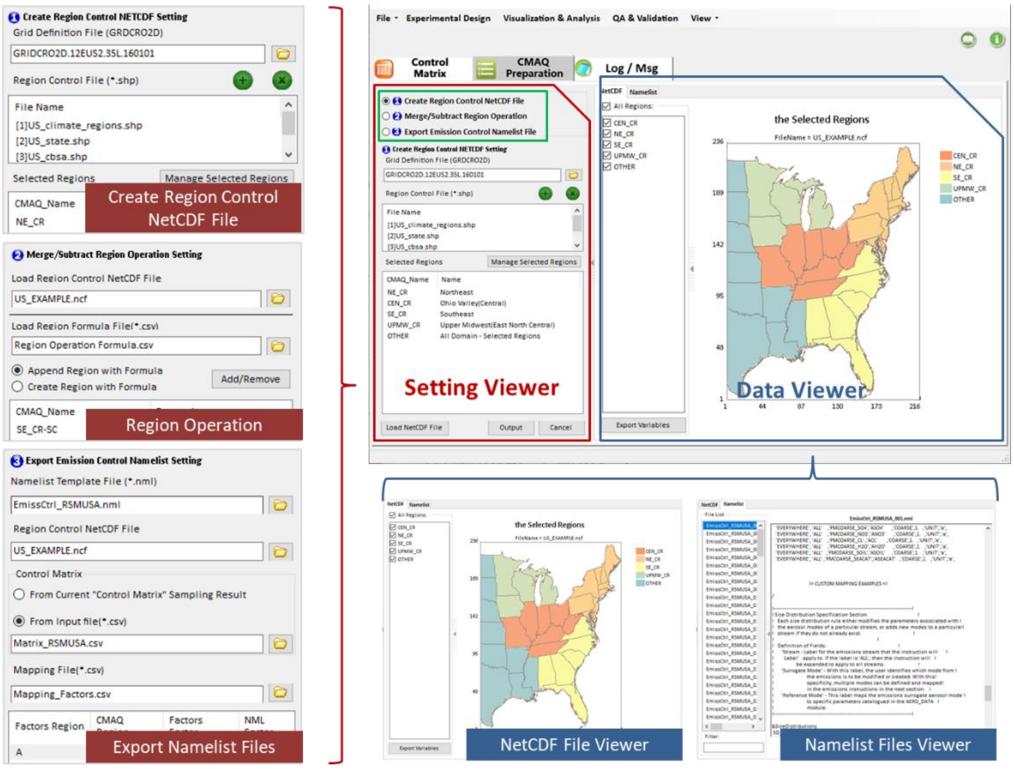


Fig. 33 Main Functions in CMAQ Preparation Module

5.2.1 Create Region Control NetCDF File

The **Create Region Control NetCDF File** module is used to create region control NetCDF files for the CMAQ module. To create a region control NetCDF file, the following operations are needed.

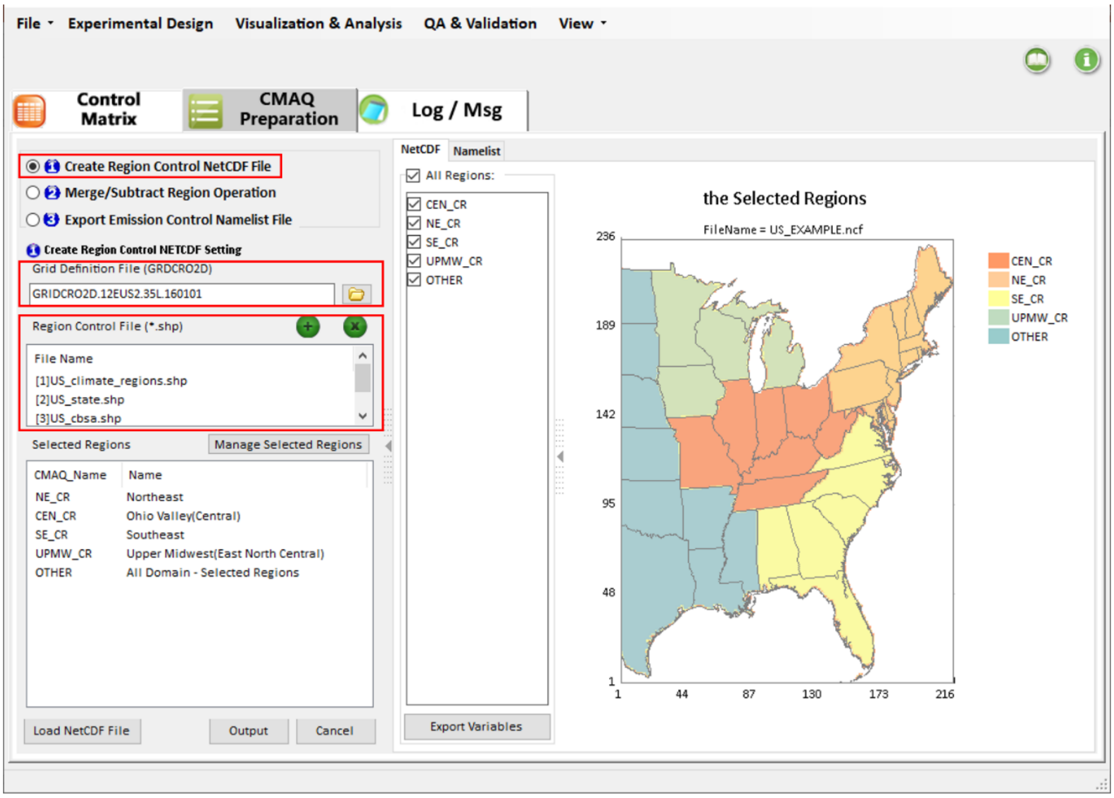


Fig. 34 GUI of Create Region Control NetCDF File

- **Load Grid Definition File (GRDCRO2D):** Click the browse file icon to select the grid definition file. This file usually comes from the CMAQ model.
- **Load region control ESRI Shapefile (*.shp):** Click the "+" icon to add a region control shapefile or click the "X" icon to remove loaded region control shapefile.
- **Manage Selected Regions:** Click this button to open the region management dialog. Under this dialog, users can select regions of interest and drag into the selected regions panel on the right. If the selected regions are not needed already, users can select them and click the "Delete" key on the keyboard. User's interested regions once set up, click the "OK" button to return the main page, and the selected regions will be listed in the "Selected Regions" panel. Note that users can also define a special region called "Other" by clicking the "Define Other" button. This region usually is defined as those regions that are outside the selected regions but inside the model domain (All Domain – the selected regions).

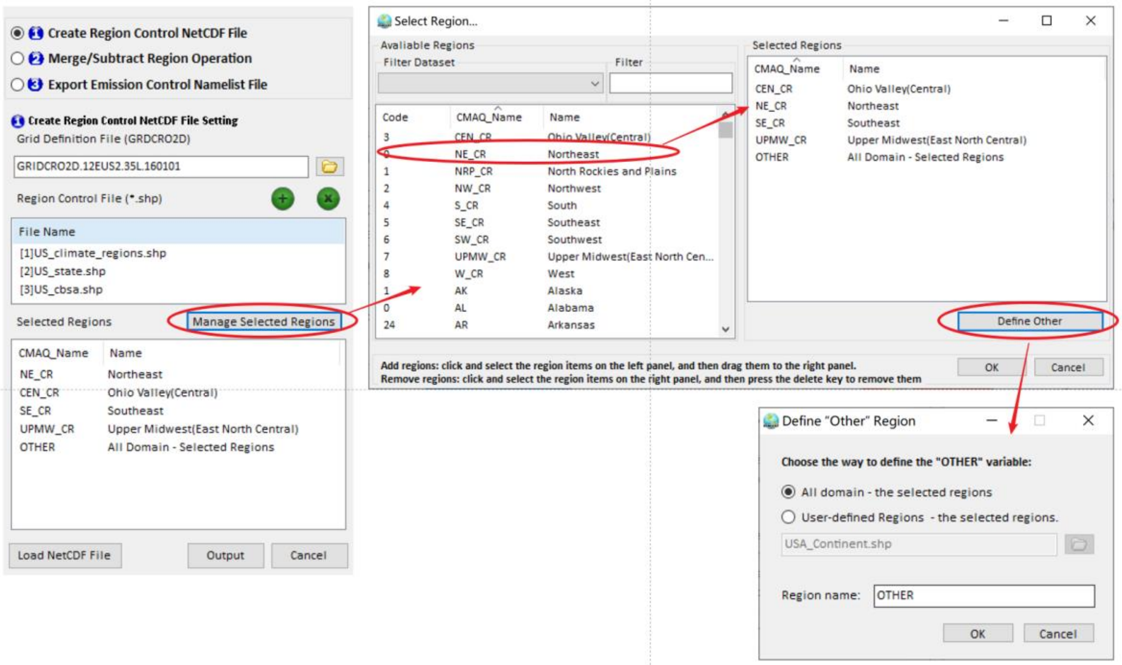


Fig. 35 Operation for Manage Selected Regions

➢ **Create region control NetCDF File**: All settings mentioned are done, click the **Output** button, and a region control NetCDF file will be created and the result will be visualized in the right panel under "NetCDF" tab page. Note that users can also load previously created region control NetCDF files by clicking the **Load NetCDF File** button.

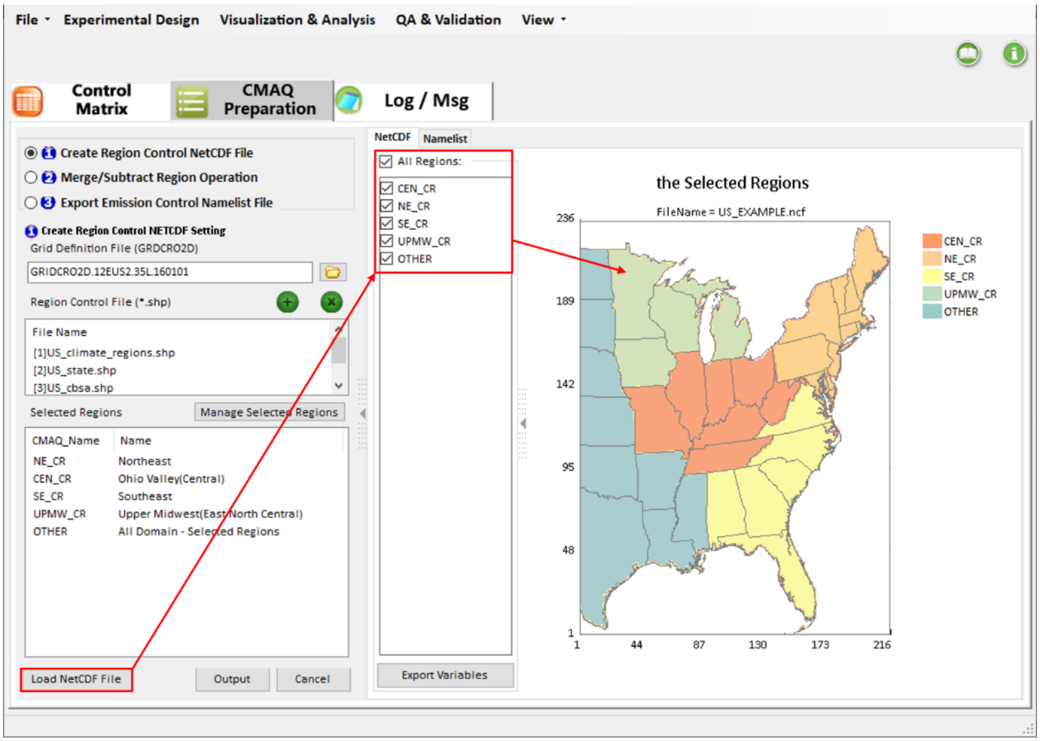


Fig. 36 Example for Load NetCDF File

5.2.2 Merge/Subtract Region Operation

The **Merge/Subtract Region Operation** module allows users to merge or subtract those regions created in the last module ("Create Region Control NetCDF File").Under this module, it includes the following operations: (1) Load Region Control NetCDF File, (2)Load Region Formula File(*.csv)(3)Add/Remove Regions;

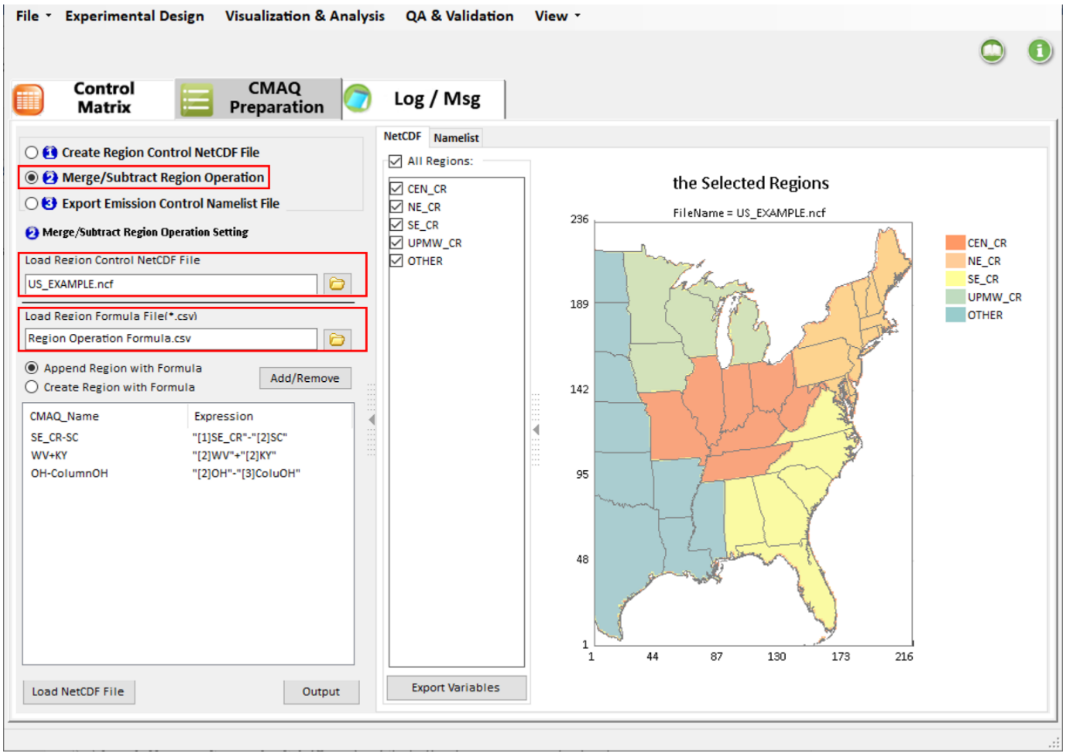


Fig. 37 GUI of Merge/Subtract Region Operation

- **Load Region Control NetCDF File**: Click the browser icon to load the NetCDF file created in the last module.
- **Load Region Formula File(*.csv)**: Click the browser icon to load a region formula file. This file defines some regions with formula.
- **Add/Remove Regions:** Click the "Add/Remove" button to open a dialog to define the region with formula. In this dialog, users can define a region by using an expression under "Formula Editor". Double-click the regions on the left panel to add them into "Formula Editor" on right. While the edit finished, click the "Add" button to commit the formula to the "Selected Regions" panel.

