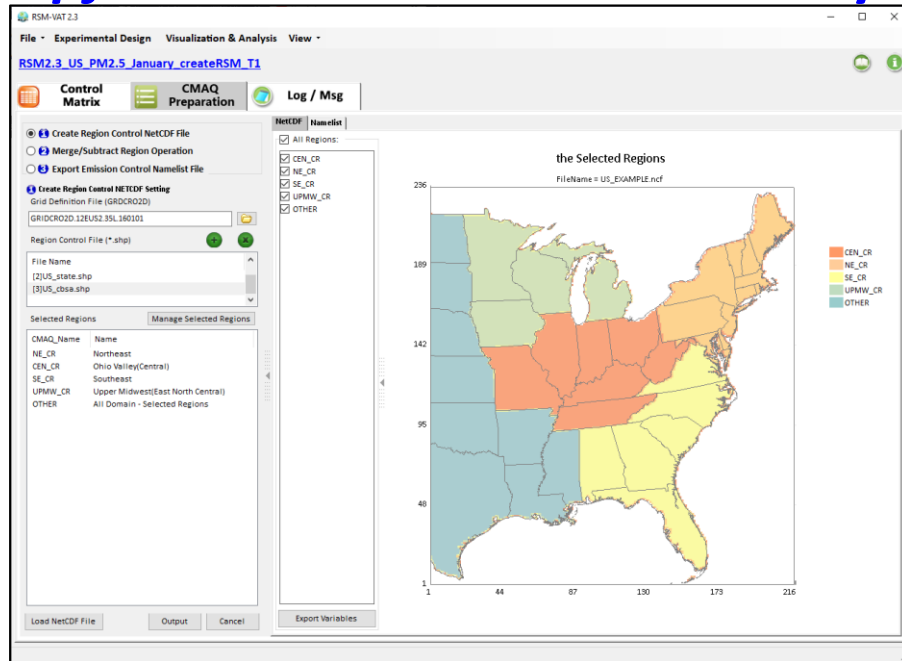
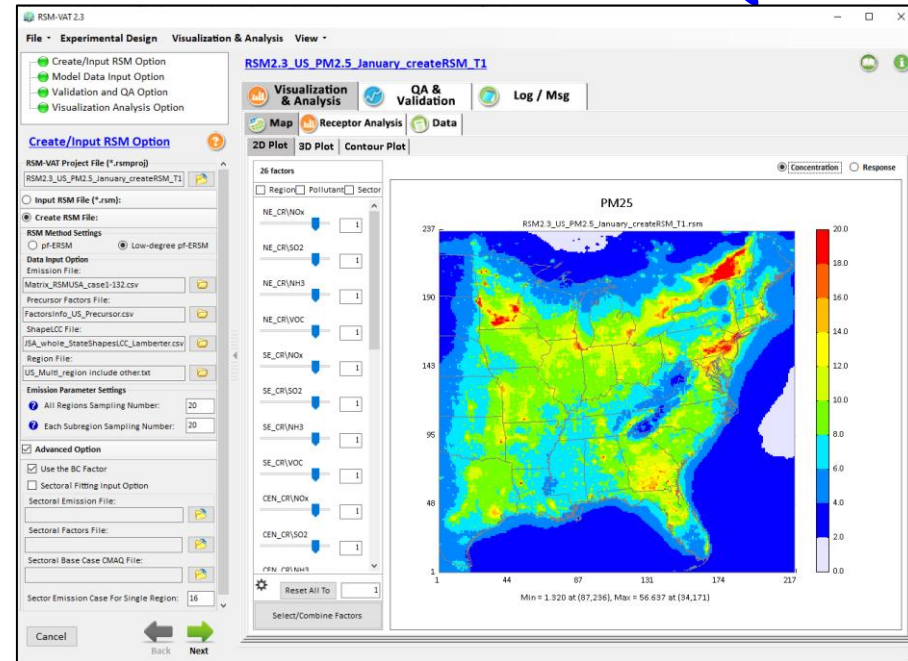


Development and Evolution of Response Surface Model (RSM) *and* RSM-VAT Demo (EUS pilot case)

“pf-RSM” EUS CMAQ Case study



RSM-VAT Demo & QA



Carey Jang and James Kelly, OAQPS/AQAD/AQMG,
08/12/2020

Outline

1. *Development and Evolution of RSM*

- Traditional *RSM*
- Extended Multi-Region RSM (*E-RSM*)
- Polynomial Function RSM (*pf-RSM*)
- “Deep Machine Learning” “Indicator-based” *pf-RSM*
(*DeepRSM*) (under development)

2. *RSM-VAT Tutorial/Demo & QA*

- CMAQ “Eastern US” 12-km pilot case based on *pf-RSM*
- QA results: “Out-of-Sample” validation

The “RSM-VAT 2.4” package (“RSM-VAT 2.4 Setup.exe” & “Data.exe”: run both to install) is available at the Google Drive (or EPA’s “ScienceFTP2” site upon request):

https://drive.google.com/open?id=1XI3VqtlRXeBt_FrfHpuCZYumxjqMR9hL

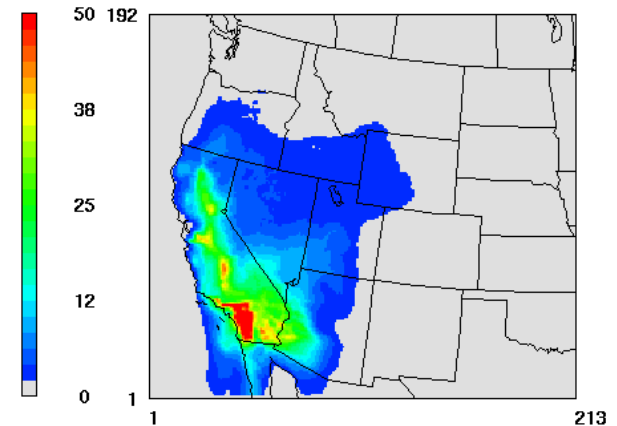
Reduced Form Modeling Techniques:

Source Contribution & Control/Response Modeling

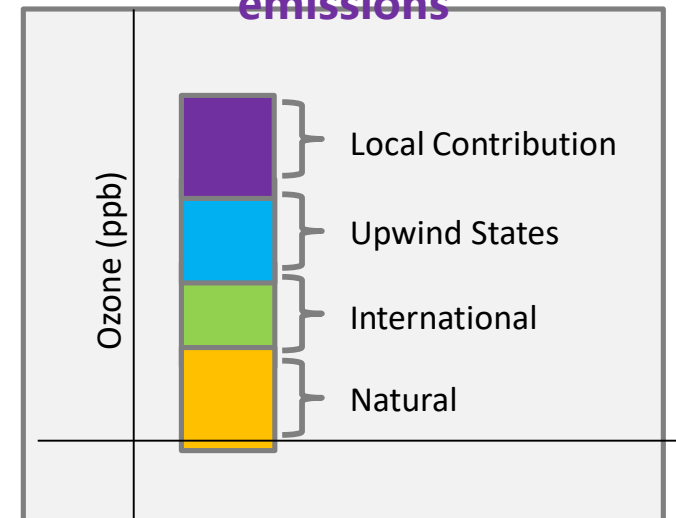
- **“Source Contribution” Assessment**
 - **Source Apportionment Modeling (Chem. approximation)**
 - CAMx’s OSAT/PSAT/APCA, CMAQ’s ISAM & TSSA, etc.
 - **Source/Receptor Sensitivity Modeling (Math. approximation)**
 - Decoupled Direct Method (DDM/HDDM), Adjoint, etc.
- **“Control Response” Assessment of emissions reduction (Control efficacy)**
 - **Zero-Out (Brute Force) Modeling**
 - **Response Surface Modeling (RSM): Provide “real-time” AQ response of emissions control**
 - Previous USA applications: REMSAD (PM_{2.5}):2008, CAMx (O₃):2009, CMAQ (EGU RSM): 2011 (Math./Stat. approximation)
 - Evolving into Extended RSM (*ERSM*):2015, Polynomial Functions RSM (*pf-RSM*):2018, Deep Machine Learning/Indicator RSM (*DeepRSM*):2020 (Math. & Chem. approximation)

Source Contribution Analysis for Policy Assessment

- Transport rules or Transport SIPS:
 - Assess “significant contribution” of sources in upwind states to downwind states
- NAAQS Area designations:
 - Provide analysis for States to assess impacts from boundaries
- Exceptional events demonstrations:
 - Assess impacts of special events such as fire
- Inform control strategy development:
 - O3, PM2.5, Reg haze SIPs & RIAs
- Single source Impact assessments:
 - PSD/NSR permitting
- Sector impact assessments:
 - EGU, Transportation, Industrial Boiler, etc.
- Characterizing international contribution:
 - 179b demonstrations



U.S. EPA Source apportionment modeling for assessing source contributions to PM2.5 & O3 from emissions



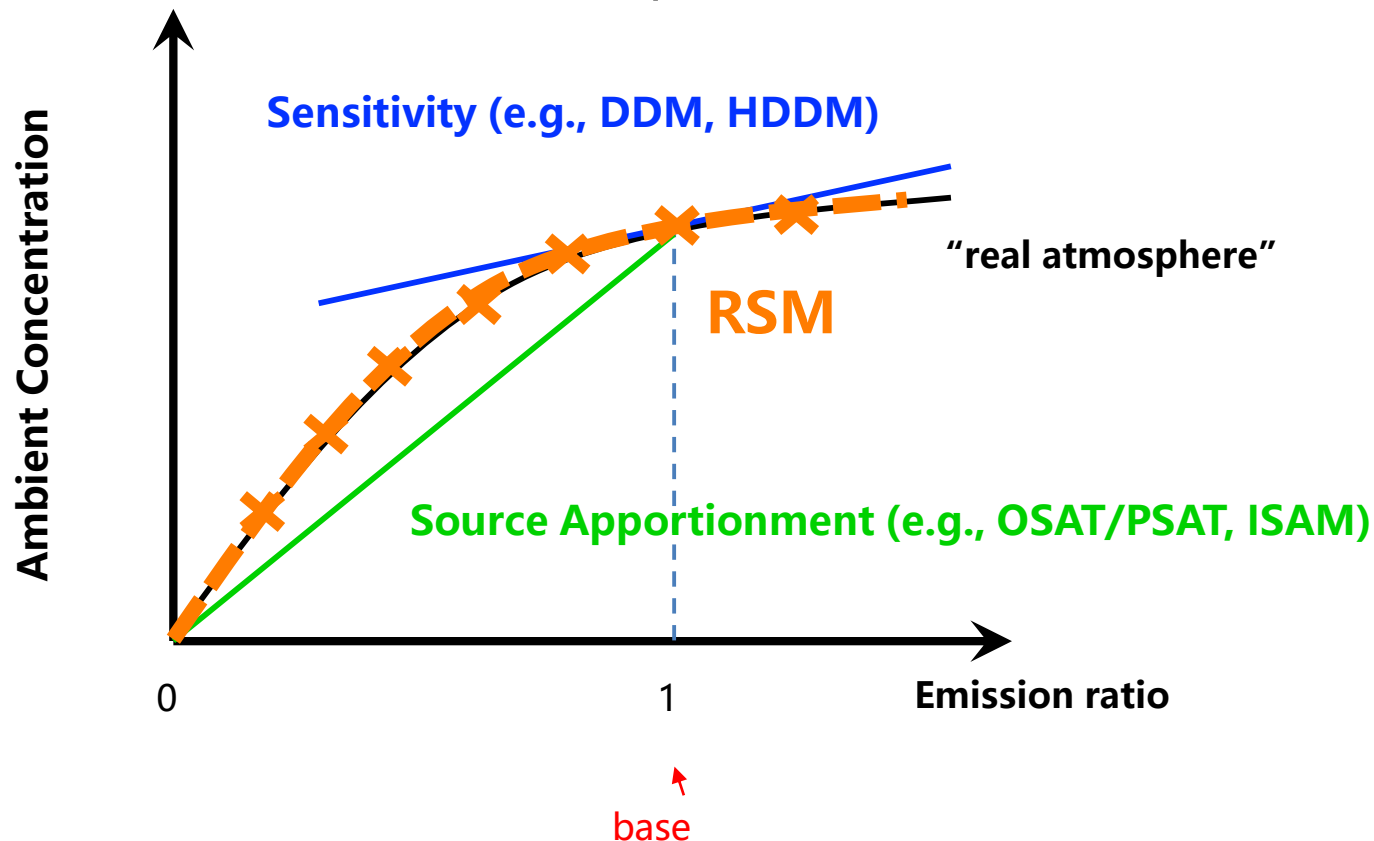
Ozone Source Contribution (example, not to scale)

(Courtesy of Dr. Kirk Baker)

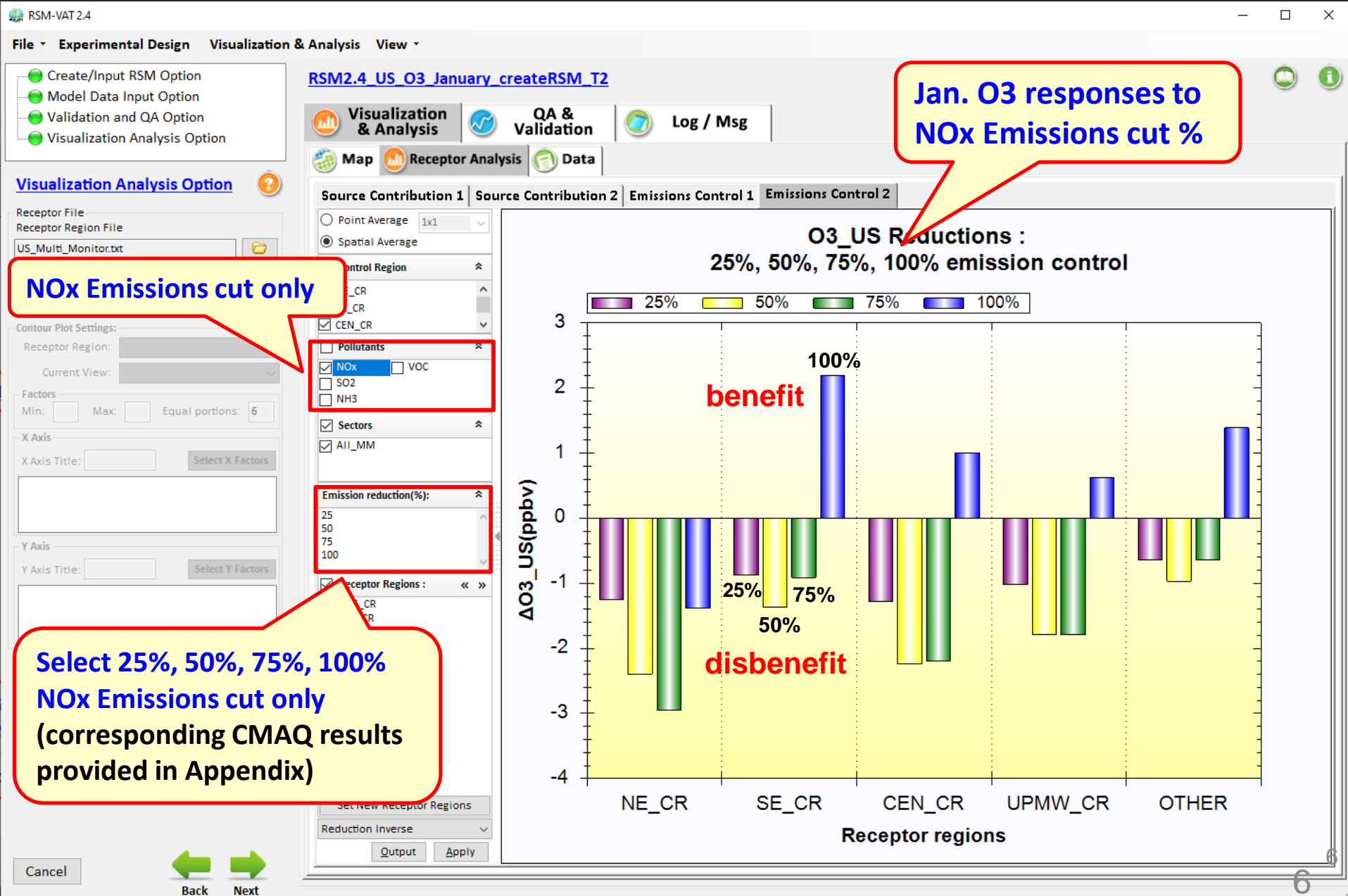
RSM: Real-time estimate of air quality responses

Response Surface Model (RSM):

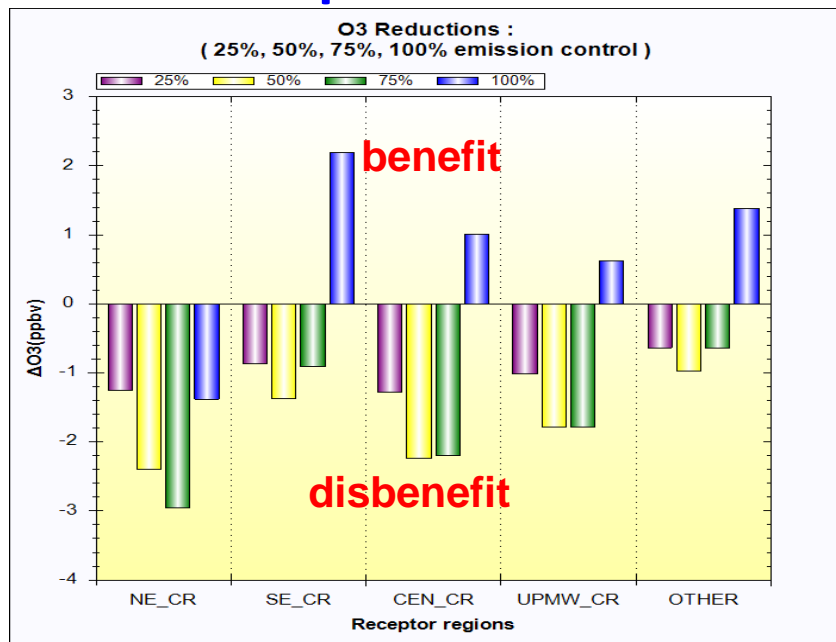
- A reduced form meta-model built upon multiple “brute force” AQ model simulations to explore “real-time” response relationship between **emission changes** and AQ (O₃ & PM_{2.5} species)
- **Major advantages:** provide “**real-time**” & improved “**non-linear**” relationship of emissions control and AQ response



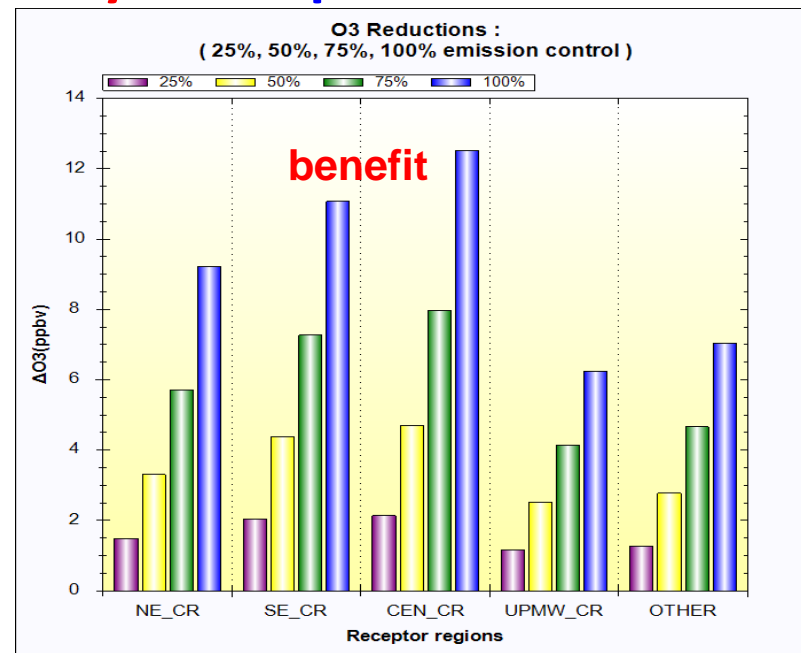
RSM example: “O3” & “PM_SO4” non-linear chemistry



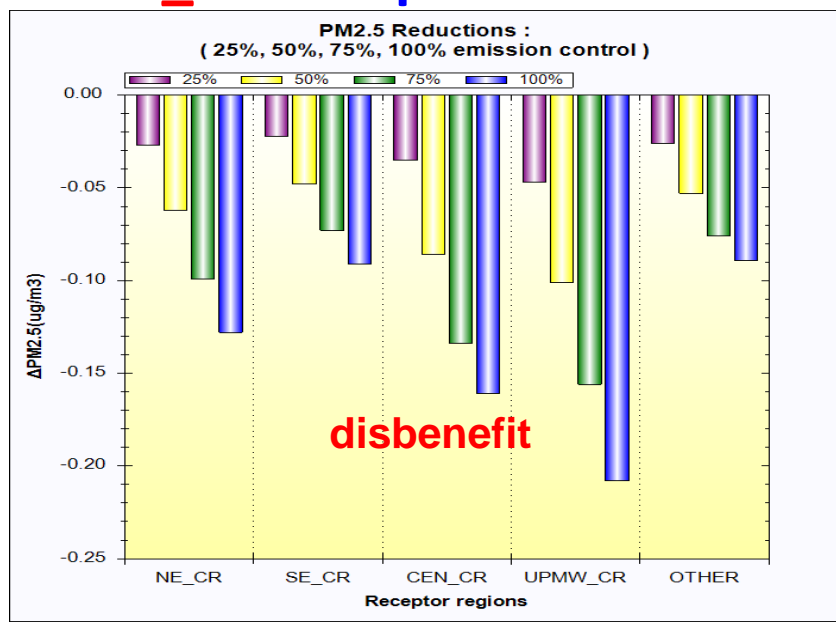
Jan. O₃ responses to NO_x cut



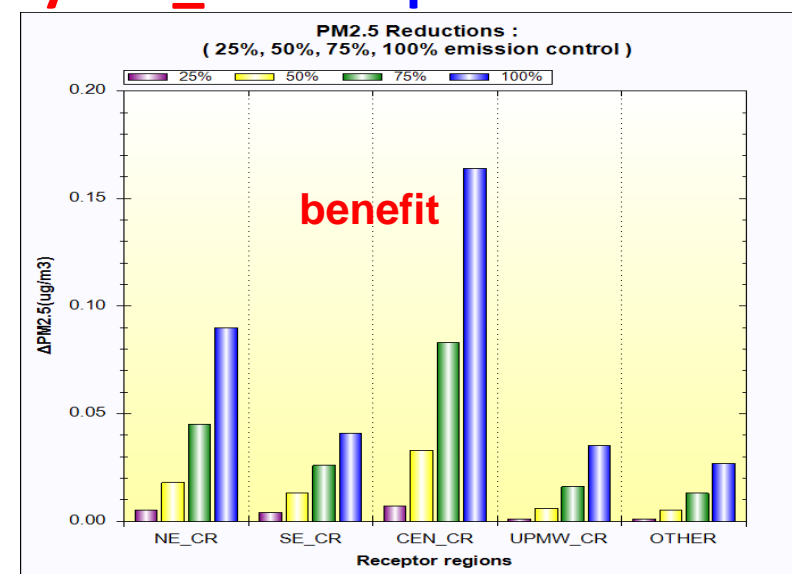
July O₃ responses to NO_x cut



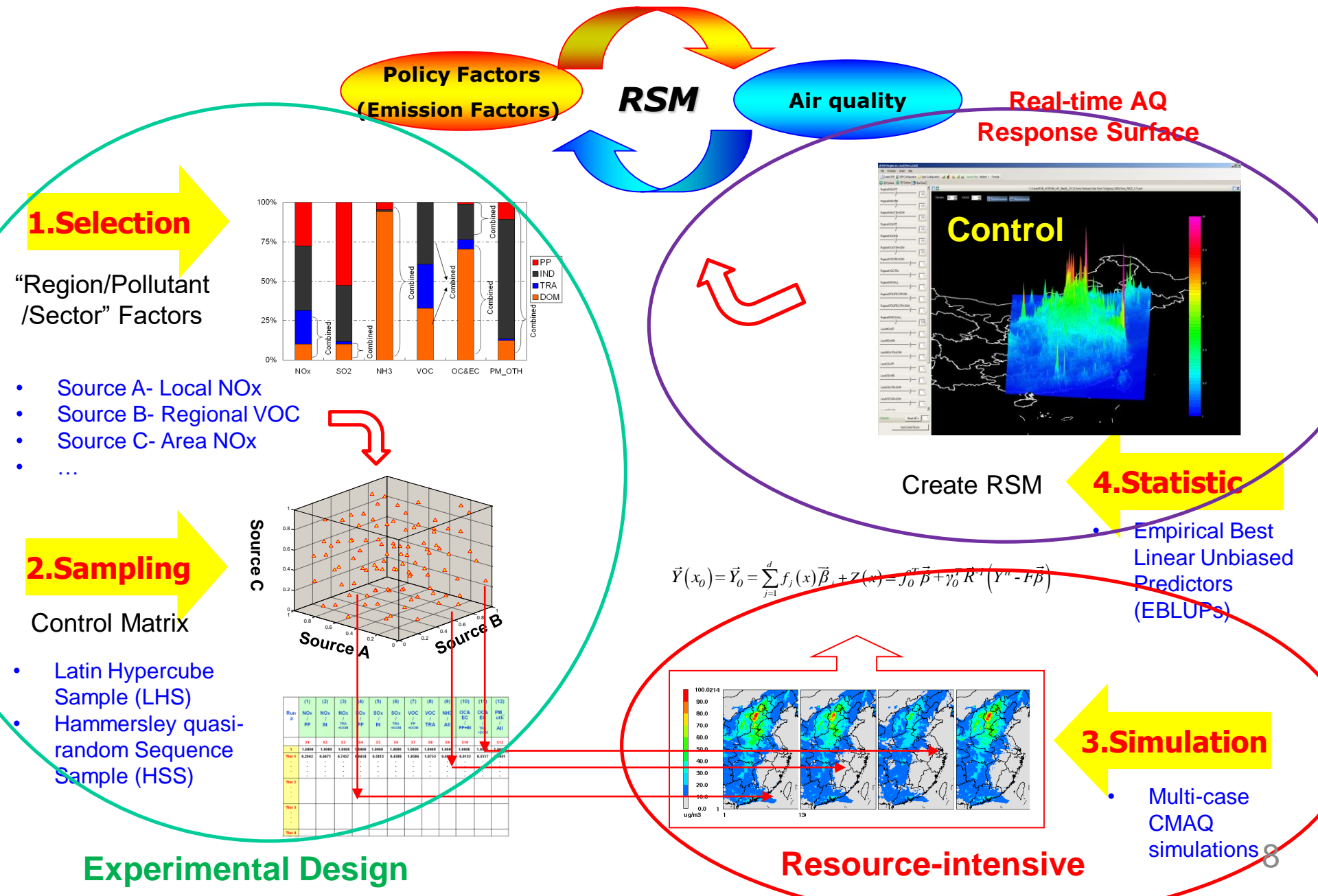
Jan. PM_{2.5} responses to NO_x cut



July PM_{2.5} responses to NO_x cut



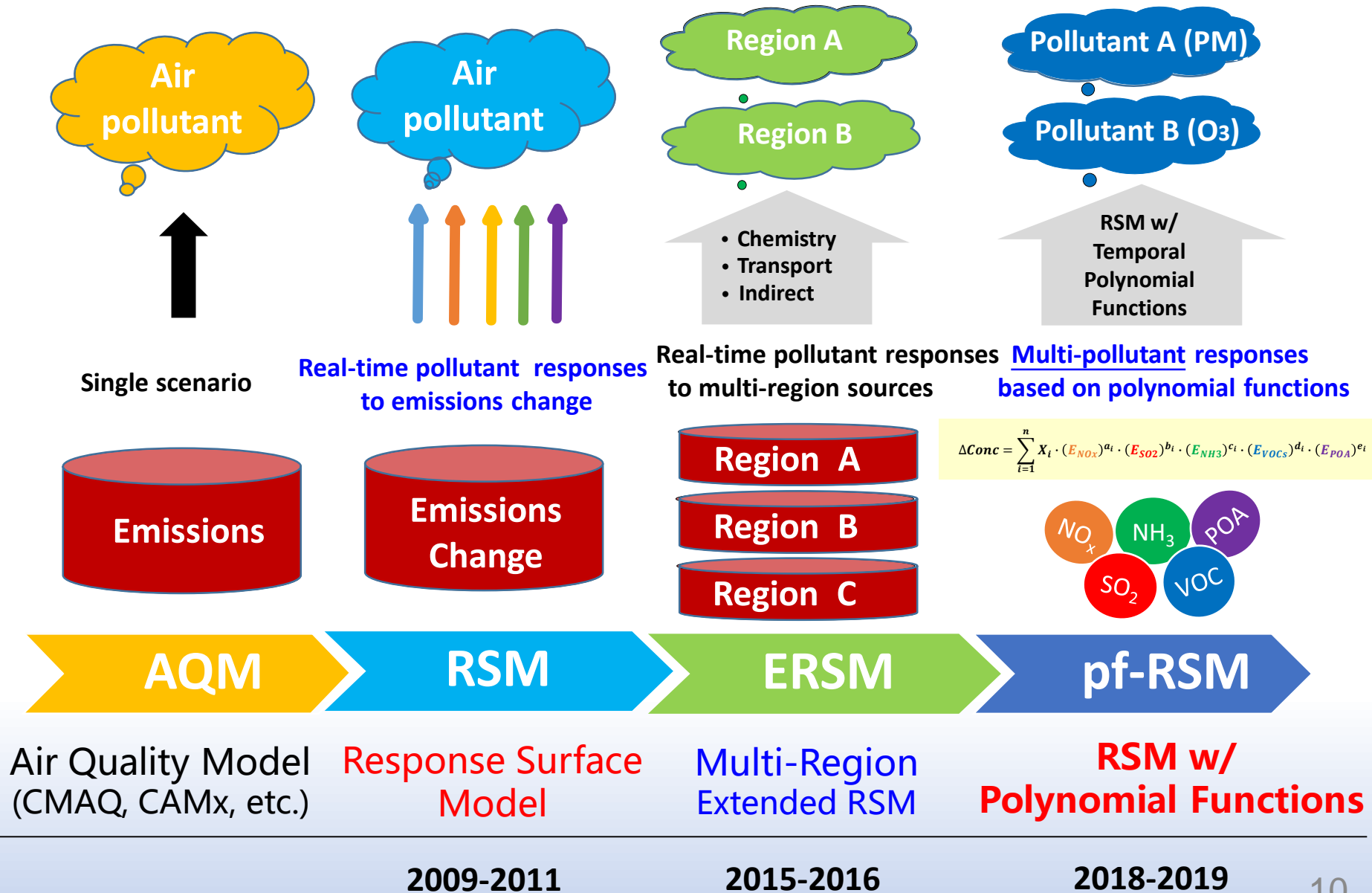
"4S" Steps in RSM (Traditional RSM)



Motivation for New RSM Development:

**How to reduce # of model simulations
while maintaining RSM accuracy?**

New RSM Development: “*pf-RSM*” & “*DeepRSM*”



“pf-RSM” Methodology

Polynomial Functions

$$\text{pf-RSM: } \Delta \text{Conc} = \sum_{i=1}^n X_i \cdot (E_{\text{NOx}})^{a_i} \cdot (E_{\text{SO2}})^{b_i} \cdot (E_{\text{NH3}})^{c_i} \cdot (E_{\text{VOCs}})^{d_i} \cdot (E_{\text{POA}})^{e_i}$$

Chemistry:
Degree of
Non-linearity

1. Degree
Examination

$\max(a_i)$

$\max(b_i)$

$\max(c_i)$

$\max(d_i)$

$\max(e_i)$

Chemistry:
Term of
Interactions

2. Term
Selection

n

a

b

c

d

e

Model:

3. Sampling
optimization

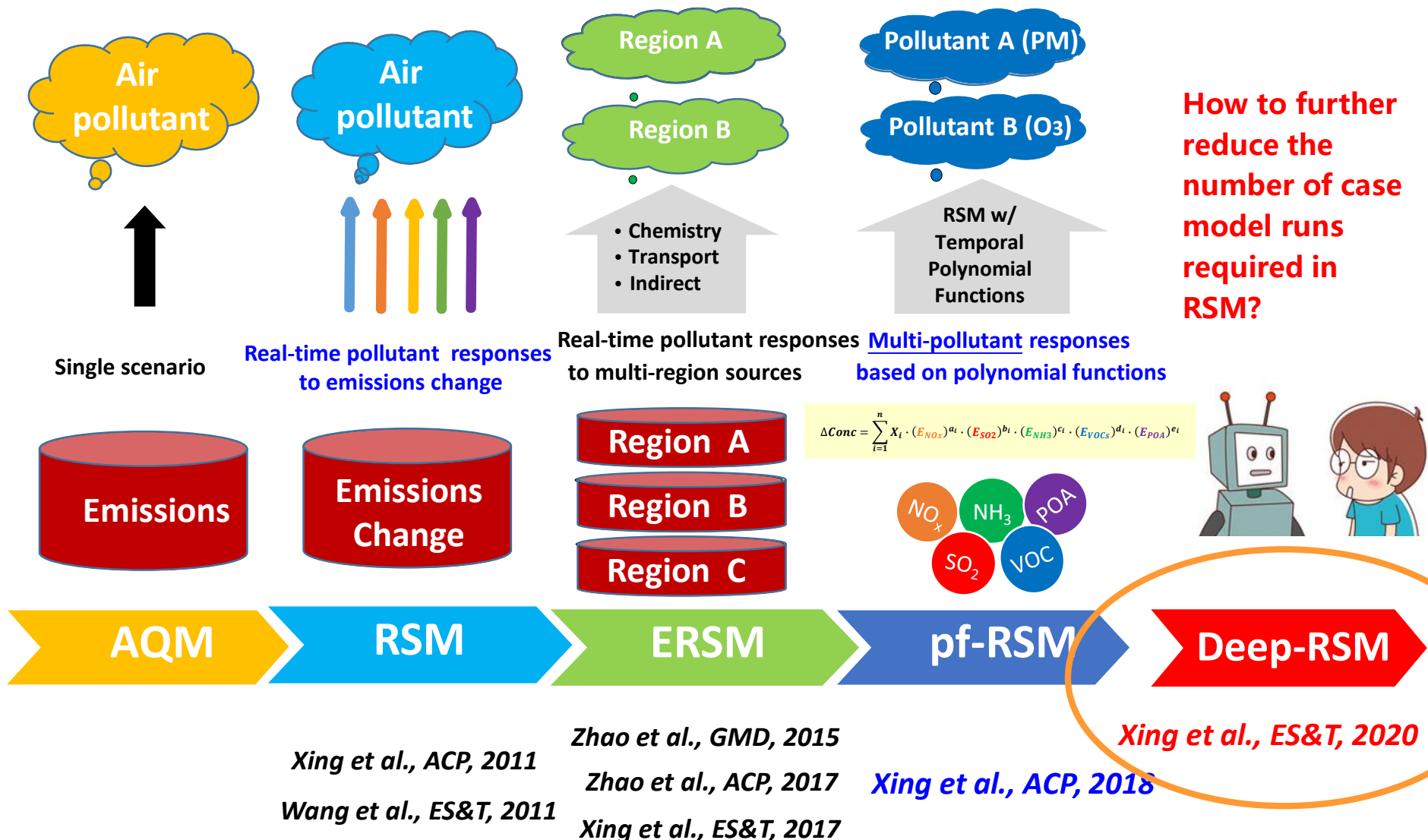
X

Number and distributions of Training Samples

Only 3rd step involved in training samples (i.e., model runs), and thus significantly reduces # of model runs required for accuracy (20~30 runs per control region)

“pf-RSM” : Response Surface Model based on Polynomial Functions (Temporal & multi-region RSM)

DeepRSM: Machine Learning w/ Indicator-RSM



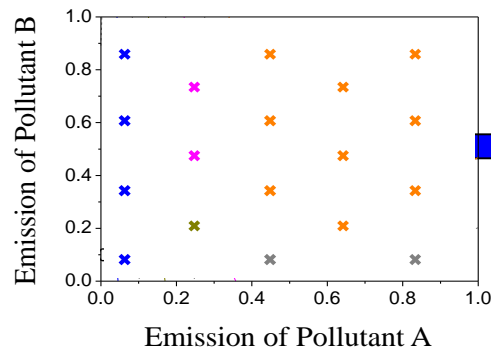
Machine Learning “DeepRSM”

DeepRSM: “Deep Learning” “Indicator-based” pf-RSM

Use 18
Species
indicators
and
deep learning
CNN
to predict
PM_{2.5} & O₃
response to
emissions
control

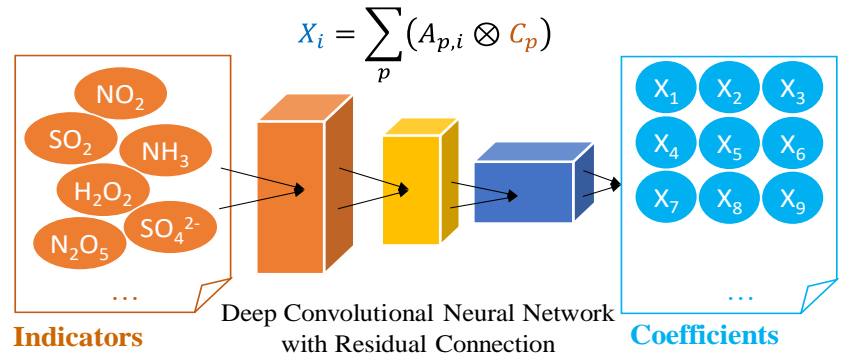
Response function of PM_{2.5} and O₃ concentrations to precursor emission change:
$$\Delta Conc = \sum_{i=1}^n X_i \cdot (E_{NOx})^{a_i} \cdot (E_{SO2})^{b_i} \cdot (E_{NH3})^{c_i} \cdot (E_{VOCs})^{d_i}$$

pf-RSM: Fitted with >20 chemical transport model simulations based on randomly sampled emission control scenarios



More efficient

DeepRSM: Predicted by indicators (i.e., a combination of concentrations of species p) based on two chemical transport model simulations (i.e., baseline and fully-controlled emission scenarios)



of model runs needed for maintaining RSM accuracy in predicting control responses per selected control region

Traditional RSM	“pf-RSM”	“DeepRSM”
>100s	20~30	2

Xing et. al., ES&T, 2020 (Further details please see Appendix A)

Outline

1. *Development and Evolution of RSM*

- Traditional *RSM*
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- “Deep Machine Learning” Indicator-based *pf-RSM* (*DeepRSM*)

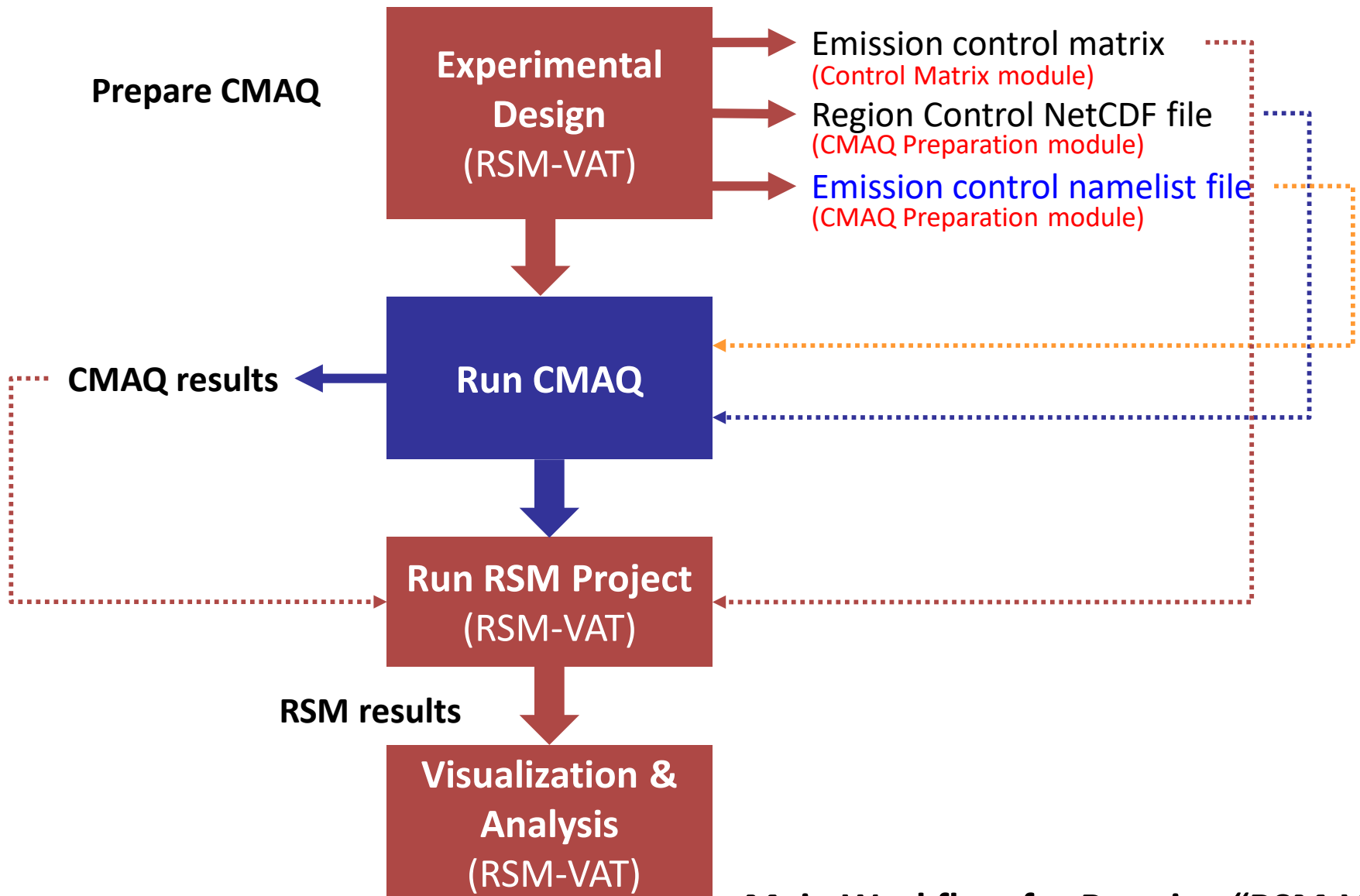
2. *RSM-VAT Tutorial & Demo*

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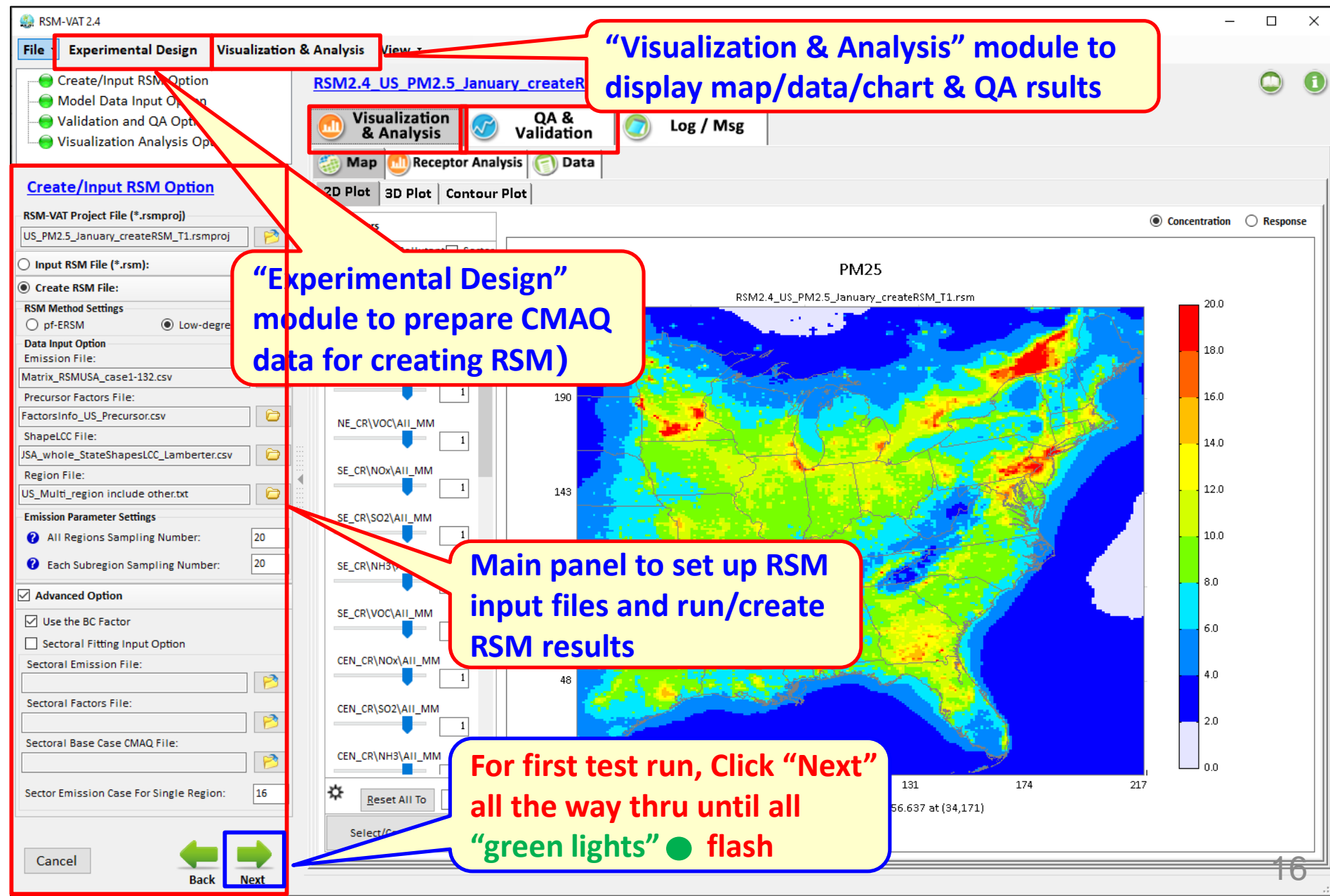
https://drive.google.com/open?id=1XI3VqtlRXeBt_FrfHpuCZYumxjqMR9hL 14

Workflow to Create RSM in “RSM-VAT”



Main Workflow for Running “RSM-VAT”

RSM-VAT: Main Page & Key Modules



Experimental Design: CMAQ EUS Case using “*pf-RSM*”

- 5 regions (CR: climate region)

A: Northeast (NE_CR); B: Southeast (SE_CR); C: Central (CEN_CR); D: Upper Midwest (UPMW_CR); E: Other

- 5 Pollutants

- 4 non-linear pollutant (NO_x, NH₃, SO₂, VOCs) factors + 1 Primary PM factor

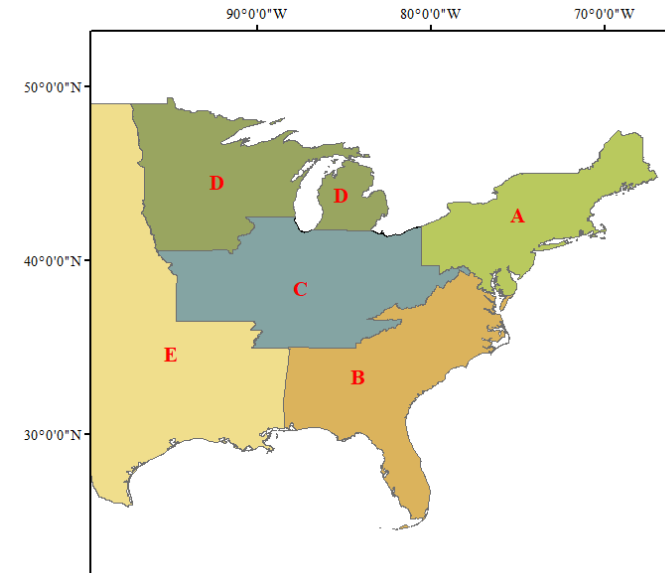
- 1 Sector

- All manmade (All_MM)

- 26 factors = 5 Pollutants * 5 regions * 1 Sector + 1 BC

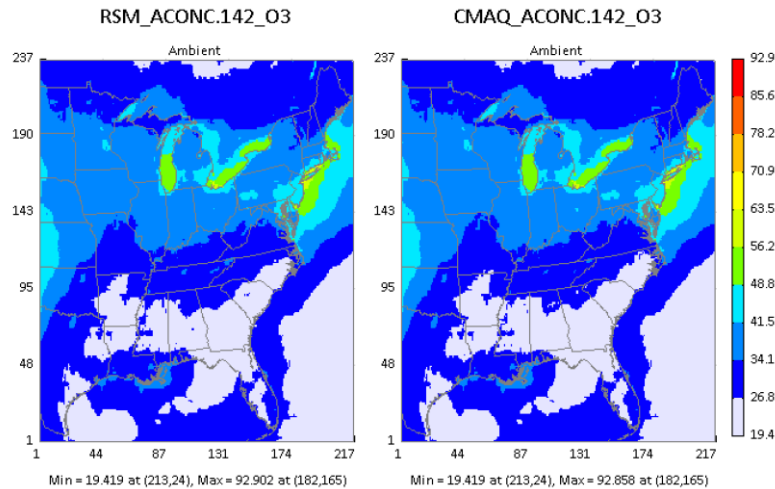
- 147 CMAQ simulation cases (12-km, January & July)

- 1 base case
- 120 cases for non-linear factors = 20 cases * (all region + 5 regions), created by Hammersley quasi-random Sequence Sample (HSS) method (0 ~ 1.2)
- 10 cases for linear Primary PM factors = 5 regions * 2 (0 and 0.5)
- 1 Clean Boundary Conditions
- 15 cases for “out-of-sample” validation (*QA for pf-RSM*)

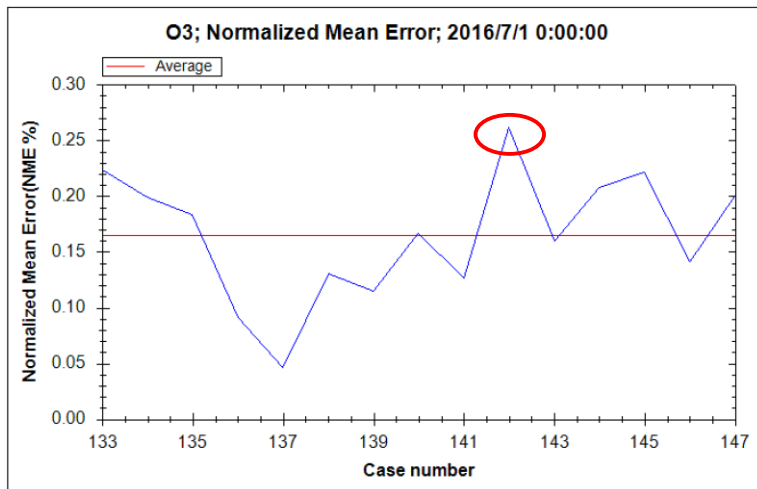
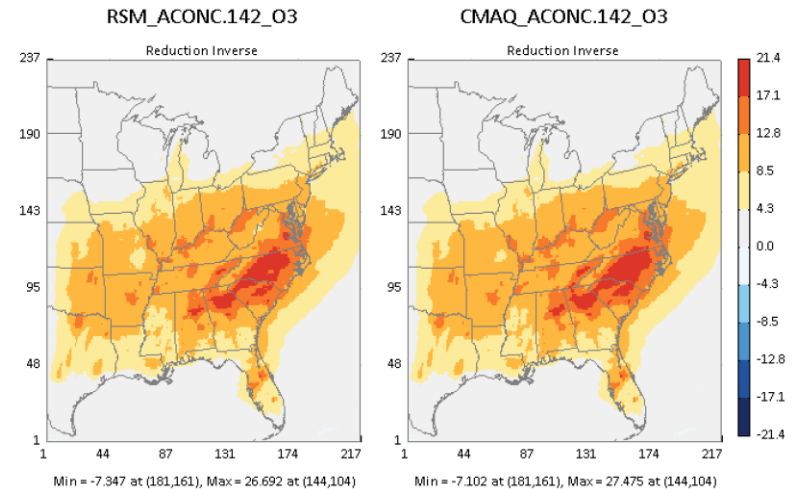


“Out-of-Sample” Validation: O₃ Conc. & Response (July, O₃-8hr avg.): Worst #1

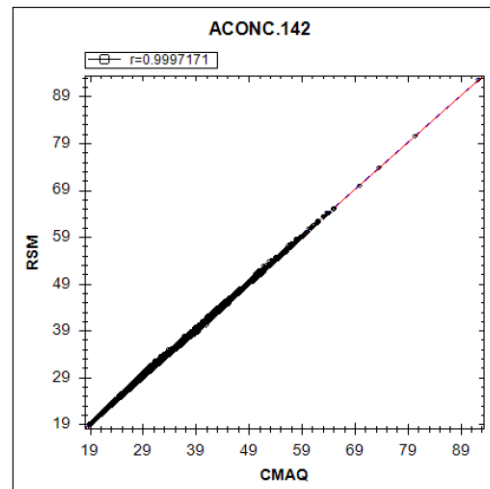
O₃ Conc: RSM vs. CMAQ



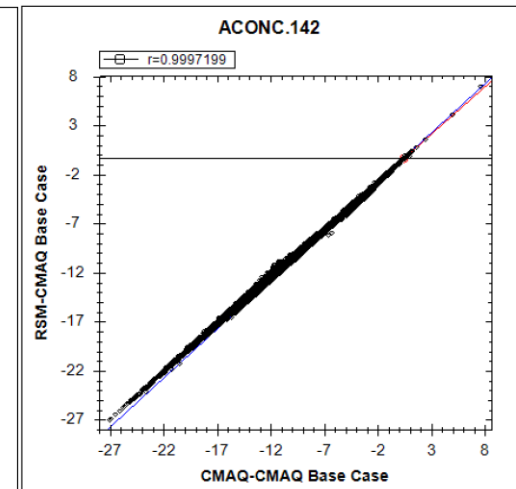
O₃ Response: RSM vs. CMAQ



All “Out-of-Sample” runs:
Normalized Mean Error



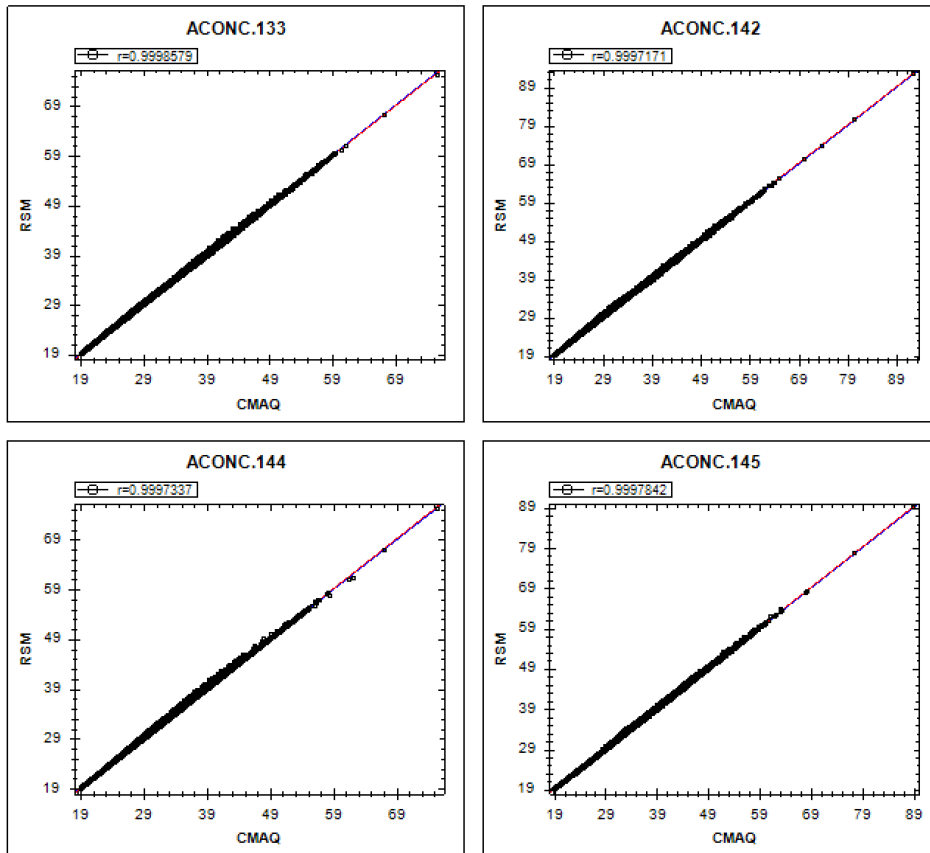
Predicted O₃ Concentration
(RSM vs. CMAQ)



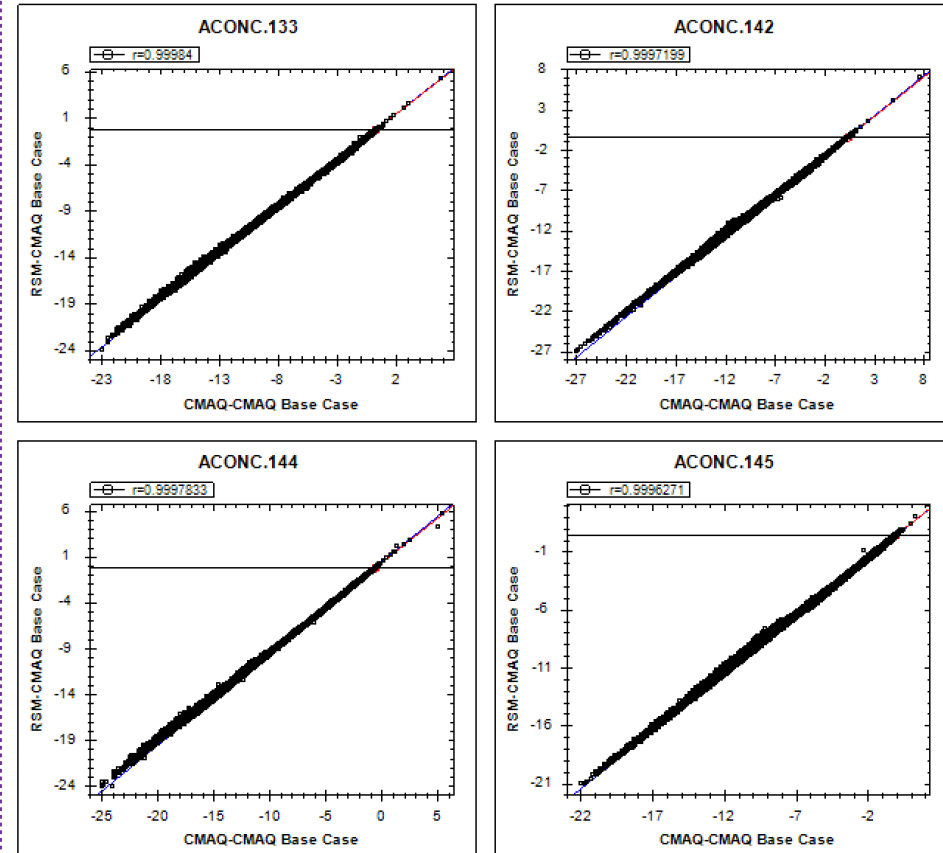
Predicted O₃ Response
(RSM vs. CMAQ)

“Out-of-Sample” Validation: O₃ Conc. & Response **(July, O₃-8hr avg. , US): Worst 4 cases**

Predicted O₃ Conc. **(RSM vs. CMAQ)**



Predicted O₃ Responses (O₃) **(RSM-Base vs. CMAQ-Base)**

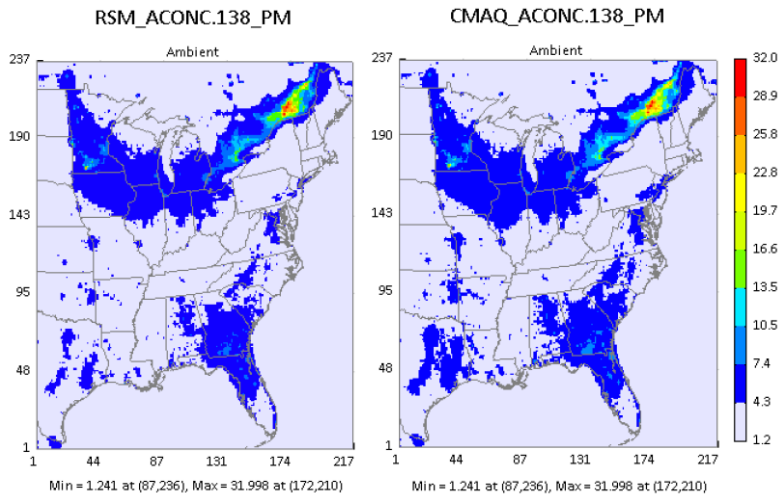


Please see “Appendix B” for additional “out-of-sample” validation slides

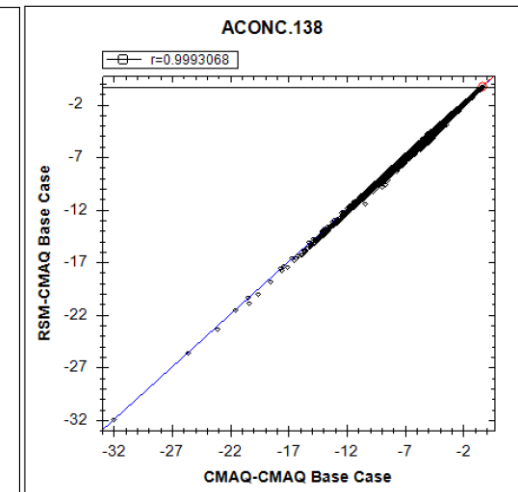
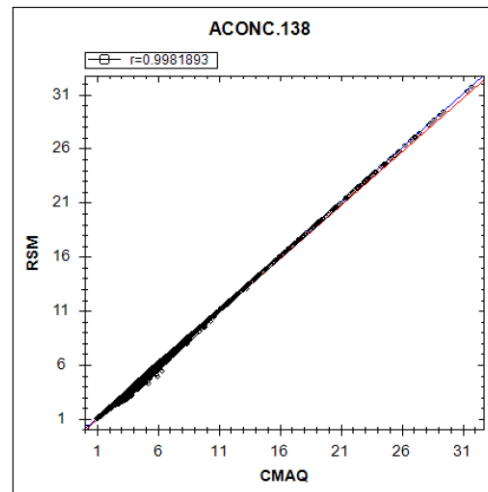
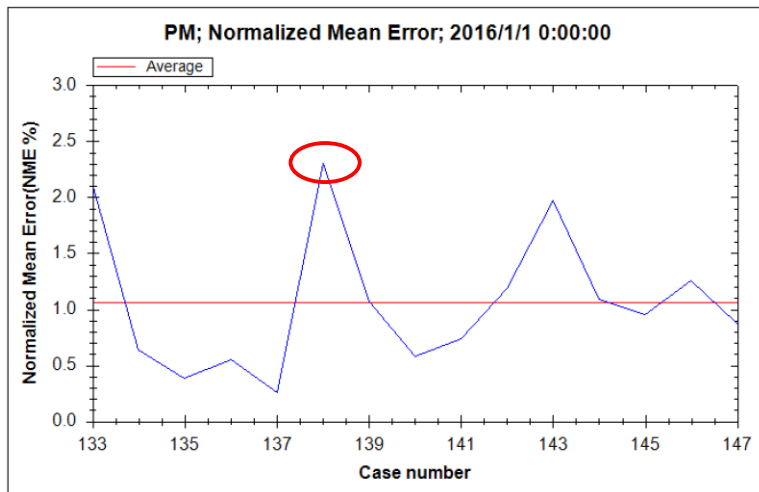
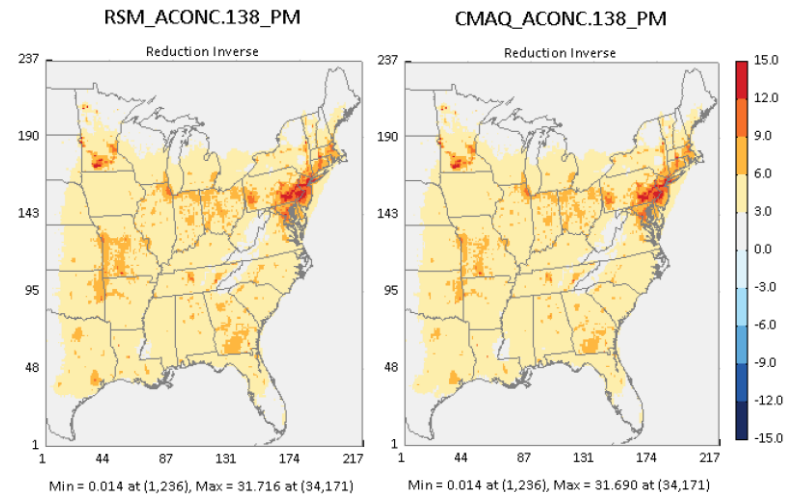
“Out-of-Sample” Validation: PM_{2.5} Conc. & Response

(Jan., PM_{2.5} monthly avg.): Worst Case #1

PM_{2.5} Conc: RSM vs. CMAQ



PM_{2.5} Response: RSM vs. CMAQ

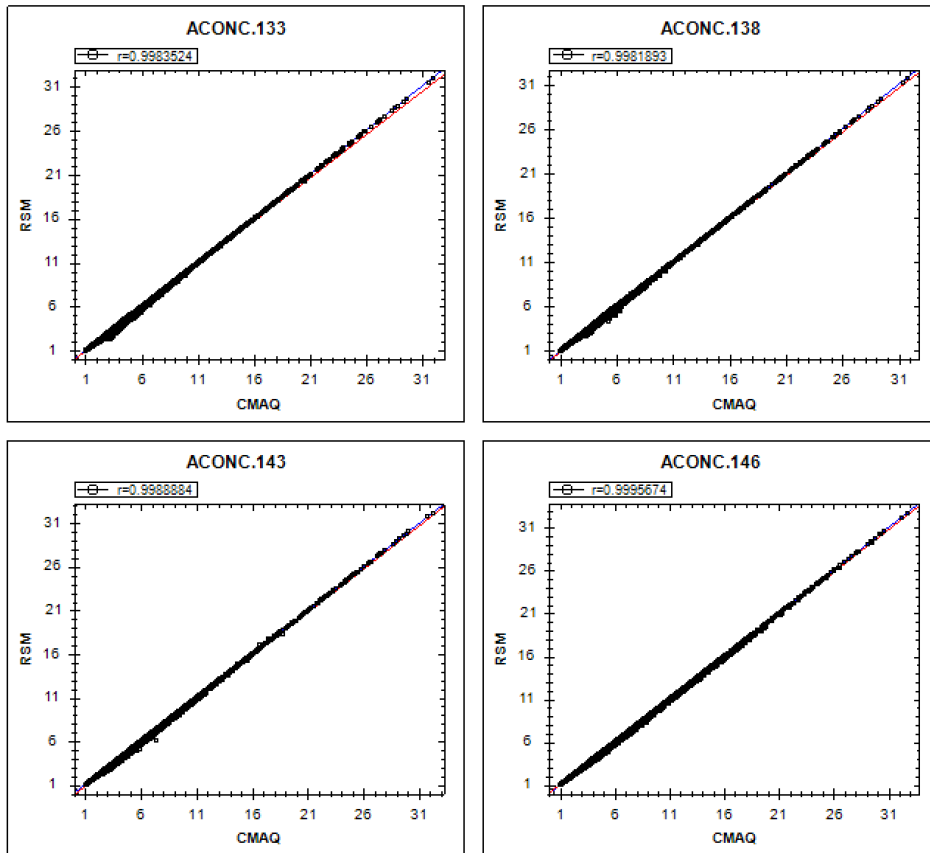


**All “Out-of-Sample” runs:
Normalized Mean Error**

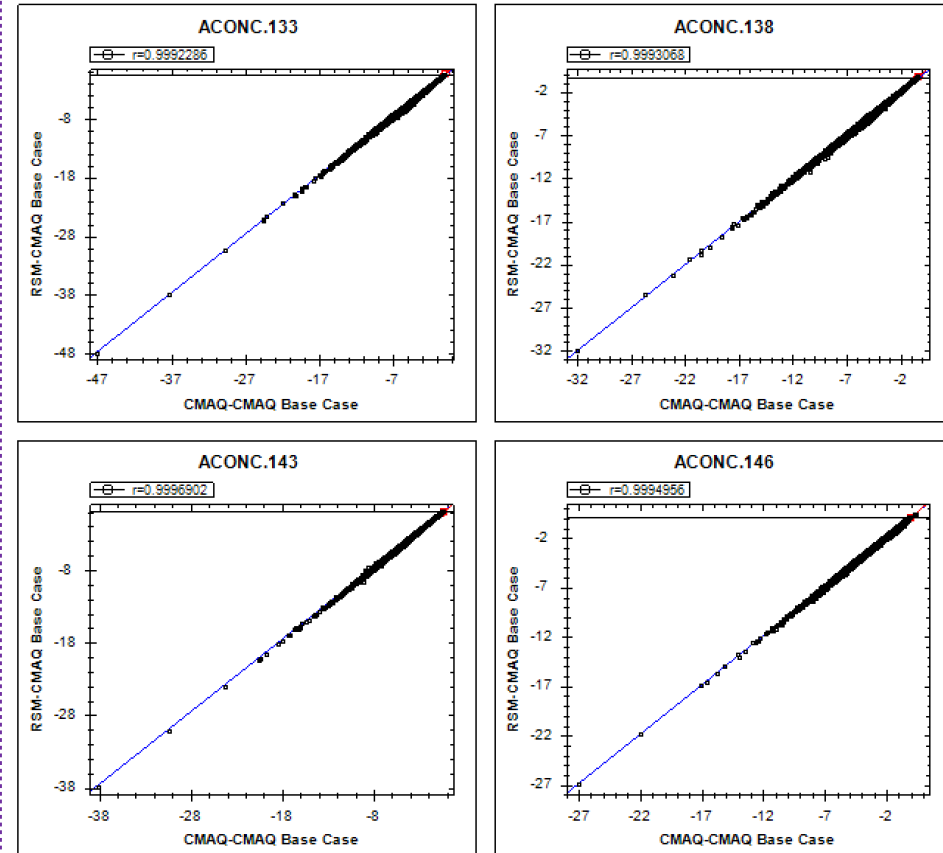
**Predicted PM_{2.5} Concentration Predicted PM_{2.5} Response
(RSM vs. CMAQ) (RSM vs. CMAQ)**

“Out-of-Sample” Validation: PM_{2.5} Conc. & Response **(Jan., PM_{2.5} monthly avg., US): Worst 4 cases**

Predicted PM_{2.5} Conc. **(RSM vs. CMAQ)**



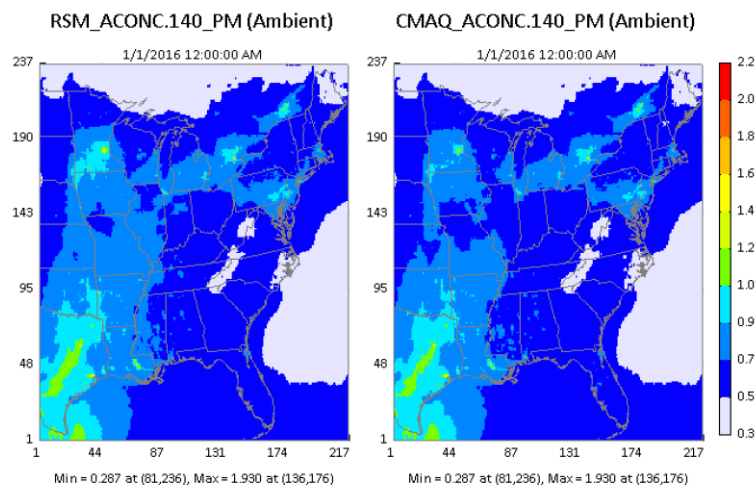
Predicted PM_{2.5} Responses **(RSM-Base vs. CMAQ-Base)**



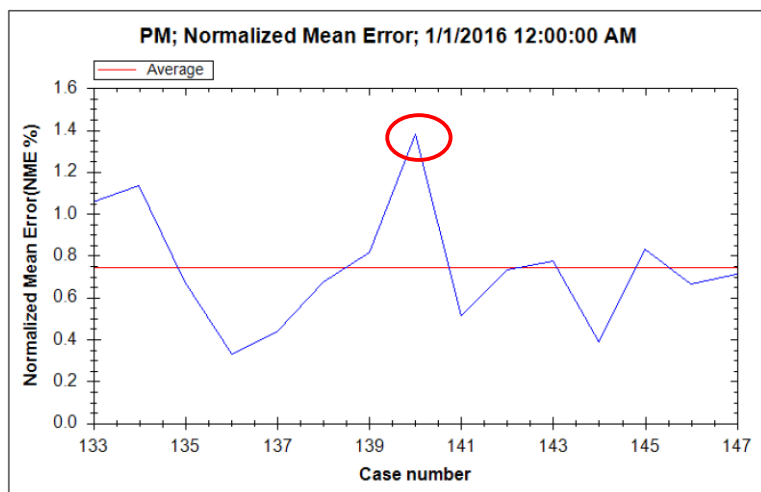
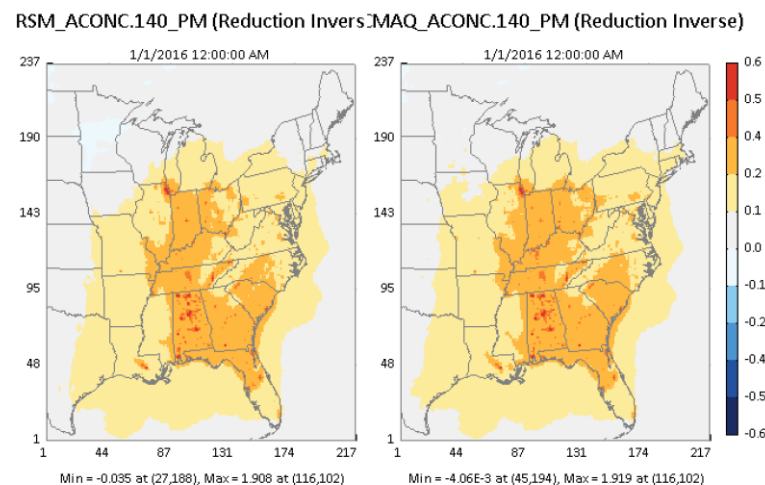
Please see “Appendix B” for additional “out-of-sample” validation slides

“Out-of-Sample” Validation: PM_{SO₄} Conc. & Responses (Jan., PM_{SO₄} monthly avg., US): Worst #1

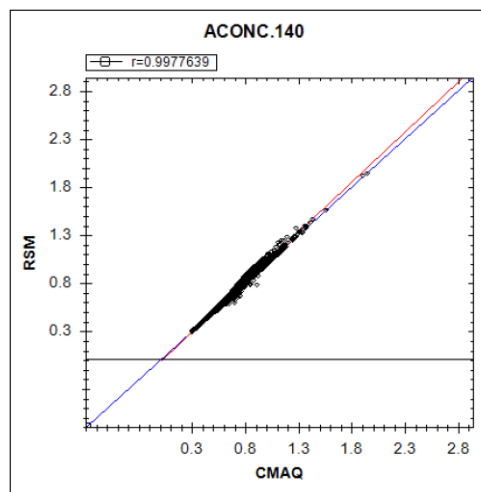
PM_{2.5} Conc: RSM vs. CMAQ



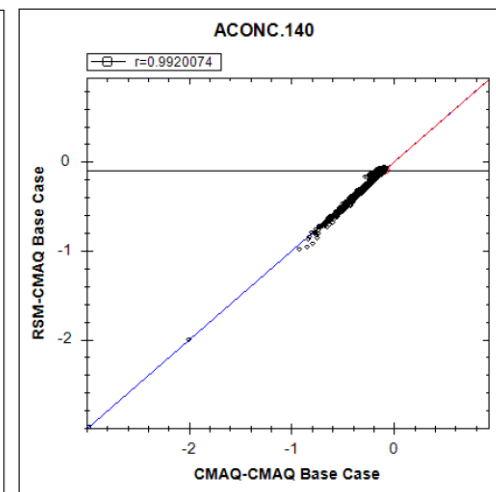
PM_{2.5} Response: RSM vs. CMAQ



All “Out-of-Sample” runs:
Normalized Mean Error



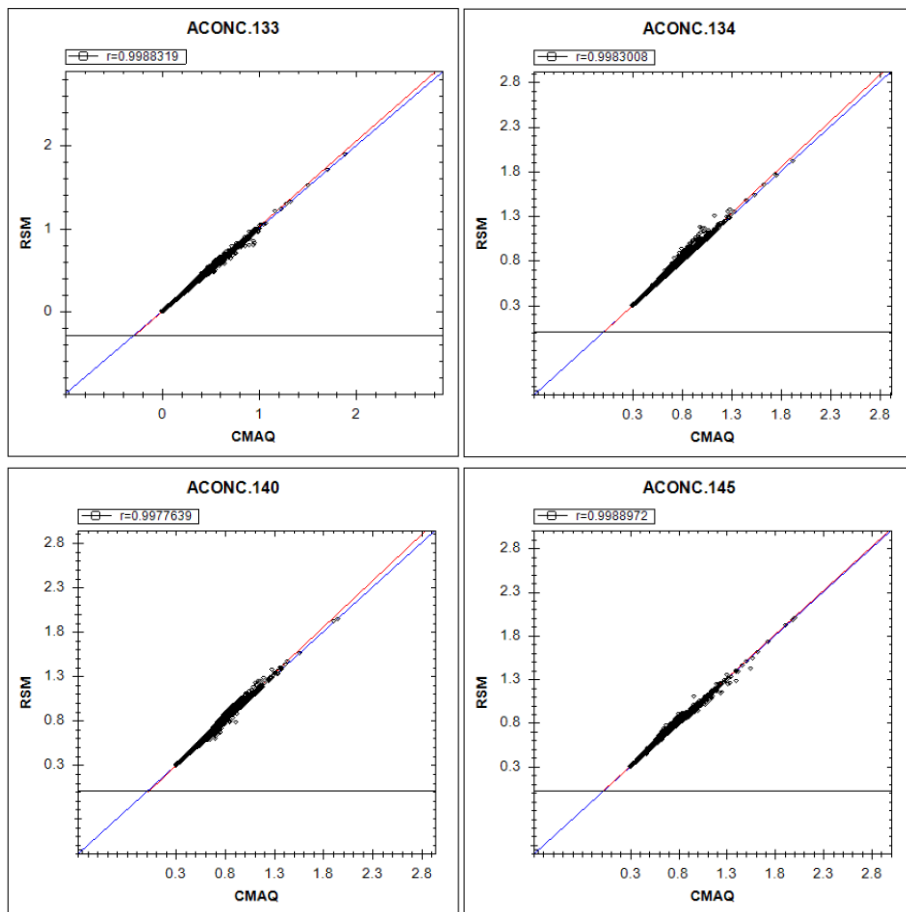
Predicted PM_{2.5} Concentration
(RSM vs. CMAQ)