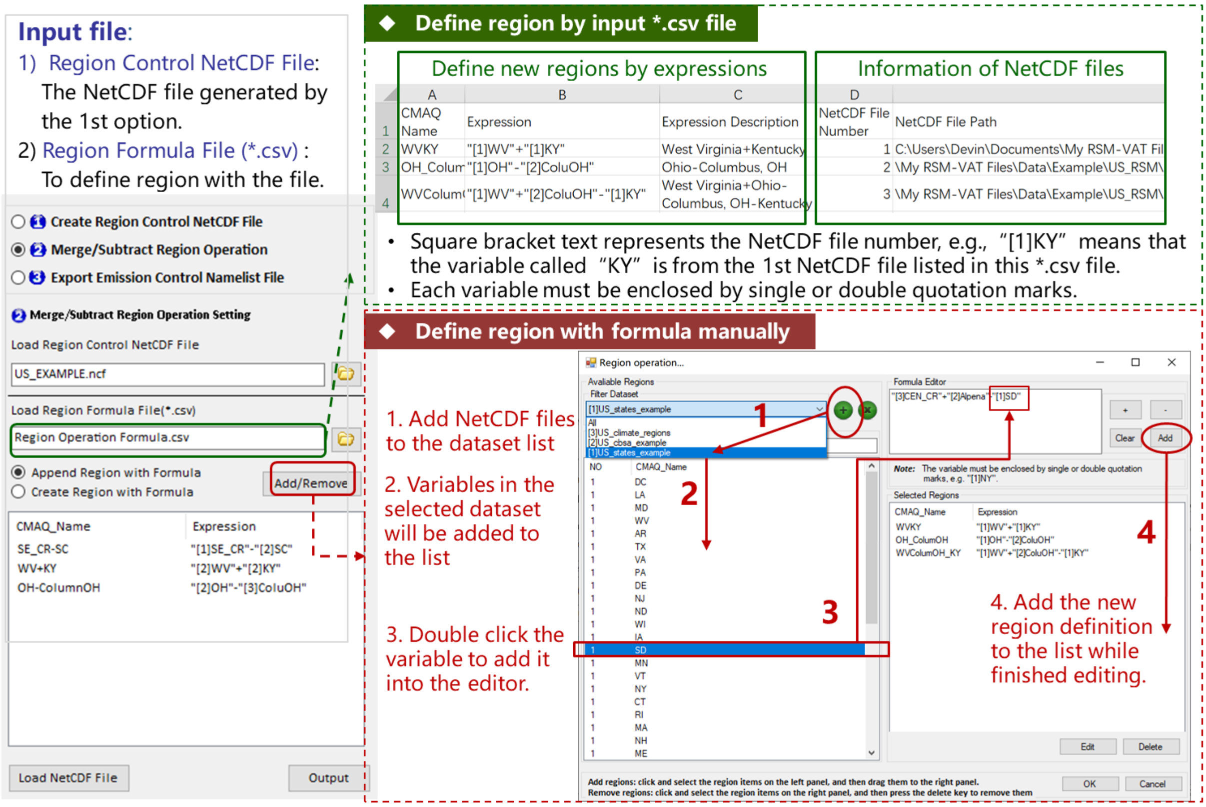


Fig. 38 Example for Using Merge/Subtract Region Operation Module

➢ **Create Region Control NetCDF File:** Once the above settings finished, click the "Output" button to create the new region control NetCDF file, and the file will be visualized in the right panel under "NetCDF" tab page**.** Note that users can also load previously created region control NetCDF files by clicking the "Load NetCDF File" button.

5.2.3 Export Emission Control Namelist File

Under the "Export Emission Control Namelist File" module, it provides users a function to output a series of Namelist files based on the emission control matrix, and these Namelist files will be used as input for CMAQ 5.3 or later. In this module, the following steps are needed. There are (1) Set Namelist Template File,(2) Set Region Control NetCDF File, (3) Set Control Matrix, and (4) Set Mapping File.

➢ **Set Namelist Template File:** This file will be used as a template to output a series of new Namelist files based on the input emission control matrix, as shown in Fig. 39. This file is available at: https://github.com/USEPA/CMAQ/blob/master/DOCS/Users_Guide/Tutorials/CMAQ_UG_tutorial_emissions.md.

- **Set Region Control NetCDF File**: This file is created from the 1st or 2nd module mentioned above. The region variables in the final output Namelist file will be obtained from this file.
- **Set Control matrix**: It provides two options for users, one is using the control matrix created in the Control Matrix module, and the other is coming from the user's input.
- **Set Mapping File:** This file is used to make the region, sector, and pollutant variables in the emission control matrix to be consistent with those in the Namelist template file, as shown in Fig. 40.

```
                         !> CUSTOM MAPPING EXAMPLES <!

   'NE_CR', 'ALL_MM'          ,'ALL'     ,'NOx'         ,'GAS'   ,0.8,'UNIT','m',
   'SE_CR', 'ALL_MM'          ,'ALL'     ,'NOx'         ,'GAS'   ,0.8,'UNIT','m',
   'CEN_CR', 'ALL_MM'          ,'ALL'     ,'NOx'         ,'GAS'   ,0.8,'UNIT','m',
   'UPMW_CR', 'ALL_MM'          ,'ALL'     ,'NOx'         ,'GAS'   ,0.8,'UNIT','m',
   'OTHER', 'ALL_MM'          ,'ALL'     ,'NOx'         ,'GAS'   ,0.8,'UNIT','m',
/

!------------------------------------------------------------------------------!
! Size Distribution Specification Section                                      !
!   Each size distribution rule either modifies the parameters associated with !
!   the aerosol modes of a particular stream, or adds new modes to a particular!
!   stream if they do not already exist.                                       !
!                                                                              !
!   Definition of Fields:                                                      !
!      'Stream - Label for the emissions stream that the instruction will      !
!        Label'   apply to. If the label is 'ALL', then the instruction will   !
!                 be expanded to apply to all streams.                         !
!      'Surrogate Mode' - With this label, the user identifies which mode from !
!                         the emissions is to be modified or created. With this!
!                         specificity, multiple modes can be defined and mapped!
!                         in the emissions instructions in the next section.   !
!      'Reference Mode' - This label maps the emissions surrogate aerosol mode !
!                         to specific parameters catalogued in the AERO_DATA   !
!                         module.                                              !
!------------------------------------------------------------------------------!
```

Fig. 39 Namelist Template File Example

Factors_Region	CMAQ_Region	Factors_Sector	NML_Secto
A	NE_CR	All_MM	ALL_MM
B	SE_CR		
C	CEN_CR		
D	UPMW_CR		
E	OTHER		

Fig. 40 Mapping File Example

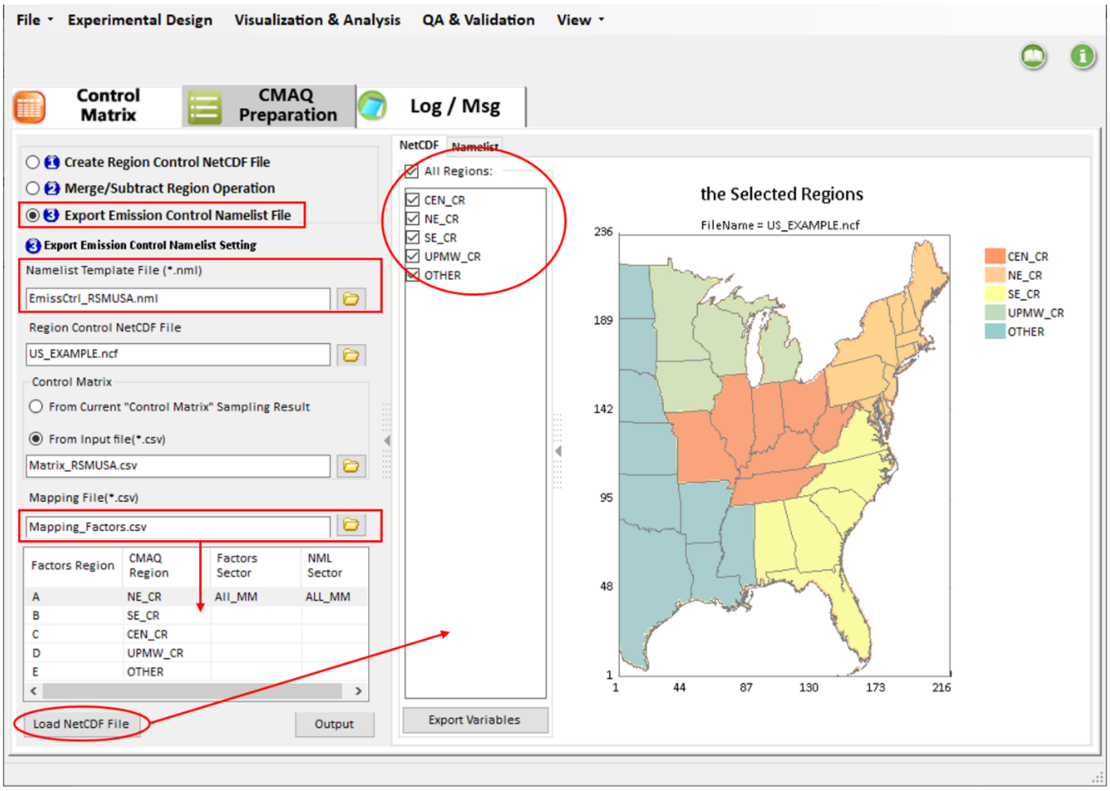


Fig. 41 Example for Using Export Emission Control Namelist File

➢ **Create Emission Control Namelist File**: Once all settings above are done, click the "Output" button, and a series of emission control Namelist files will be exported to the user-specified directory and listed in the Namelist tab page. Under Namelist tab page, users can click any of Namelist files to view or edit it.

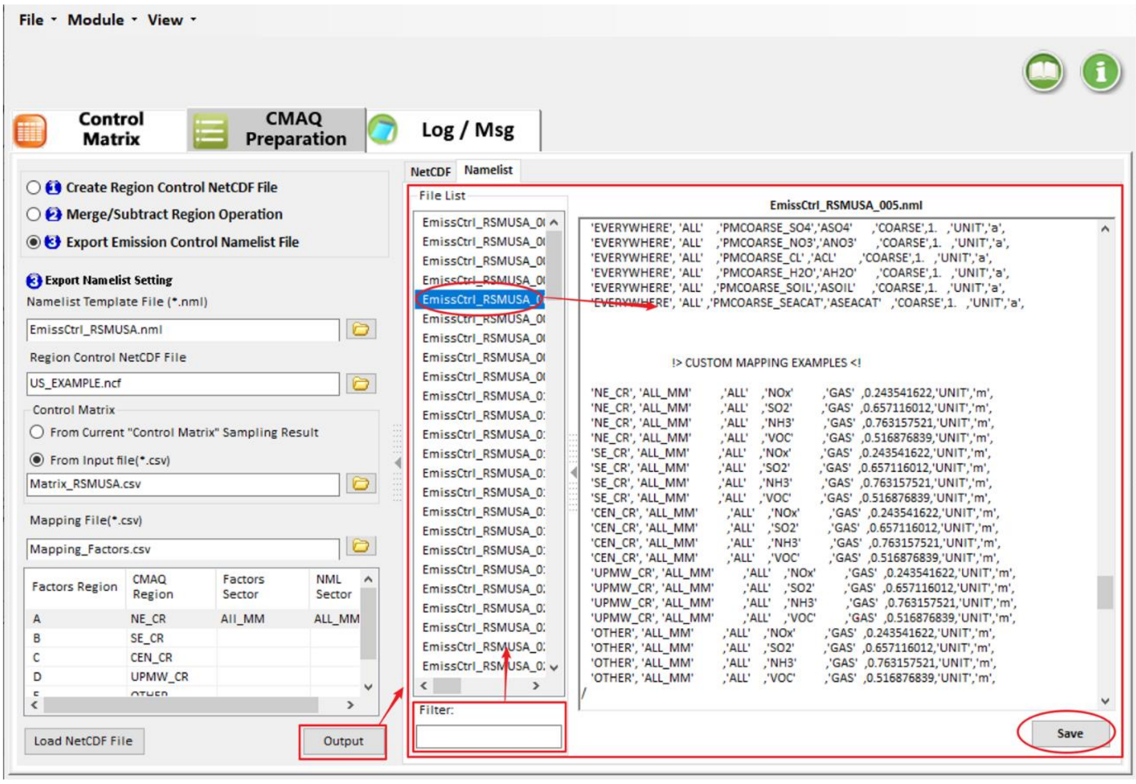


Fig. 42 Results for Output Namelist Files

6 Create RSM Project

There are four steps of input options for inputting different data or configuring the calculation parameters, including Create/ Input RSM Option, Model Data Input Option, Validation and QA Option, and Visualization Analysis Option.

6.1 Create/ Input RSM Option

The Create/ Input RSM Option includes **RSM-VAT Project File**, **Input RSM File, Create RSM File,** and **Advanced Option**, as shown in Fig. 43.