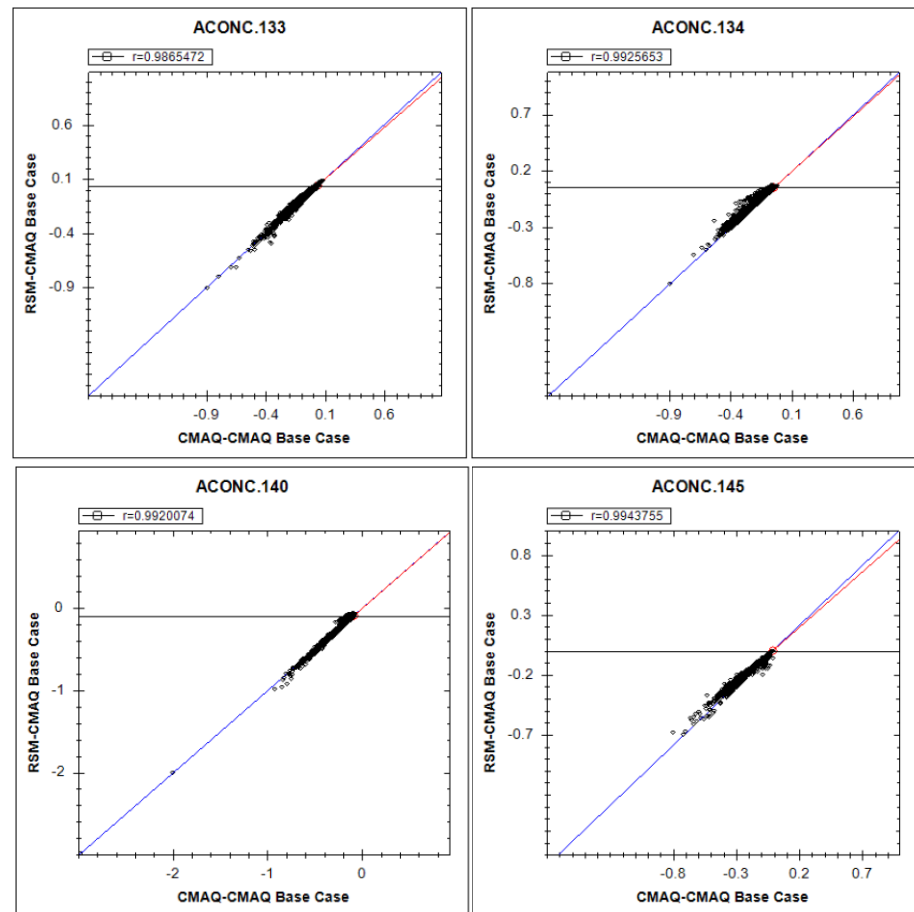
Predicted PM₅ Response
(RSM vs. CMAQ)

“Out-of-Sample” Validation: PM_{SO_4} Concentration & Response (Jan., PM_{SO_4} monthly avg.): Worst 4 cases

Predicted $\text{PM}_{2.5}$ Conc. (RSM vs. CMAQ)



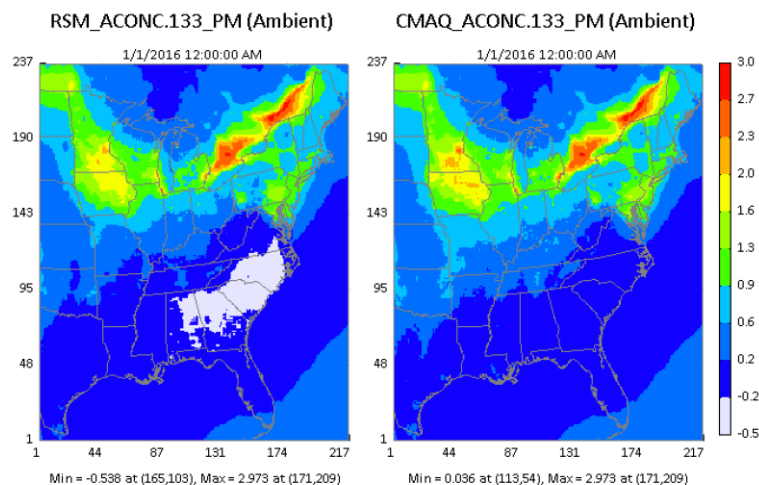
Predicted $\text{PM}_{2.5}$ Responses (RSM-Base vs. CMAQ-Base)



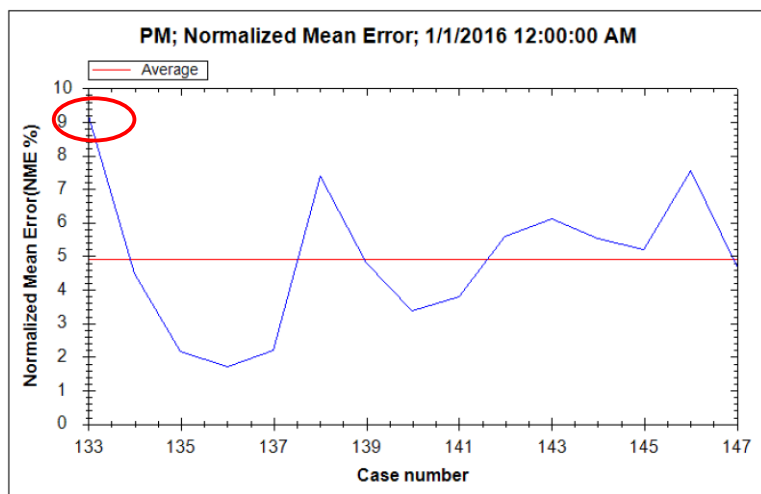
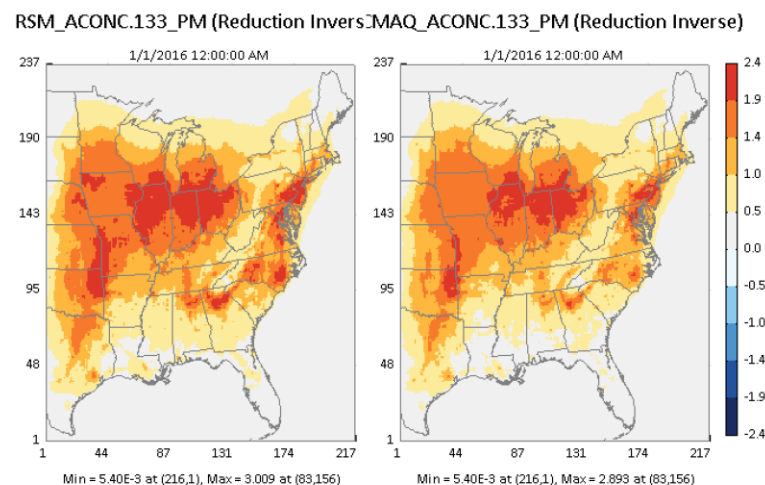
Please see “Appendix B” for additional “out-of-sample” validation slides

“Out-of-Sample Validation”: PM_{NO₃} Conc. & Responses (Jan., PM_{NO₃} monthly avg., US): Worst #1

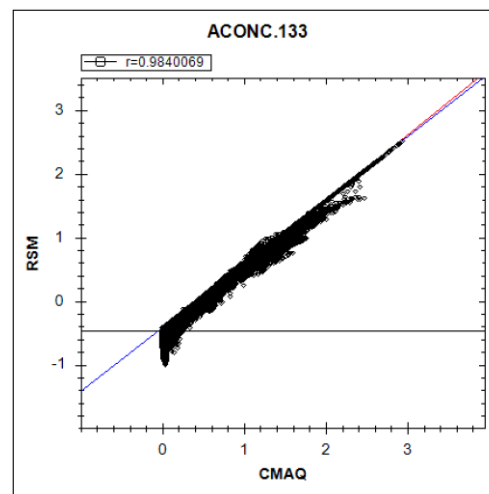
PM_{2.5} Conc: RSM vs. CMAQ



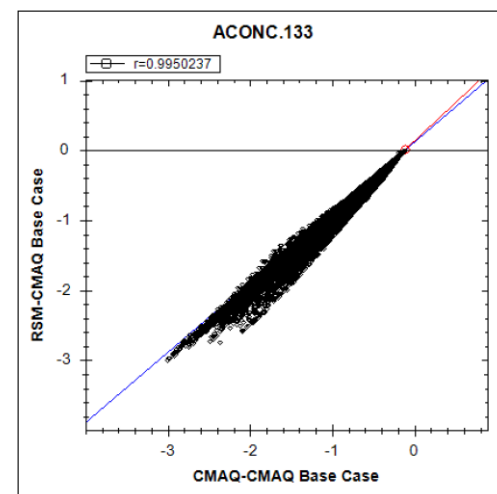
PM_{2.5} Response: RSM vs. CMAQ



All “Out-of-Sample” runs:
Normalized Mean Error



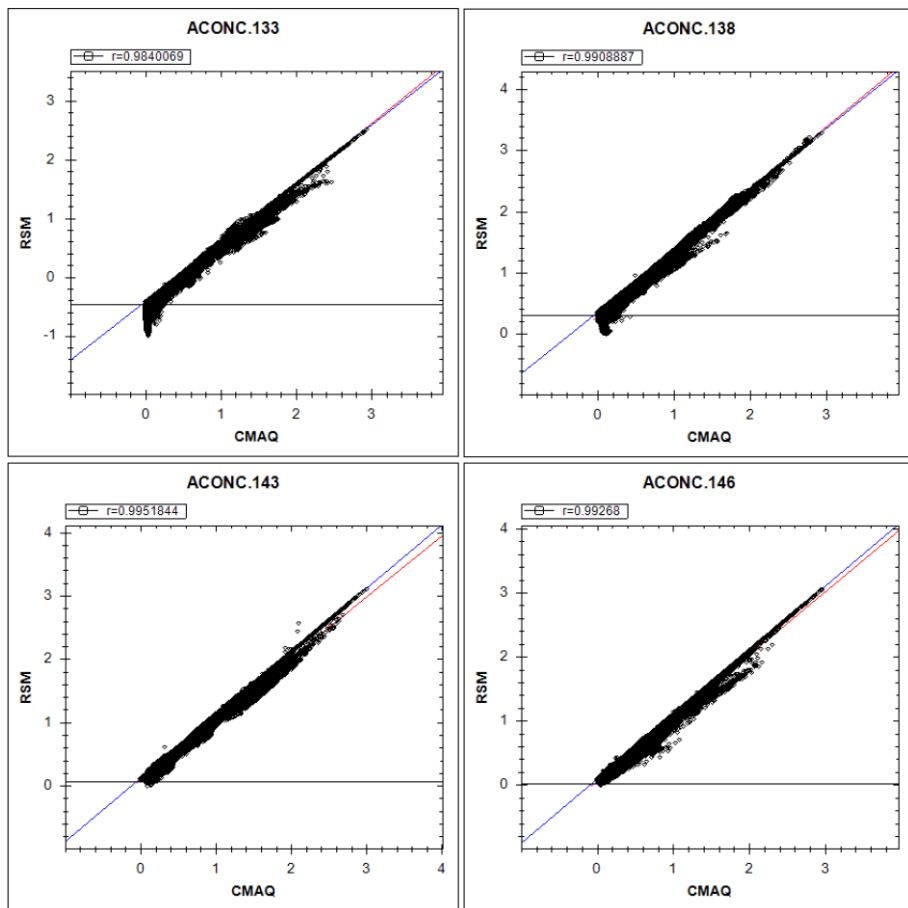
Predicted PM_{2.5} Concentration
(RSM vs. CMAQ)



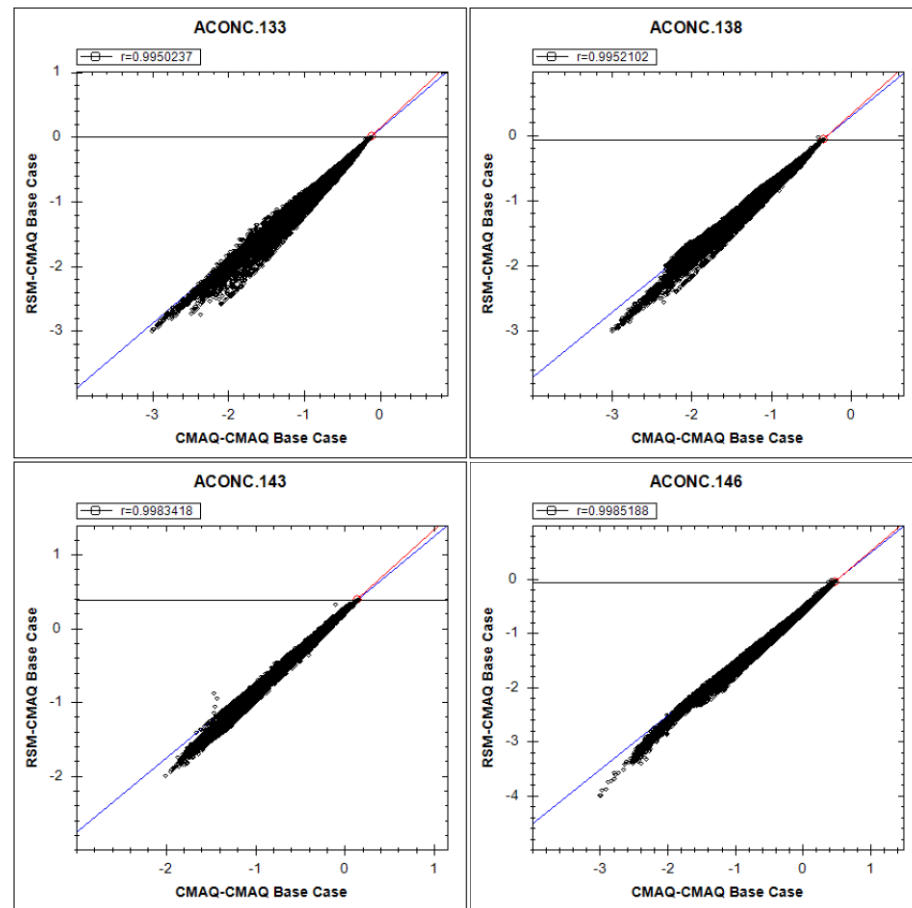
Predicted PM₅ Response
(RSM vs. CMAQ)

“Out-of-Sample” Validation: PM_{NO₃} Concentration & Response (Jan., PM_{NO₃} monthly avg.): **Worst 4 cases**

Predicted PM_{2.5} Conc. (RSM vs. CMAQ)



Predicted PM_{2.5} Responses (RSM-Base vs. CMAQ-Base)



Please see “Appendix B” for additional “out-of-sample” validation slides

“RSM-VAT” Demo

Main GUI:

1. Launch/open PM2.5 Jan. project
2. Main GUI -> File/Analysis/View
3. Menu: VA/QA/Log&Msg
4. Traffic Light: Each module & input files
5. Help: Online User's Manual

Module -> Experimental Design module

1. “Control Matrix” creation
2. “CMAQ Preparation”
 - Create Region (default CR, State & CBSA)
 - Merge/Subtract
 - Export Control Namelist File

V/A module:

1. MAP -> 2D/3D/Contour
2. Conc./Response toggle
3. Radio button: Control %: Set & Reset
4. NOx/SO2/NH3 & Primary PM
5. Output to SMAT/BenMAP/CSV & color legend
6. Chart: EC 1 & 2: NOx: 25/50/75/100%

7. Region/Pollutant/Sector checked
8. Chart: SC 1: NOx, 20%/40%/60%/80%/100%
9. SC2: NOx & Primary PM

QA/Validation module:

1. OOSV: RSM vs. CMAQ
 - “Conc.” toggle “to Response”
2. OOSV: Comparison Plot
 - “Ambient” to “Reduction”
 - Show Difference Plot
 - Adjust legend/scale
3. “CMAQ Viewer”: O3 & PM2.5 species

O3 July case:

1. Launch/open O3 July project
2. V/A->MAP: Concs & Response toggle
3. V/A-> Chart: NOx: 25/50/75/100%
4. QA/Validation:
 - OOSA: RSM vs. CMAQ
 - OOSA: Comparison Plot

Discussion & Next Steps

Next Steps:

- Implement “*DeepRSM*” under RSM-VAT
- Conduct “*DeepRSM*” U.S. pilot case studies under 2016 or 2017 modeling platform (CMAQ & CAMx?)

Potential Applications & Projects

- Hemispheric CMAQ applications
- Inter-comparisons with APCA (O₃/PM) & DDM/HDDM (O₃)

Potential Issue:

- No current year funding for RSM development; Need new funding to support “*DeepRSM*” pilot project under new GSA contract starting Oct. 1st, 2020

Appendix A:

"DeepRSM" Supplemental information

Appendix B:

RSM CMAQ EUS Case "QA":

pf-RSM "Out-of-Sample" Validation

Appendix C:

RSM-VAT Demo & Tutorial:

EUS 12-km Case using "pf-RSM"

DeepRSM Publication (2020)

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Deep Learning for Prediction of the Air Quality Response to Emission Changes

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

Cite this: *Environ. Sci. Technol.* 2020, 54, 8589–8600

Publication Date: June 17, 2020

<https://doi.org/10.1021/acs.est.0c02923>

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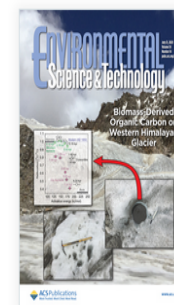
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James T. Kelly

Office of Air Quality Planning and Standards, U.S.
Environmental Protection Agency, Research
Triangle Park, North Carolina 27711, United States

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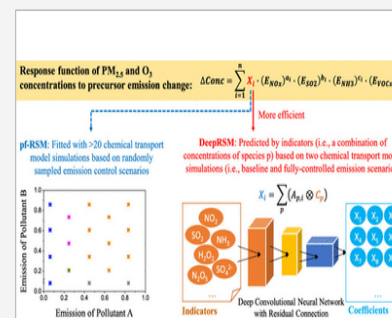
PDF (4 MB)

Supporting Info (1)

SUBJECTS: Precursors, Environmental chemistry, Environmental modeling,

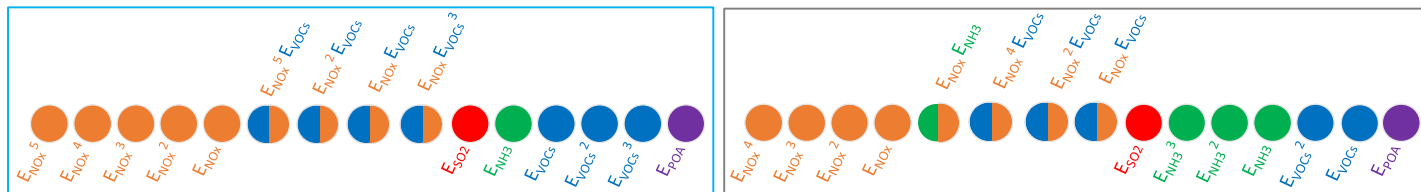
Abstract

Efficient prediction of the air quality response to emission changes is a prerequisite for an integrated assessment system in developing effective control policies. Yet, representing the nonlinear response of air quality to emission controls with accuracy remains a major barrier in air quality-related decision making. Here, we demonstrate a novel method that combines deep learning approaches with chemical indicators of pollutant formation to quickly estimate the coefficients of air quality response functions using ambient concentrations of 18 chemical indicators simulated with a comprehensive atmospheric chemical transport model (CTM). By requiring only two CTM simulations for model application, the new method significantly enhances the computational efficiency compared to existing methods that achieve lower accuracy despite requiring 20+ CTM simulations (the benchmark statistical model). Our results demonstrate the utility of deep learning approaches for capturing the nonlinearity of atmospheric chemistry and physics and the prospects of the new method to support effective policymaking in other environment systems.

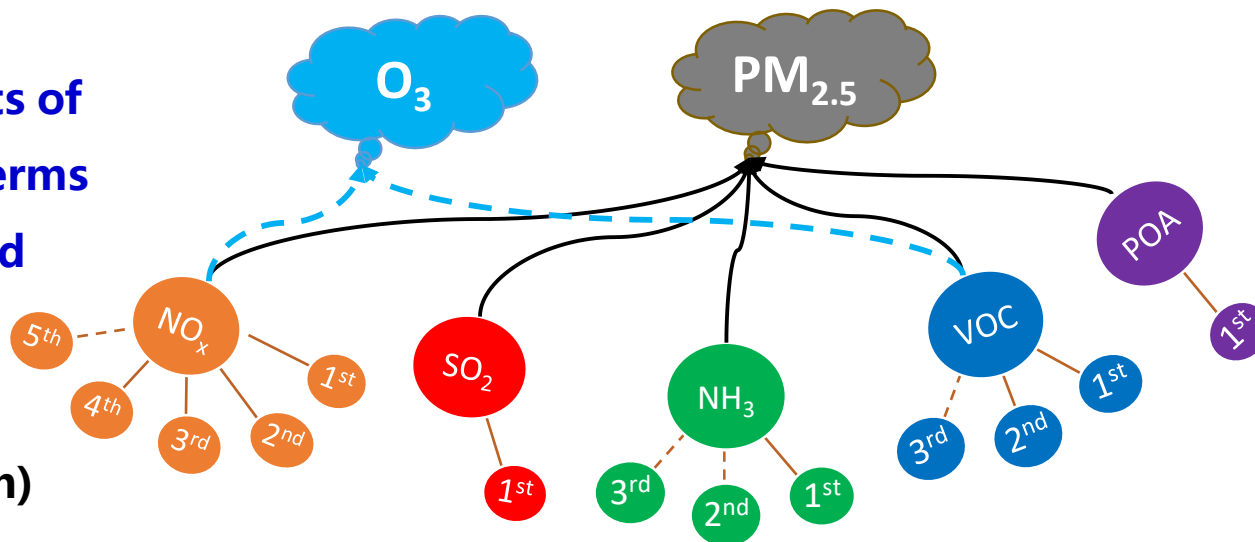


RSM with polynomial functions: *pf-RSM*

$$\Delta Conc = \sum_{i=1}^n X_i \cdot (E_{NOx})^{a_i} \cdot (E_{SO2})^{b_i} \cdot (E_{NH3})^{c_i} \cdot (E_{VOCs})^{d_i} \cdot (E_{POA})^{e_i}$$



14 coefficients of polynomial terms can be derived from 20~30 samples (per control region)

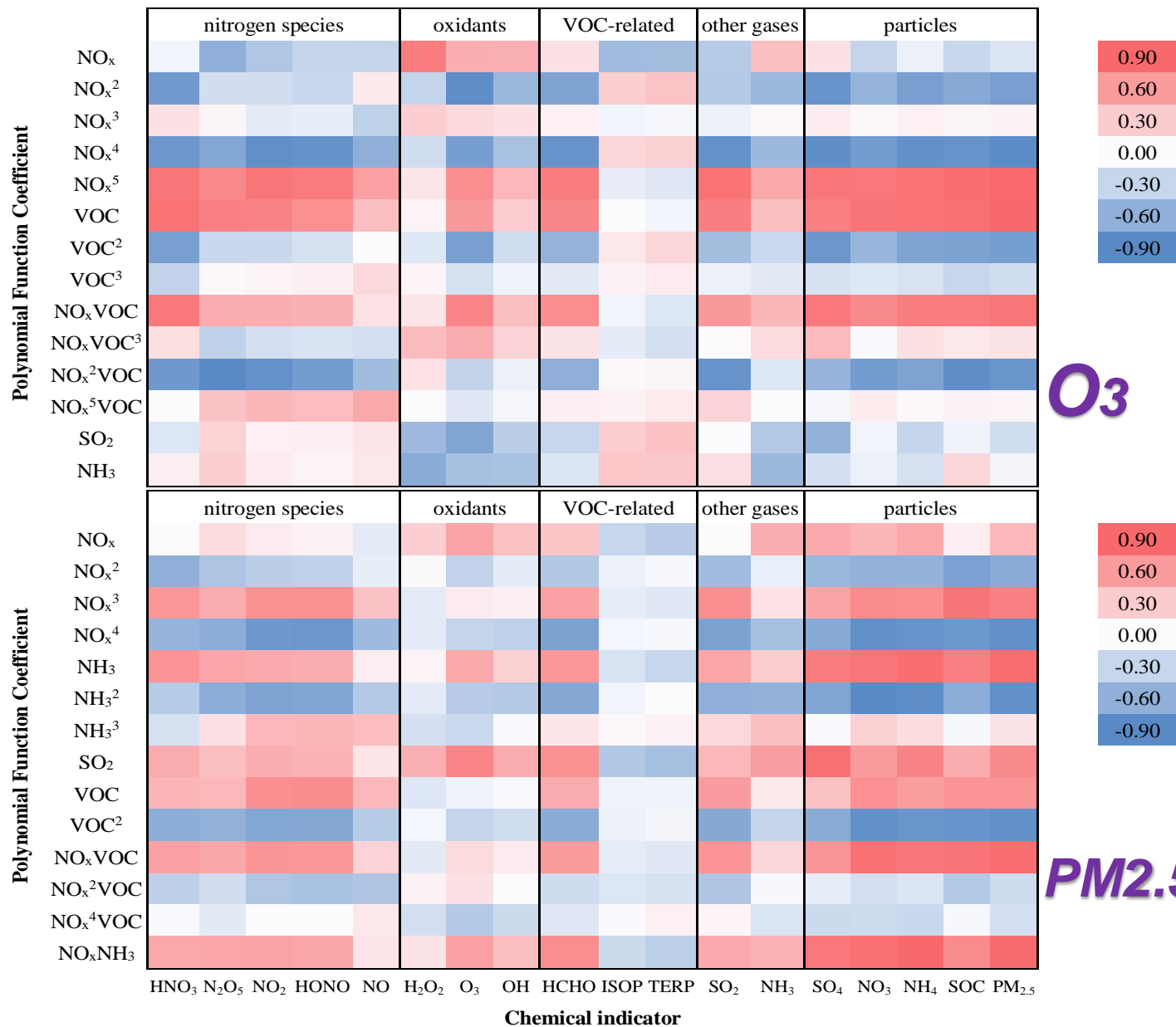


High order for NO_x and VOC

Linear behavior for SO_2 and POA

Xing et al., ACP, 2018

“Indicator-based” DeepRSM



14 coefficients of terms in in responding to 18 chemical indicators for O₃ and PM_{2.5} (example)

Appendix B:

QA for RSM CMAQ EUS Case:

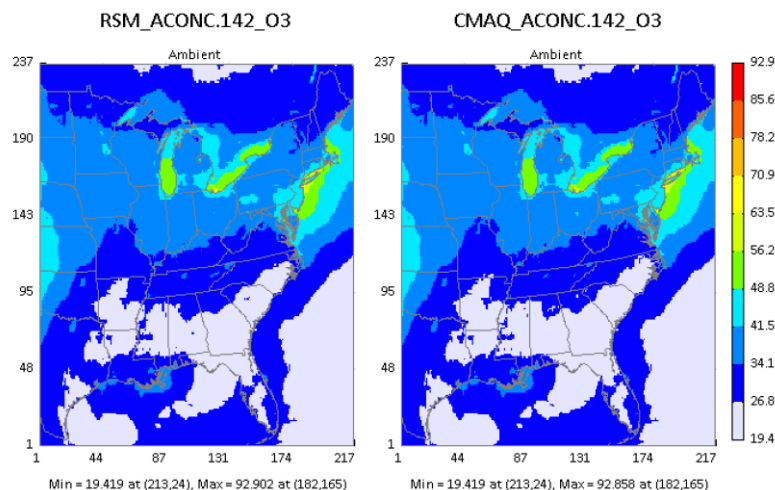
pf-RSM "Out-of-Sample" Validation

- 1. O₃ July 8-hr avg.***
- 2. PM_{2.5} July monthly avg.***
- 3. PM_{2.5} Jan. monthly avg.***
- 4. PM__SO₄ Jan. monthly avg.***
- 5. PM__NO₃ Jan. monthly avg.***

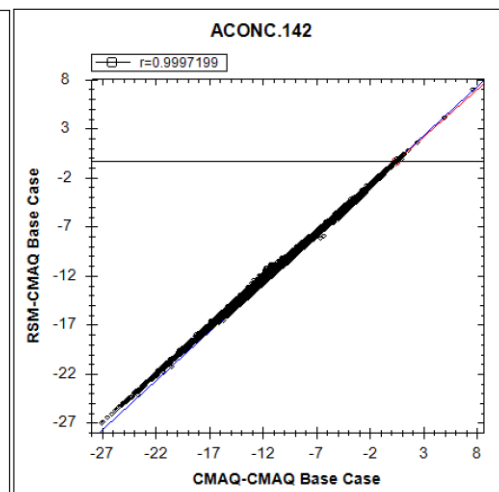
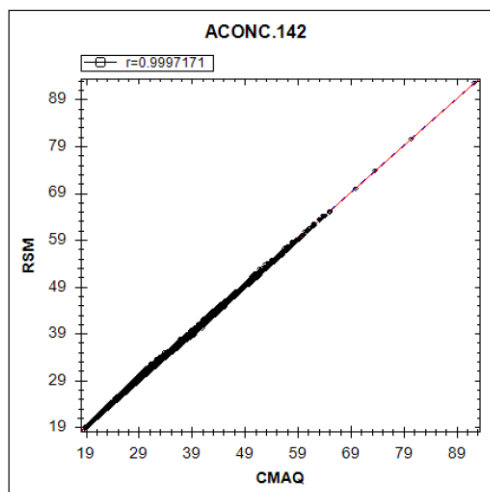
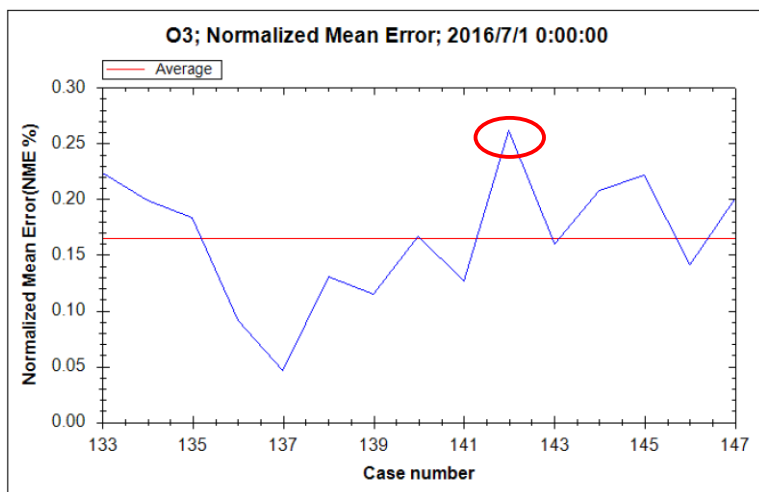
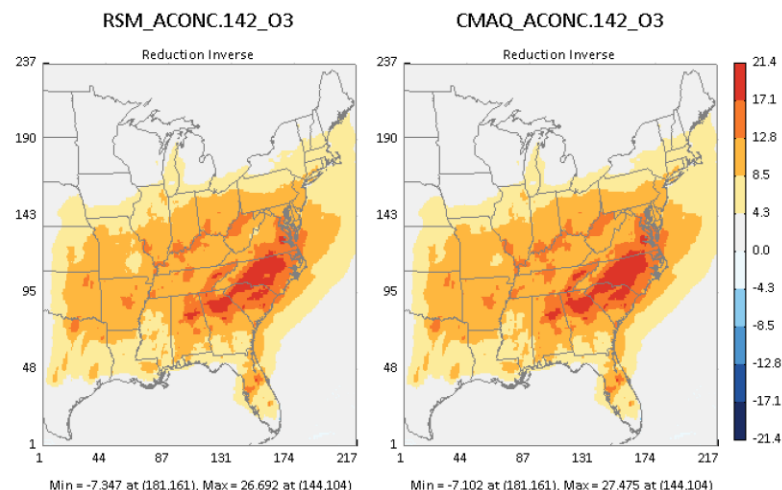
July, O₃-8hr avg. , US

Out-of-Sample Validation: Predicted O₃ Concentrations & Responses (July, O₃-8hr avg. , US) Worst 1

O₃ Conc: RSM vs. CMAQ



O₃ Response: RSM vs. CMAQ



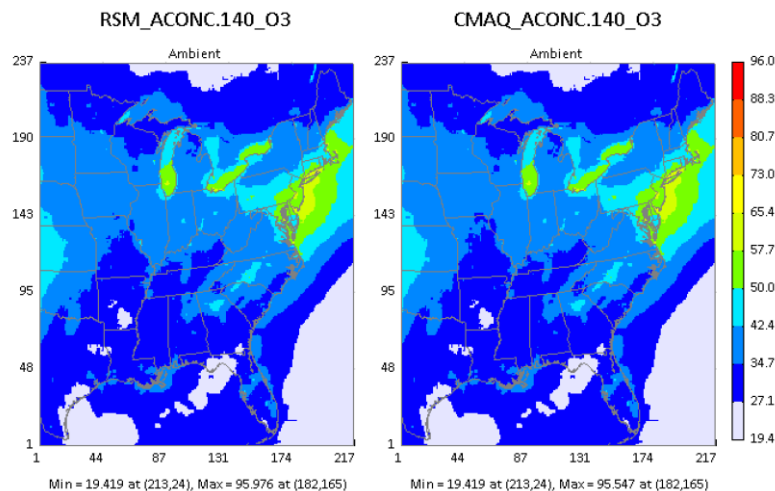
All “Out-of-Sample” runs:
Normalized Mean Error

Predicted O₃ Concentration
(RSM vs. CMAQ)

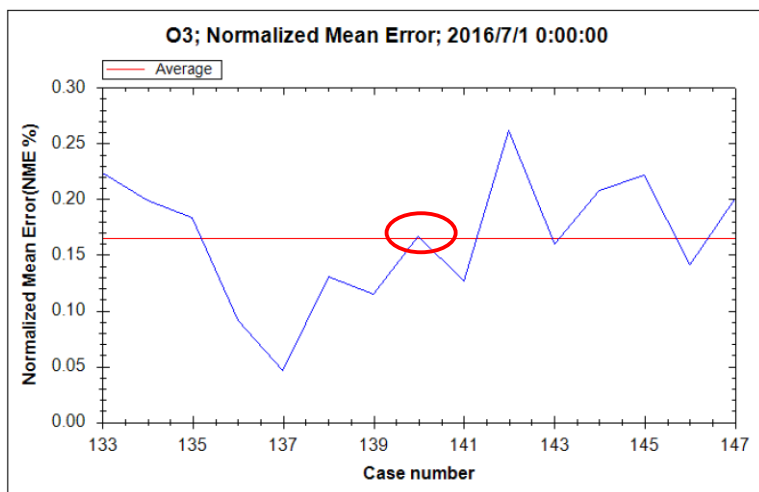
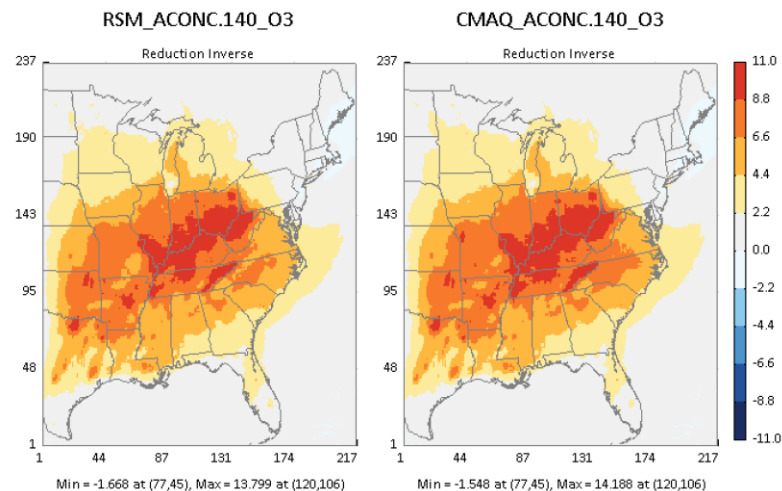
Predicted O₃ Response
(RSM vs. CMAQ)

Out-of-Sample Validation: Predicted O₃ Concentrations & Responses (July, O₃-8hr avg. , US) Typical 1

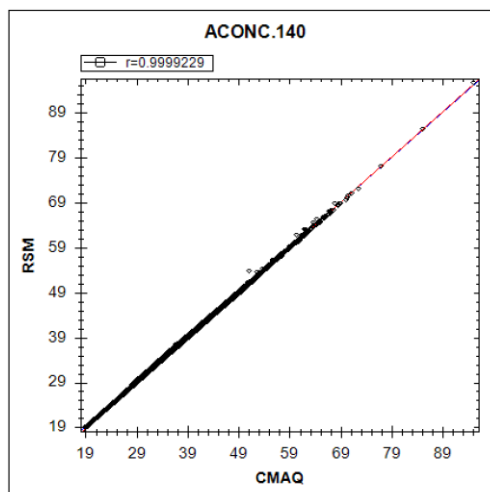
O₃ Conc: RSM vs. CMAQ



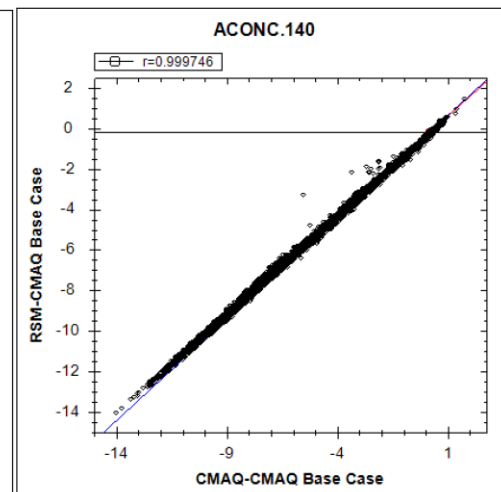
O₃ Response: RSM vs. CMAQ



All “Out-of-Sample” runs:
Normalized Mean Error



Predicted O₃ Concentration
(RSM vs. CMAQ)

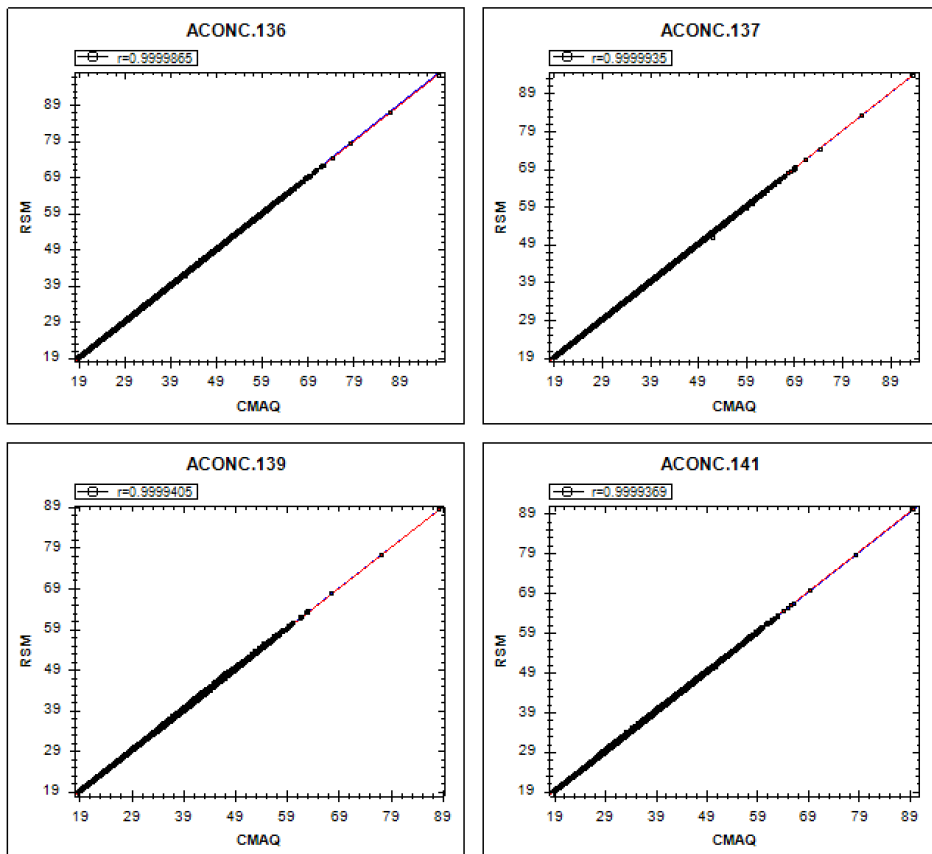


Predicted O₃ Response
(RSM vs. CMAQ)

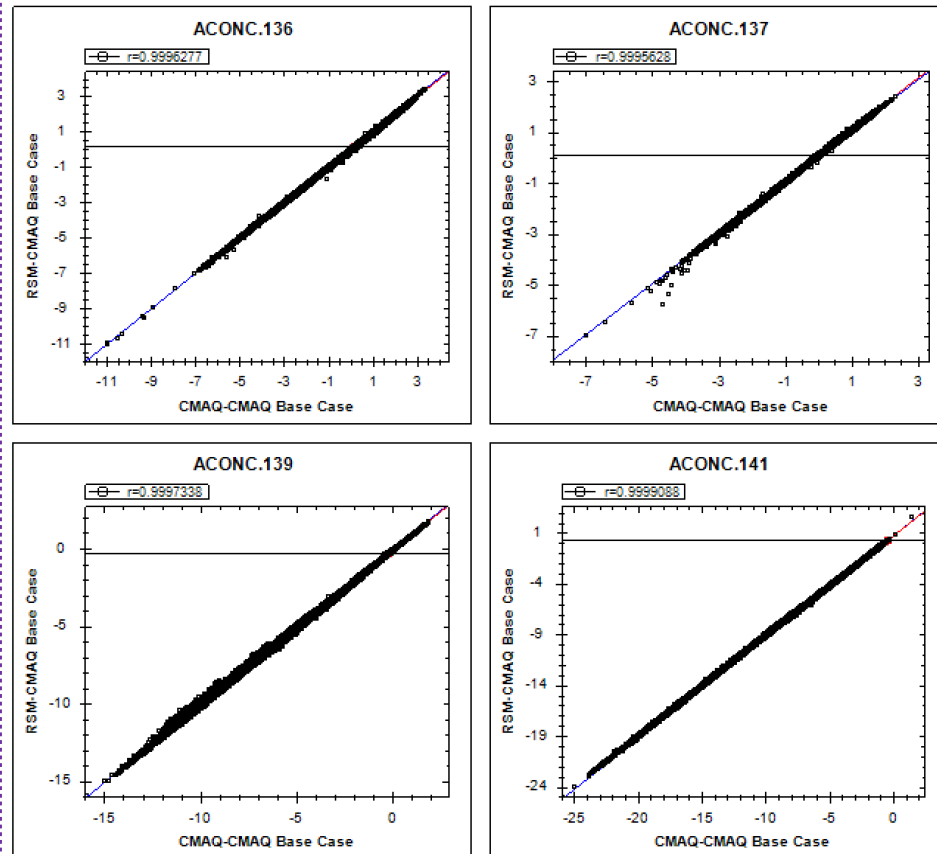
Out-of-Sample Validation: Concentration Comparison

(July, O₃-8hr avg. , US) Best 4

Predicted O₃ Conc.
(RSM vs. CMAQ)



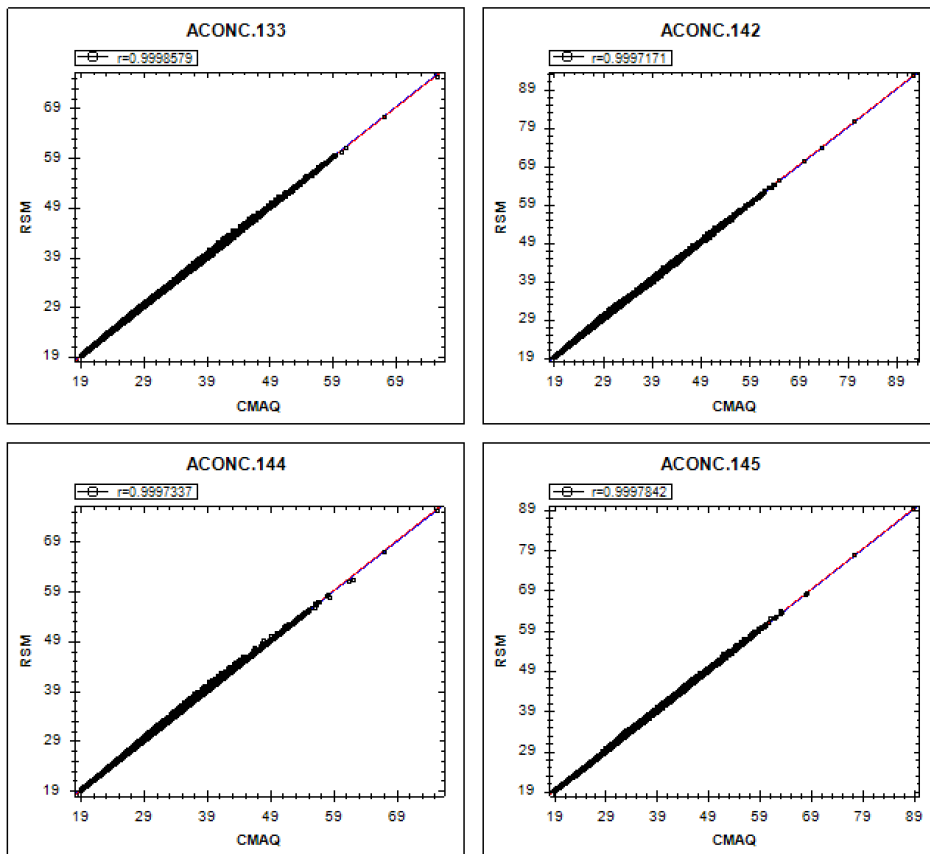
Predicted O₃ Responses (O₃)
(RSM-Base vs. CMAQ-Base)



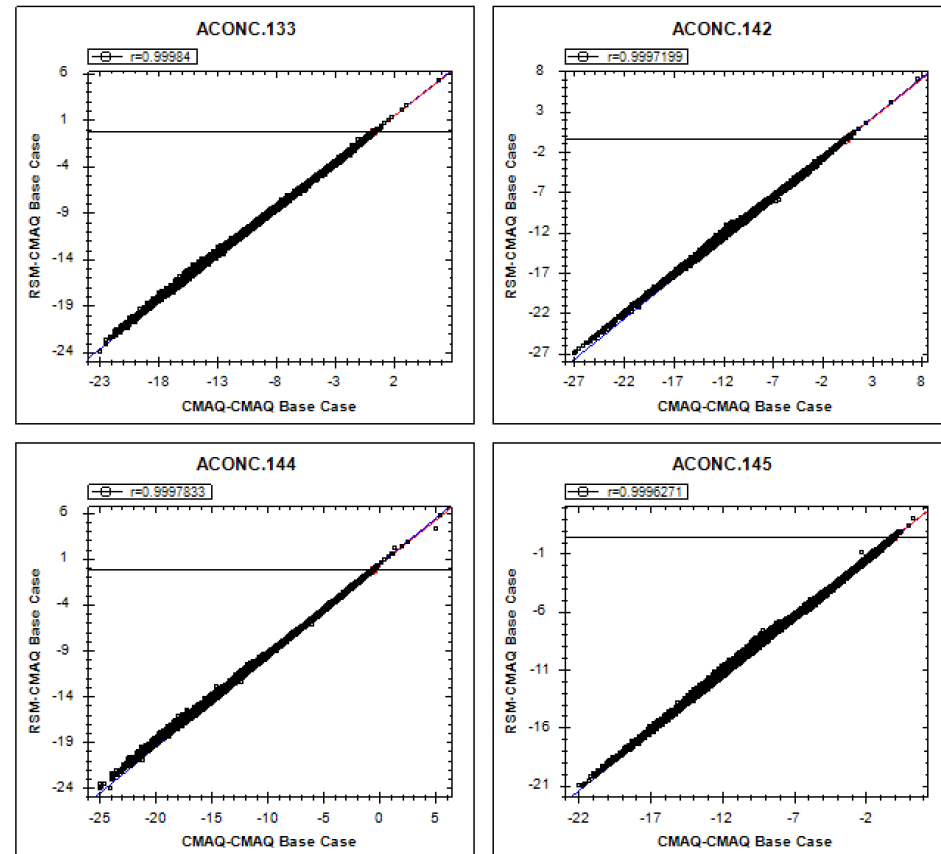
Out-of-Sample Validation: Concentration Comparison

(July, O₃-8hr avg. , US) Worst 4

Predicted O₃ Conc. (RSM vs. CMAQ)



Predicted O₃ Responses (O₃) (RSM-Base vs. CMAQ-Base)

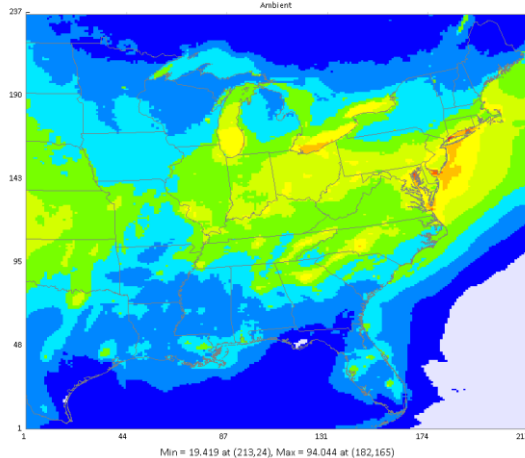


Out-of-Sample Validation: Predicted Concentrations (July, O₃-8hr avg. , US) Best 1

RSM

RSM_ACONC.137_O3

Ambient

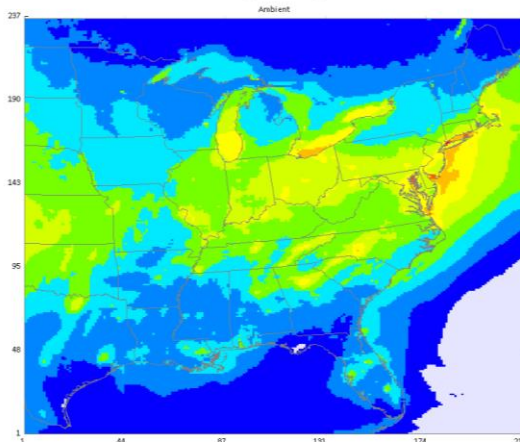


Min = 19.419 at (213,24), Max = 94.044 at (182,165)

CMAQ

CMAQ_ACONC.137_O3

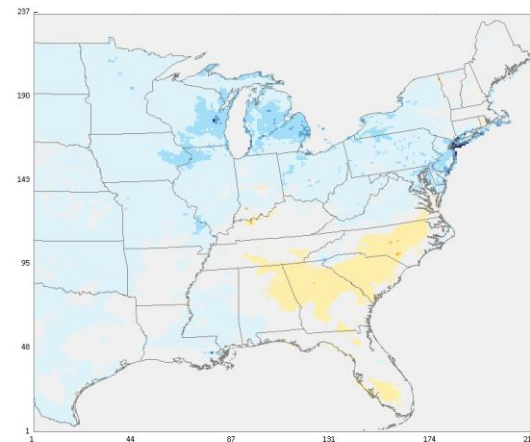
Ambient



Min = 19.419 at (213,24), Max = 94.319 at (182,165)

Delta

Delta_ACONC.137_O3

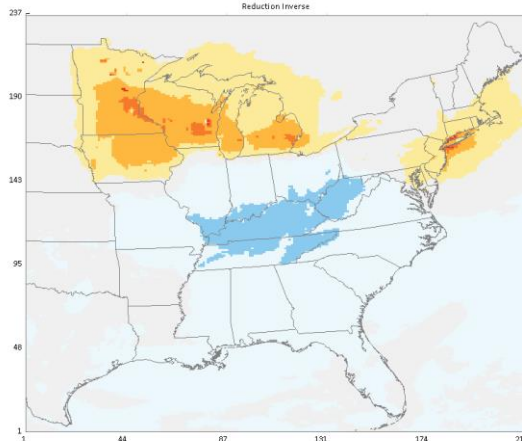


Min = -1.172 at (181,161), Max = 0.224 at (94,120)

Base - RSM

RSM_ACONC.137_O3

Reduction Inverse

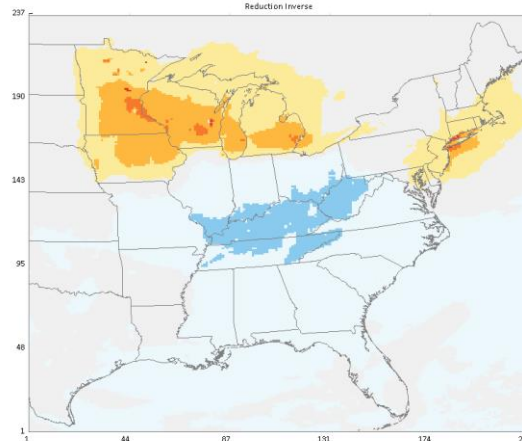


Min = -2.274 at (122,106), Max = 7.129 at (44,193)

Base - CMAQ

CMAQ_ACONC.137_O3

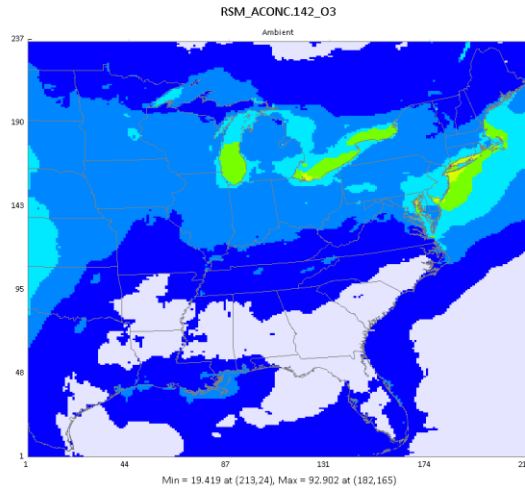
Reduction Inverse



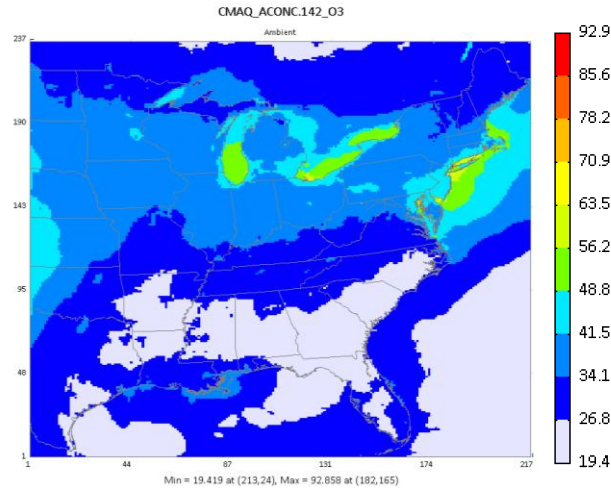
Min = -2.249 at (121,106), Max = 7.078 at (44,193)

Out-of-Sample Validation: Predicted Concentrations (July, O₃-8hr avg. , US) Worst 1

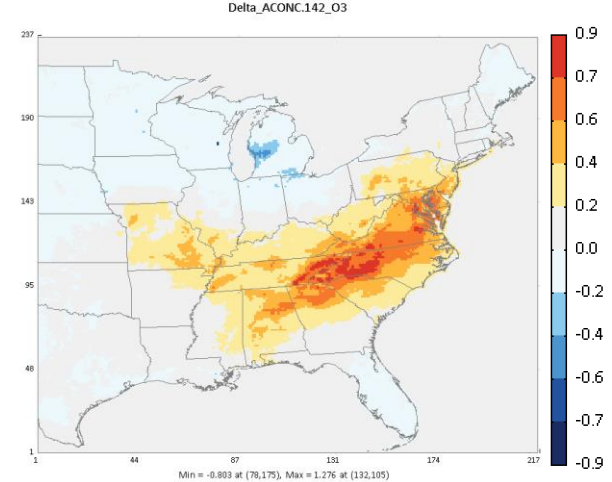
RSM



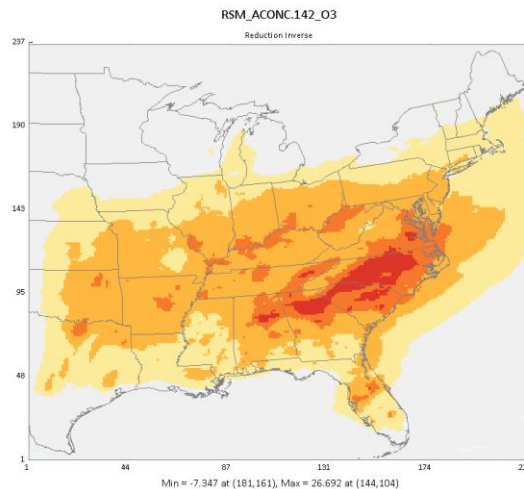
CMAQ



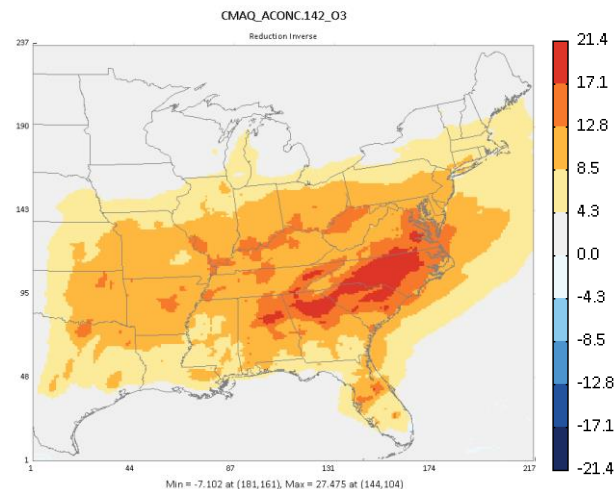
Delta



Base - RSM



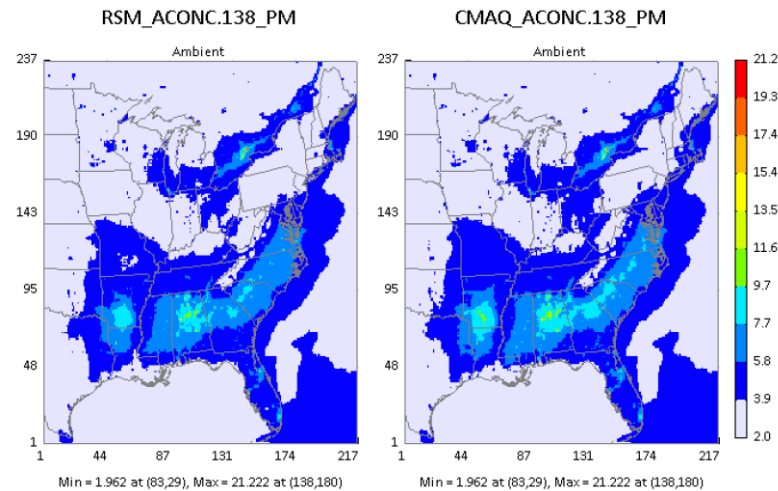
Base - CMAQ



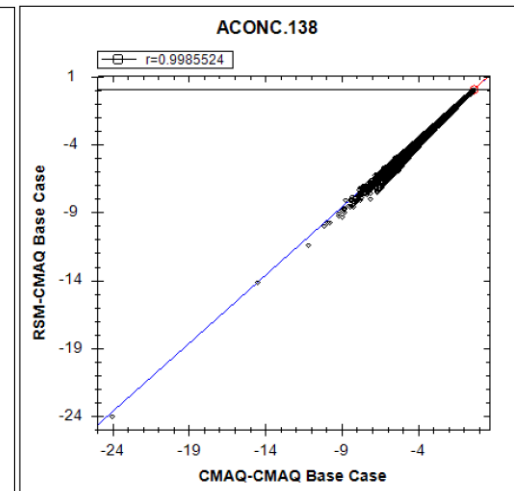
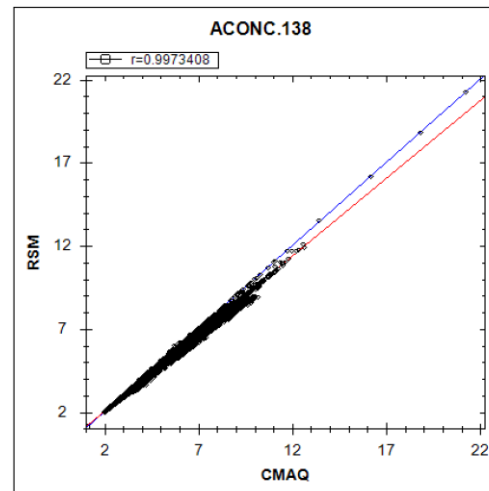
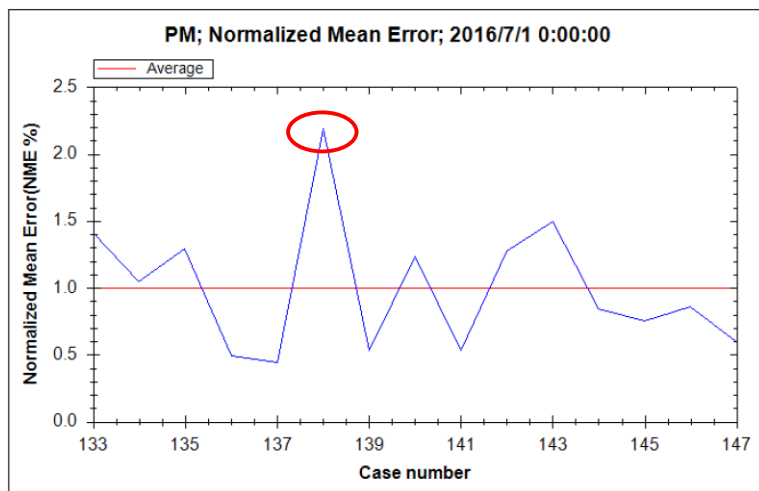
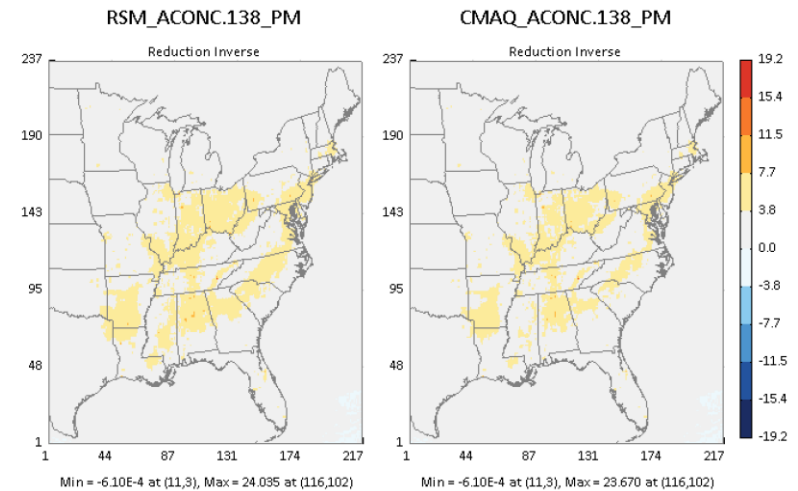
July, PM_{2.5} monthly avg., US

Out-of-Sample Validation: Predicted PM_{2.5} Concentrations & Responses (July, PM_{2.5} monthly avg., US) Worst 1

PM_{2.5} Conc: RSM vs. CMAQ



PM_{2.5} Response: RSM vs. CMAQ

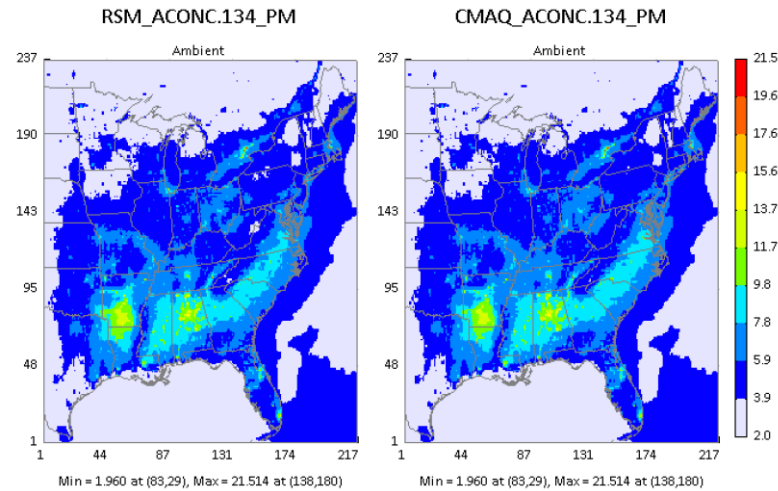


All “Out-of-Sample” runs:
Normalized Mean Error

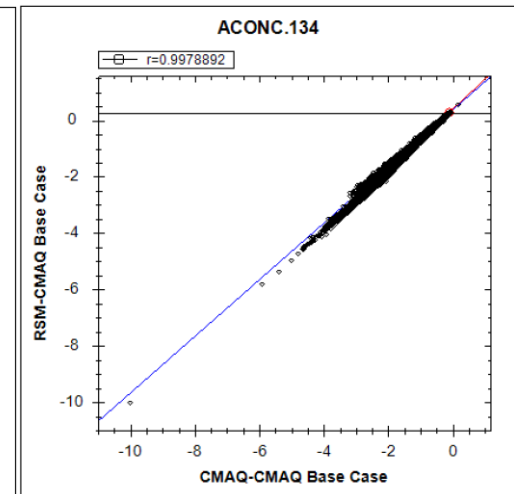
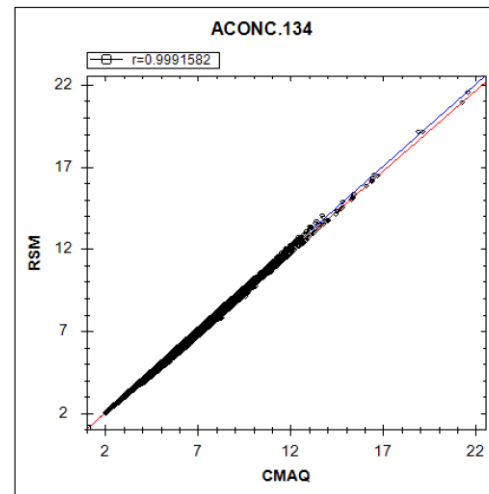
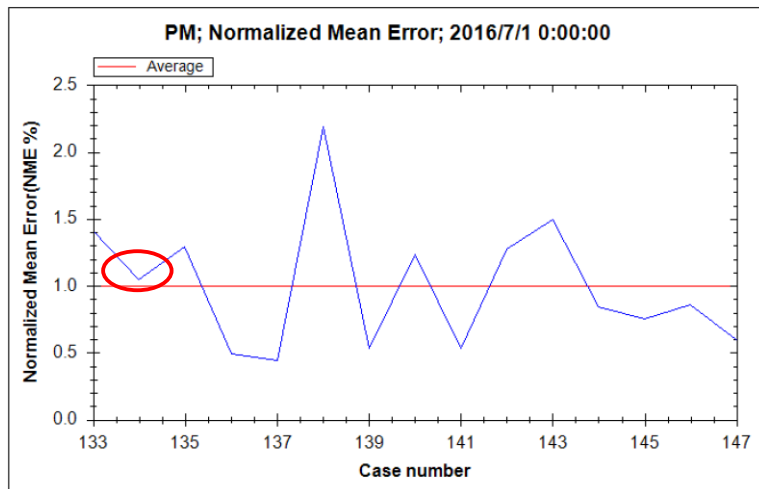
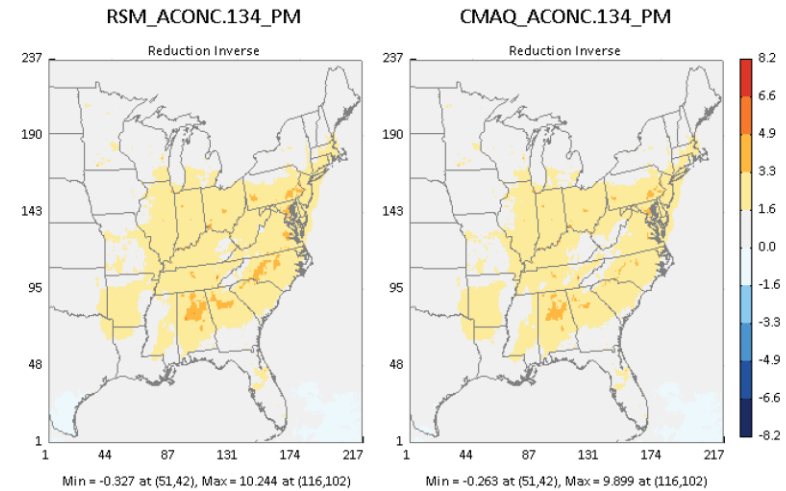
Predicted PM_{2.5} Concentration Predicted PM_{2.5} Response
(RSM vs. CMAQ) (RSM vs. CMAQ)

Out-of-Sample Validation: Predicted PM_{2.5} Concentrations & Responses (July, PM_{2.5} monthly avg., US) Typical 1

PM_{2.5} Conc: RSM vs. CMAQ



PM_{2.5} Response: RSM vs. CMAQ

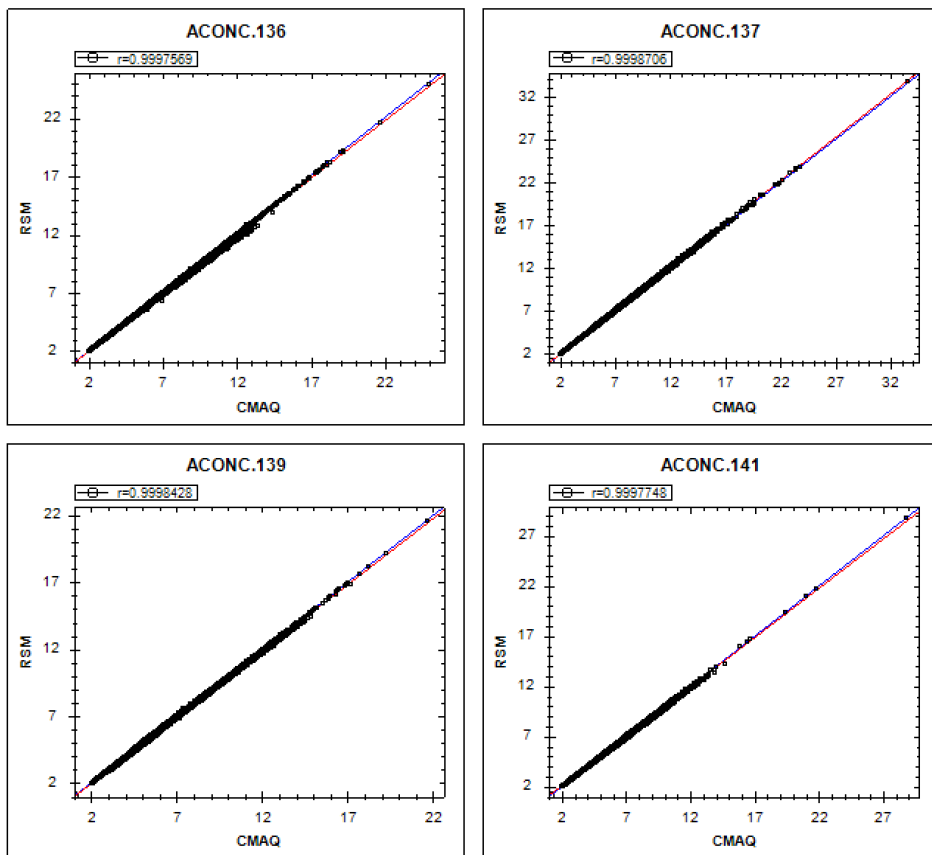


All “Out-of-Sample” runs:
Normalized Mean Error

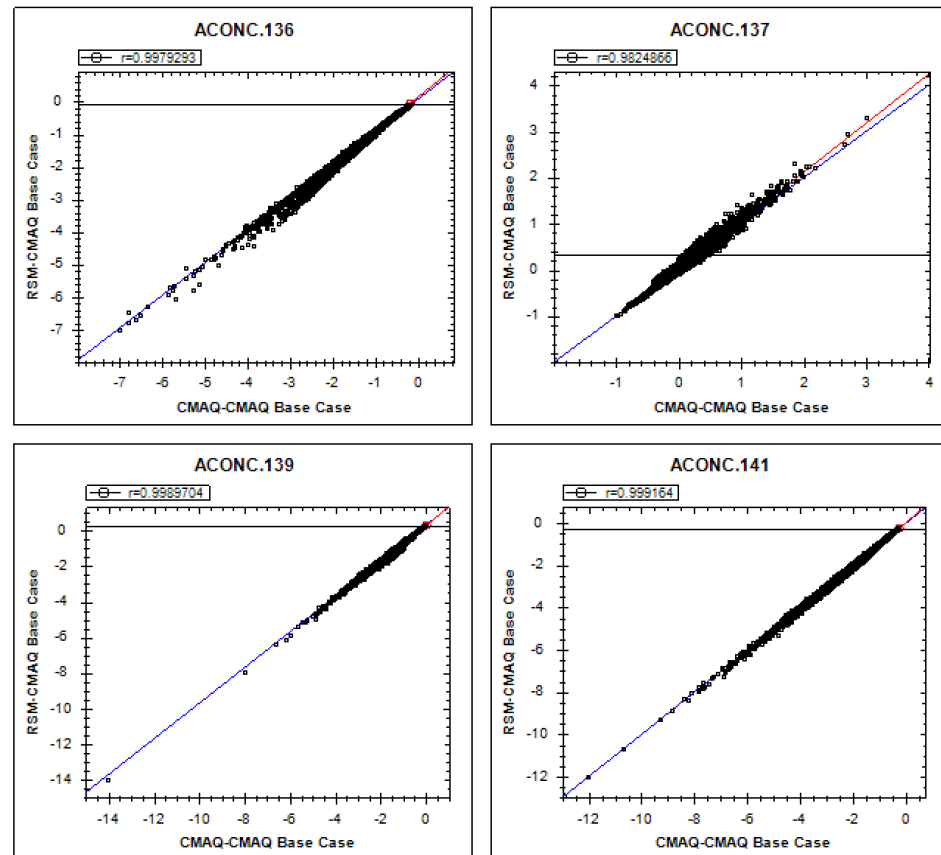
Predicted PM_{2.5} Concentration Predicted PM_{2.5} Response
(RSM vs. CMAQ) (RSM vs. CMAQ)

Out-of-Sample Validation: Concentration Comparison (July, PM_{2.5} monthly avg., US) Best 4

Predicted PM_{2.5} Conc. (RSM vs. CMAQ)



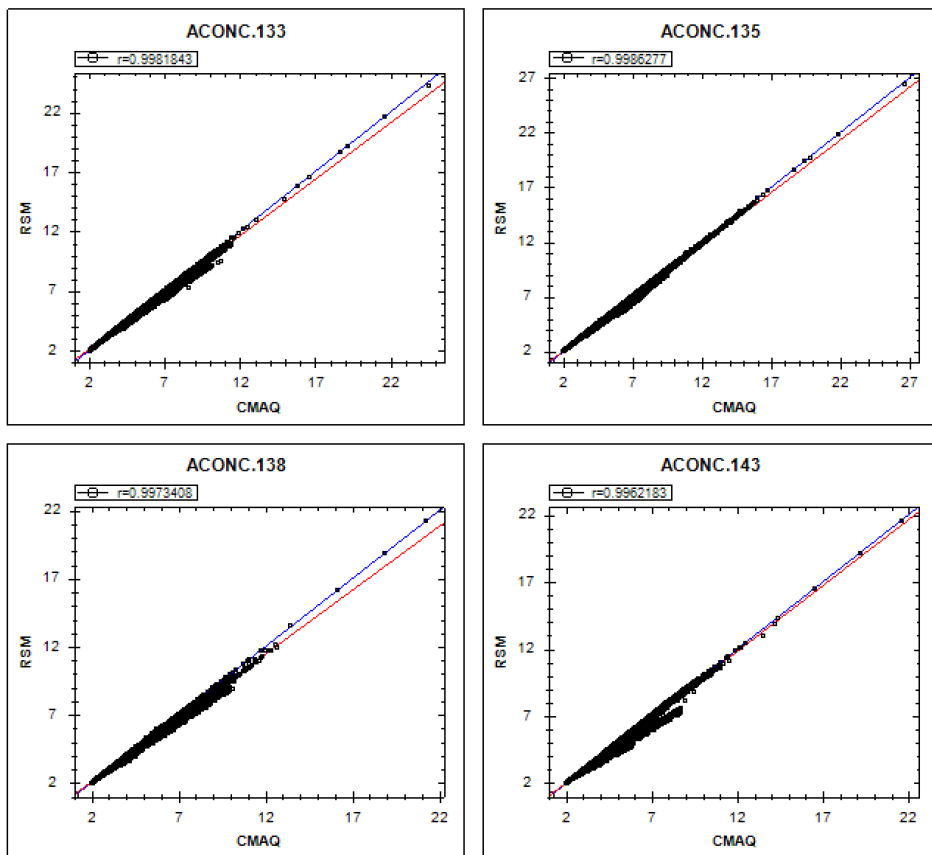
Predicted PM_{2.5} Responses (RSM-Base vs. CMAQ-Base)