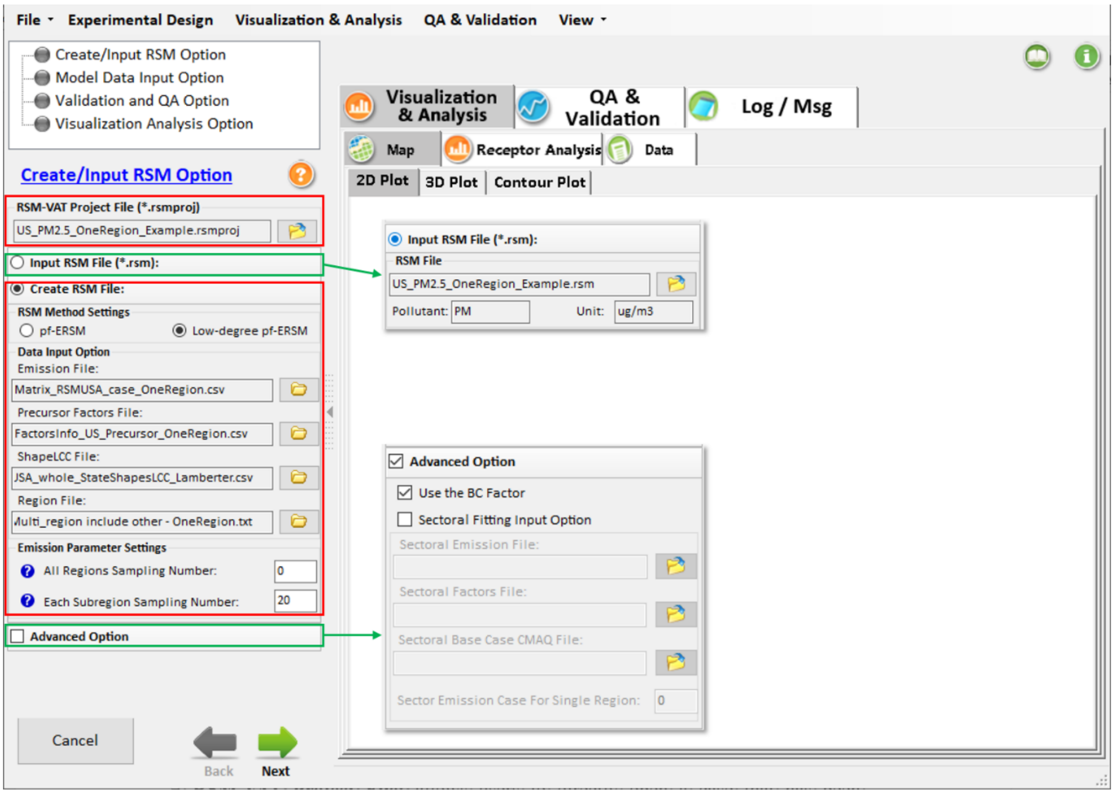


Fig. 43 Create/ Input RSM Option

➢ **RSM-VAT Project File:** allows users to directly open a rsm project that has been successfully run without having to run again (US_PM2.5_Jan.rsmproj).

➢ **Input RSM File:** allows users to directly open an already fitted RSM file. Also, the Create RSM File option will be unavailable if the Input RSM File option is chosen. This option will be time-saving because it dosenot need to create RSM again.

➢ **Create RSM File:** allows users to select RSM methods according to their needs and then set related files that need to be fitted, including Emission File, Precursor Factors File, ShapeLCC File, and Region File. This option for RSM run is a little time-consuming compared with the Input RSM File option because the fitting process for creating the RSM file is computational.

➢ **Emission Parameter Settings:** allows users to set the sampling number for the regions and subregions. The values of All Regions Sampling Number and Each Subregion Sampling Number should correspond to the input Emission File.

➢ **Advanced Option:** allows users to perform source contribution analysis by using related sectoral files. For example, it allows users to identify which emission sources contributes the most to the target pollutant concentration and then make control strategies.

Click on the “Next” green arrow at the bottom right of Data Input setting window to the next option.

6.2 Model Data Input Option

The Model Data Input Option includes **Model Data Input Option**, **Target Pollutant**, **Precursor Pollutant**, **Fitting Parameter Setting,** and **Plot Type**, as shown in Fig. 44.

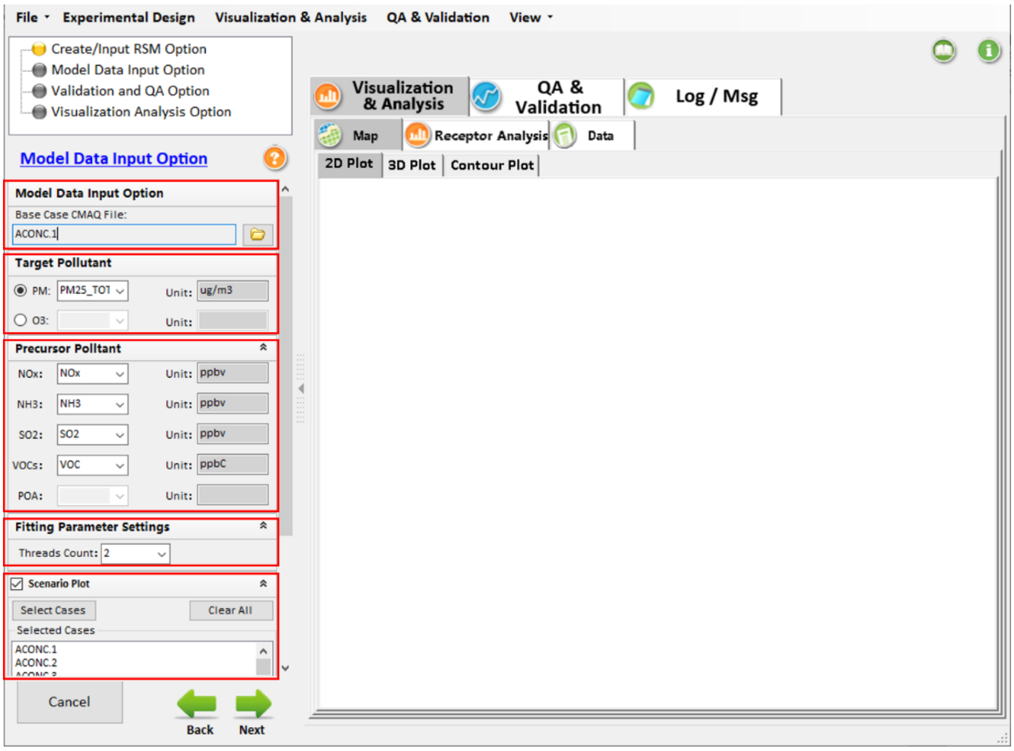


Fig. 44 Model Data Input Option

➢ **Model Data Input Option:** allow users to set the file path of the Base Case CMAQ File, where all CMAQ simulation files are located.

➢ **Target Pollutant:** allows the user to set the pollutant that will be modeled, e.g., $PM_{2.5}$ or O_3.

➢ **Precursor Pollutant:** allows the user to specify the precursor species.

➢ **Fitting Parameter Settings:** allows the user to set the number of threads called during the fitting process.

➢ **Scenario Plot:** allow the user to select CMAQ cases to check the CMAQ simulations by chekcing the Scenario Plot option.

Click on the "Next" green arrow at the bottom right of Data Input setting window to proceed to the next option.

6.3 Validation and QA Option

The Validation and QA Option includes Validation Types, Out of Sample Input

Option, and Cross Validation Input Option, as shown in Fig. 45. This option is used to validate the reliability and rationality of created RSM.

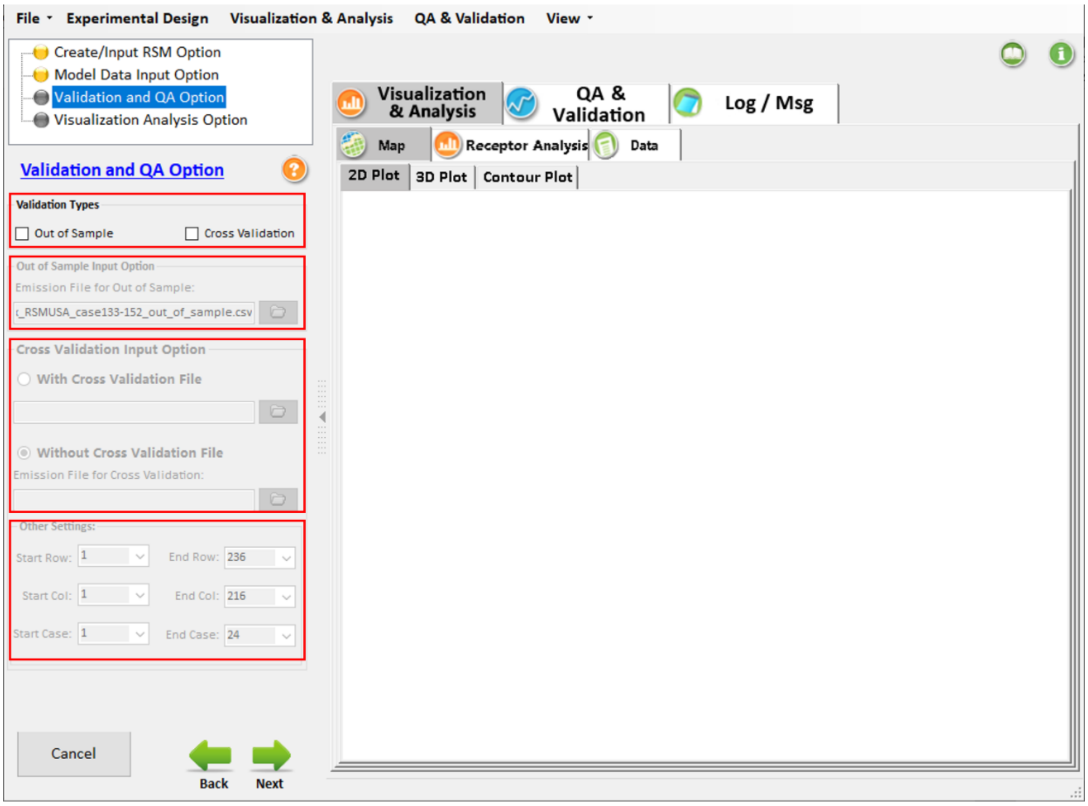


Fig. 45 Validation and QA Option

➢ **Validation Types:** allows users to choose the ways of validation, including Out of Sample and Cross Validation. These two options are optional for users.

➢ **Out of Sample Input Option:** once this option is checked, users should prepare and input an out of sample emission file. Note that the CMAQ runs in this emission file are not included in the RSM creation.

➢ **Cross Validation Input Option:** once this option is checked, users should input an emission file for Cross Validation. Note that one of the CMAQ runs in this emission file is left out for creating the RSM and the RSM predicted data are then verified against the CMAQ results that are left out. This comparison process is sequentially carried out for all CMAQ runs in this emission file.

Click on the "Next" green arrow at the bottom right of Data Input setting window to proceed to the next option.

6.4 Visualization Analysis Option

The Visualization Analysis Option allows users to set **Receptor File** and **Plot Types**, as shown in Fig. 46. Onced the Contour Plot option is checked under the **Plot**

Types, users should set up control factors for X axis and Y axis, respectively. And the results will be shown in "Contour Plot" once it is selected under **Visualization & Analysis →Map.**

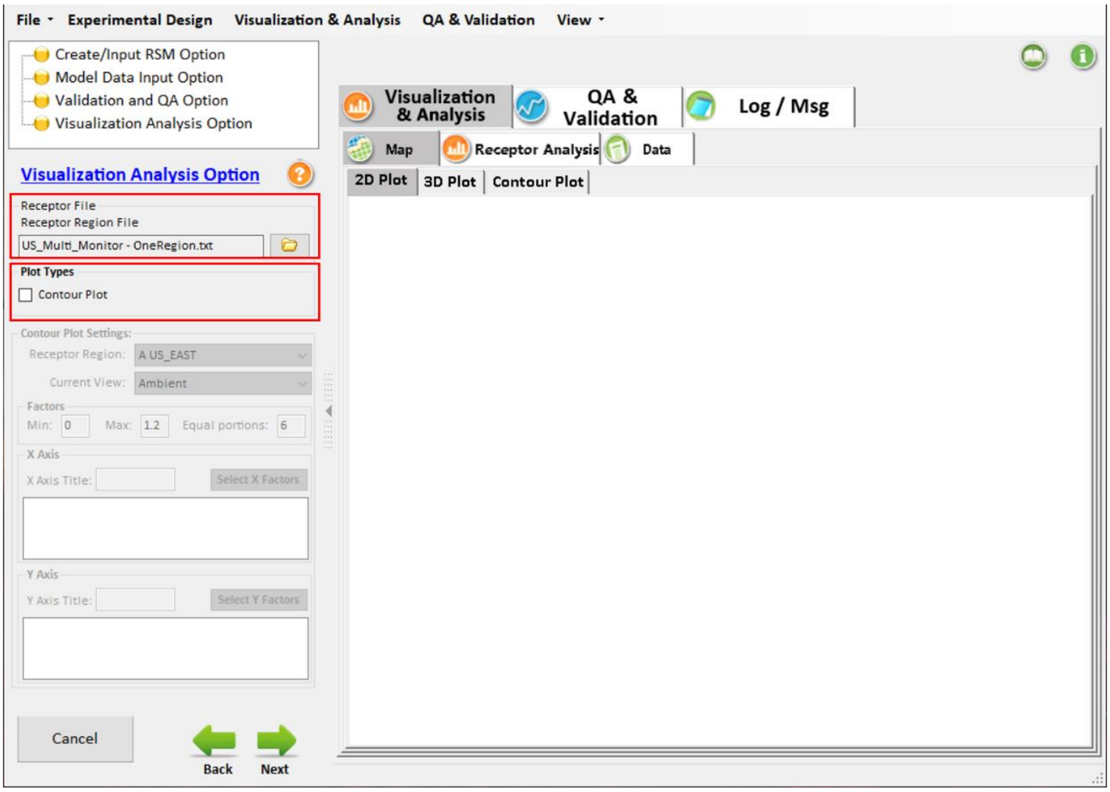


Fig. 46 Visualization Analysis Option

Click on the "Next" green arrow at the bottom right of Data Input setting window to proceed to save and run RSM-VAT. Users can view the running messages through "**Log/Msg**", as shown in Fig. 47.