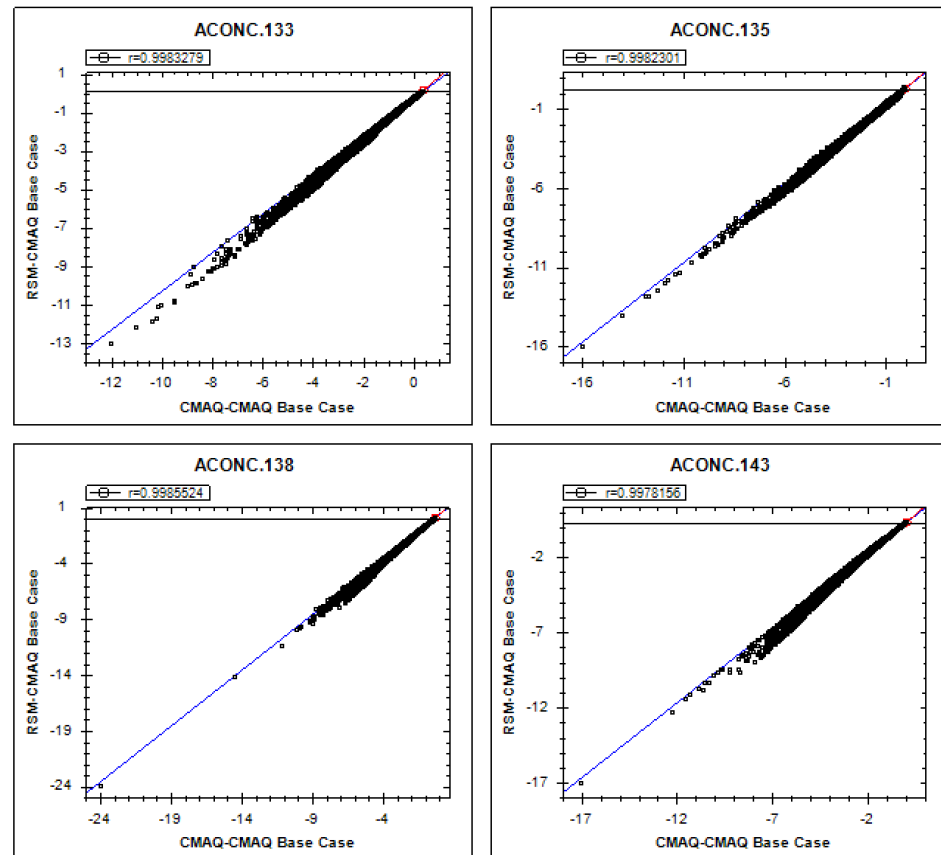
Out-of-Sample Validation: Concentration Comparison

(July, PM_{2.5} monthly avg., US) Worst 4

Predicted PM_{2.5} Conc. (RSM vs. CMAQ)

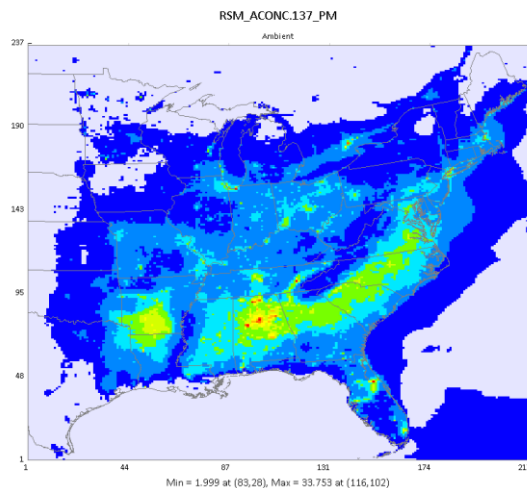


Predicted PM_{2.5} Responses (RSM-Base vs. CMAQ-Base)

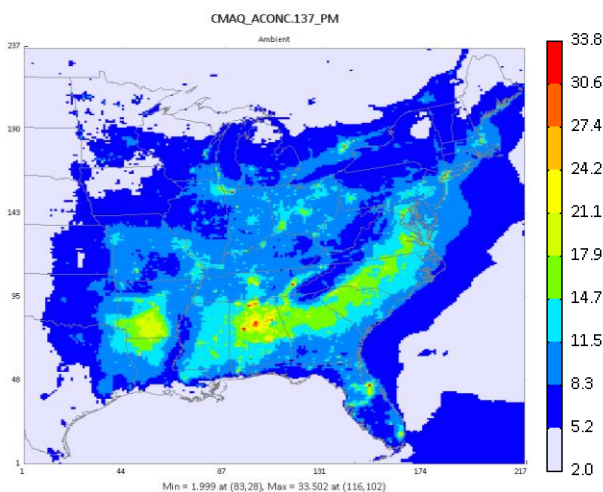


Out-of-Sample Validation: Predicted Concentrations (July, PM_{2.5} monthly avg., US) Best 1

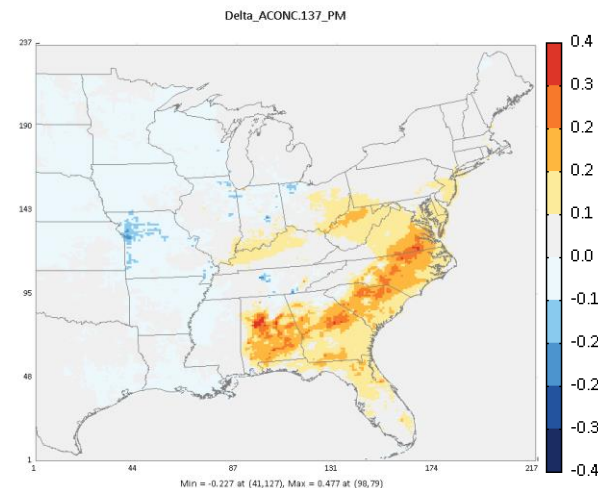
RSM



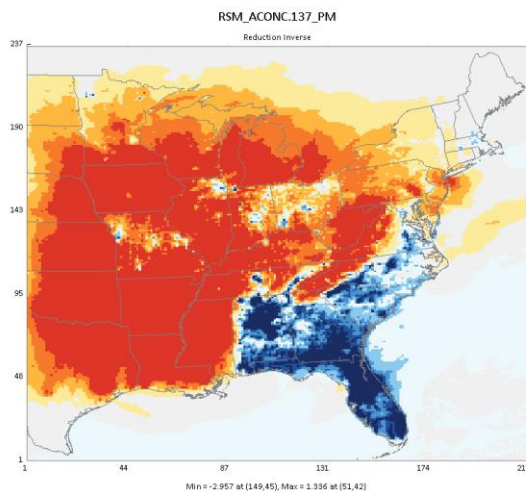
CMAQ



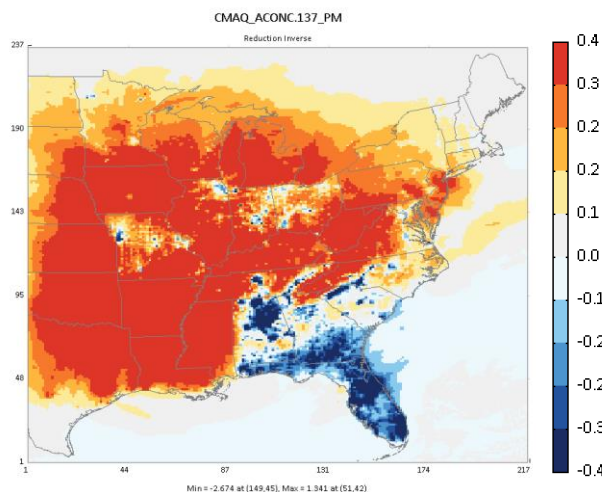
Delta



Base - RSM



Base - CMAQ

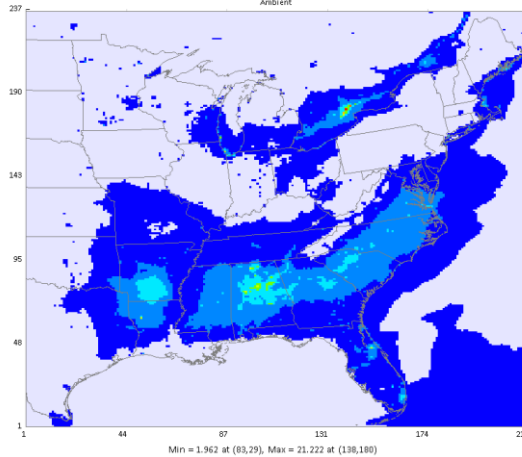


Out-of-Sample Validation: Predicted Concentrations (July, PM_{2.5} monthly avg., US) Worst 1

RSM

RSM_ACONC.138_PM

Ambient

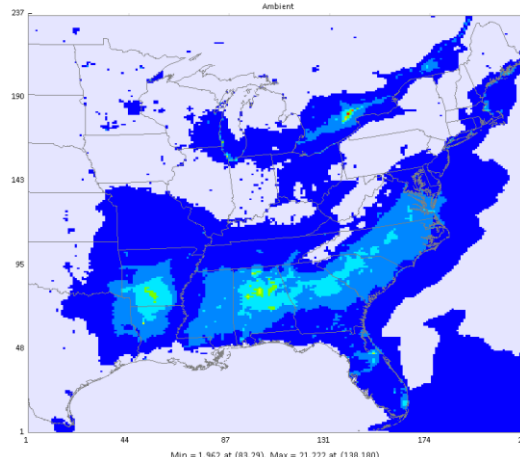


Min = 1.962 at (83,29), Max = 21.222 at (138,180)

CMAQ

CMAQ_ACONC.138_PM

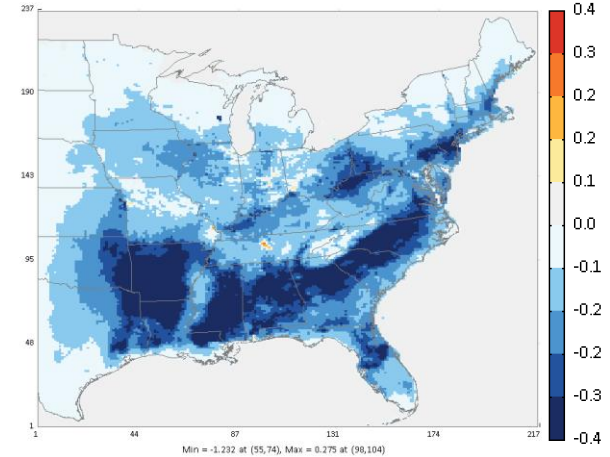
Ambient



Min = 1.962 at (83,29), Max = 21.222 at (138,180)

Delta

Delta_ACONC.138_PM

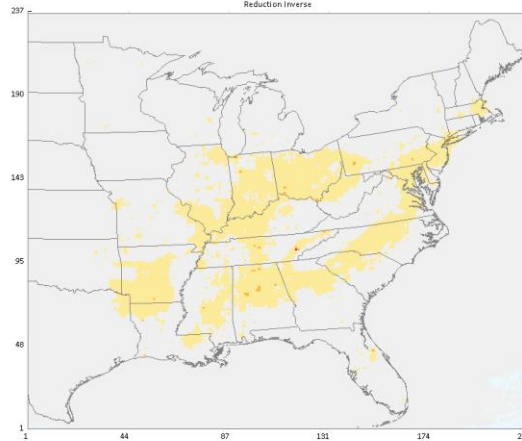


Min = -1.232 at (55,74), Max = 0.275 at (98,104)

Base - RSM

RSM_ACONC.138_PM

Reduction Inverse

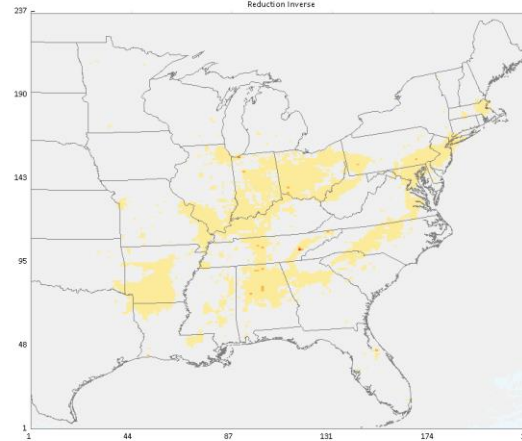


Min = -6.10E-4 at (11,3), Max = 24.095 at (116,102)

Base - CMAQ

CMAQ_ACONC.138_PM

Reduction Inverse

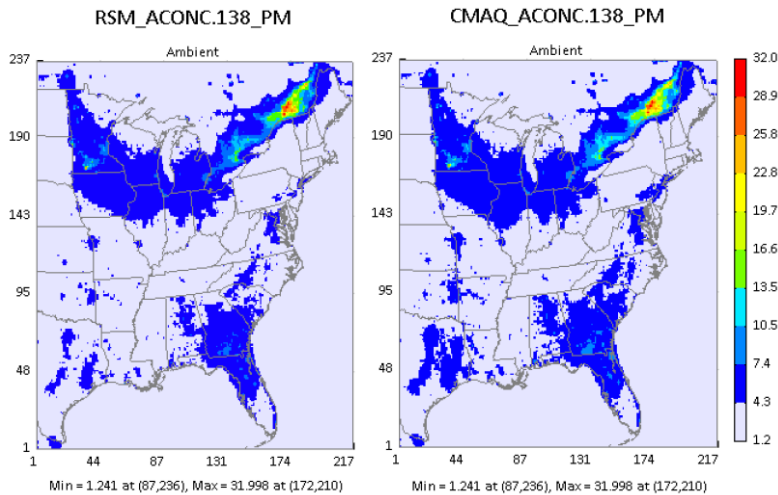


Min = -6.10E-4 at (11,3), Max = 23.670 at (116,102)

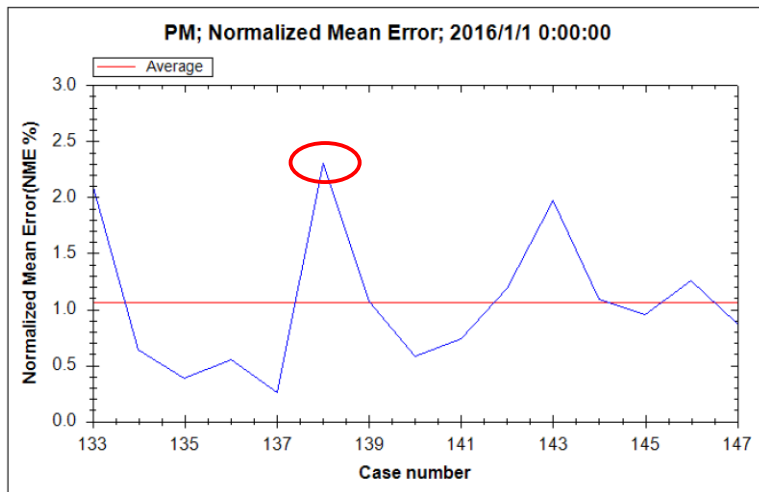
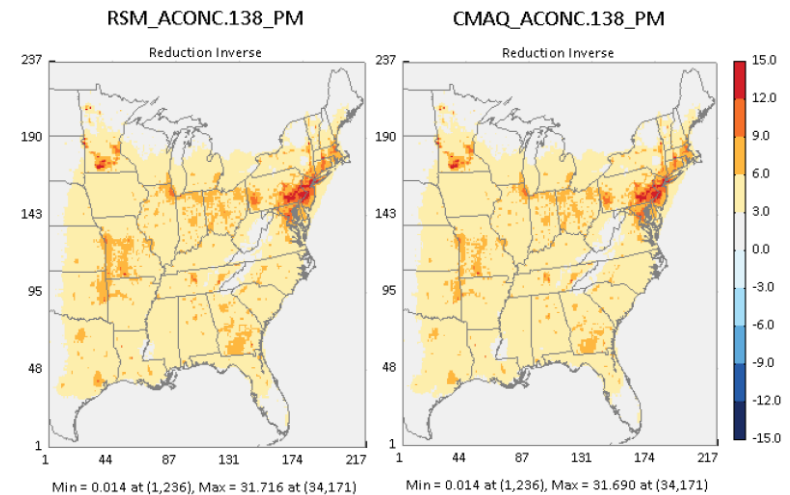
Jan., PM_{2.5} monthly avg., US

Out-of-Sample Validation: Predicted PM_{2.5} Concentrations & Responses (Jan., PM_{2.5} monthly avg., US) Worst 1

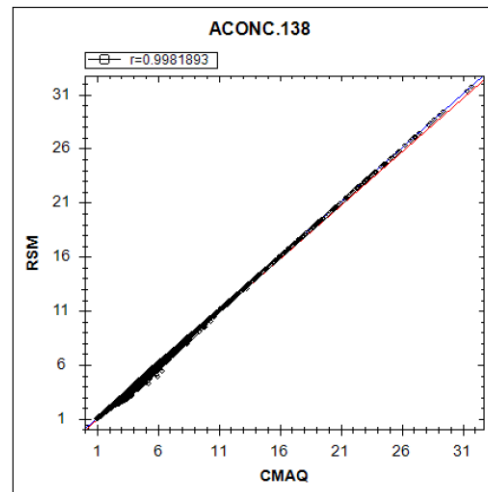
PM_{2.5} Conc: RSM vs. CMAQ



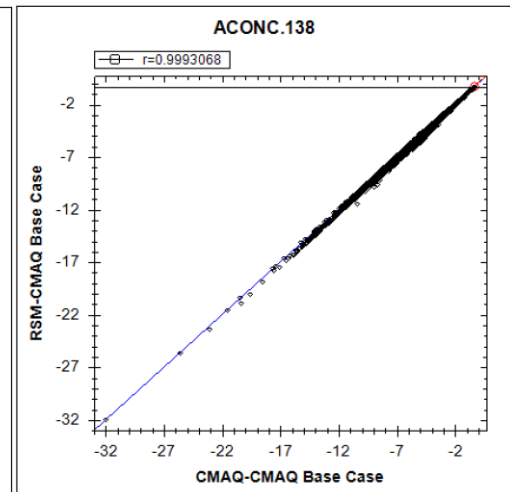
PM_{2.5} Response: RSM vs. CMAQ



All “Out-of-Sample” runs:
Normalized Mean Error



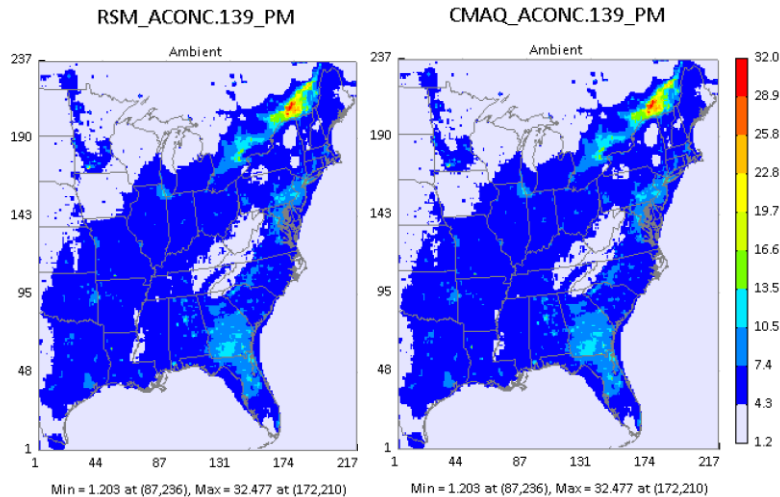
Predicted PM_{2.5} Concentration
(RSM vs. CMAQ)



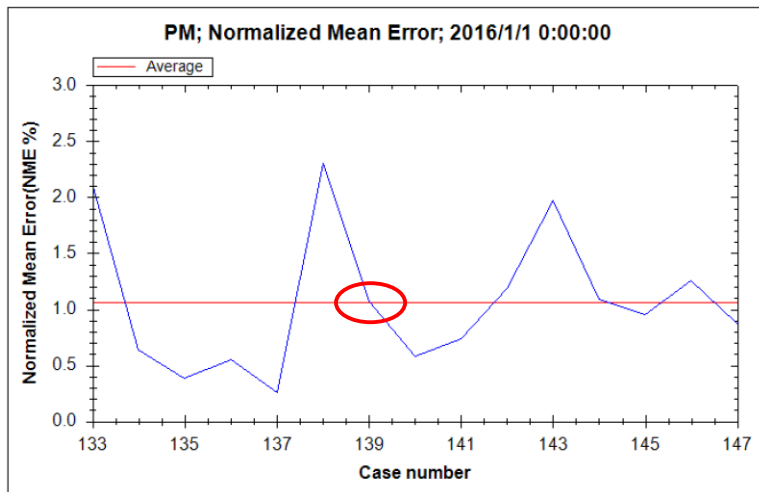
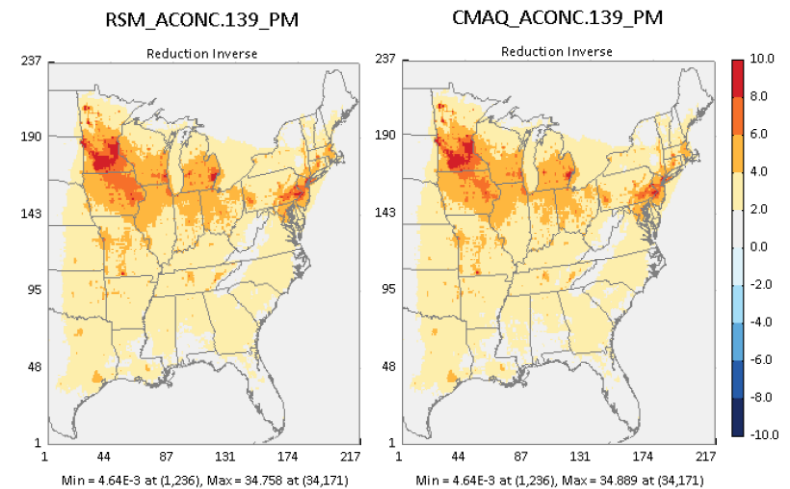
Predicted PM₅ Response
(RSM vs. CMAQ)

Out-of-Sample Validation: Predicted PM_{2.5} Concentrations & Responses (Jan., PM_{2.5} monthly avg., US) Typical 1

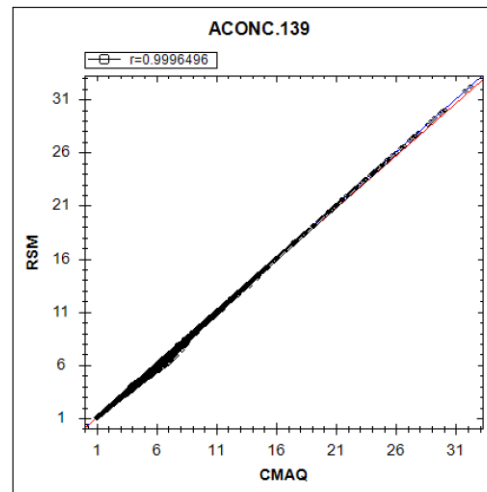
PM_{2.5} Conc: RSM vs. CMAQ



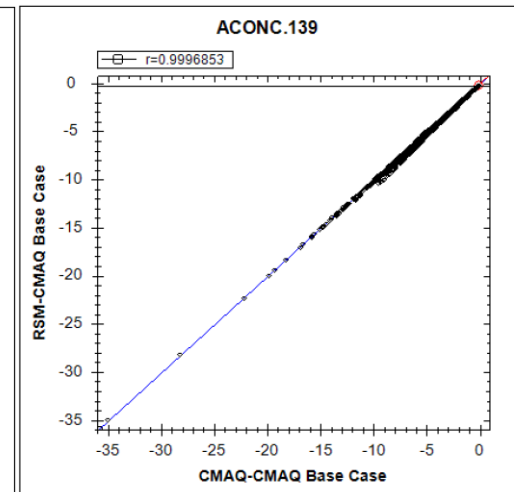
PM_{2.5} Response: RSM vs. CMAQ



All “Out-of-Sample” runs:
Normalized Mean Error



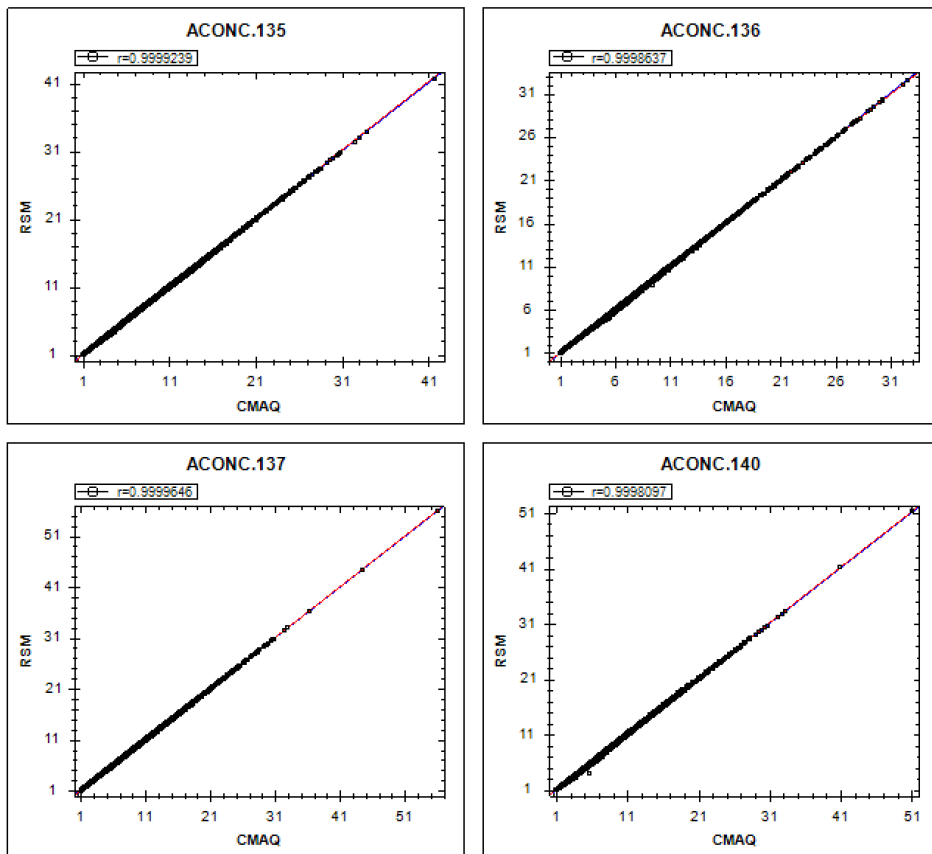
Predicted PM_{2.5} Concentration
(RSM vs. CMAQ)



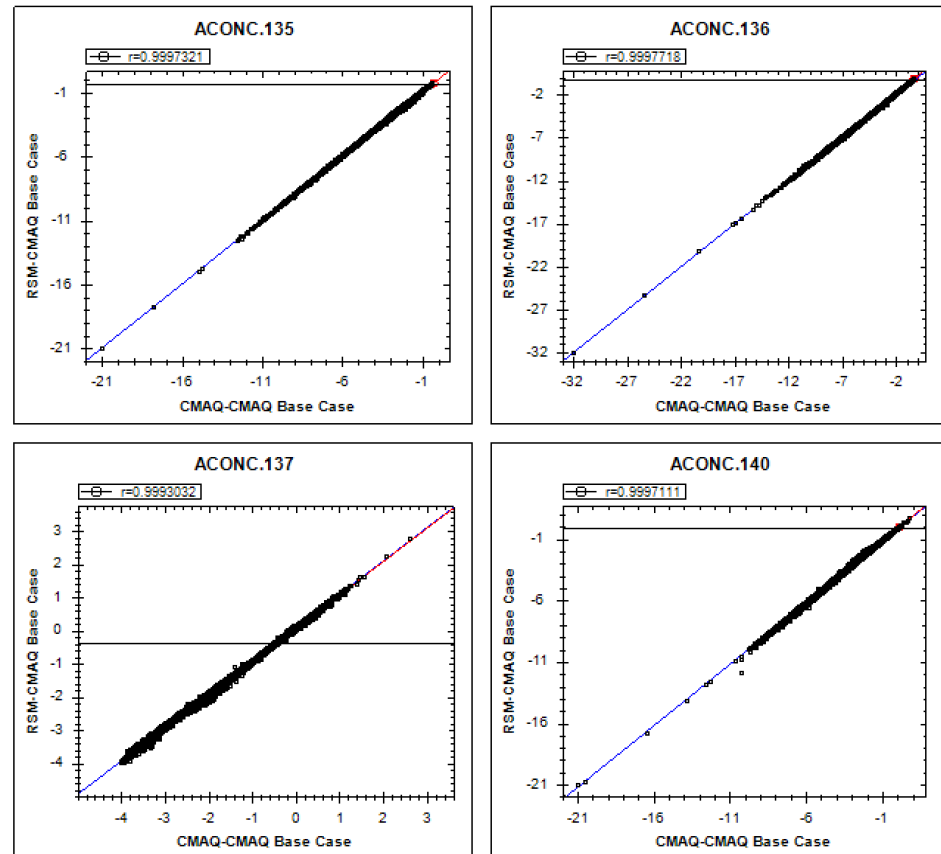
Predicted PM₅ Response
(RSM vs. CMAQ)

Out-of-Sample Validation: Concentration Comparison (Jan., PM_{2.5} monthly avg., US) Best 4

Predicted PM_{2.5} Conc. (RSM vs. CMAQ)

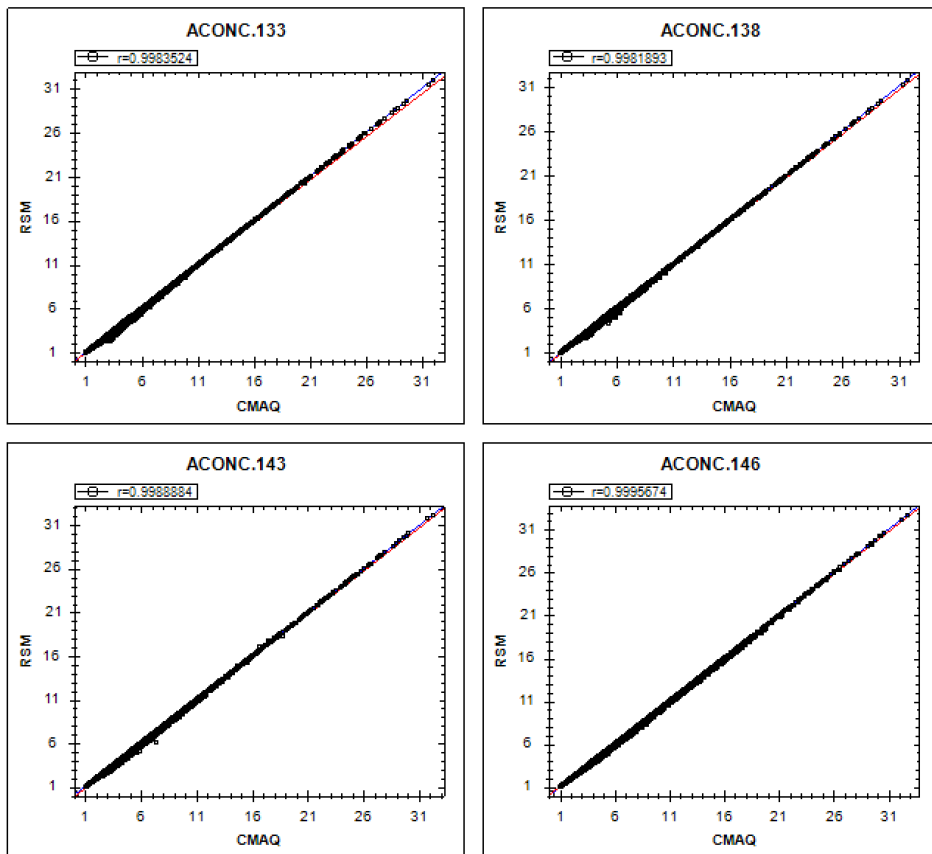


Predicted PM_{2.5} Responses (RSM-Base vs. CMAQ-Base)

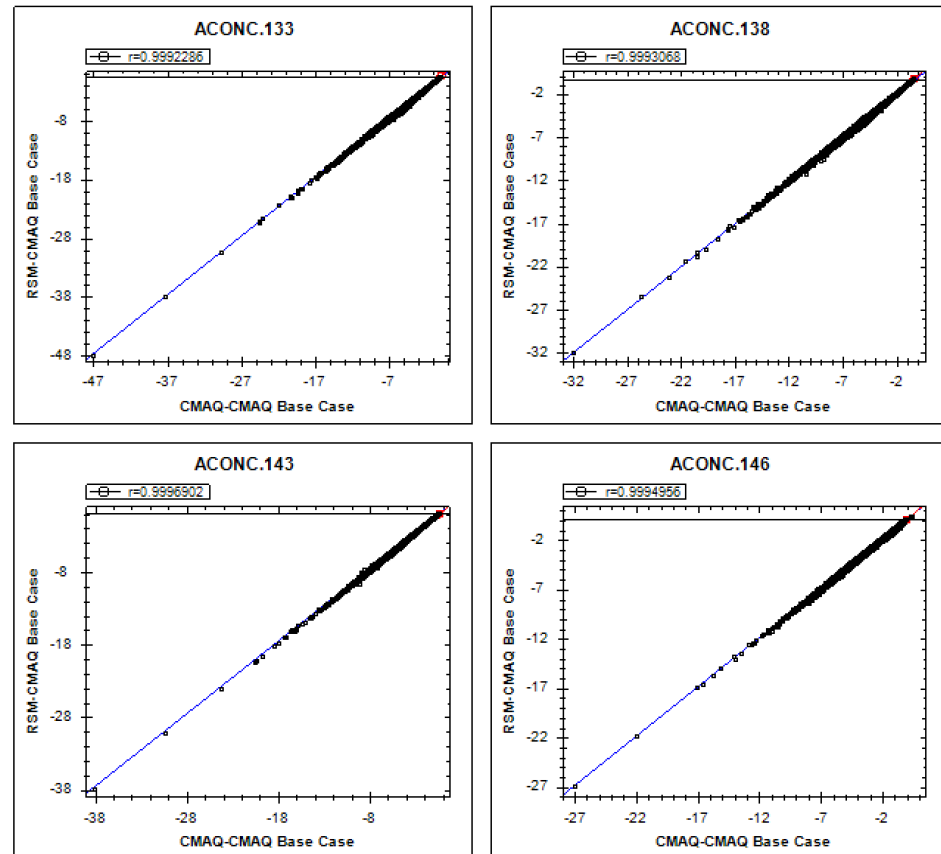


Out-of-Sample Validation: Concentration Comparison (Jan., PM_{2.5} monthly avg., US) Worst 4

Predicted PM_{2.5} Conc. (RSM vs. CMAQ)

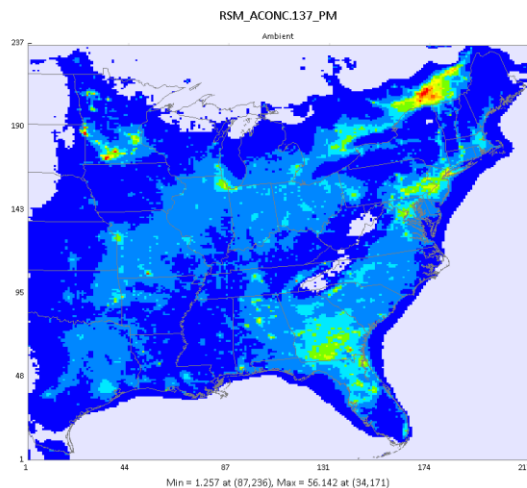


Predicted PM_{2.5} Responses (RSM-Base vs. CMAQ-Base)

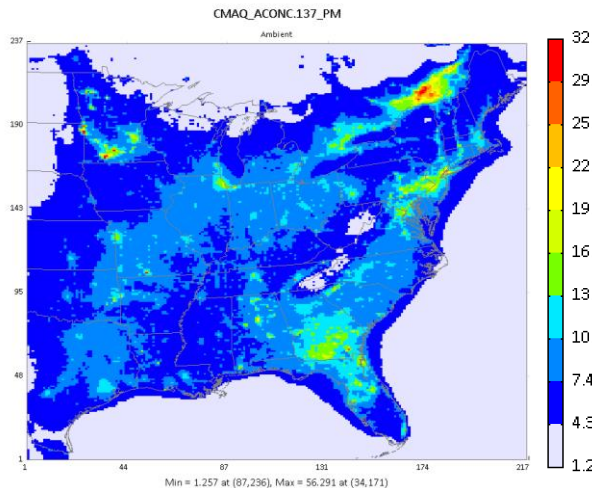


Out-of-Sample Validation: Predicted Concentrations (Jan., PM_{2.5} monthly avg., US) Best 1

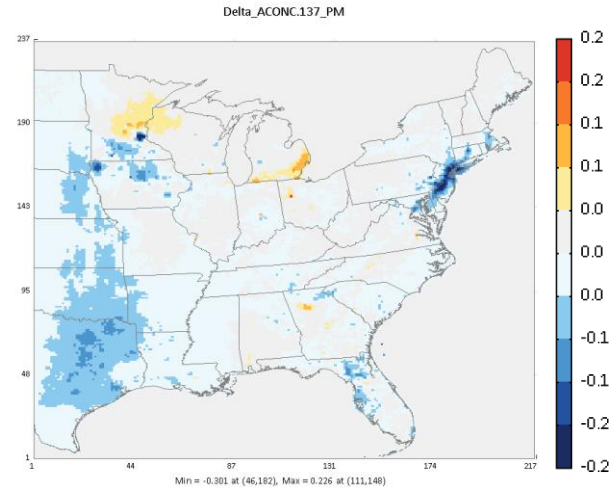
RSM



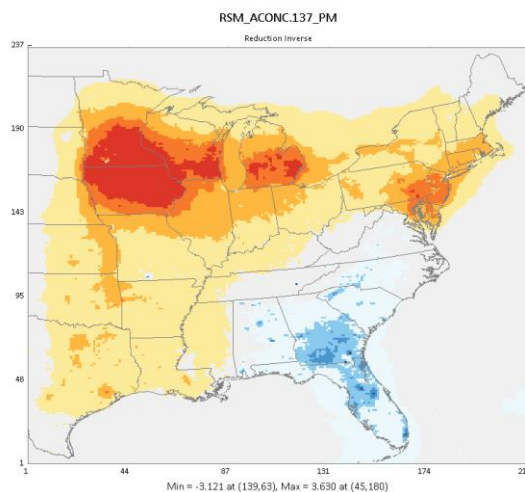
CMAQ



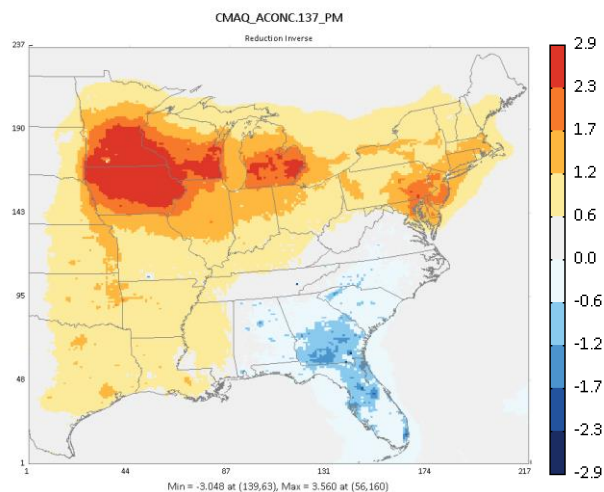
Delta



Base - RSM



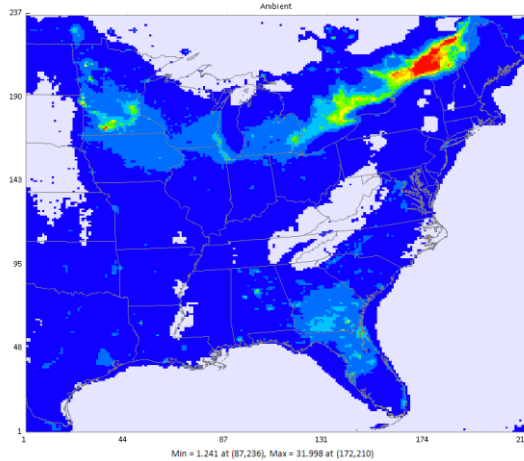
Base - CMAQ



Out-of-Sample Validation: Predicted Concentrations (Jan., PM_{2.5} monthly avg., US) Worst 1

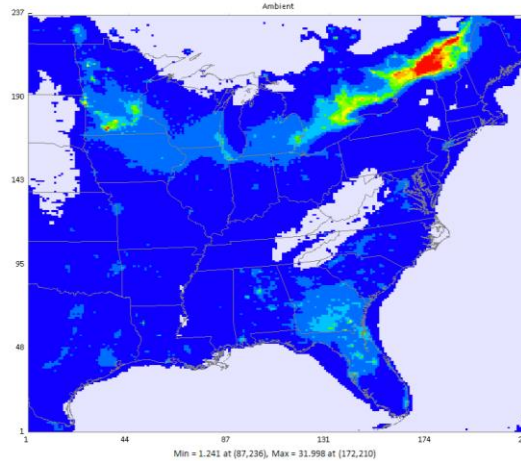
RSM

RSM_ACONC.138_PM



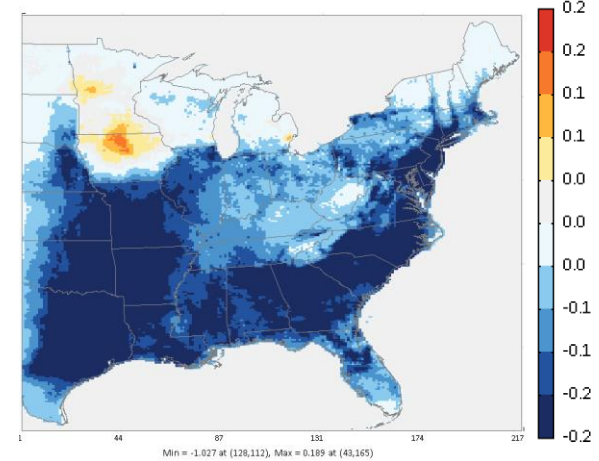
CMAQ

CMAQ_ACONC.138_PM



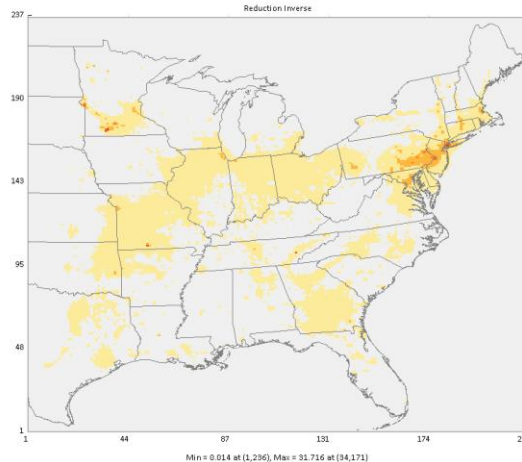
Delta

Delta_ACONC.138_PM



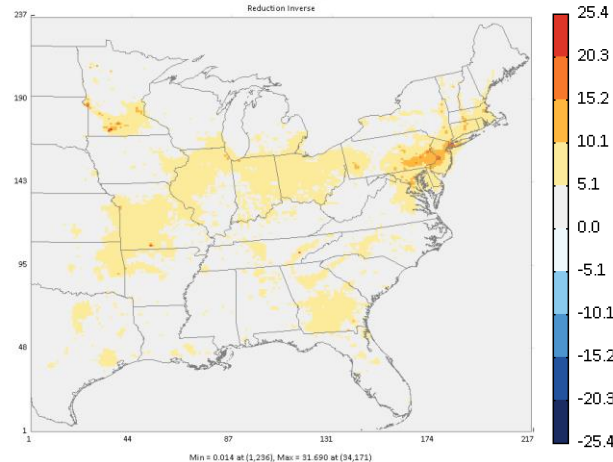
Base - RSM

RSM_ACONC.138_PM



Base - CMAQ

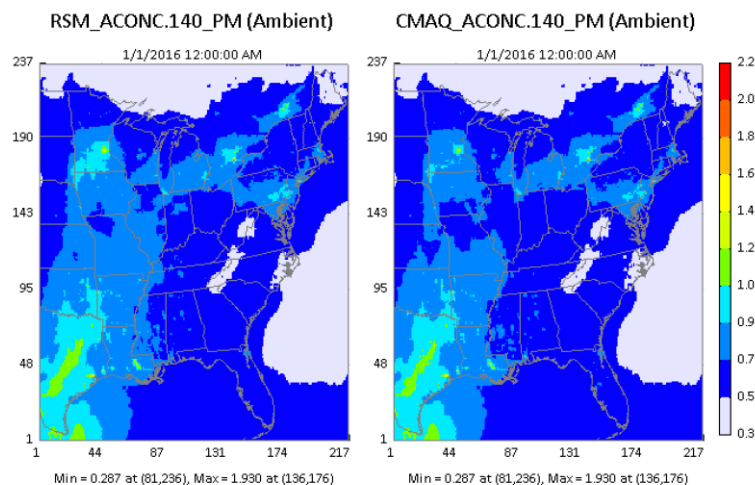
CMAQ_ACONC.138_PM



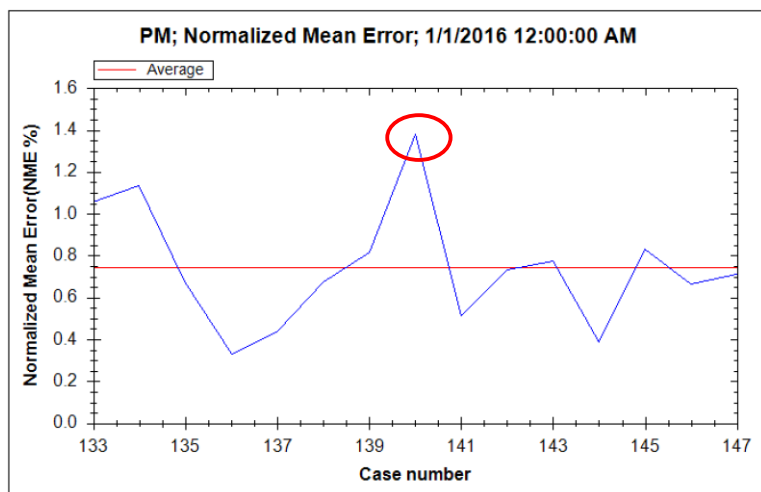
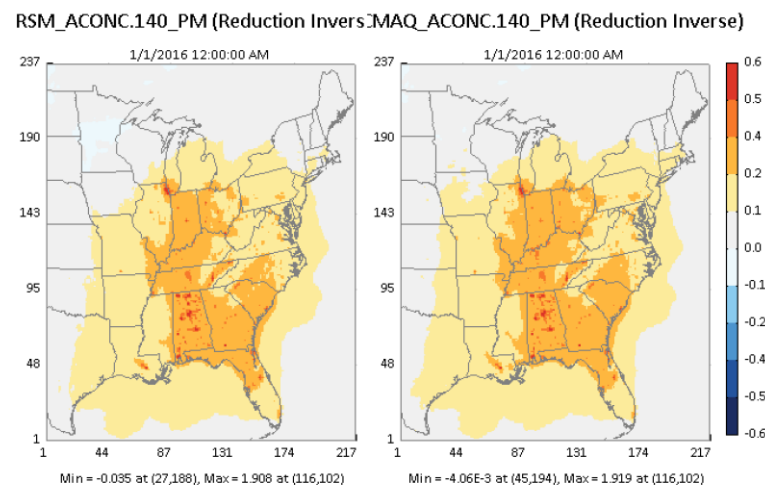
Jan., PM_SO₄ monthly avg., US

Out-of-Sample Validation: PM_{SO₄} Conc. & Responses (Jan., PM_{SO₄} monthly avg., US) Worst 1

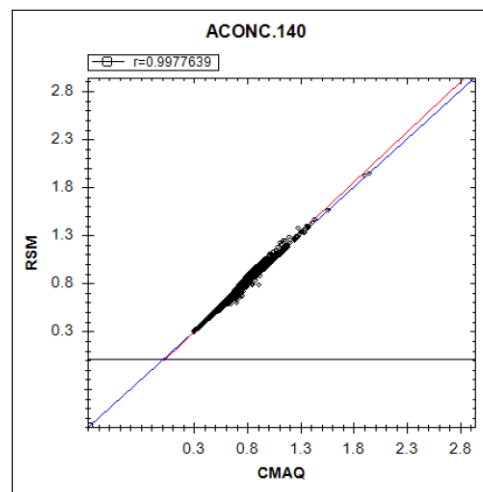
PM_{2.5} Conc: RSM vs. CMAQ



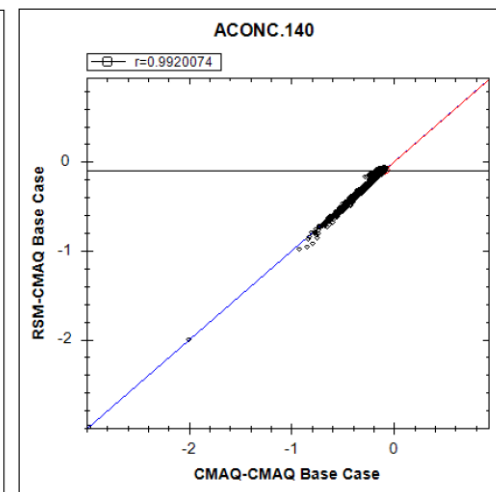
PM_{2.5} Response: RSM vs. CMAQ



All “Out-of-Sample” runs:
Normalized Mean Error



Predicted PM_{2.5} Concentration
(RSM vs. CMAQ)

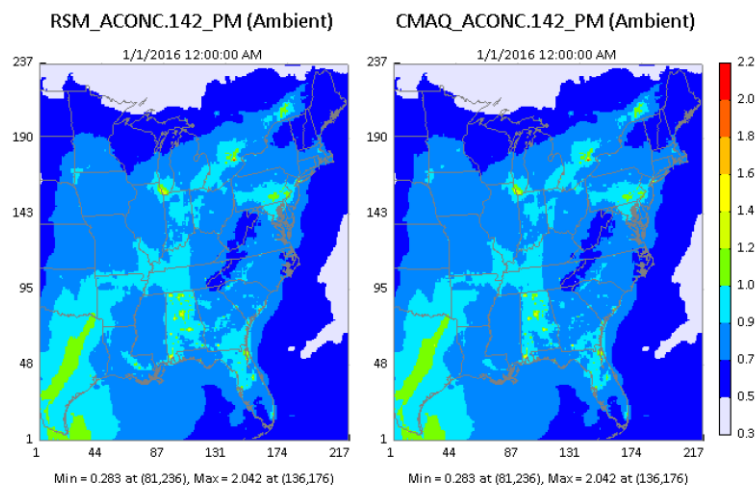


Predicted PM₅ Response
(RSM vs. CMAQ)

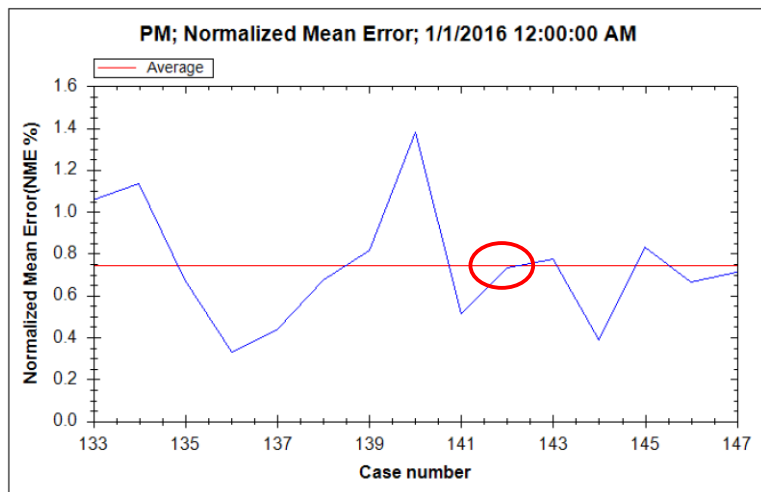
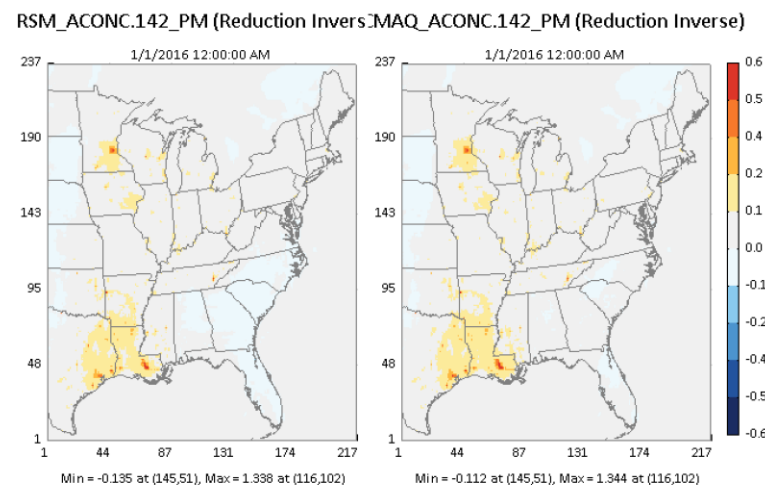
Out-of-Sample Validation: PM_{SO₄} Conc. & Responses

(Jan., PM_{SO₄} monthly avg., US) Typical 1

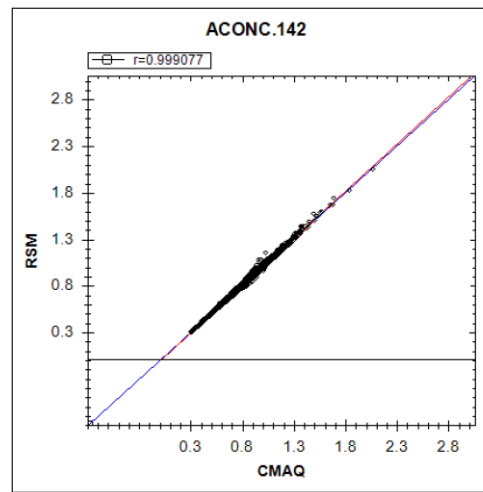
PM_{2.5} Conc: RSM vs. CMAQ



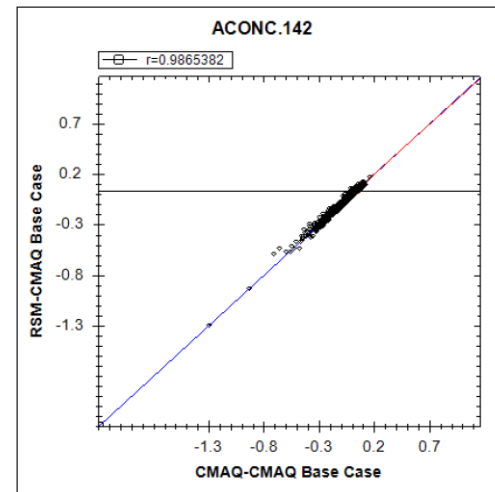
PM_{2.5} Response: RSM vs. CMAQ



All “Out-of-Sample” runs:
Normalized Mean Error



Predicted PM_{2.5} Concentration (RSM vs. CMAQ)

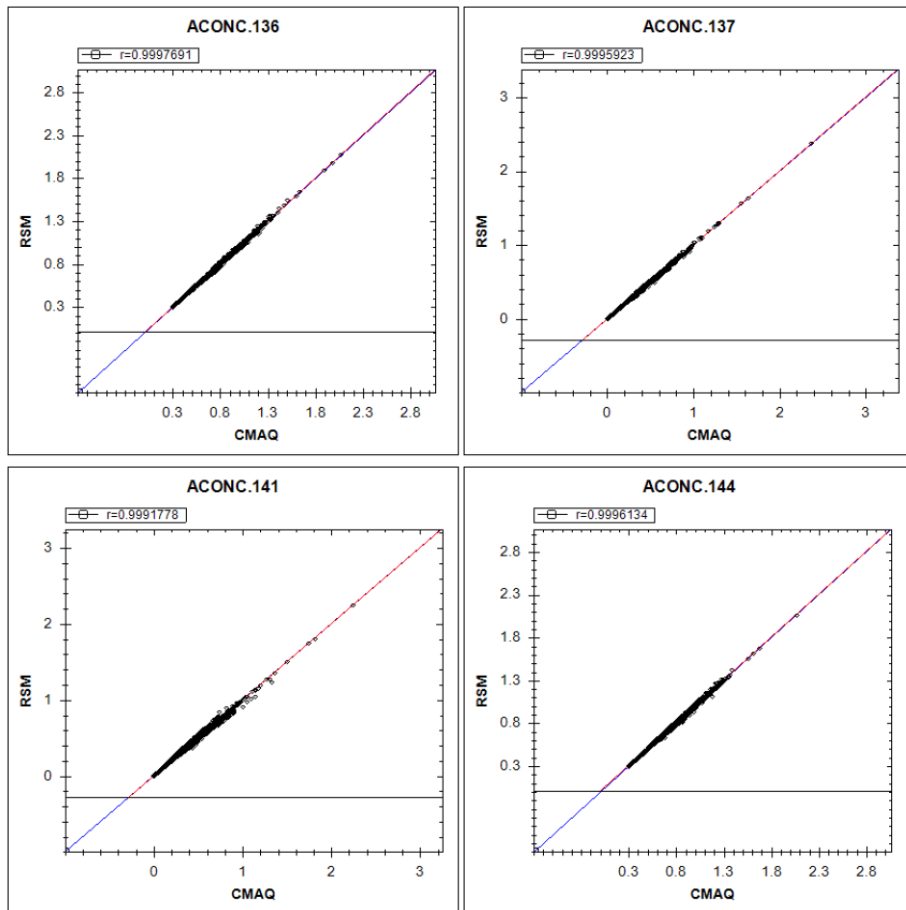


Predicted PM₅ Response (RSM vs. CMAQ)

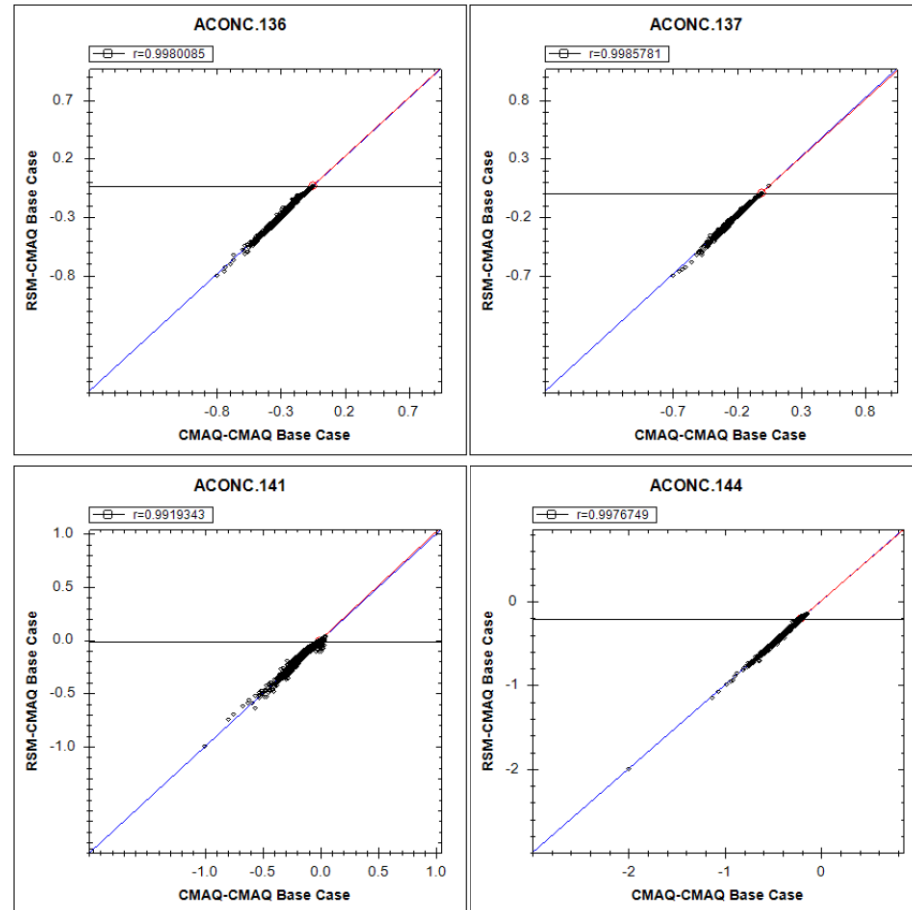
Out-of-Sample Validation: Concentration Comparison

(Jan., PM_{SO₄} monthly avg., US) Best 4

Predicted PM_{2.5} Conc. (RSM vs. CMAQ)

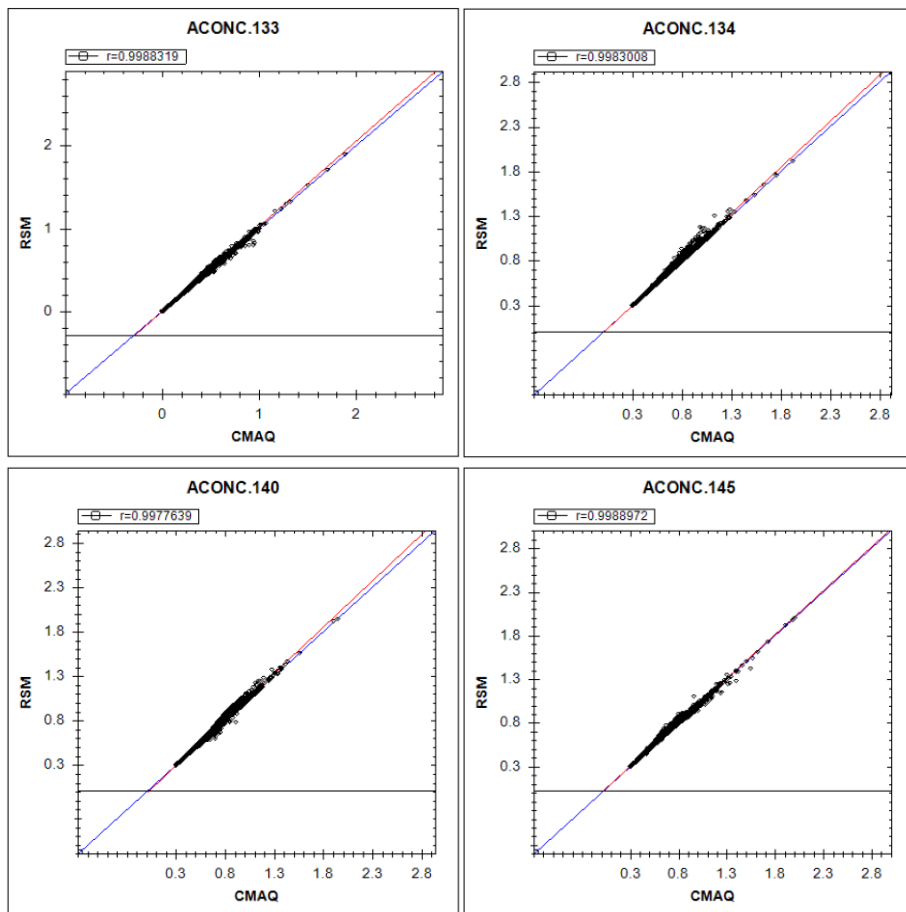


Predicted PM_{2.5} Responses (RSM-Base vs. CMAQ-Base)

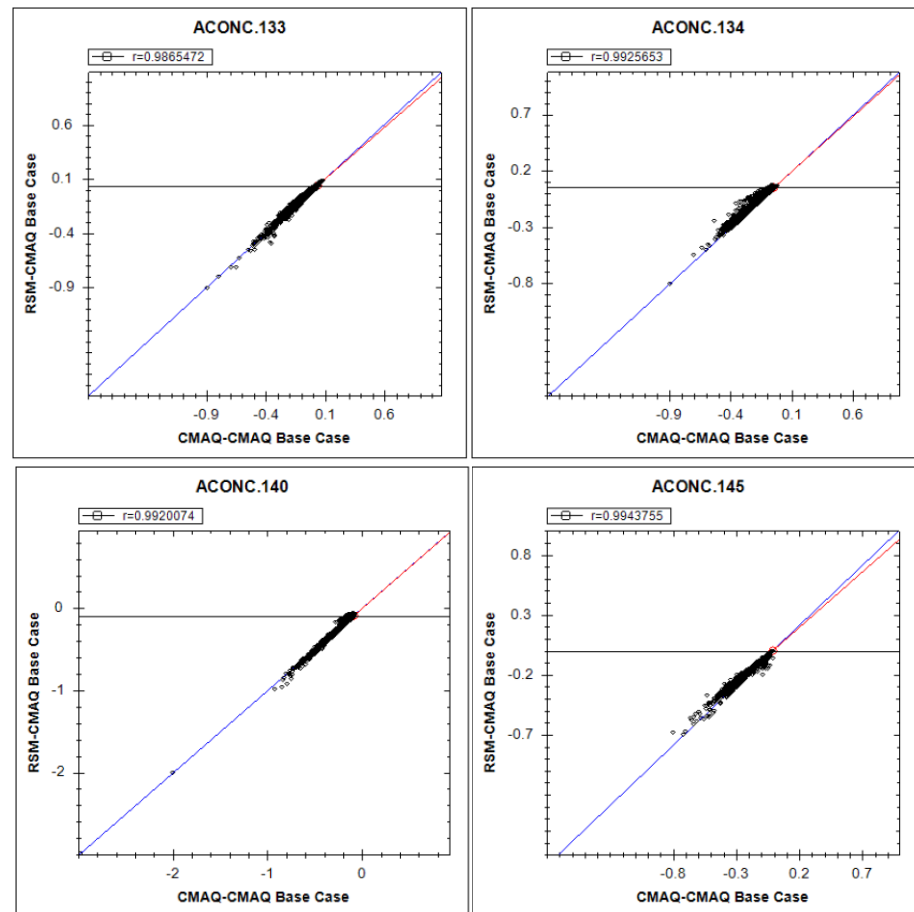


Out-of-Sample Validation: Concentration Comparison (Jan., PM_{SO₄} monthly avg., US) Worst 4

Predicted PM_{2.5} Conc. (RSM vs. CMAQ)



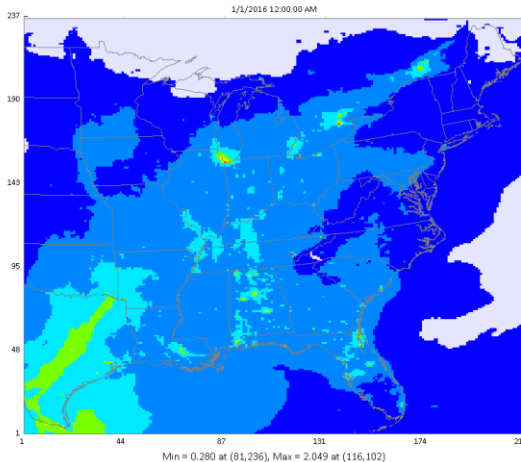
Predicted PM_{2.5} Responses (RSM-Base vs. CMAQ-Base)



Out-of-Sample Validation: Predicted Concentrations (Jan., PM_{SO₄} monthly avg., US) Best 1

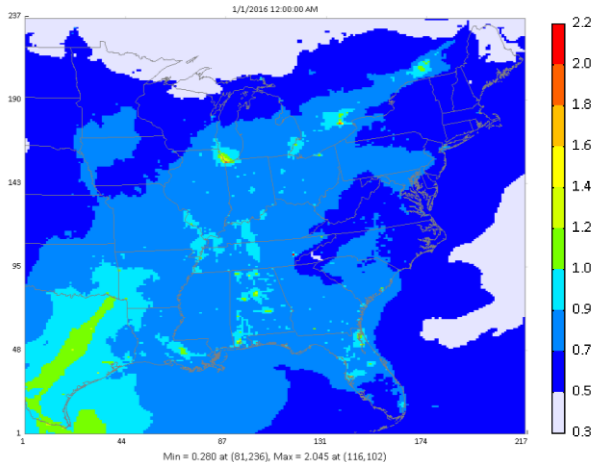
RSM

RSM_ACONC.136_PM (Ambient)



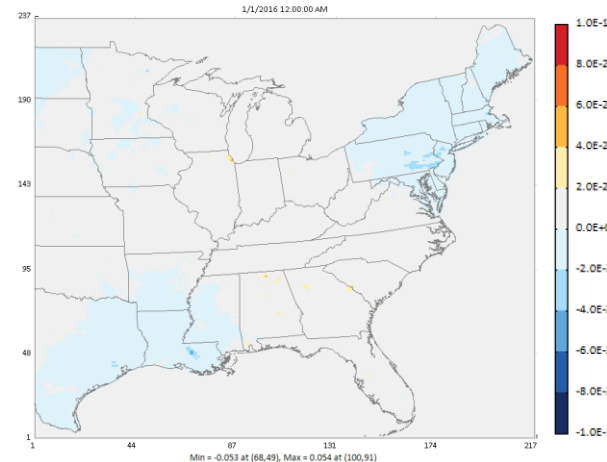
CMAQ

CMAQ_ACONC.136_PM (Ambient)



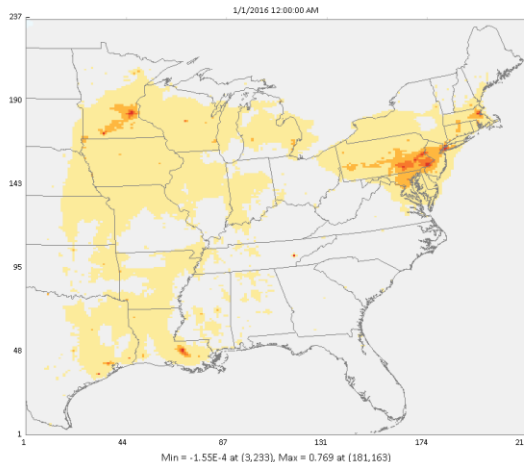
Delta

Delta_ACONC.136_PM (Reduction Inverse)



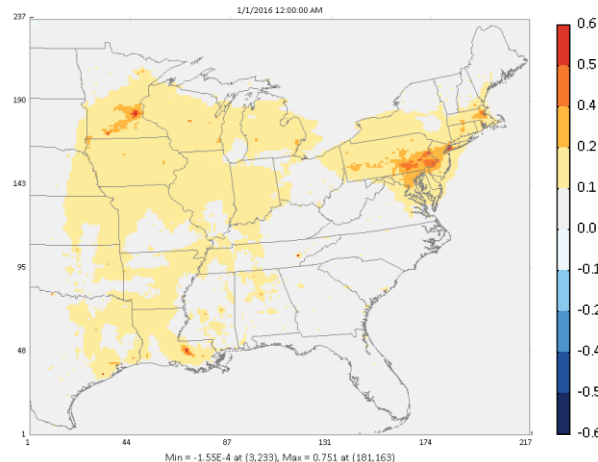
Base - RSM

RSM_ACONC.136_PM (Reduction Inverse)



Base - CMAQ

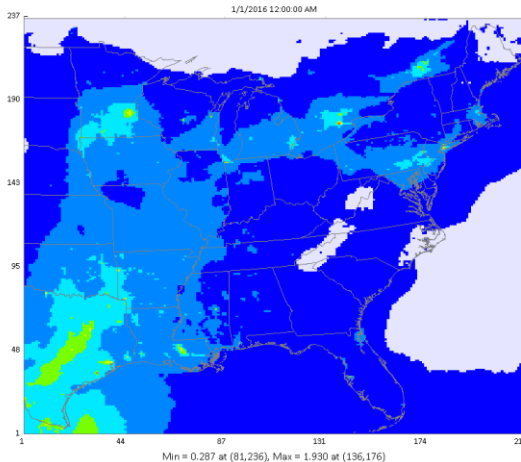
CMAQ_ACONC.136_PM (Reduction Inverse)



Out-of-Sample Validation: Predicted Concentrations (Jan., PM_{SO₄} monthly avg., US) Worst 1

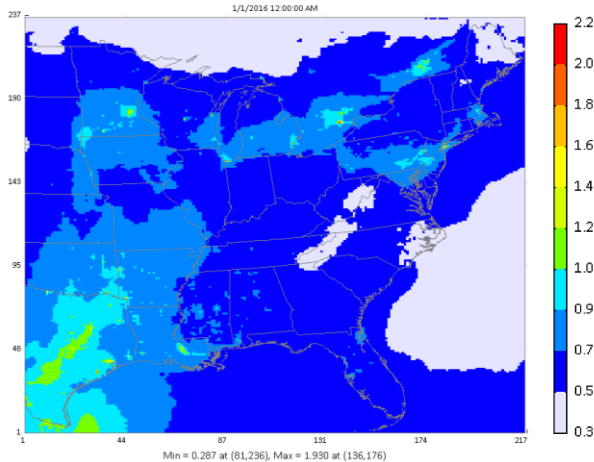
RSM

RSM_ACONC.140_PM (Ambient)



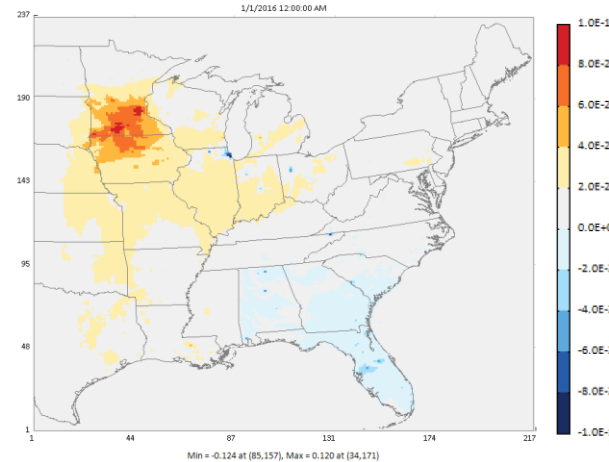
CMAQ

CMAQ_ACONC.140_PM (Ambient)



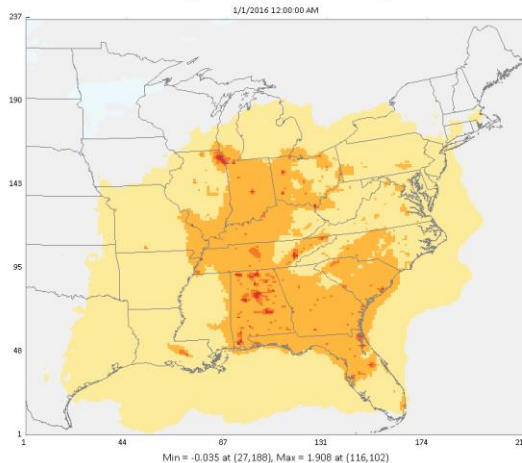
Delta

Delta_ACONC.140_PM (Reduction Inverse)



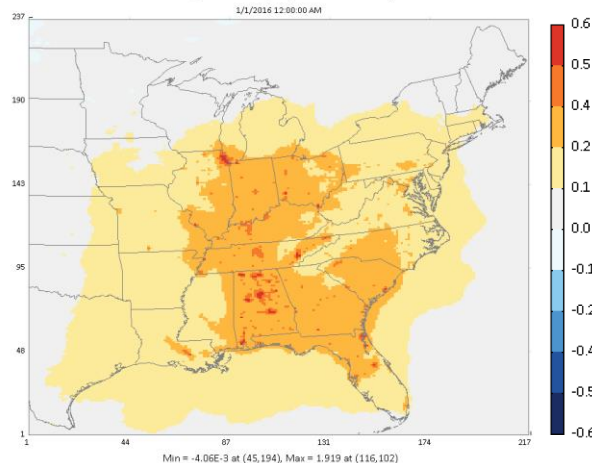
Base - RSM

RSM_ACONC.140_PM (Reduction Inverse)



Base - CMAQ

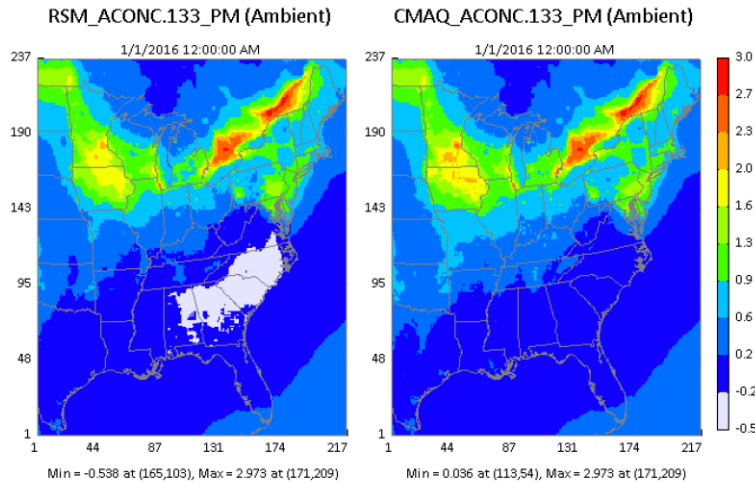
CMAQ_ACONC.140_PM (Reduction Inverse)



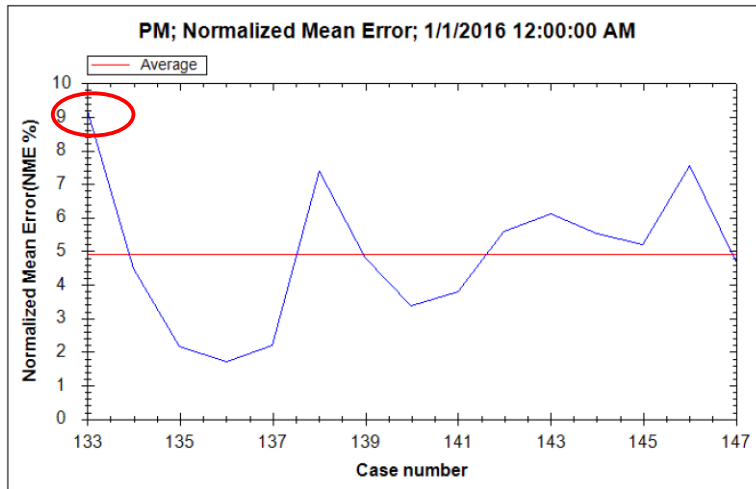
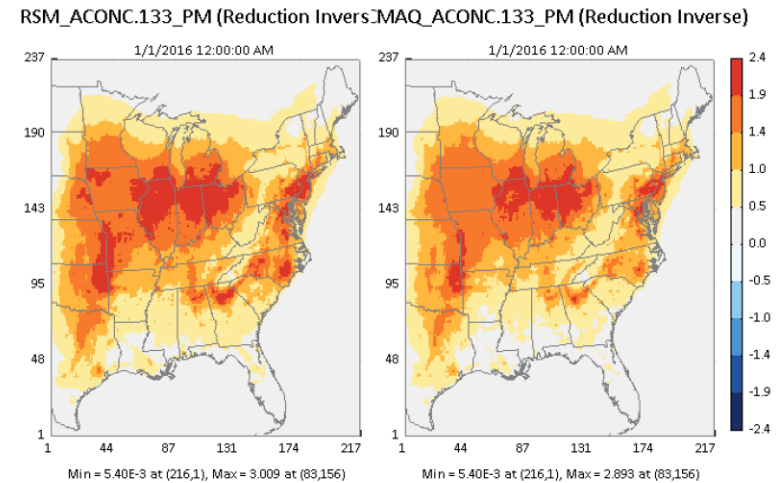
Jan., PM_{NO₃} monthly avg., US