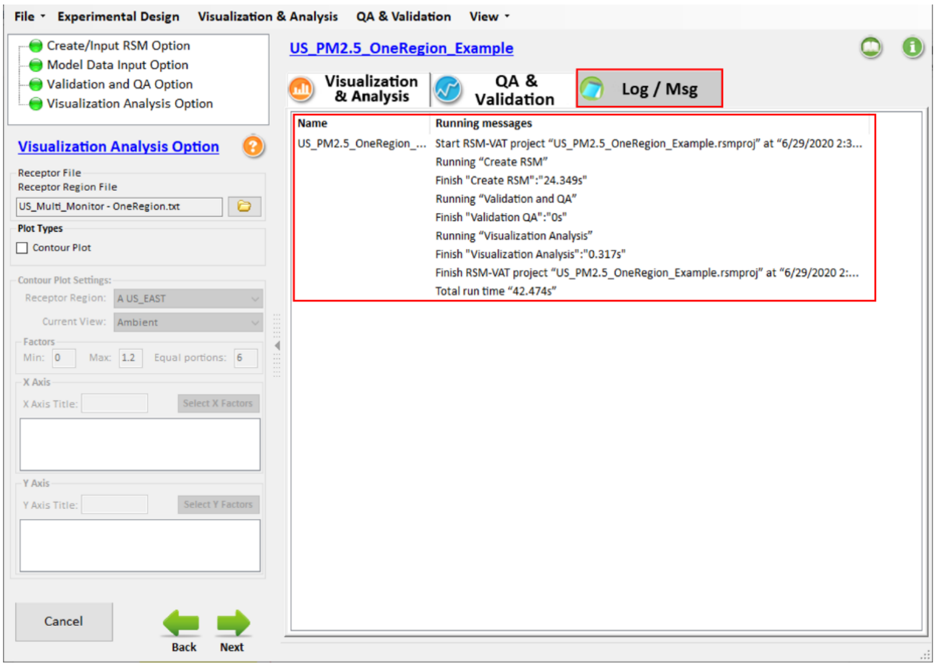


Fig. 47 Running Messages

7 Visualization & Analysis for RSM Results

When RSM project is created, the QA & Validation of Created RSM will be shown in "QA & Validation" module, and the RSM results will be shown in Visulization & Analysis module by multiple visualization types, including **MAP**, **Chart, or Data**, as shown in Fig. 48.

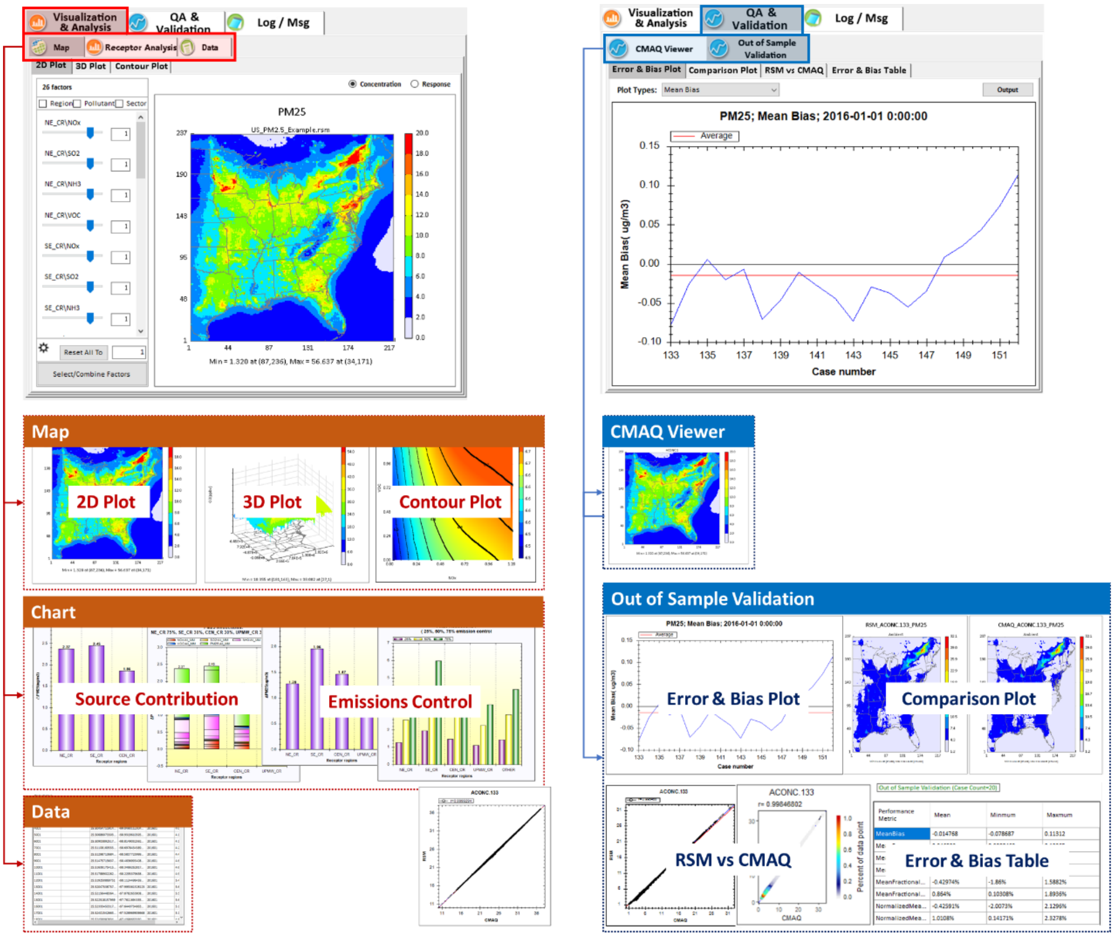


Fig. 48 Data Viewer of RSM-VAT Results

7.1 QA & Validation

Uncertainties associated with RSM come from two key areas: (1) inherent uncertainties from the air quality model (CMAQ) due to uncertainties of modeling sciences and formulation, computational approximation, and input data, including both emission and meteorological data;and (2) statistical representation of RSM model to simulate the responses of the air quality model(CMAQ) due to preset control scenarios. The model was validated using a number of techniques (e.g., OOS, CV), while recognizing and acknowledging these uncertainties associated with the application of the RSM.

The QA & Validation module includes **Out of Sample Validation, Cross Validation** and **CMAQ Viewer**, as shown in Fig. 49. This module is mainly used to examine and validate the RSM model performance. Among them, **Out of Sample Validation** is conducted to evaluate the performance of RSM, which compares the predicted values derived from the response surface models with the CMAQ simulations of a set of model runs that are outside of the experimental design and are not used in developing the predictive model. The same evaluation metrics (Table 3) were used for both **Out of Sample** Validation and **Cross Validation** methods. **CMAQ Viewer** is a tool for displaying and comparing the RSM predicted results to the CMAQ simulations.

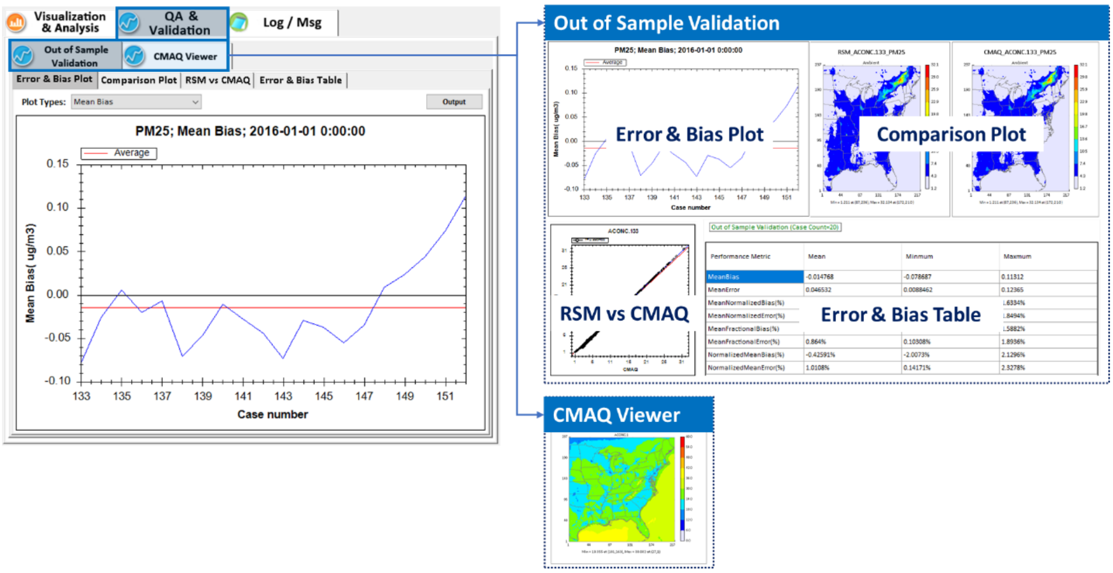


Fig. 49 QA & Validation

Table 3 Evaluation Metrics of RSM (Response Surface Model)

Performance Metric	Equation
Mean Bias (MB, ug/m^3)	$MB = \frac{1}{N}\sum_{i=1}^{N}(Cri - Cci)$
Mean Error (ME, ug/m^3)	$MB = \frac{1}{N}\sum_{i=1}^{N}(Cri - Cci)$
Mean Normalized Bias (MNB, $-100\% \sim +\infty$)	$MNB = \frac{1}{N}\sum_{i=1}^{N}(\frac{Cri - Cci}{Cci})$
Mean Normalized Error (MNE, $0\% \sim +\infty$)	$MNE = \frac{1}{N}\sum_{i=1}^{N}\lvert\frac{Cri - Cci}{Cci}\rvert$
Mean Fractional Bias (MFB,-200% to +200%)	$MFB = \frac{1}{N}\sum_{i=1}^{N}\frac{(Cri - Cci)}{(\frac{Cri + Cci}{2})}$

Mean Fractional Error	$MFE = \frac{1}{N}\sum_{i=1}^{N}\frac{\lvert Cri - Cci \rvert}{(\frac{Cri + Cci}{2})}$
(MFE, 0% to +200%)	
Normalized Mean Bias	$NMB = \underline{\sum_{i=1}^{N}(Cri - Cci)}\sum_{i=1}^{N}Cci$
(NMB, $-100\% \sim +\infty$)	
Normalized Mean Error	$NMB = \underline{\sum_{i=1}^{N}\lvert Cri - Cci \rvert}\sum_{i=1}^{N}Cci$
(NME, $0\% \sim +\infty$)	

N is the number of grid cells, Cri is the RSM predicted value in grid i, and Cci is the CMAQ value in grid i.

7.1.1 Out of Sample Validation

7.1.1.1 Error & Bias Plot

Under **Error & Bias Plot** module, it provides multiple statistical plots (e.g., MB, ME, MNB, MNE, MFB, MFE, etc.) for validating the RSM performance in different aspects. Users can also configure the plot according to their preferences, as shown in Fig. 50.

Fig. 50 Error & Bias Plot of Out of Sample Validation

7.1.1.2 Comparison Plot

Under the **Comparison Plot** module, visual inspection of prediction maps was conducted to confirm overall spatial comparability in the predicted versus modeled outputs for each of the CMAQ experimental design runs. Users can also set specific plot types and perform different operations on map (e.g., zoom in or zoom out domain), as shown in Fig. 51.

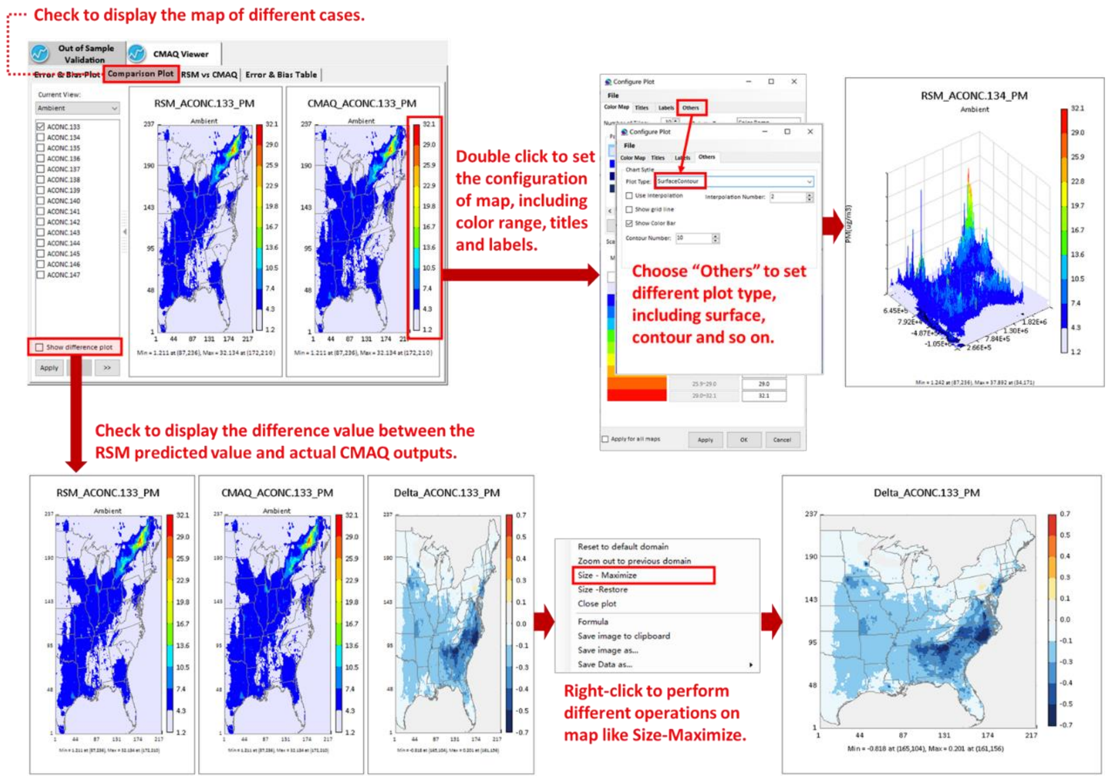


Fig. 51 Comparison Plot

7.1.1.3 RSM vs CMAQ

In RSM vs CMAQ module, it shows the correlation between RSM and CMAQ by scatter plots, denisity scatter plots. Users can also configure the plots according to their preferences, as shown in Fig. 52.