Out-of-Sample Validation: PM_{NO₃} Conc. & Responses (Jan., PM_{NO₃} monthly avg., US) Worst 1

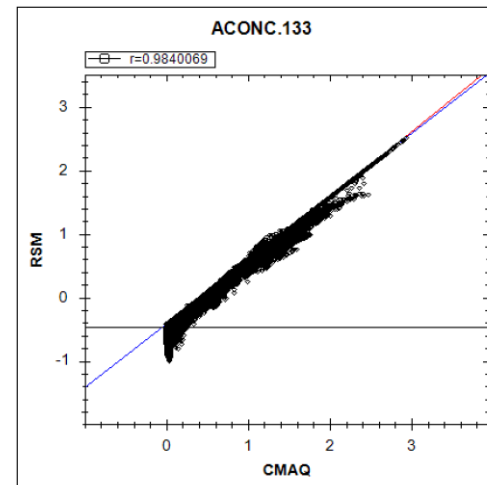
PM_{2.5} Conc: RSM vs. CMAQ



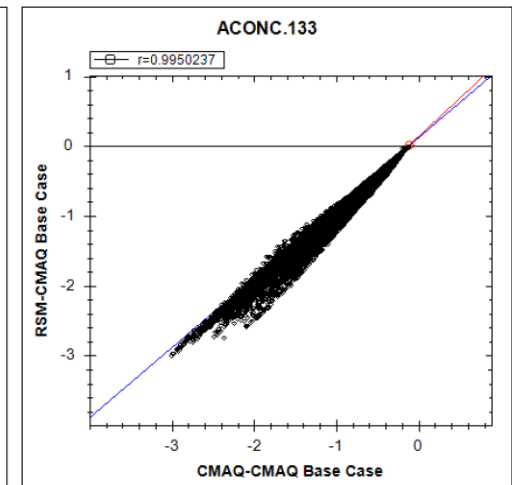
PM_{2.5} Response: RSM vs. CMAQ



All “Out-of-Sample” runs:
Normalized Mean Error



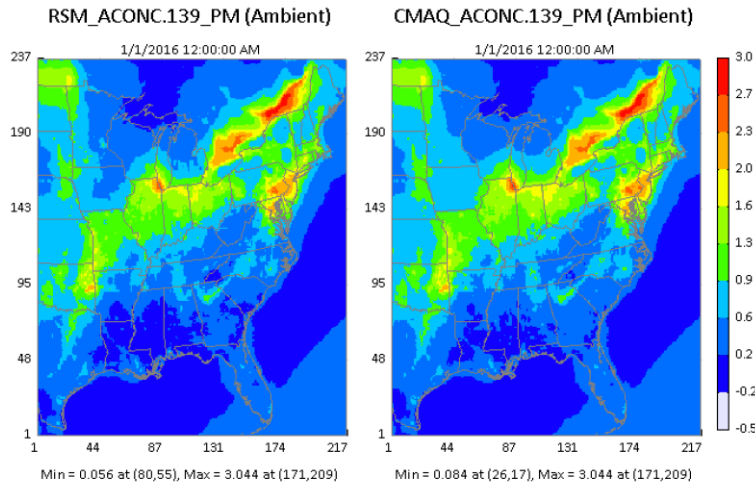
Predicted PM_{2.5} Concentration
(RSM vs. CMAQ)



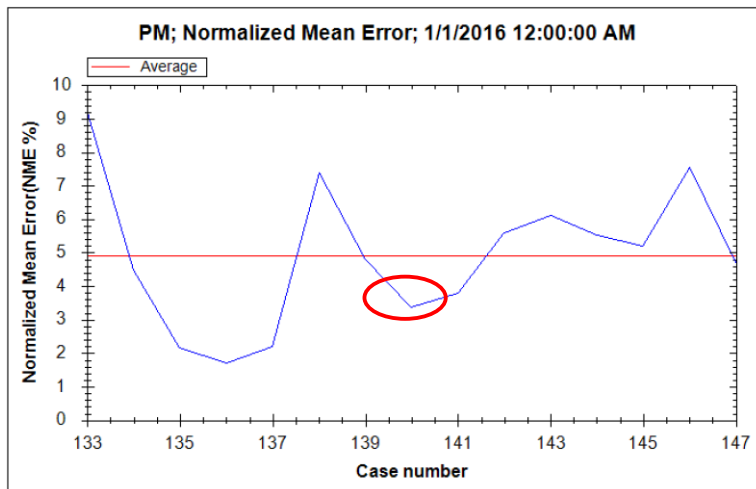
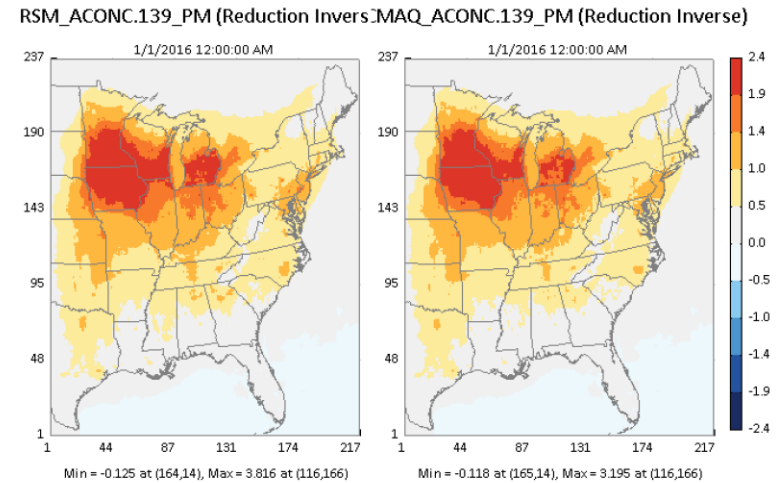
Predicted PM₅ Response
(RSM vs. CMAQ)

Out-of-Sample Validation: PM_{NO₃} Conc. & Responses (Jan., PM_{NO₃} monthly avg., US) Typical 1

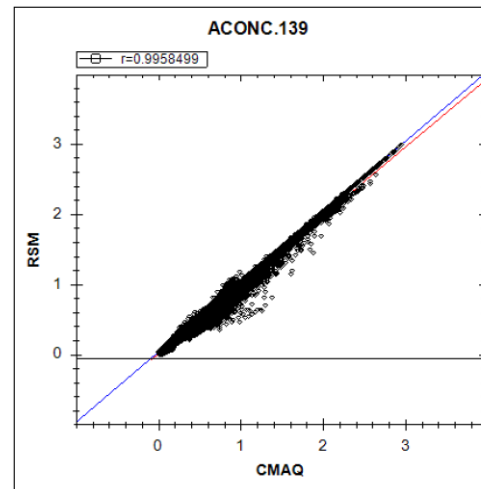
PM_{2.5} Conc: RSM vs. CMAQ



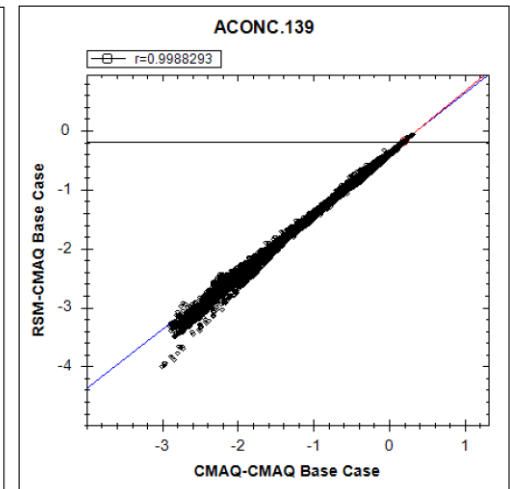
PM_{2.5} Response: RSM vs. CMAQ



All “Out-of-Sample” runs:
Normalized Mean Error



Predicted PM_{2.5} Concentration
(RSM vs. CMAQ)

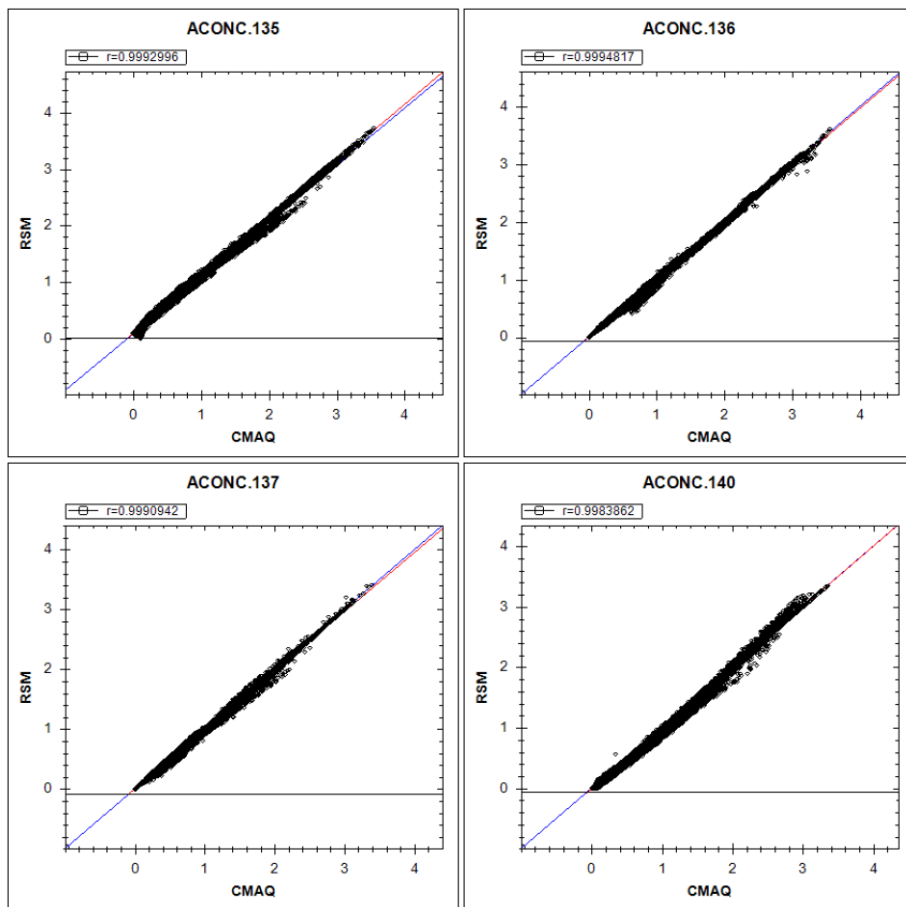


Predicted PM₅ Response
(RSM vs. CMAQ)

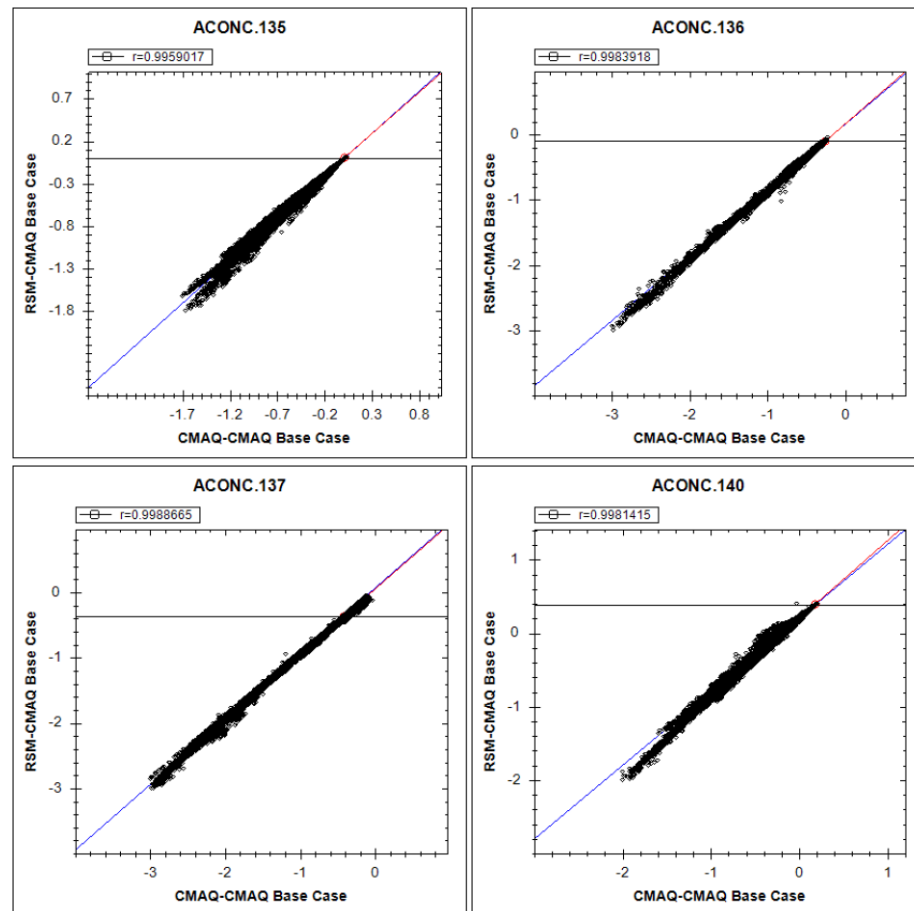
Out-of-Sample Validation: Concentration Comparison

(Jan., PM_{NO₃} monthly avg., US) Best 4

Predicted PM_{2.5} Conc. (RSM vs. CMAQ)

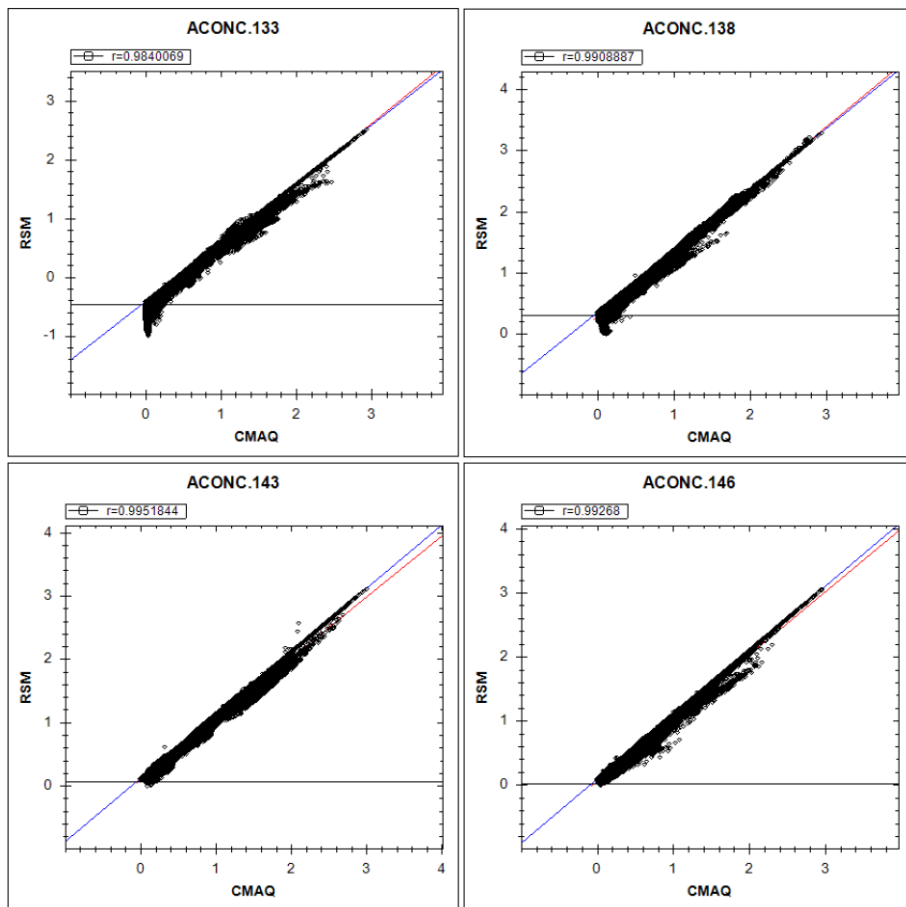


Predicted PM_{2.5} Responses (RSM-Base vs. CMAQ-Base)

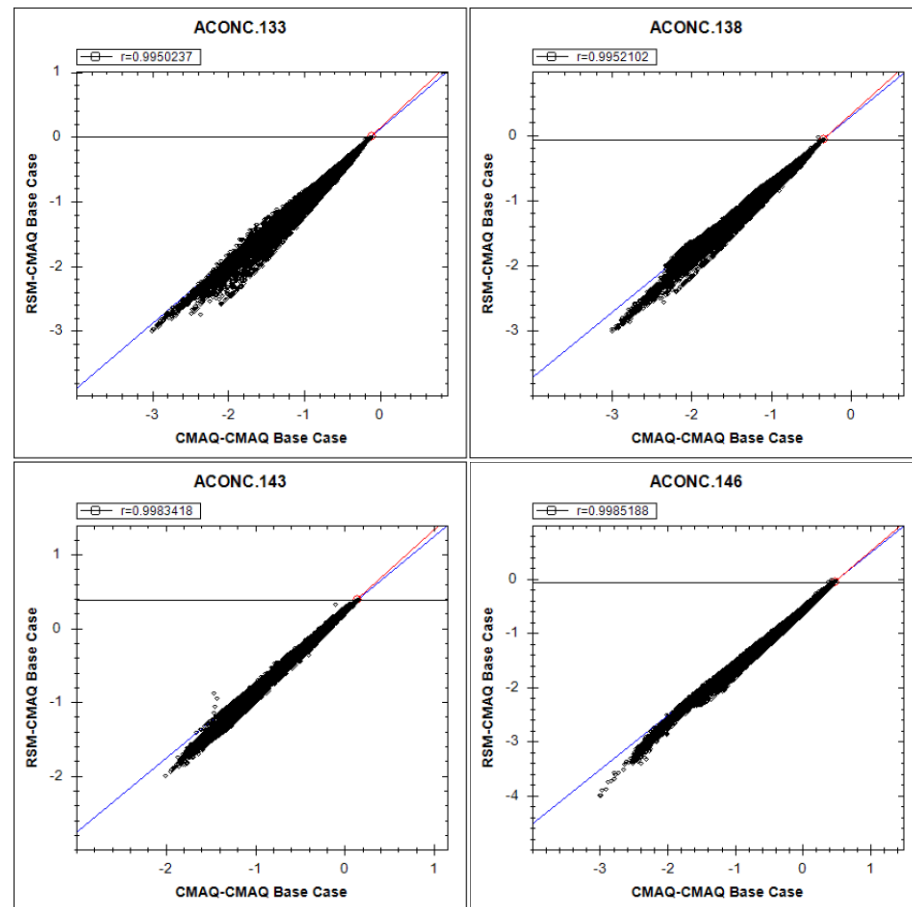


Out-of-Sample Validation: Concentration Comparison (Jan., PM_{NO₃} monthly avg., US) Worst 4

Predicted PM_{2.5} Conc. (RSM vs. CMAQ)



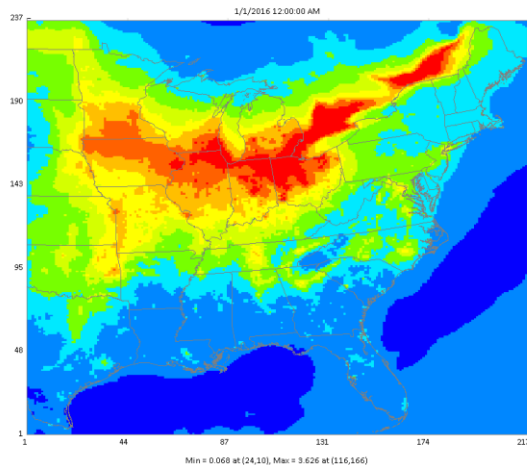
Predicted PM_{2.5} Responses (RSM-Base vs. CMAQ-Base)



Out-of-Sample Validation: Predicted Concentrations (Jan., PM_{NO₃} monthly avg., US) Best 1

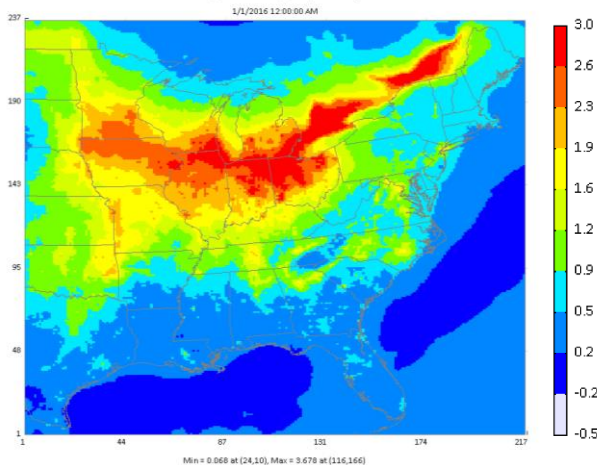
RSM

CMAQ_ACONC.136_PM (Ambient)



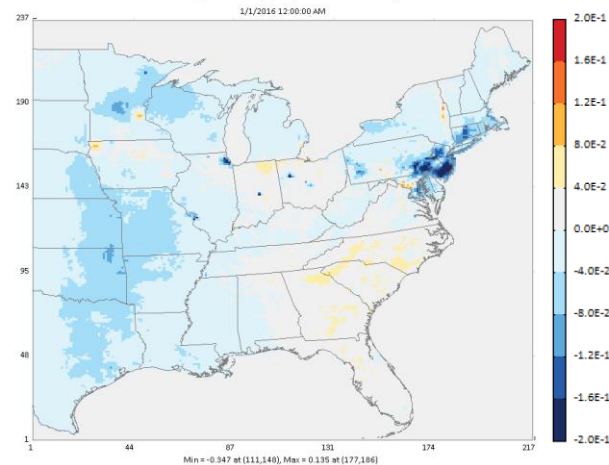
CMAQ

RSM_ACONC.136_PM (Ambient)



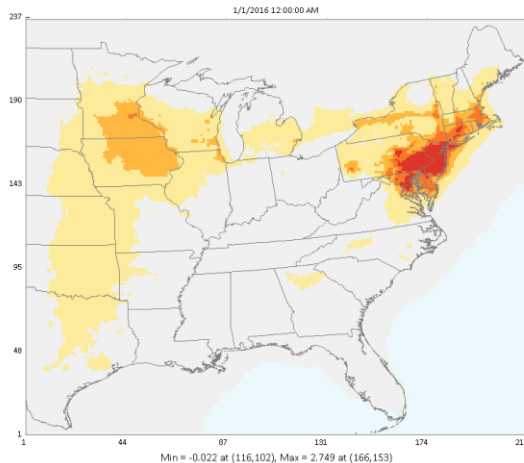
Delta

Delta_ACONC.136_PM (Reduction Inverse)



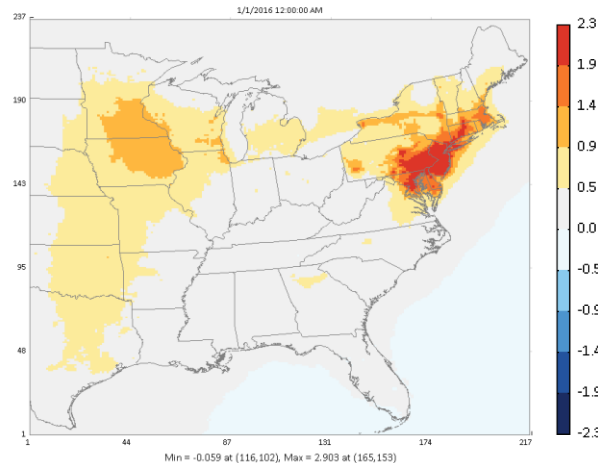
Base - RSM

CMAQ_ACONC.136_PM (Reduction Inverse)



Base - CMAQ

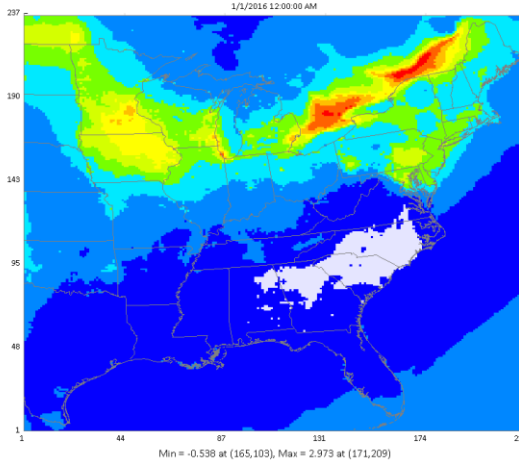
RSM_ACONC.136_PM (Reduction Inverse)



Out-of-Sample Validation: Predicted Concentrations (Jan., PM_{NO₃} monthly avg., US) Worst 1

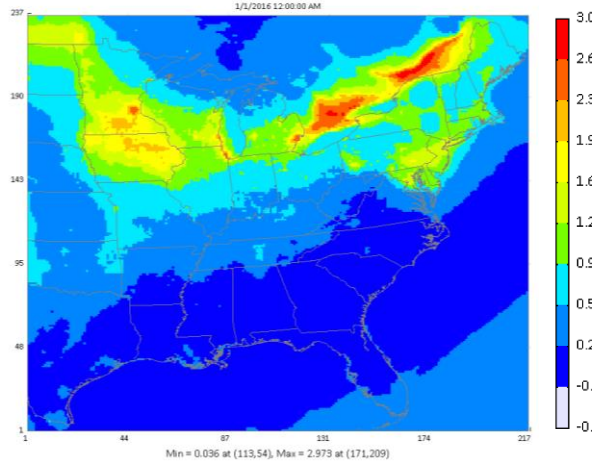
RSM

RSM_ACONC.133_PM (Ambient)



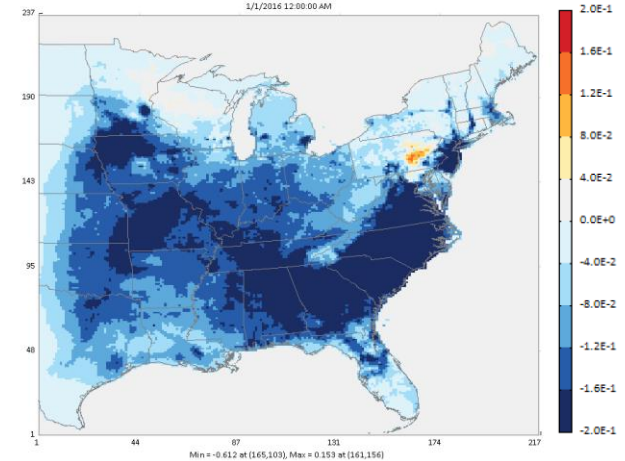
CMAQ

CMAQ_ACONC.133_PM (Ambient)



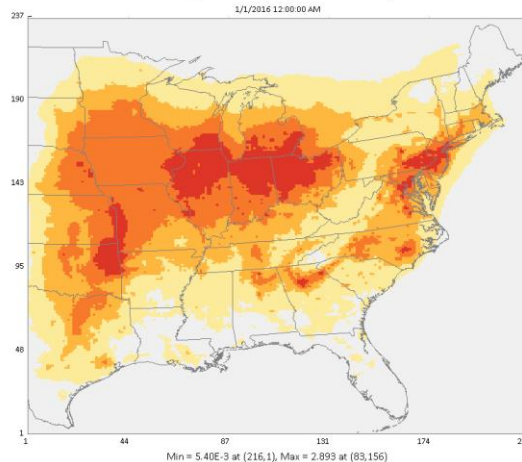
Delta

Delta_ACONC.133_PM (Reduction Inverse)



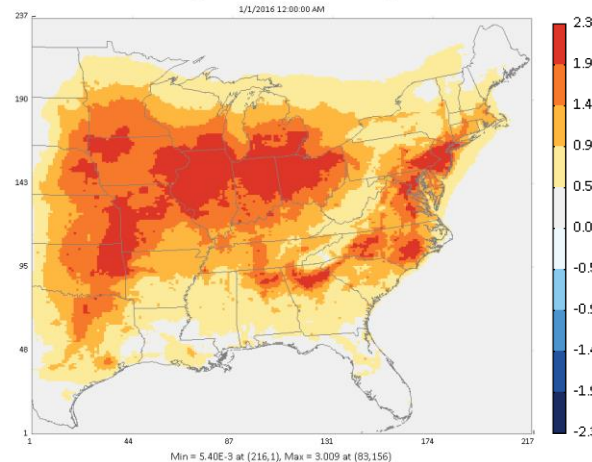
Base - RSM

CMAQ_ACONC.133_PM (Reduction Inverse)



Base - CMAQ

RSM_ACONC.133_PM (Reduction Inverse)

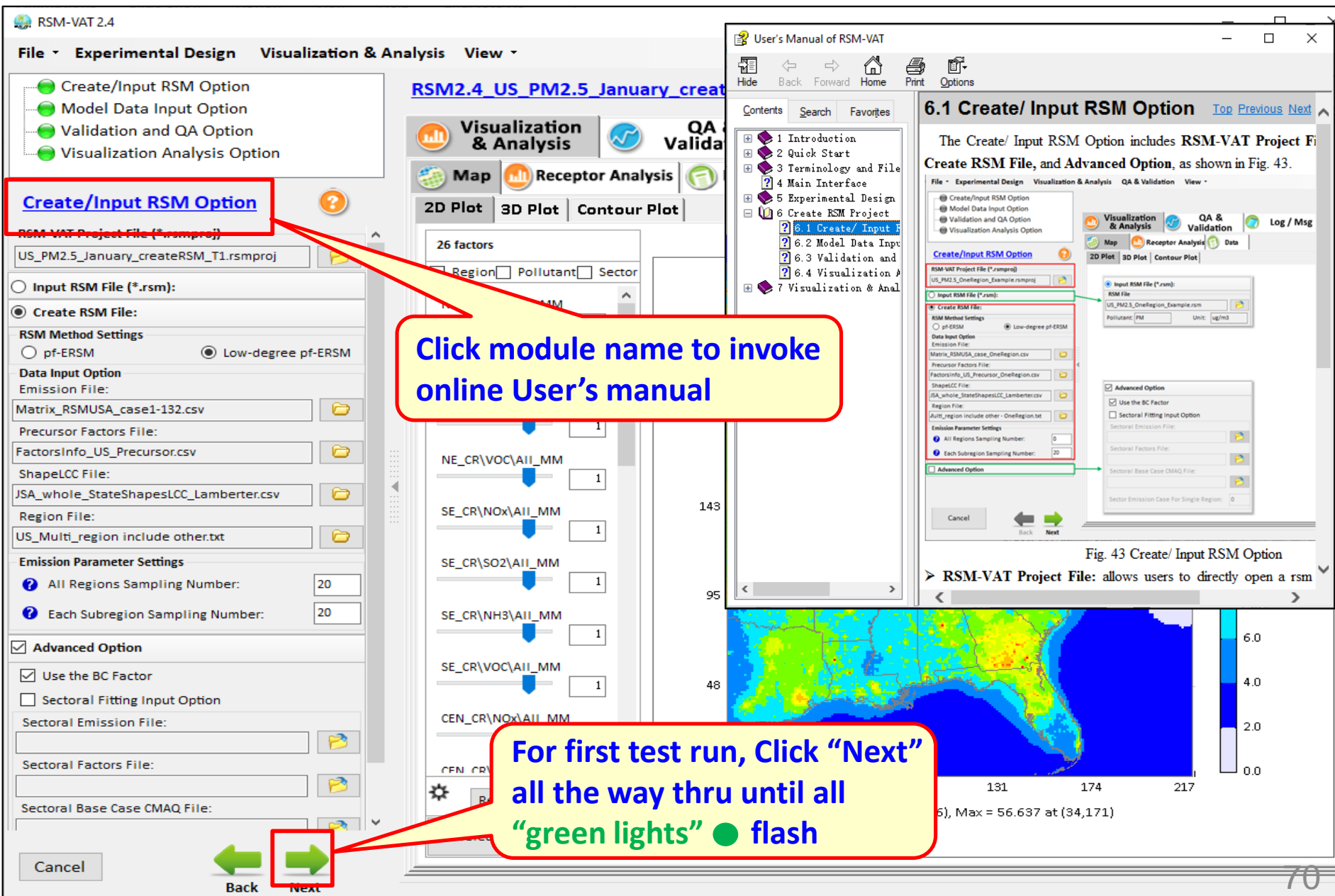


Appendix C:

RSM-VAT Demo & Tutorial:

EUS 12-km Case using "pf-RSM"

RSM-VAT: Launching Page & User's Manual



RSM-VAT 2.4

File Experimental Design Visualization & Analysis View

- Create/ Input RSM Option
- Model Data Input Option
- Validation and QA Option
- Visualization Analysis Option

Create/ Input RSM Option

RSM-VAT Project File (*.rsmproj)

US_PM2.5_January_createRSM_T1.rsmproj

Input RSM File (*.rsm):

Create RSM File:

RSM Method Settings

pf-ERSM Low-degree pf-ERSM

Data Input Option

Emission File:

Matrix_RSMUSA_case1-132.csv

Precursor Factors File:

FactorsInfo_US_Precursor.csv

ShapeLCC File:

JSA_whole_StateShapesLCC_Lamberter.csv

Region File:

US_Multi_region include other.txt

Emission Parameter Settings

All Regions Sampling Number: 20

Each Subregion Sampling Number: 20

Advanced Option

Use the BC Factor

Sectoral Fitting Input Option

Sectoral Emission File:

Sectoral Factors File:

Sectoral Base Case CMAQ File:

Cancel Back Next

User's Manual of RSM-VAT

Hide Back Forward Home Print Options

Contents Search Favorites

- 1 Introduction
- 2 Quick Start
- 3 Terminology and File
- 4 Main Interface
- 5 Experimental Design
- 6 Create RSM Project
- 6.1 Create/ Input RSM Option
- 6.2 Model Data Input
- 6.3 Validation and QA
- 6.4 Visualization & Analysis
- 7 Visualization & Analysis

6.1 Create/ Input RSM Option Top Previous Next

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

File Experimental Design Visualization & Analysis QA Validation View

Visualization & Analysis QA Validation Log / Msg

Map Receptor Analysis Data

2D Plot 3D Plot Contour Plot

26 factors

Region Pollutant Sector

NE_CR\VOC\All_MM 1

SE_CR\NOx\All_MM 1

SE_CR\SO2\All_MM 1

SE_CR\NH3\All_MM 1

SE_CR\VOC\All_MM 1

CEN_CR\NOx\All_MM 1

CFN_CR\NOx\All_MM 1

143

95

48

6.0

4.0

2.0

0.0

131 174 217

6), Max = 56.637 at (34,171)

Fig. 43 Create/ Input RSM Option

RSM-VAT Project File: allows users to directly open a rsm

Cancel Back Next

Back Next

Click module name to invoke online User's manual

For first test run, Click "Next" all the way thru until all "green lights" flash

1. Create/Input RSM Option 2. Model Data Input Option 3. Validation & Q/A Option 4. Vis./Analysis Option

RSM-VAT 2.4

File Experimental Design Visualization

Create/Input RSM Option
Model Data Input Option
Validation and QA Option
Visualization Analysis Option

Create/Input RSM Option

RSM-VAT Project File (*.rsmproj)

Input RSM File (*.rsm):

Create RSM File:

RSM Method Settings
pf-ERSM
Low-degree pf-ERSM

Data Input Option
Emission File:
Matrix_RSMUSA_case1-132.csv
Precursor Factors File:
FactorsInfo_US_Precursor.csv
ShapeLCC File:
JSA_whole_StateShapesLCC_Lamberter.csv
Region File:
US_Multi_region include other.txt

Emission Parameter Settings
All Regions Sampling Number: 20
Each Subregion Sampling Number: 20

Advanced Option
Use the BC Factor
Sectoral Fitting Input Option
Sectoral Emission File:
Sectoral Factors File:
Sectoral Base Case CMAQ File:

Cancel Back Next

RSM-VAT 2.4

File Experimental Design Visualization

Create/Input RSM Option
Model Data Input Option
Validation and QA Option
Visualization Analysis Option

Model Data Input Option

Model Data Input Option

Base Case CMAQ File:
ACONC.1

Target Pollutant
PM: PM25_TOT Unit: ug/m3
O3: Unit:

Precursor Pollutant
NOx: NOx Unit: ppbv
NH3: NH3 Unit: ppbv
SO2: SO2 Unit: ppbv
VOC: VOC Unit: ppbC
POA: Unit:

Fitting Parameter Settings
Threads Count: 2

Scenario Plot
Select Cases
Selected Cases
ACONC.1
ACONC.2
ACONC.3
ACONC.4
ACONC.5
ACONC.6
ACONC.7
ACONC.8

Cancel Back Next

RSM-VAT 2.4

File Experimental Design Visualization

Create/Input RSM Option
Model Data Input Option
Validation and QA Option
Visualization Analysis Option

Validation and QA Option

Validation Types
Out of Sample Cross Validation

Out of Sample Input Option
Emission File for Out of Sample:
r_RSMUSA_case133-152_out_of_sample.csv

Cross Validation Input Option
With Cross Validation File
Without Cross Validation File
Emission File for Cross Validation:

Other Settings:
Start Row: 1 End Row: 236
Start Col: 1 End Col: 216
Start Case: 1 End Case: 132

Cancel Back Next

RSM-VAT 2.4

File Experimental Design Visualization

Create/Input RSM Option
Model Data Input Option
Validation and QA Option
Visualization Analysis Option