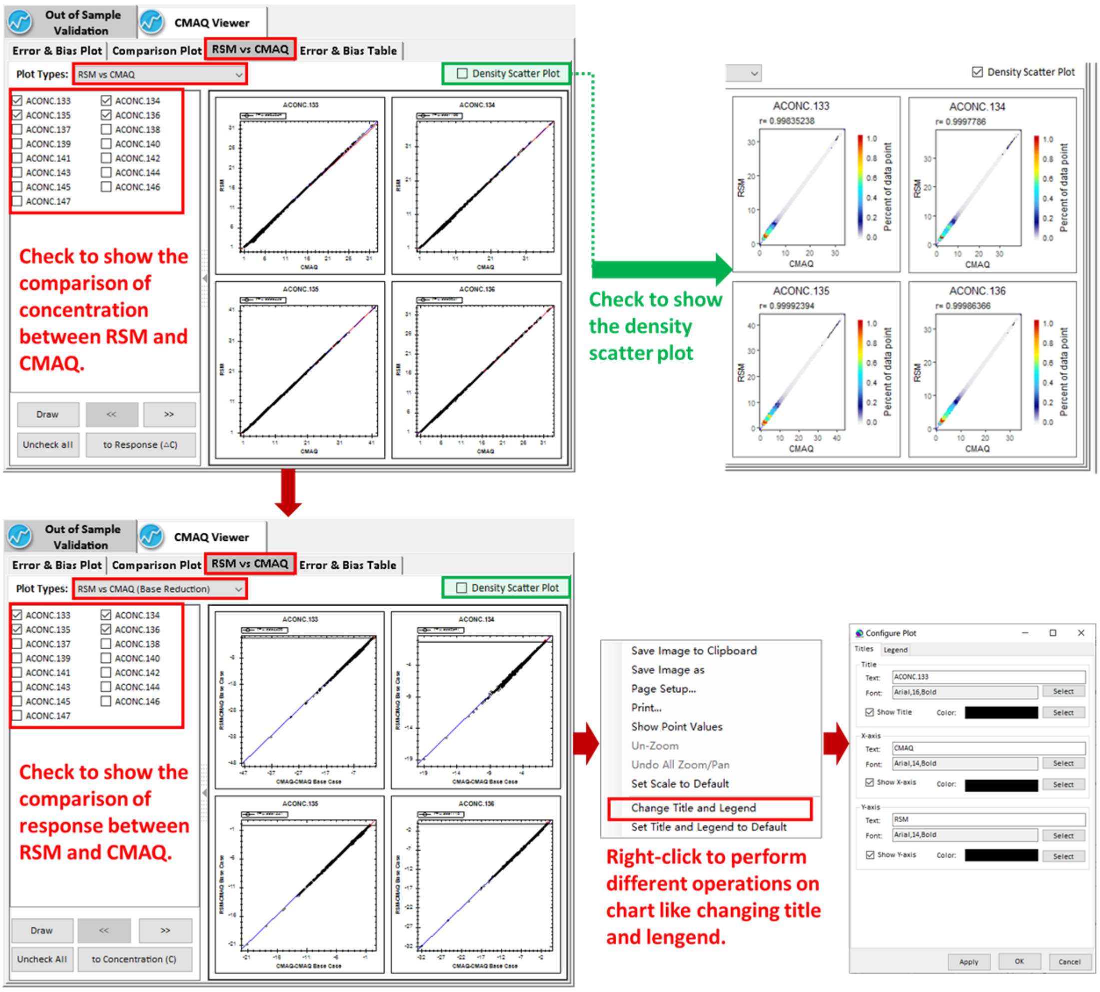


Fig. 52 RSM vs CMAQ of Out of Sample Validation

This module provides two kinds of plot types for users to view the comparison of the results between RSM and CMAQ. **RSM vs CMAQ** shows the comparison of the concentration between RSM and CMAQ, while **RSM vs CMAQ (Base Reduction)** shows the comparison of the response between RSM and CMAQ, where CMAQ-CMAQ Base Case and RSM-CMAQ Base Case are plotted as abscissa and ordinate respectively.

7.1.1.4 Error & Bias Table

The **Error & Bias Table** module summarizes the values of those statistical metrics listed in Table 3 to characterize the performance of created RSM,e.g., mean bias, mean normalized bias, and normalized mean bias, and so on. Users can export data for further study, as shown in Fig. 53.

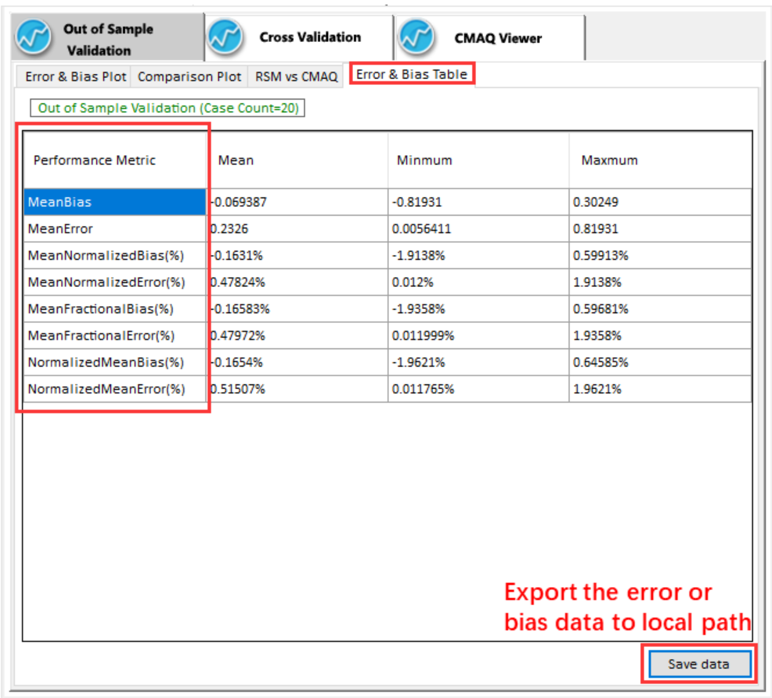


Fig. 53 Error & Bias Table of Out of Sample Validation

7.1.2 Cross Validation

Cross Validation is used to evaluate overall RSM performance. For each iterative run, one of the experimental model runs is left out of the model estimation, and the RSM is then computed and used to predict the omitted run. If Cross Validation option is checked in the "Validation and QA Option", Cross Validation tab will be listed under "QA & Validation" module. The predictive performance of the RSM is also evaluated using a standard set of model performance statistical indices over all grid cells, e.g., MB, ME, MNB, MNE.etc. And it also provides Error & Bias Plot, Comparison Plot, RSM vs CMAQ scatter plot , and Error & Bias Table functions, which are similar to that of Out of Smaple validation. So we will not elaborate it again here.

7.1.3 CMAQ Viewer

Under CMAQ Viewer module, it provides functions for users to visualize and examine the CMAQ simulations. Users can also set specific plot types and perform different operations on map (e.g., zoom in or zoom out domain), as shown in Fig. 54.

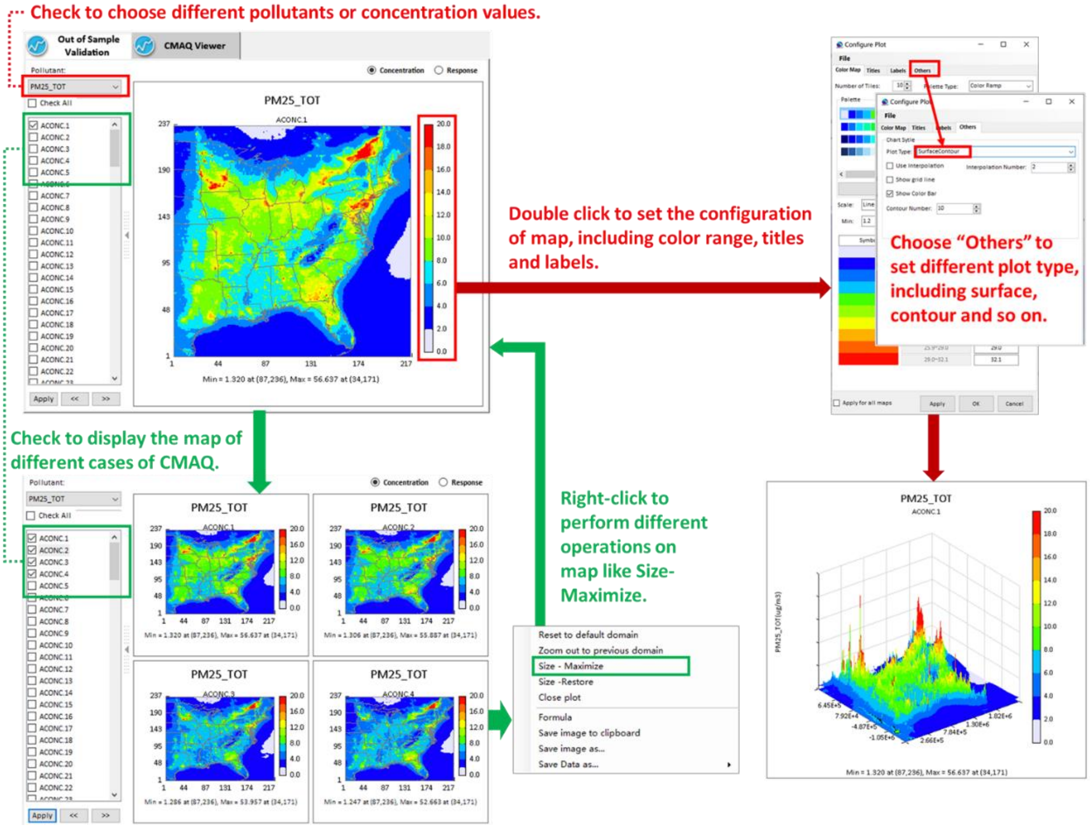


Fig. 54 CMAQ Viewer

7.2 Visualization & Analysis

RSM-VAT provides a series of visualization and analysis functions for supporting decision making, including 2D and 3D maps for instant overview of air quality response, bar/pie charts for quantitatively analyzing and comparing the effectiveness of emission reduction, and contour plots for dynamically description of the nonlinear or linear relationship between two single/groups of emission control factors.

7.2.1 Map

Under Map module, users are allowed to show the concentration that responds in real-time to the emission reduction control with specific plot type. 2D map can identify these changes in different administrative regions intuitively, while The 3D map has an instant three-dimensional visual effect for the air quality changes. Users can also perform different operations on map (e.g., size-maximize or size-restore), using the menu brought up by right-clicking on the map, as shown in Fig. 55.

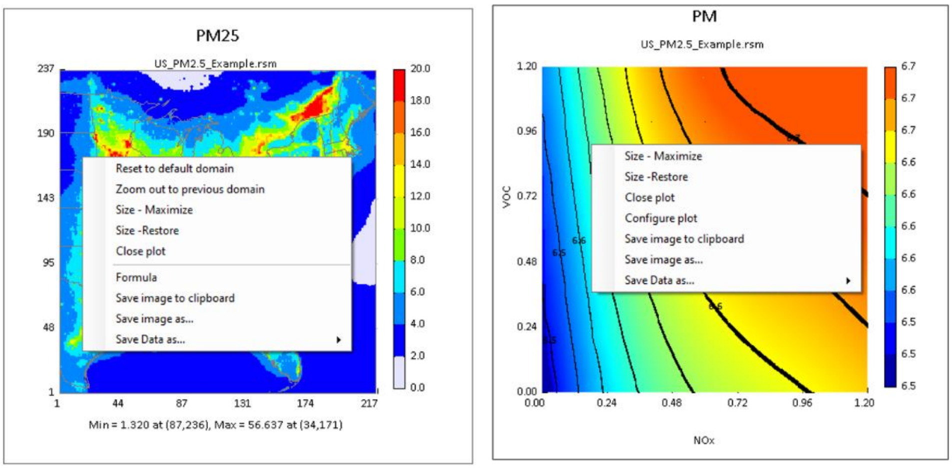


Fig. 55 Right-click on Map to Perform Different Operations on Map Results

7.2.1.1 2D Plot

User can click the **2D Plot** tab to view the 2D distribution of pollutant concentration in real-time. In this module, users are allowed to set the value of emission control factors and get the corresponding 2D concentration in response to the set emission controls as shown in Fig. 56. For example, the user will be able to change any control factor (e.g., NE_CR NOx levels) and see the impacts on $PM_{2.5}$.

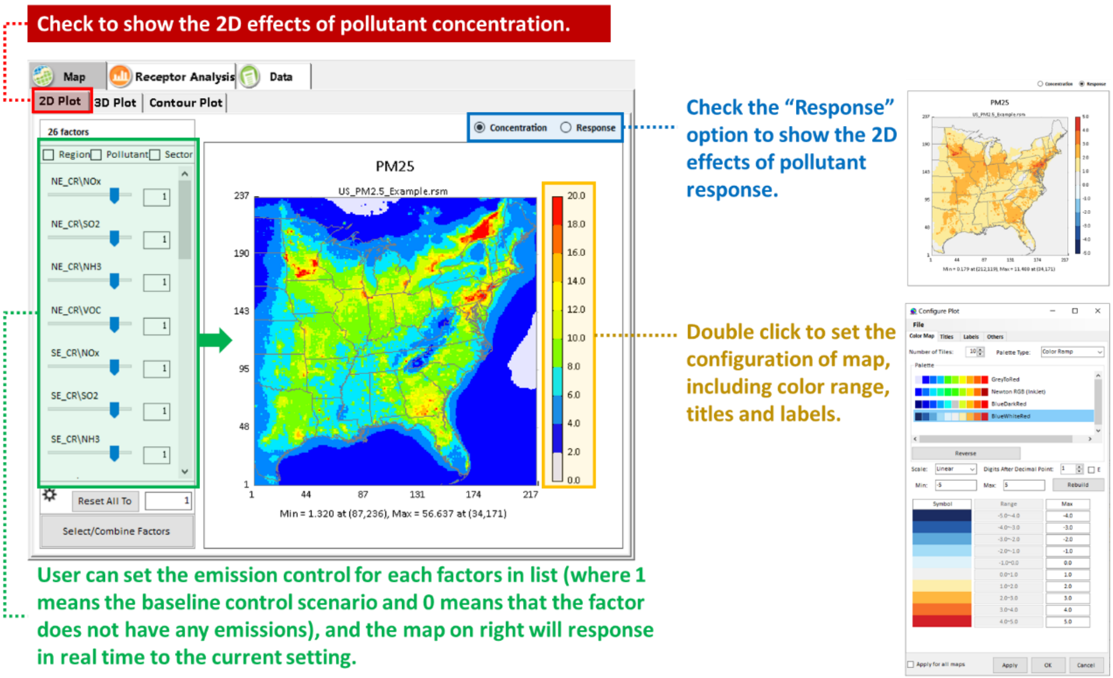


Fig. 56 2D Plot Viewer in the Map Module

Change emissions of control factors: The panel (green line) on the left lists all control factors. Users are able to change any control factor (e.g., NE_CR NOx levels) and see the impacts on air quality changes (e.g., PM2.5 or O3) by dragging the slide bar or inputting value in the text box. Besides, users can also set all control factors to a same control level, e.g., 0.5 by clicking "Reset All To" button.

Customize control factors: it allows users to flexibly group/combine specific factors by checking Region/Pollutant/Sector in the top of the control factors panel. Users are also allowed to customize these control factors by clicking "Select/Combine Factors" button. When "Select/Combine Factors" is clicked, it will show a "Select/Combine Factors" window, and provide two ways to customize control factors in this window.

1) **Using pre-defined control filters**: all existing control factors can be classified by pre-defined filters, including "Region", "Pollutant" and "Sector". Users can select interested filter to re-organized control factors and get the corresponding air quality surfaces by changing these new defined factors, as shown in Fig. 57.

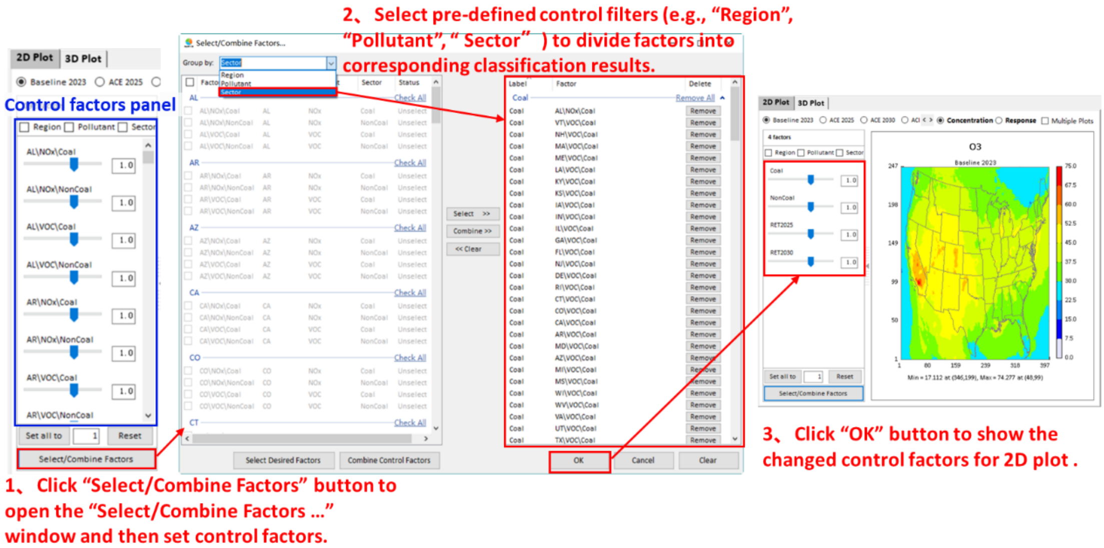
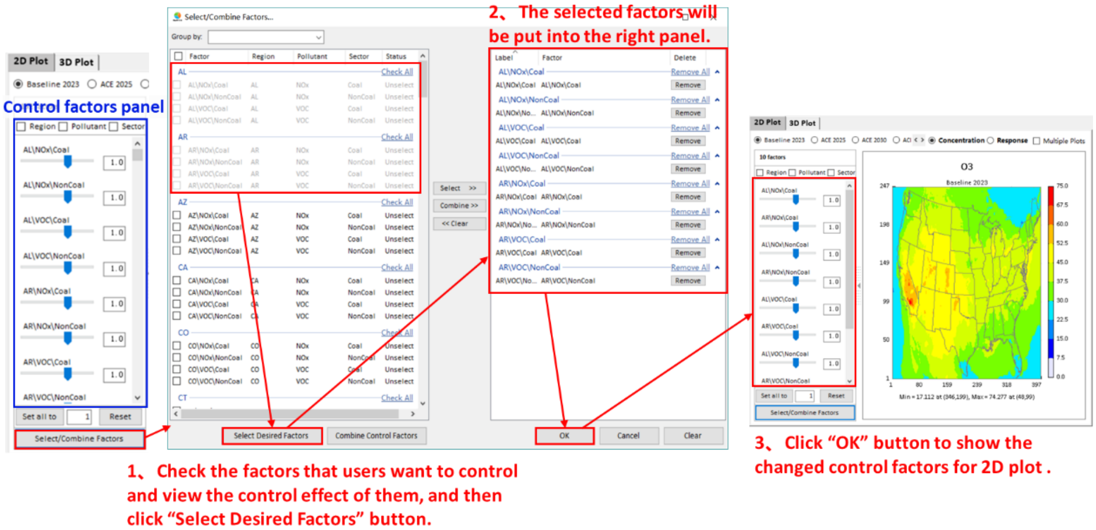
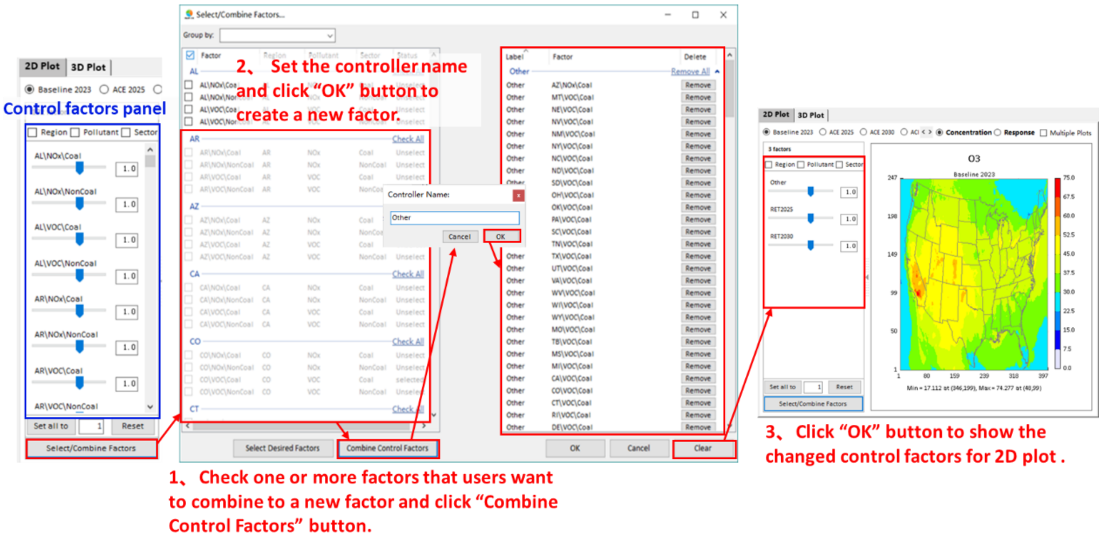


Fig. 57 Pre-defined control filter

2) **User-defined control method**: it provides two kinds of ways to define control factors as needed. a) **Select interested factors only.** This means that those factors you want to control will be selected and listed in control factors panel while those unselected factors will be kept as baseline (equal to 1). To do this, users just need to check the interested factors from the left panel of Fig. 58(a), and then click "Select Desired Factors" to move these factors to right panel and finally click "OK" to return control factors panel. b) Select any combination of factors. This means that you can combine one or more factors to form a new factor by using "Combine Control Factors", as shown in Fig. 58(b).



(a) Select interested factors only



(b) Select any combination of factors

Fig. 58 User-defined control method

7.2.1.2 3D Plot

User can click the **3D Plot** tab to view the 3D distribution of pollutant concentration in real-time. In this module, users are allowed to set the value of emission factors and get the corresponding 2D concentration in response to the set emissions as shown in Fig. 59.

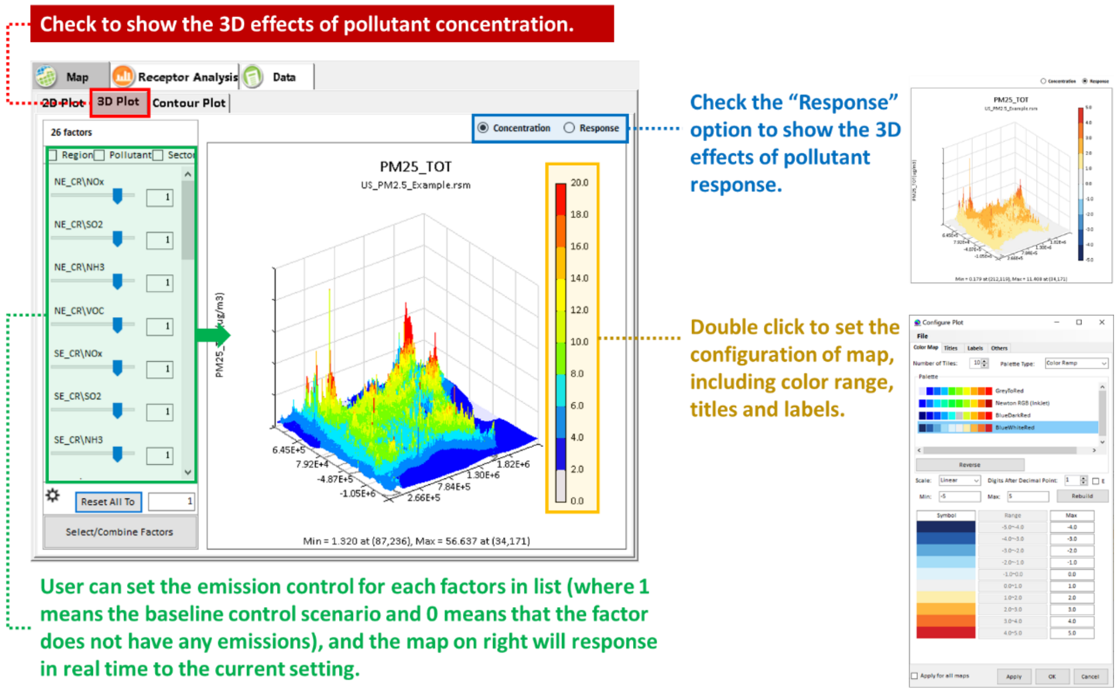


Fig. 59 3D Plot Viewer in the Map Module

7.2.1.3 Contour Plot

User can click the **Contour Plot** tab to view the 2D contour plot of pollutant concentration. This module can help users study the sensitivity among different precursors, e.g.,O_3 response of NOx and VOCs emissions control.In this module, users can draw the contour plot of pollutant concentration based on the specified emission factors as shown in Fig. 60.

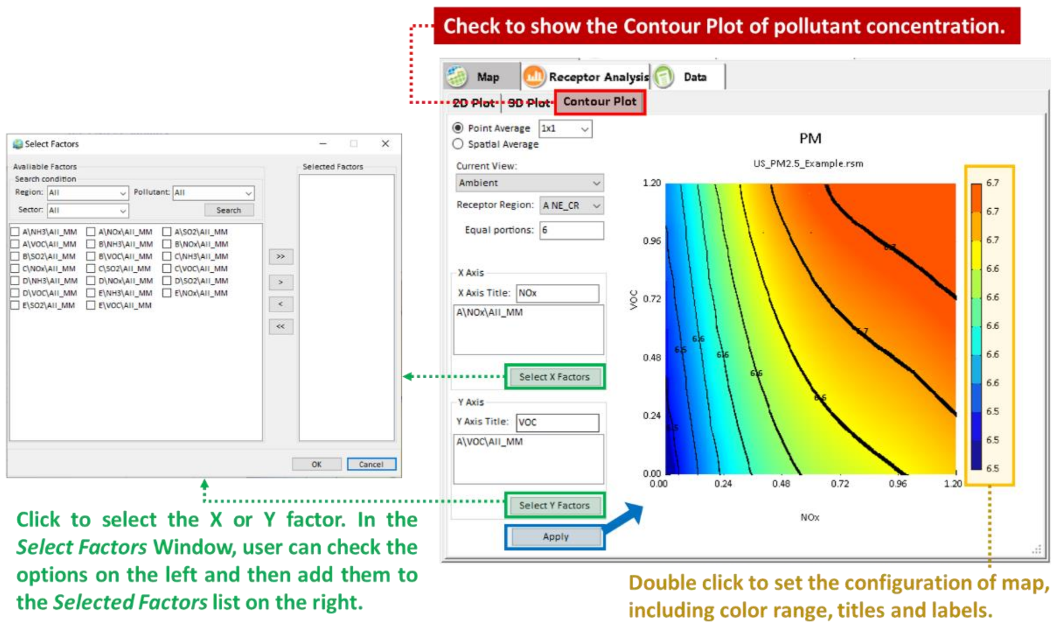


Fig. 60 Contour Plot Viewer in the Map Module

7.2.2 Chart

Under Chart module, it provides 4 kinds of charts for users to anlysis the response to different emission controls. There are (1) Source Contribution 1, (2) Source Contribution 2, (3) Emission Control 1 and (4) Emission Control 2.

7.2.2.1 Source Contribution 1

Under **Source Contribution 1** module, it provides functions for users to analyze the source contribution to target pollutant (e.g., $PM_{2.5}$, O_3) in selected receptors from the different emission controls. As shown in Fig. 61, the left panel is the configuration options of **Source Contribution 1,** while the right panel shows the pollutant reductions under current configuration of emissions control.

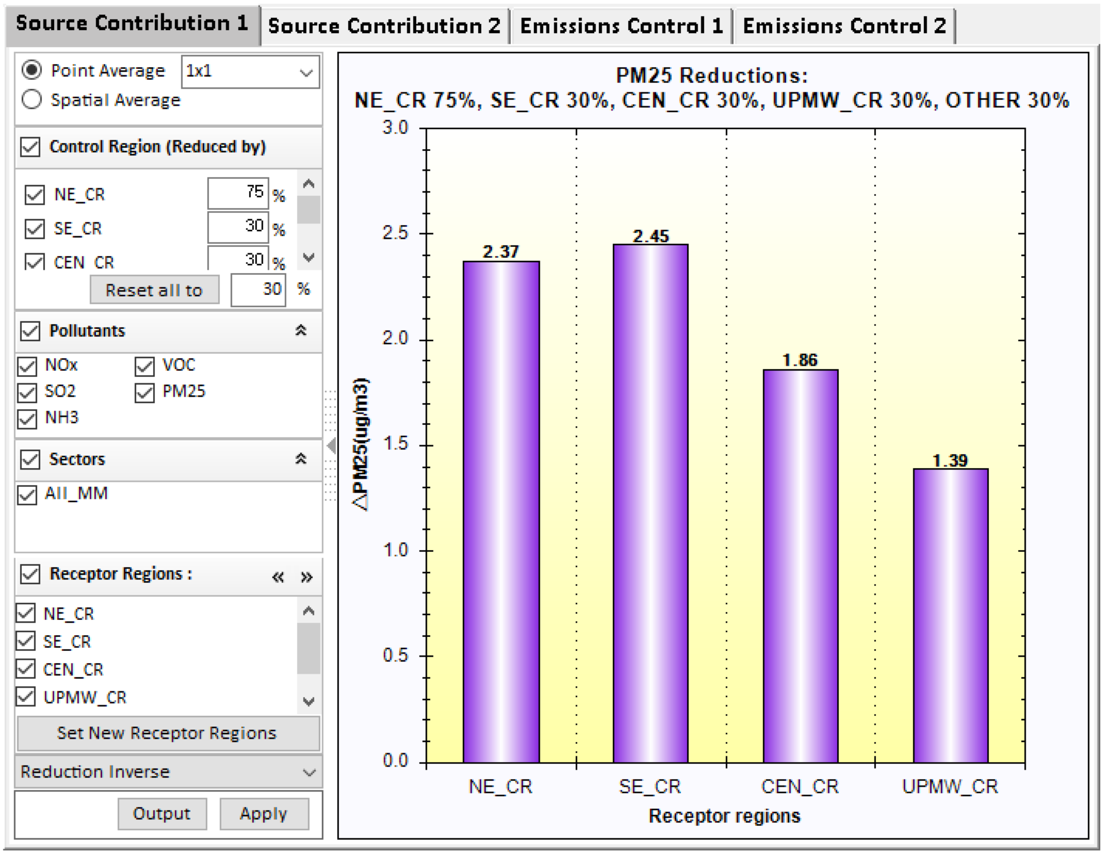


Fig. 61 Example of Source Contribution 1

The configuration options available in this module include:

Point Average: This option specifies how many model grid cells at the monitor locations to use in the calculation of mean concentration for specified receptor regions. A drop down menu provides options to use 1x1, 3x3, 5x5, and 7x7 arrays of model grid cells. The default is to use a 1x1 array of grid cells at the monitor locations.

Spatial Average: This option averages pollutant concentration in those grid cells that located in specified receptor regions, respectively.

Control Region (Reduced by): It lists all control regions and supports to set emission reductions for each control region. "Reset all to" button allows users reset a same emission reductions for all control region.

Pollutants: It lists all precusours (including primary PM for $PM_{2.5}$) that come from emission control matrix.

Sectors: It lists all sectors (e.g., Points, Mobiles,etc) that come from emission control matrix.

Receptor Regions: This option lists all receptor regions that come from the "Receptor Region File" in "Visualization Analysis Option" module by default.Under this option, it also provides a option for users to set up new receptor regions. For example, users can click the "Set New Receptor Regions" to open a receptor region configuration window to select desired states or CBSA regions by selecting the default file "US_STATE.txt" or "US_CBSA.txt" and then checking the regions of interest on the right panel, and then click "OK" or "Apply to All Charts" to show the corresponding response results of new receptor regions (Fig. 62).Note that "OK" button only takes effect in current chart, but "Apply to All Charts" button applies to all charts under Receptor Analysis module. Users can also add new receptor regions by importing receptor region files in the specified format according to their needs (Fig. 63). Besides, users can extract the desired regions for further study (Fig. 64).

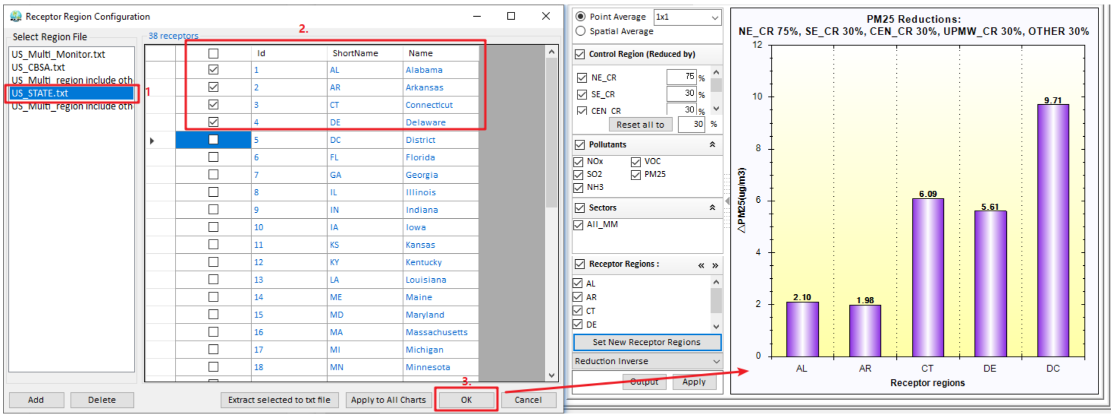


Fig. 62 Set up new receptors regions

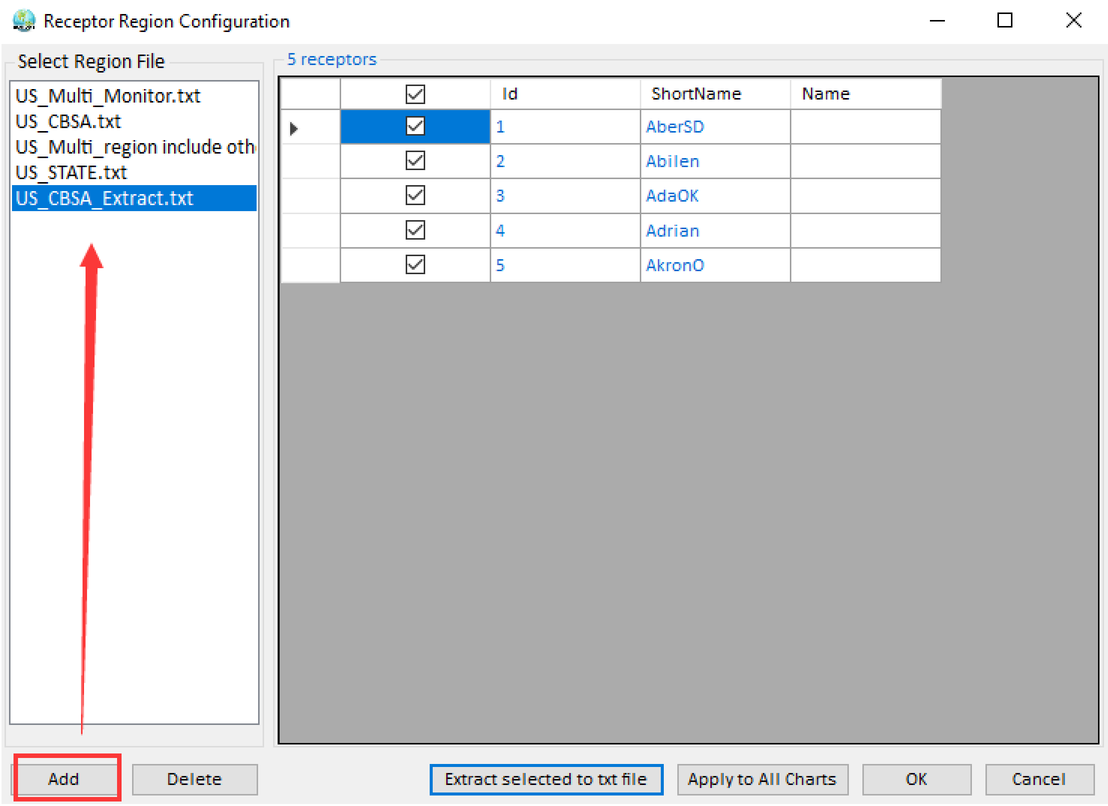


Fig. 63 Load a receptor region file

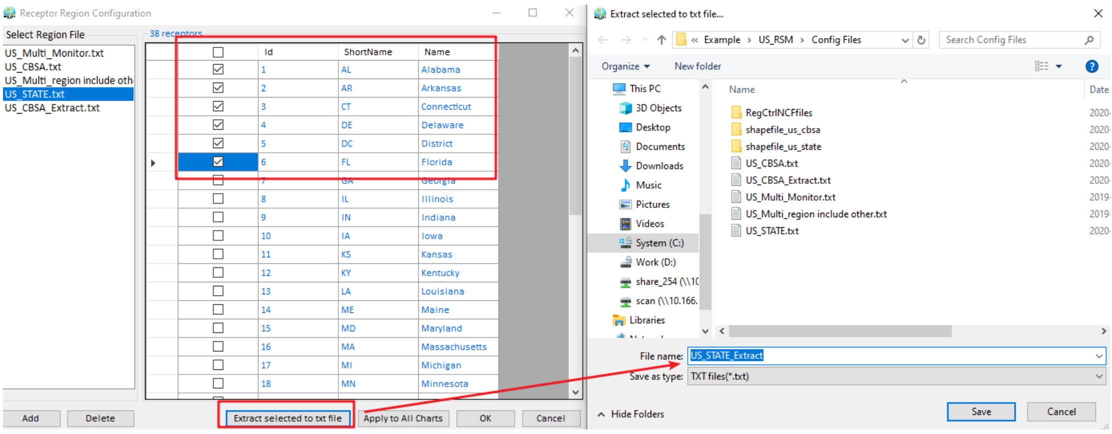


Fig. 64 Extract selected regions to text file.

Response type: A drop down menu on the bottom of this module configuration panel provides three response types: **Ambient, Reduction, and Reduction Inverse**. **Ambient** option means the chart on the right will show as absolute concentration of each receptor. **Reduction** option means that the chart on the right will show as "RSM Prediction" –"Baseline CMAQ concentration" , while **Reduction Inverse** option is the reverse of **Reduction**.

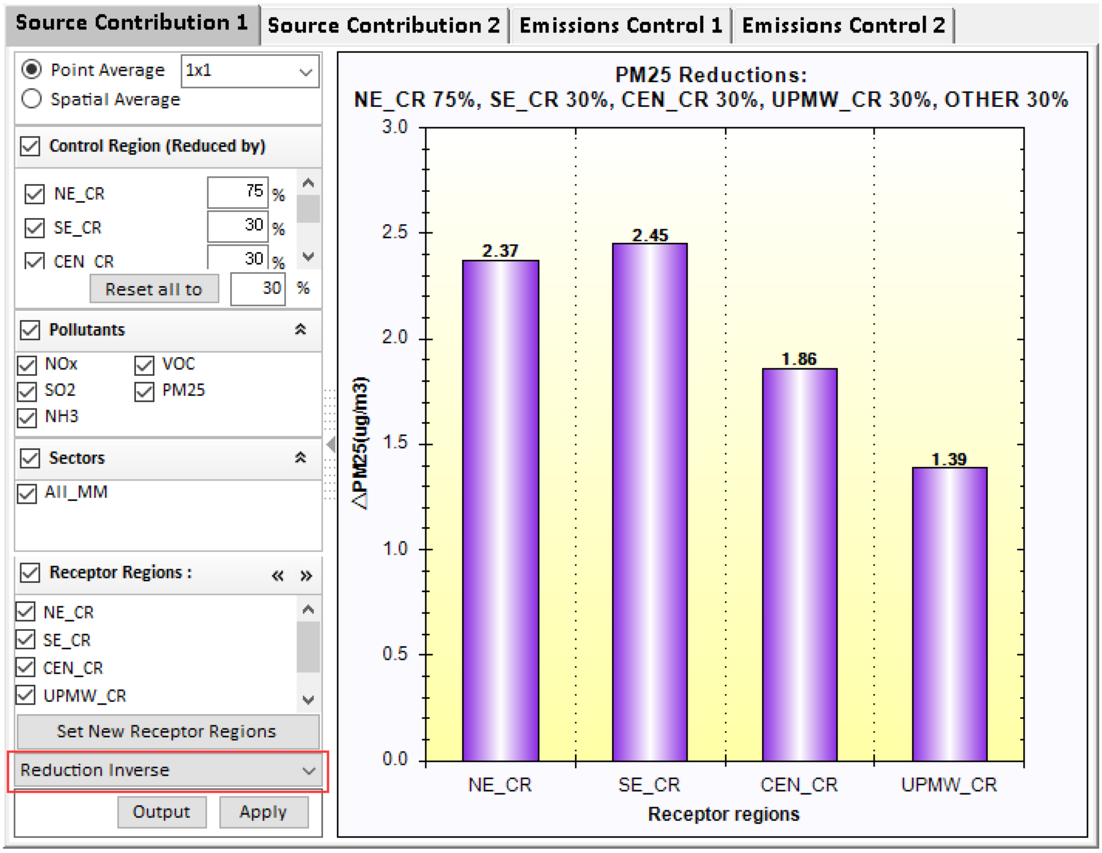


Fig. 65 Response Type in Source Contribution 1

Output: Click this button to output current results to "*.csv" file for further study.

Apply: Click this button to make the settings effective and draw chart.

7.2.2.2 Source Contribution 2

Under this module, it allows user to compare the cumulative/cluster impacts and the different source contributions to $PM_{2.5}$ or O_3 decrease caused by control factors (a control factor means a combination of region, pollutant, sector, e.g., NE_CR/NOx/All_MM) emission reductions under different emission control scenarios. As shown in Fig. 61, the configuration options in the left panel is similar to that of **Source Contribution 1**.The difference is that it provides three types of charts for visualization on the bottom of the configuration options, there are (1)Stack chart, (2)Cluster chart and (3)Pie chart.

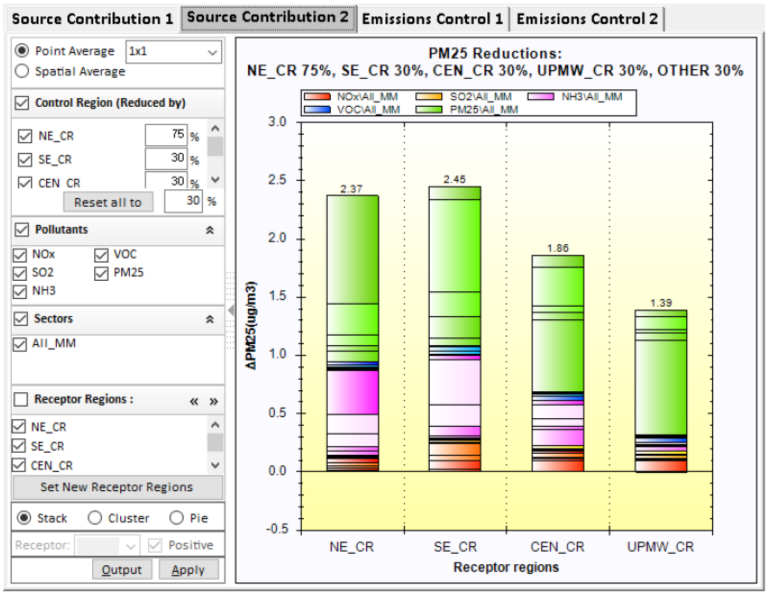


Fig. 66 Example of Source Contribution 2

Stack chart: This option shows the cumulative impacts of $PM_{2.5}$ or O_3 decrease (Air quality improvements) caused by the emission control scenario from current configuration options. For example, Fig. 61 shows the ambient $PM_{2.5}$ concentration of Northeast climate region(NE_CR) could be reduced by 2.37 μ g/m^3 under the emission control scenario of NE_CR 75%, SE_CR 30%, CEN_CR 30%, UPMW_CR 30% and OTHER 30%. And the emission sources from primary $PM_{2.5}$ (PM2.5/All_MM) contributes almost 60% to $PM_{2.5}$ Reduction in NE_CR rececptor.

Cluster chart: This option shows the cluster impacts of $PM_{2.5}$ or O_3 decrease (Air quality improvements) caused by the emission control scenario from current configuration options as shown in Fig. 67.

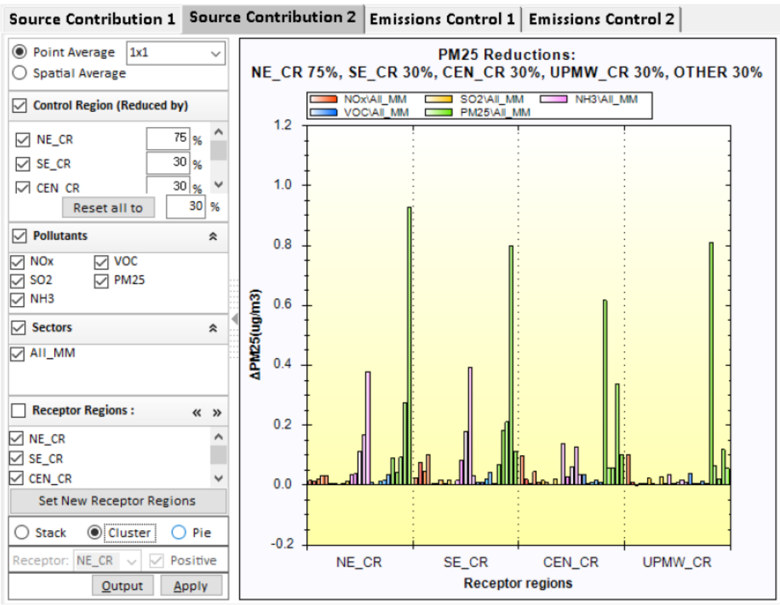


Fig. 67 Cluster chart in Source Contribution 2

Pie chart: This option shows the source contributions to $PM_{2.5}$ or O_3 in a selected receptor region caused by the emission control scenario from current configuration options. As shown in Fig. 68, the drop down menu of **Receptor** option on the bottom of configuration panel only takes effect in checked **Pie** option. It lists all receptor regions from **Receptor Regions** list panel, and uses the first item as default. Fig. 68 shows that the emission sources from NE_CR primary $PM_{2.5}$ (A,PM25,All_MM) have a greater impact (~23.04%) on $PM_{2.5}$ Reduction of NE_CR compared to other control factors.

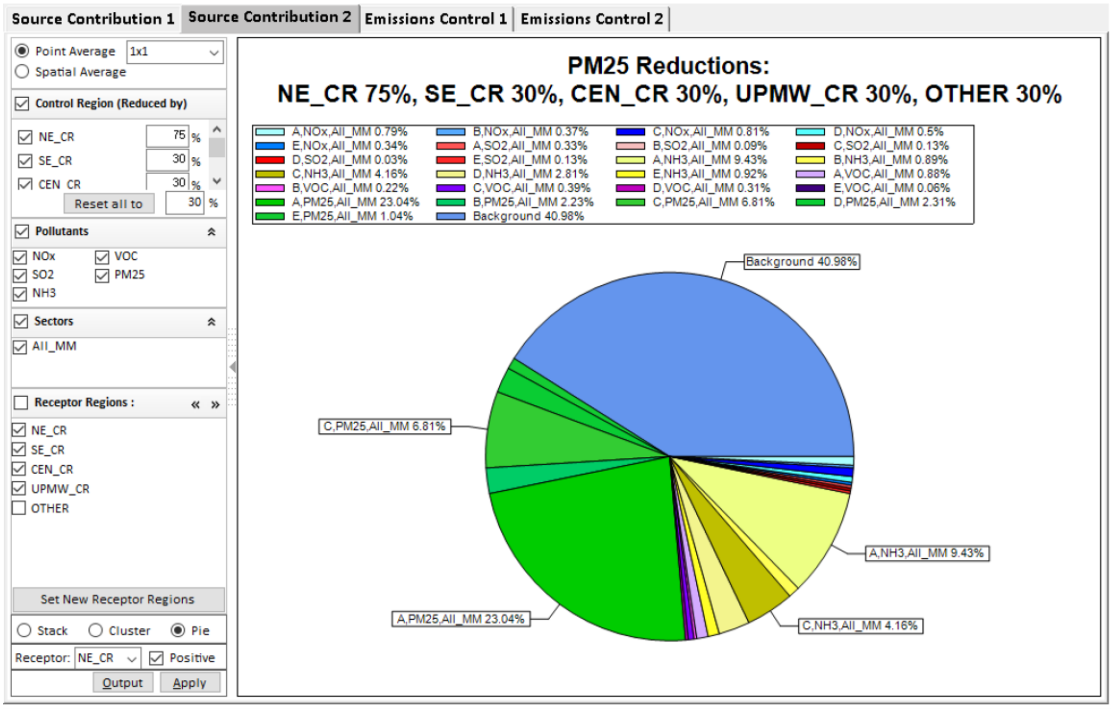


Fig. 68 Pie chart in Source Contribution 2

7.2.2.3 Emission Control 1

Under this module, it allows user to compare the emission source contributions to $PM_{2.5}$ or O_3 decrease caused by changing each control factor emissions. As shown in Fig. 69, the configuration options in the left panel is similar to that of **Source Contribution 1**.The difference is that it allows users to control changing each control factor emission under the control factors panel. Under the control factors panel, users are allowed to to flexibly change the input control factor emission and show the corresponding response value of concentrations in real-time. The panel lists all control factors. The sliders could be dragged to change the emission of each control factor. Users can also group/combine specific factors by checking **Region/Pollutant/Sector** on the top of the control factors panel or by clicking the **Select/Combine Factors** button to custom control factors of insterest.

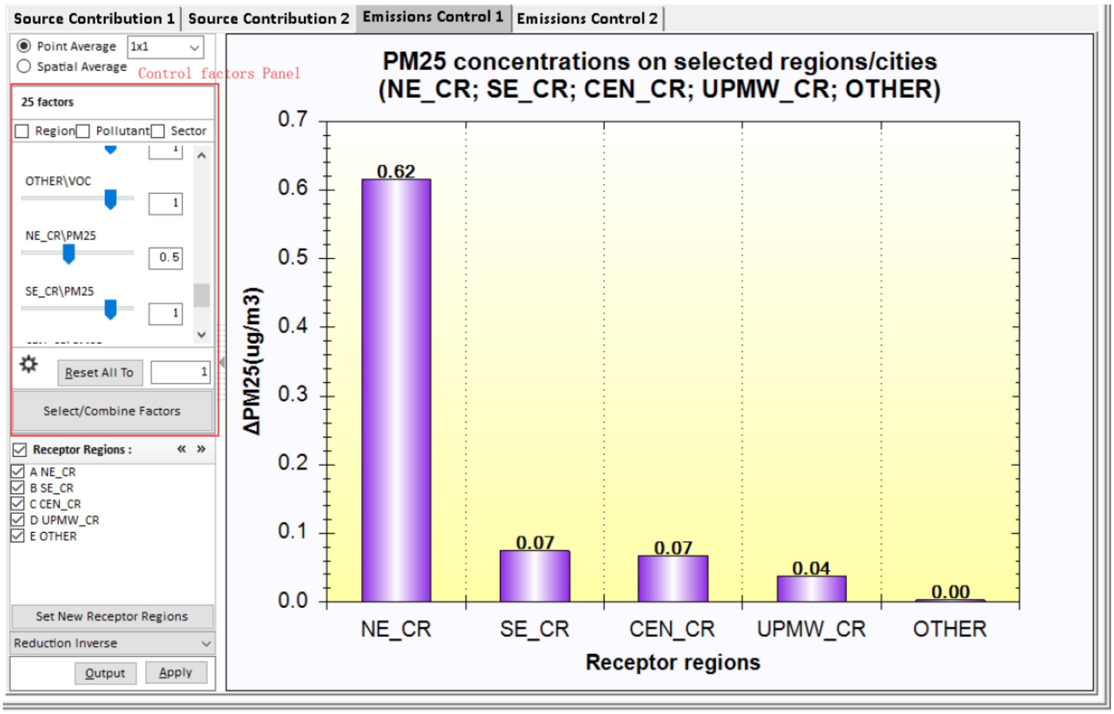


Fig. 69 Example of Emission Control 1

7.2.2.4 Emission Control 2

Under this module, it allows user to compare the emission source contributions to $PM_{2.5}$ or O_3 decrease under various emission reductions at a time. As shown in Fig. 70, the configuration options in the left panel is similar to that of **Source Contribution 1**. The difference is that it allows users to input multiple emission reductions at a time under the **Emission Reduction** panel. Fig. 70 shows PM2.5 reductions of NE_CR, SE_CR,CEN_CR,UPMW_CR and OTHER receptor regions under 25%, 50%,75% emission controls.

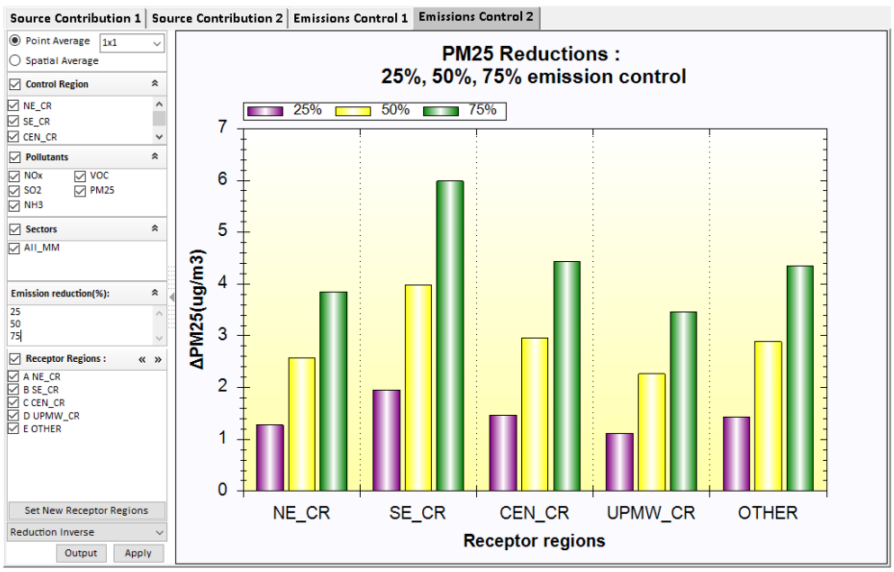


Fig. 70 Example of Emission Control 2

Note that in the above charts under Chart module, RSM-VAT provides a right-click menu on charts which allow users to right-click to perform different operations on the chart like changing title and legend as shown in Fig. 55.

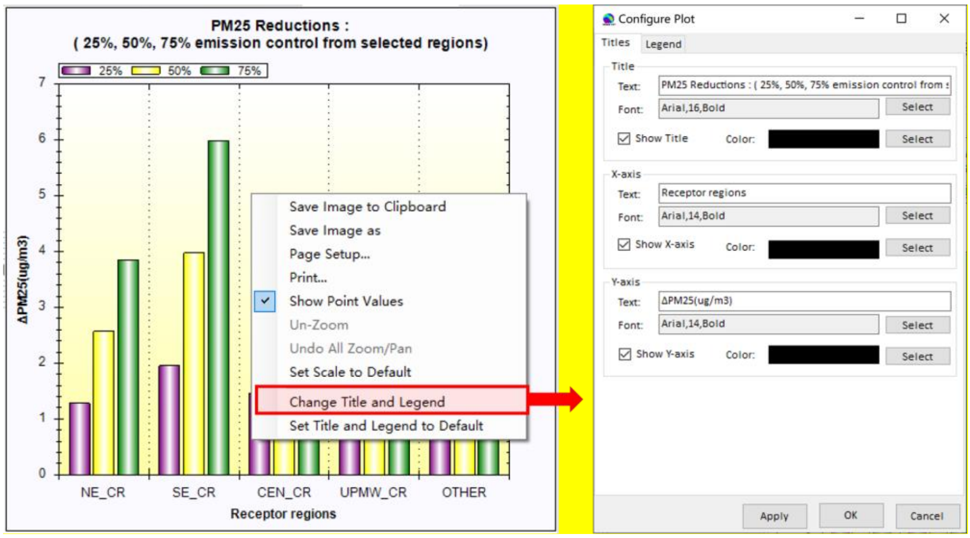


Fig. 71 Right-click menu on Chart

7.2.3 Data

The Data module provides detailed information(e.g.,Latitude, Longitude, ambient concentration) of all grid cells in the model domain. Users can check the fields of interest to show or export data for further study, e.g.,as input for SMAT-CE, as shown in Fig. 72.

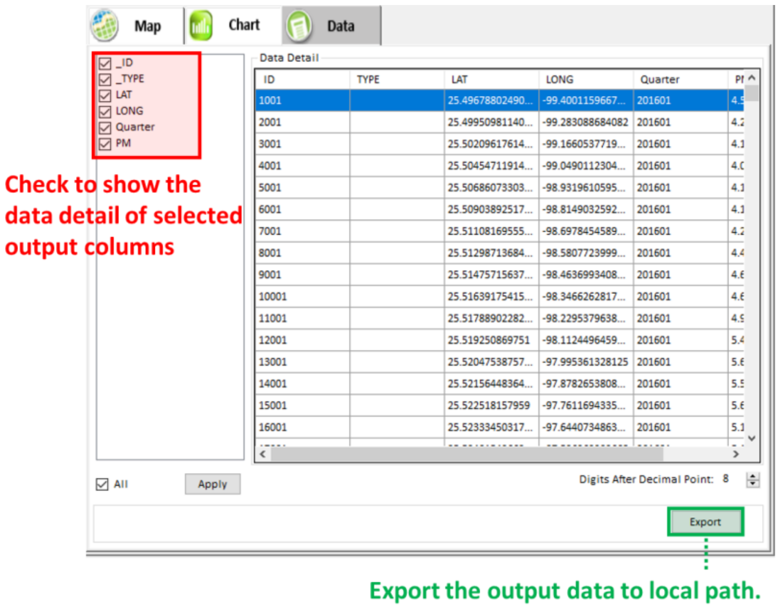


Fig. 72 Data Detail Results and Configuration