Visualization Analysis Option

Receptor File
Receptor Region File
US_Multi_Monitor.txt

Plot Types
Contour Plot

Contour Plot Settings:
Receptor Region: A NE_CR
Current View: Ambient

Factors
Min: 0 Max: 1.2 Equal portions: 6

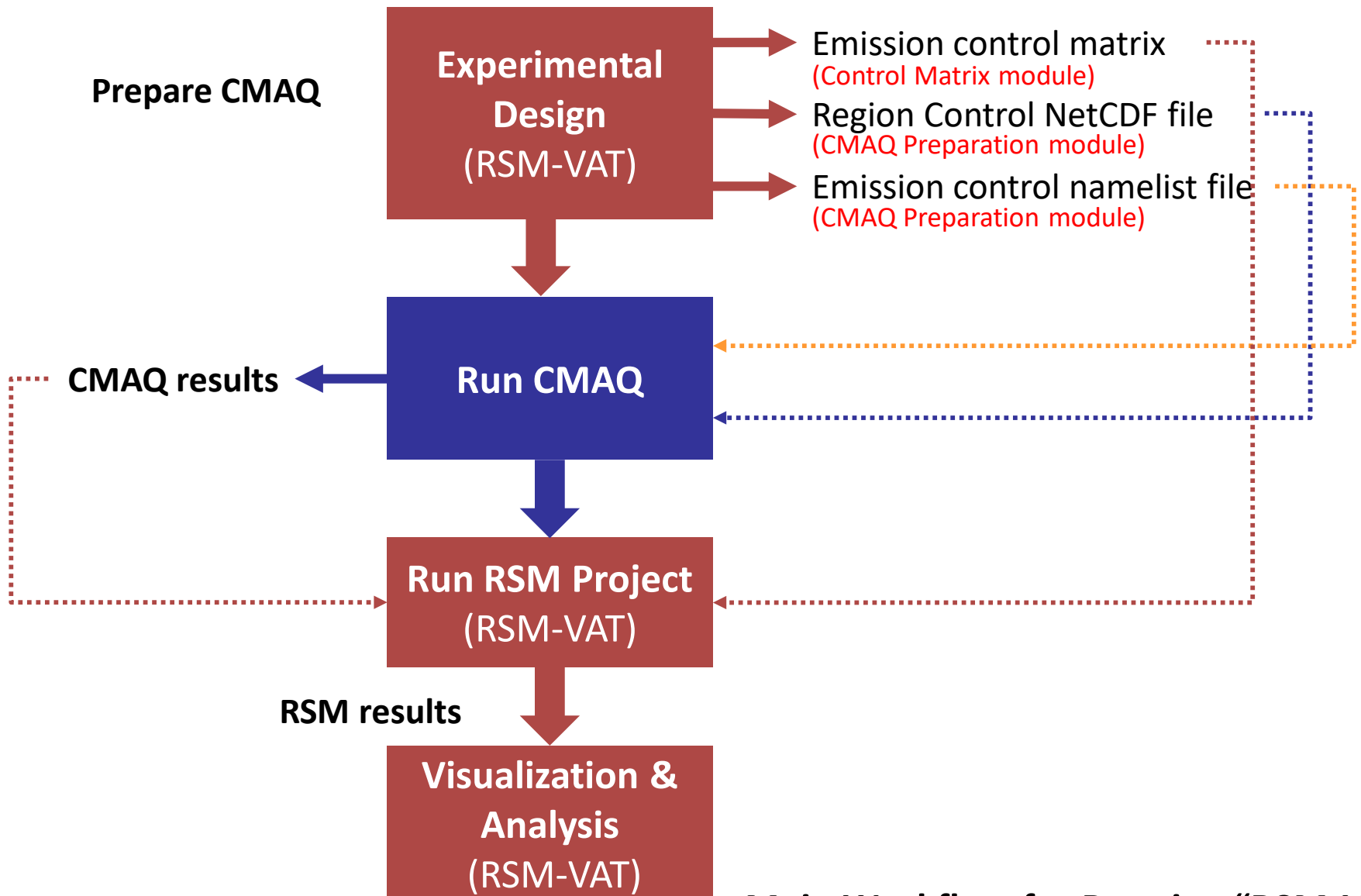
X Axis
X Axis Title: Select X Factors

Y Axis
Y Axis Title: Select Y Factors

Cancel Back Next

Running RSM-VAT to create RSM

Workflow to Create RSM in “RSM-VAT”



Main Workflow for Running “RSM-VAT”

Experimental Design

Running “Single Region” RSM

Note: *Default RSM case is “5 Climate Regions” in RSM-VAT*

RSM-VAT: Experimental Design Module

RSM-VAT 2.4

File **Experimental Design** Visualization & Analysis View

RSM2.4 US_PM2.5 January_createRSM_T1

Control Matrix CMAQ Preparation Log / Msg

☐ Create Region Control NetCDF File
☒ Merge/Subtract Region Operation
☐ Export Emission Control Namelist File

Merge/Subtract Region Operation Setting

Load Region Control NetCDF File
US_EXAMPLE.ncf

☒ Load Region Formula File(*.csv)
Region Operation Formula.csv

☒ Append Region with Formula
☐ Create Region with Formula

Add/Remove

CMAQ_Name	Expression
SE_CR-SC	"[1]SE_CR"- "[2]SC"
WV+KY	"[2]WV"+"[2]KY"
OH-ColumnOH	"[2]OH"- "[3]ColuOH"

Output Reg Ctrl NetCDF File

Reg Ctrl NetCDF EmissCtrl Namelist

☒ All Regions:
☒ CEN_CR
☒ NE_CR
☒ SE_CR
☒ UPMW_CR
☒ OTHER

the Selected Regions
FileName = US_EXAMPLE.ncf

236
189
142
95
48
1

1 44 87 130 173 216

Export Variables for Mapping File

Example Data

Default case for Experimental Design is for “5 Climate Region”, but you can run “One Region” case & “Sector” case with the following setup:

- Input Data for Experimental Design and RSM runs for OneRegion:
C:\Users\...\Documents\My RSM-VAT Files\Data\Example\US_RSM – OneRegion

Experimental Design projects (.expproj):

1. US_PM2.5_MultiRegion_Example.expproj
2. US_PM2.5_OneRegion_Example.expproj
3. US_PM2.5_Sector_OneRegion_Example.expproj

RSM projects (.rsmproj):

1. US_PM2.5_OneRegion_Example.rsmproj
2. US_PM2.5_Sector_OneRegion_Example.rsmproj

Note:

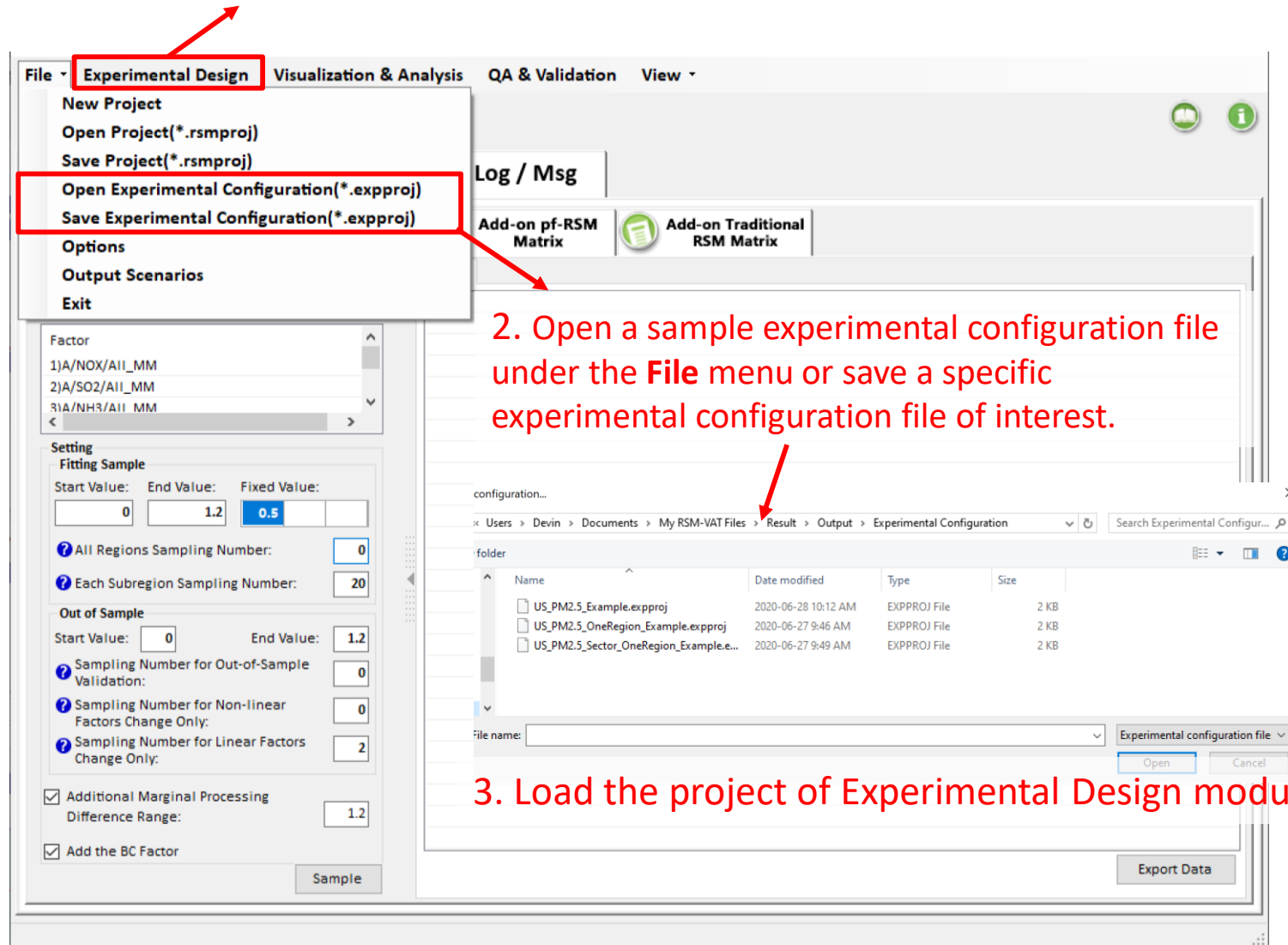
- **“US_PM2.5_MultiRegion_Example.expproj”**: the example project of experimental design module for multi-region RSM, while the corresponding input data (*C:\Users\...\Documents\My RSM-VAT Files\Data\Example\US_RSM*) and RSM project (.rsmproj) has been run and packaged in our last version of RSM, as shown here.

<input type="checkbox"/> US_PM2.5_July.rsmproj	2020-04-20 12:16	RSMPROJ :	56,064 KB
<input type="checkbox"/> US_PM2.5_January.rsmproj	2020-04-20 12:12	RSMPROJ :	56,064 KB

- **“US_PM2.5_OneRegion_Example”** : the example project of experimental design module for single-region RSM, in which all regions were merged into one region;
- **“US_PM2.5_Sector_OneRegion_Example”**: the example project of experimental design module for sectoral single-region RSM, in which the sources of NO_x were divided into ‘Points’, ‘Mobile’ and ‘Others’

Experimental Design

1. Click **Experimental Design** menu to switch to this module.



Steps for Experimental Design

Option 1 (recommended and used in our example case)

Step 1:

Create the emission control matrix for single-region RSM



Step 2:

Create region control NetCDF file based on region control shapefile (.shp) that consisted of multiple regions



Step 3:

Create the new single-region NetCDF file through merging the regions in the NetCDF file generated in Step 2 using RSM-VAT



Step 4:

Export Emission Control Namelist file based on the emission control matrix and single-region NetCDF file generated in step 1 and step 3 respectively

Option 2 (not recommended because the Step 3 is time-consuming)

Create the emission control matrix for single-region RSM



Create single-region shapefile (.shp) that consisted of only one region using **ArcGIS**



Create the single-region NetCDF file based on the single-region shapefile (.shp) generated in Step 2



Export Emission Control Namelist file based on the emission control matrix and single-region NetCDF file generated in step 1 and step 3 respectively

Control Matrix for Single Region

➤ Step 1: Create emission control matrix for RSM

Key Settings for single region matrix:

All Regions Sampling Number: 0

Each subregion Sampling Number: 20

Sampling Setting: see more tips by hovering the mouse over the icon ?

File Experimental Design Visualization & Analysis QA & Validation View

Control Matrix CMAQ Preparation Log / Msg

pf-RSM Matrix Traditional RSM Matrix Add-on pf-RSM Matrix Add-on Traditional RSM Matrix

Factors File (*.csv) Sectoral Factor File (*.csv)

FactorsInfo_US_OneRegion.csv

Factor

1)A/NOx/AII_MM

2)A/SO2/AII_MM

3)A/NH3/AII_MM

4)A/VOC/AII_MM

5)A/PM25/AII_MM

Setting

Fitting Sample

Start Value: End Value: Fixed Value:

0 1.2 0 0.5

All Regions Sampling Number: 0

Each Subregion Sampling Number: 20

Out of Sample

Start Value: End Value:

0 1.2

Sampling Number for Out-of-Sample Validation: 19

Sampling Number for Non-linear Factors Change Only: 0

Sampling Number for Linear Factors Change Only: 0

Additional Marginal Processing

Difference Range: 1.2

Add the BC Factor

Sample

Export Data

1. Get sampling result.

2. Save the sampling results as a .csv file to local path.

CMAQ Preparation for Single Region

➤ Step 2: Create region control NetCDF file based on region control shapefile (.shp)

File ▾ Experimental Design Visualization & Analysis QA & Validation View ▾

Control Matrix CMAQ Preparation Log / Msg

☒ 1 Create Region Control NetCDF File

☐ 2 Merge/Subtract Region Operation

☐ 3 Export Emission Control Namelist File

1. Select the step ①.

Create Region Control NETCDF Setting

Grid Definition File (GRDCRO2D)
GRIDCRO2D.12EUS2.35L160101

Region Control File (*.shp)
File Name
[1]US_climate_regions.shp
[2]US_state.shp
[3]US_cbsa.shp

Selected Regions **Manage Selected Regions**

CMAQ_Name	Name
CEN_CR	Ohio Valley(Central)
NE_CR	Northeast
SE_CR	Southeast
UPMW_CR	Upper Midwest(East North Central)
OTHER	The Whole User-defined Region - Select...

2. Click to select those regions that used to merge (CEN_CR, NE_CR, SE_CR, UPMW_CR, OTHER)

NetCDF **Namelist**

☒ All Regions:

- ☒ CEN_CR
- ☒ NE_CR
- ☒ SE_CR
- ☒ UPMW_CR
- ☒ OTHER

the Selected Regions
FileName = US_EXAMPLE.ncf

236
189
142
95
48
1

1 44 87 130 173 216

Legend:
CEN_CR
NE_CR
SE_CR
UPMW_CR
OTHER

Load NetCDF File **Output** Cancel Export Variables

3. Click to start generating NetCDF file for selected regions.

CMAQ Preparation for Single Region

Mange Selected Regions:

Click to select those regions that used to merge (CEN_CR,NE_CR,SE_CR,UPMW_CR,OTHER)

The screenshot displays the CMAQ Preparation software interface. The main window has a menu bar (File, Experimental Design, Visualization & Analysis, QA & Validation, View) and a toolbar with icons for Control Matrix, CMAQ Preparation, and Log / Msg. The left panel shows three options: 'Create Region Control NetCDF File' (selected), 'Merge/Subtract Region Operation', and 'Export Emission Control Namelist File'. Below these are settings for 'Create Region Control NETCDF Setting', including a 'Grid Definition File (GRDCRO2D)' and a 'Region Control File (*.shp)'. A list of 'Selected Regions' is shown, with a red circle around the 'Manage Selected Regions' button. The central panel shows a 'NetCDF Namelist' window with a 'Select Region...' dialog. This dialog has a 'Filter Dataset' dropdown set to 'US_climate_regions' and a table of available regions. A red box highlights the table, and a red arrow points from the 'Manage Selected Regions' button to it. The table lists regions with their codes, CMAQ names, and names. The right panel shows a 'Selected Regions' window with a table of selected regions. A green box highlights the 'OTHER' region, and a green arrow points from the 'Define Other' button in the 'Define "Other" Region' dialog to it. The dialog has a 'Choose the way to define the "OTHER" variable:' section with two options: 'All domain - the selected regions' and 'User-defined Regions - the selected regions.' (selected). A text box shows 'USA_Continent.shp' and a 'Region name:' field shows 'OTHER'. The 'Define Other' button is circled in green. At the bottom, there are buttons for 'Load NetCDF File', 'Output', 'Cancel', and 'Export Variables'.

File Experimental Design Visualization & Analysis QA & Validation View

Control Matrix CMAQ Preparation Log / Msg

Create Region Control NetCDF File
Merge/Subtract Region Operation
Export Emission Control Namelist File

Create Region Control NETCDF Setting
Grid Definition File (GRDCRO2D)
GRDCRO2D.12EUS2.35L.160101
Region Control File (*.shp)
File Name
[1]US_climate_regions.shp
[2]US_state.shp
[3]US_cbsa.shp
Selected Regions
Manage Selected Regions

NetCDF Namelist

Select Region...

Available Regions
Filter Dataset US_climate_regions Filter

Code	CMAQ Name	Name
3	CEN_CR	Ohio Valley(Central)
0	NE_CR	Northeast
1	NRP_CR	North Rockies and Plains
2	NW_CR	Northwest
4	S_CR	South
5	SE_CR	Southeast
6	SW_CR	Southwest
7	UPMW_CR	Upper Midwest(East North Central)
8	W_CR	West

Drag the regions to the right panel to add regions.

Selected Regions

CMAQ Name	Name
CEN_CR	Ohio Valley(Central)
NE_CR	Northeast
SE_CR	Southeast
UPMW_CR	Upper Midwest(East North Central)
OTHER	The Whole User-defined Region - Select...

Define "Other" Region

Choose the way to define the "OTHER" variable:

☐ All domain - the selected regions
☒ User-defined Regions - the selected regions.

USA_Continent.shp

Region name: OTHER

Click to define Other region.

Define Other

Add regions: click and select the region items on the left panel, and then drag them to the right panel.
Remove regions: click and select the region items on the right panel, and then press the delete key to remove them

Load NetCDF File Output Cancel Export Variables

CMAQ Preparation for Single Region

- **Step 3: Get the new NetCDF file for Single Region through merge operation on the generated NetCDF file from step ①.**

1. Select the step ②.

2. Edit formula for region operation.

3. Click to start generating NetCDF file

Use the NetCDF file generated from step ① as the input.

US_EXAMPLE_MERGE
FileName = US_EXAMPLE_MERGE.ncf

US_EXAMPLE

81

CMAQ Preparation for Single Region

Edit formula for region operation (merge regions)

Control Matrix **CMAQ Preparation**

☐ 1 Create Region Control NetCDF File
☒ 2 Merge/Subtract Region Operation
☐ 3 Export Emission Control Namelist File

Merge/Subtract Region Operation Setting

Load Region Control NetCDF File
US_EXAMPLE.ncf

Load Region Formula File(*.csv)
Region Operation Formula.csv

☐ Append Region with Formula
☒ Create Region with Formula

Add/Remove

CMAQ_Name	Expression
US_EXAMPLE	"[4]CEN_CR"+"[4]NE_CR"+"[4]...

Region operation...

Available Regions
Filter Dataset
[4]US_EXAMPLE

Filter

File NO.	CMAQ_Name
4	CEN_CR
4	NE_CR
4	SE_CR
4	UPMW_CR
4	OTHER

Formula Editor

"[4]CEN_CR"+"[4]NE_CR"+"[4]SE_CR"+"[4]U
PMW_CR"+"[4]OTHER"

Note: The variable must be enclosed by single or double quotation marks, e.g. "[1]NY".

Selected Regions

CMAQ_Name	Expression
US_EXAMPLE	"[4]CEN_CR"+"[4]NE_CR"+"[4]SE_CR"+"[4]U...

Edit formula for region operation.

Double-click the regions to add them into the formula editor.

Add formula: double-click the regions on the left panel to add them into the "Formula Editor" on right. While the edit finished, click the "Add" button to commit the formula to the "Selected Regions" panel.

OK Cancel

CMAQ Preparation for Single Region

➤ Step 4: Export Emission Control Namelist file.

1. Select the step ③.

2. Click to export namelist files.

Use the NetCDF file generated from step ② as the input.

NetCDF Namelist

File List

EmissCtrl_RSMUSA_OneRegion.nml

EVERYWHERE, 'ALL', 'PMCOARSE_SO4', 'ASO4', 'COARSE', 1, 'UNIT', 'a',
EVERYWHERE, 'ALL', 'PMCOARSE_NO3', 'ANO3', 'COARSE', 1, 'UNIT', 'a',
EVERYWHERE, 'ALL', 'PMCOARSE_CL', 'ACL', 'COARSE', 1, 'UNIT', 'a',
EVERYWHERE, 'ALL', 'PMCOARSE_H2O', 'AH2O', 'COARSE', 1, 'UNIT', 'a',
EVERYWHERE, 'ALL', 'PMCOARSE_SOIL', 'ASOIL', 'COARSE', 1, 'UNIT', 'a',
EVERYWHERE, 'ALL', 'PMCOARSE_SEACAT', 'ASEACAT', 'COARSE', 1, 'UNIT', 'a',

!> CUSTOM MAPPING EXAMPLES <!

'US_EXAMPLE_MERGE', 'ALL_MM', 'ALL', 'NOx', 'GAS', 0.432514006, 'UNIT', 'm',
'US_EXAMPLE_MERGE', 'ALL_MM', 'ALL', 'SO2', 'GAS', 0.041362158, 'UNIT', 'm',
'US_EXAMPLE_MERGE', 'ALL_MM', 'ALL', 'NH3', 'GAS', 0.188971141, 'UNIT', 'm',
'US_EXAMPLE_MERGE', 'ALL_MM', 'ALL', 'VOC', 'GAS', 0.978930682, '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.

Factors Region	CMAQ Region	Factors Sector	NMI Sect
A	US_EXAMPLE_MERGE	All_MM	ALL_

Load NetCDF File

Output

Save

Experimental Design (Single Region with sectors)

Control Matrix for Single Region with sectors

➤ Step 1: Create sectoral emission control matrix for RSM

Key Settings for Single Region with sectors:

Fixed Value: 0

Only the precursors that contain different sectors are needed to be listed in the sectoral file

The screenshot shows the CMAQ software interface with the 'Control Matrix' tab selected. The 'Factors File (*.csv)' option is chosen, and the file path is set to 'ctorsInfo_US_Sector_Precursor_OneRegion.csv'. The 'Fixed Value' is set to 0. The 'Sample' button is highlighted with a red circle and an arrow pointing to the 'Export Data' button, which is also highlighted with a green circle.

Setting Fitting Sample

Start Value: 0 End Value: 1.2 Fixed Value: 0

Out of Sample

Start Value: 0 End Value: 1.2

Sampling Number for Out-of-Sample Validation: 0

Sampling Number for Non-linear Factors Change Only: 0

Sampling Number for Linear Factors Change Only: 0

☒ Additional Marginal Processing

Difference Range: 1.2

Data

Run	1)A/NOx/Mobi...	2)A/NOx/Poin...	3)A/NOx/Others
1	1	1	1
2	0	1	1
3	1	0	1
4	1	1	0
5	0	0	0

Note:
If only part of the precursors are divided into multiple sectors(e.g., NOx/Mobile, NOx/Points, SO₂/All_MM), the OOS matrix for sectors could be generated through checking the "Factors File", as shown in the next slide

1. Get sampling result. **2. Save the sampling results as a .csv file to local path.**

(\\My RSM-VAT Files\\Data\\Example\\US_RSM - OneRegion\\Config Files\\FactorsInfo_US_Sector_Precursor_OneRegion.csv)

Control Matrix for Single Region with sectors

➤ Create out-of-sample emission control matrix for sectors

The screenshot shows the 'Control Matrix' tab in the CMAQ software. The 'Factors File (*.csv)' radio button is selected, and the file 'FactorsInfo_US_Sector_OneRegion_OOS.csv' is loaded. The 'Factor' list on the left includes '1)A/NOx/Mobile', '2)A/NOx/Points', and '3)A/NOx/Others'. The 'Setting' section includes 'Fitting Sample' and 'Out of Sample' options. The 'Out of Sample' section has 'Start Value' set to 0 and 'End Value' set to 1.2. The 'Additional Marginal Processing' checkbox is checked, and the 'Difference Range' is set to 1.2. The 'Sample' button is highlighted with a red circle and an arrow pointing to it. The 'Export Data' button is highlighted with a green circle. The 'Data' table on the right shows the results of the sampling process.

Run	1)A/NOx/Mobile	2)A/NOx/Points	3)A/NOx/Others	4)A/SO2/All MM	5)A/NH3/All MM	6)A/VOC/All MM
1	1	1	1	1	1	1
2	0.549653590893444	0.580242287900109	1.19151983445934	0.88082283651302	0.218987776461612	1.101298448790
3	0.467668218740853	0.713976754183833	0.73597568837679	0.818790559571504	0.318482390395837	0.549504530811
4	1.09202740591643	0.178840668186833	0.361200307377236	0.0977407781685852	0.577184017335968	0.665193216006
5	0.262378271843941	1.044572683532	0.549394498168601	0.682837693769392	0.912574931294806	0.160111041461
6	0.231032173477463	0.123422013857968	0.15544516942195	1.10577803482752	0.795309397664342	0.213104313147

Generating the OOS matrix for factors that contain both the sectoral precursor (e.g., NOx/Mobile) and All_MM precursor (e.g., SO₂/All)

2. Save the sampling results as a .csv file to local path.

1. Get OOS sampling result.

Export Data

CMAQ Preparation for Single Region with sectors

- Step 2: Create region control NetCDF file based on region control shapefile (.shp)
- Step 3: Get the new NetCDF file for Single Region through merge operation on the generated NetCDF file from step ①.

The above steps for single region with sectors are the same to "single region" (detailed in Slide 8 to 10)

- Step 4: Export Sectoral Emission Control Namelist file.

Use the namelist template file from EPA

Use the NetCDF file generated from step ② as the input.

The screenshot shows the CMAQ Preparation software interface. The 'Control Matrix' tab is active, and the 'Export Emission Control Namelist Setting' option is selected. A red box highlights the 'Export Emission Control Namelist Setting' option. Another red box highlights the 'EmissCtrl_USA_RSM_2ndCase_sector_OneRegion.nml' file in the 'Region Control NetCDF File' list. A third red box highlights the 'Output' button at the bottom right. The 'Namelist' tab is also visible, showing a list of files and a preview of the 'EmissCtrl_USA_RSM_2ndCase_sector_OneRegion_005.nml' file content.

1. Select the step ③.

2. Click to export namelist files.

Running RSM Project with Single Region

Note: *Default RSM case is “5 Climate Regions” in RSM-VAT*

Run RSM Project

Steps of running RSM project for single region

Create/Input RSM Option

- Create/Input RSM Option
- Model Data Input Option
- Validation and QA Option
- Visualization Analysis Option

Create/Input RSM Option

RSM-VAT Project File (*.rsmproj)

Input RSM File (*.rsm):

Create RSM File:

RSM Method Settings

☐ pf-ERSM ☒ Low-degree pf-ERSM

Data Input Option

Emission File:

Matrix_RSMUSA_case_OneRegion.csv

Precursor Factors File:

FactorsInfo_US_OneRegion.csv

ShapeLCC File:

JSA_whole_StateShapesLCC_Lamberter.csv

Region File:

Multi_region include other - OneRegion.txt

Emission Parameter Settings

All Regions Sampling Number: 0

Each Subregion Sampling Number: 20

☐ Advanced Option

Model Data Input Option

Model Data Input Option

Base Case CMAQ File:

ACONC.1

Target Pollutant

☒ PM: PM25_TOT Unit: ug/m3

☐ O3: Unit:

Precursor Polltant

NOx: NOx Unit: ppbv

NH3: NH3 Unit: ppbv

SO2: SO2 Unit: ppbv

VOCs: VOC Unit: ppbC

POA: Unit:

Fitting Parameter Settings

Threads Count: 2

☒ Scenario Plot

Select Cases

Clear All

Selected Cases

Cancel Back Next

Validation and QA Option

Log / Msg

Validation Types

☒ Out of Sample ☐ Cross Validation

Out of Sample Input Option

Emission File for Out of Sample:

_case25-43_out_of_sample_OneRegion.csv

Cross Validation Input Option

☐ With Cross Validation File

☒ Without Cross Validation File

Emission File for Cross Validation:

Other Settings:

Start Row: 1 End Row: 236

Start Col: 1 End Col: 216

Start Case: 1 End Case: 24

Cancel Back Next

Visualization Analysis Option

Receptor File

Receptor Region File

US_Multi_Monitor - OneRegion.txt

Plot Types

☐ Contour Plot

Contour Plot Settings:

Receptor Region:

Current View:

Factors:

Min: Max: Equal portions: 6

X Axis

X Axis Title: Select X Factors

Y Axis

Y Axis Title: Select Y Factors

Cancel Back Next

1. Select input files for creating Single Region RSM

2. Select regional CMAQ files and pollutants, and set fitting parameters

3. Select the input file for out-of-sample validation

4. Select the receptor region file for visualization analysis

All Regions Sampling Number:0
Each Subregion Sampling Number:20

(C:\Users\...\Documents\My RSM-VAT Files\Data\Example\US_RSM - OneRegion)

Run RSM Project

Steps of running RSM project for single region with different sectors

The screenshot displays the RSM Project software interface with four main panels highlighted by red boxes and numbered instructions:

- 1. Create/Input RSM Option:** This panel shows the 'RSM-VAT Project File (*.rsmproj)' field. Under 'Input RSM File (*.rsm):', the 'Create RSM File' radio button is selected. The 'RSM Method Settings' section has 'Low-degree pf-ERSM' selected. The 'Data Input Option' section shows 'Emission File: Matrix_RSMUSA_case_OneRegion.csv', 'Precursor Factors File: FactorsInfo_US_OneRegion.csv', 'ShapeLCC File: JSA_whole_StateShapesLCC_Lamberter.csv', and 'Region File: Multi_region include other - OneRegion.txt'. The 'Emission Parameter Settings' section has 'All Regions Sampling Number: 0' and 'Each Subregion Sampling Number: 20'. The 'Advanced Option' section is checked, with 'Use the BC Factor' and 'Sectoral Fitting Input Option' selected. The 'Sectoral Emission File: trix_RSMUSA_case_Sector_OneRegion.csv', 'Sectoral Factors File: Info_US_Sector_Precursor_OneRegion.csv', 'Sectoral Base Case CMAQ File: ACONC.1', and 'Sector Emission Case For Single Region: 4' are specified. A red arrow points to the 'Next' button.
- 2. Model Data Input Option:** This panel shows the 'Model Data Input Option' section. The 'Base Case CMAQ File: ACONC.1' is entered. The 'Target Pollutant' section has 'PM: PM25_TOT' selected with 'Unit: ug/m3'. The 'Precursor Pollutant' section has 'NOx: NOx', 'NH3: NH3', 'SO2: SO2', 'VOCs: VOC', and 'POA: ' selected with units 'ppbv', 'ppbv', 'ppbv', 'ppbC', and 'Unit: ' respectively. The 'Fitting Parameter Settings' section has 'Threads Count: 2' and 'Scenario Plot' checked. A red arrow points to the 'Next' button.
- 3. Validation and QA Option:** This panel shows the 'Validation and QA Option' section. The 'Validation Types' section has 'Out of Sample' checked. The 'Out of Sample Input Option' section has 'Emission File for Out of Sample: i-10_out_of_sample_Sector_OneRegion.csv' entered. The 'Cross Validation Input Option' section has 'Without Cross Validation File' selected. The 'Other Settings' section has 'Start Row: 1', 'End Row: 236', 'Start Col: 1', 'End Col: 216', 'Start Case: 1', and 'End Case: 387' entered. A red arrow points to the 'Next' button.
- 4. Visualization Analysis Option:** This panel shows the 'Visualization Analysis Option' section. The 'Receptor File' and 'Receptor Region File' fields are empty. The 'Plot Types' section has 'Contour Plot' selected. The 'Contour Plot Settings' section has 'Receptor Region: ' and 'Current View: ' selected. The 'Factors' section has 'Min: ', 'Max: ', and 'Equal portions: 6' entered. The 'X Axis' section has 'X Axis Title: ' and 'Select X Factors' button. The 'Y Axis' section has 'Y Axis Title: ' and 'Select Y Factors' button. A red arrow points to the 'Next' button.

Red arrows and text annotations provide additional guidance:

- Red arrow 1: '1. Keep the input files like "Single Region", and check the "Advanced Option" to select the input files for sectoral fitting' points to the 'Advanced Option' section.
- Red arrow 2: '2. Same to that of regional analysis' points to the 'Model Data Input Option' panel.
- Red arrow 3: '3. Select the input file for sectoral out-of-sample validation' points to the 'Validation and QA Option' panel.
- Red arrow 4: '4. Same to that of regional analysis' points to the 'Visualization Analysis Option' panel.

Visualization and Analysis & QA Module

RSM-VAT: Visualization & Analysis Module

RSM-VAT 2.4

File Experimental Design **Visualization & Analysis** View

Create/Input RSM Option
Model Data Input Option
Validation and QA Option
Visualization Analysis Option

Visualization & Analysis QA & Validation
Map Receptor Analysis Data

2D Plot 3D Plot Contour Plot

Toggle between "Concentration" and "Response"

☐ Concentration ☒ Response

Radio Button Panel
to control %
emissions reduction of
control policy factors
(Region/Pollutant/
Sector)

26 factors

☐ Region ☐ Pollutant ☐ Sector

NE_CR\NOx\All_MM 0.75
NE_CR\SO2\All_MM 0.75
NE_CR\NH3\All_MM 0.75
NE_CR\VOC\All_MM 0.75
SE_CR\NOx\All_MM 0.75
SE_CR\SO2\All_MM 0.75
SE_CR\NH3\All_MM 0.75
SE_CR\VOC\All_MM 0.75
CEN_CR\NOx\All_MM 0.75
CEN_CR\SO2\All_MM 0.75

Reset All To 0.75

Select/Combine Factors

PM25

RSM2.4_US_PM2.5_January_createRSM_T1.rsm

Min = 0.223 at (212,119), Max = 14.330 at (34,171)

5.0
4.0
3.0
2.0
1.0
0.0
-1.0
-2.0
-3.0
-4.0
-5.0

Back Next

RSM-VAT: Visualization & Analysis Module

RSM-VAT 2.4

File ▾ **Experimental Design** **Visualization & Analysis** **View** ▾

- Create/Input RSM Option
- Model Data Input Option
- Validation and QA Option
- Visualization Analysis Option

Create/Input RSM Option

RSM-VAT Project File (*.rsmproj)
US_PM2.5_January_createRSM_T1.rsmproj

☐ Input RSM File (*.rsm):

☒ Create RSM File:

RSM Method Settings
☐ pf-ERSM ☒ Low-degree pf-ERSM

Data Input Option
Emission File:
Matrix_RSMUSA_case1-132.csv

Precursor Factors File:
FactorsInfo_US_Precursor.csv

ShapeLCC File:
JSA_whole_StateShapesLCC_Lamberter.csv

Region File:
US_Multi_region_include_other.txt

Emission Parameter Settings
All Regions Sampling Number:
Each Subregion Sampling Number:

☒ Advanced Option
☒ Use the BC Factor
☐ Sectoral Fitting Input Option

Sectoral Emission File:
Sectoral Factors File:
Sectoral Base Case CMAQ File:

Visualization & Analysis

Map **Receptor Analysis** **Data**

2D Plot 3D Plot Contour Plot

26 factors

☐ Region ☐ Pollutant ☐ S

NE_CR\NOx\All_MM 1
NE_CR\SO2\All_MM 1
NE_CR\NH3\All_MM 1
NE_CR\VOC\All_MM 1
SE_CR\NOx\All_MM 1

Reset All To 1

Select/Combine Factors

Configure Plot

File Color Map Titles Labels Others

Number of Tiles: 10 Palette Type: Color Ramp

Palette

GreyToRed
Newton RGB (Inkjet)
BlueDarkRed
BlueWhiteRed

Reverse

Scale: Linear Digits After Decimal Point: 1 Min: 0 Max: 20 Rebuild

Symbol Range Max

0.0-2.0 2.0
2.0-4.0 4.0
4.0-6.0 6.0
6.0-8.0 8.0
8.0-10.0 10.0
10.0-12.0 12.0
12.0-14.0 14.0
14.0-16.0 16.0
16.0-18.0 18.0
18.0-20.0 20.0

Apply for all maps Apply OK Cancel

“Single click” on color bar to configure color/legend

“Right-click” to save data to BenMAP-CE & SMAT-CE format

Reset to default domain
Zoom out to previous domain
Size - Maximize
Size - Restore
Close plot
Formula
Save image to clipboard
Save image as...
Save Data as...
Excel
SMAT-CE
BenMAP-CE

Min = 1.320 at (87,236), Max = 5

Back Next

RSM-VAT: Visualization & Analysis Module

RSM-VAT 2.4

File Experimental Design Visualization & Analysis View

- Create/Input RSM Option
- Model Data Input Option
- Validation and QA Option
- Visualization Analysis Option

[Create/Input RSM Option](#)

RSM-VAT Project File (*.rsmproj)
US_PM2.5_January_createRSM_T1.rsmproj

Input RSM File (*.rsm):

Create RSM File:

RSM Method Settings
☐ pf-ERSM ☒ Low-dear

Advanced Option
☒ Use the BC Factor
☐ Sectoral Fitting Input Option

Sectoral Emission File:

Visualization & Analysis QA & Validation Log / Msg

Map Receptor Analysis Data

2D Plot 3D Plot Contour Plot

6 factors

☒ Region ☐ Pollutant ☐ Sector

CEN_CR 0.75

NE_CR 0.75

OTHER 0.75

SE_CR 0.75

UPMW_CR 0.75

BC 1

Reset All To 0.75

Select/Combine Factors

PM25

RSM2.4_US_PM2.5_January_createRSM_T1.rsm

Concentration Response

237 190 143 217

5.0 4.0 3.0 2.0 1.0 0.0 -1.0 -2.0 -3.0 -4.0 -5.0

Select/Combine Factors...

Factor	Region	Pollutant	Sector	Status
CEN_CR				Unselect
CEN_CR/NOx/Ail...	CEN_CR	NOx	Ail_MM	Unselect
CEN_CR/SO2/Ail...	CEN_CR	SO2	Ail_MM	Unselect
CEN_CR/NH3/Ail...	CEN_CR	NH3	Ail_MM	Unselect
CEN_CR/VOC/Ail...	CEN_CR	VOC	Ail_MM	Unselect
CEN_CR/PM25/Ail...	CEN_CR	PM25	Ail_MM	Unselect
NE_CR				Unselect
NE_CR/NOx/Ail...	NE_CR	NOx	Ail_MM	Unselect
NE_CR/SO2/Ail...	NE_CR	SO2	Ail_MM	Unselect
NE_CR/NH3/Ail...	NE_CR	NH3	Ail_MM	Unselect
NE_CR/VOC/Ail...	NE_CR	VOC	Ail_MM	Unselect
NE_CR/PM25/Ail...	NE_CR	PM25	Ail_MM	Unselect
OTHER				Unselect
OTHER/NOx/Ail...	OTHER	NOx	Ail_MM	Unselect
OTHER/SO2/Ail...	OTHER	SO2	Ail_MM	Unselect
OTHER/NH3/Ail...	OTHER	NH3	Ail_MM	Unselect
OTHER/VOC/Ail...	OTHER	VOC	Ail_MM	Unselect
OTHER/PM25/Ail...	OTHER	PM25	Ail_MM	Unselect
SE_CR				Unselect
SE_CR/NOx/Ail...	SE_CR	NOx	Ail_MM	Unselect
SE_CR/SO2/Ail...	SE_CR	SO2	Ail_MM	Unselect
SE_CR/NH3/Ail...	SE_CR	NH3	Ail_MM	Unselect
SE_CR/VOC/Ail...	SE_CR	VOC	Ail_MM	Unselect
SE_CR/PM25/Ail...	SE_CR	PM25	Ail_MM	Unselect
UPMW_CR				Unselect
UPMW_CR/NOx/Ail...	UPMW_CR	NOx	Ail_MM	Unselect
UPMW_CR/SO2/Ail...	UPMW_CR	SO2	Ail_MM	Unselect

Select Desired Factors Combine Control Factors

OK Cancel Clear

Cancel Back Next

Allow to flexibly select "Region", "Pollutant" and/or "Sector" of control policy factors

Allow to customize control policy factors

RSM-VAT: Receptor Analysis -> Source Contribution

RSM-VAT 2.4

File Experimental Design Visualization & Analysis View

Create/Input RSM Option
Model Data Input Option
Validation and QA Option
Visualization Analysis Option

Create/Input RSM Option

RSM-VAT Project File (*.rsmproj)
US_PM2.5_January_createRSM_T1.rsmproj

Input RSM File (*.rsm):
Create RSM File:
RSM Method Settings
pf-ERSM Low-degree pf-ERSM
Data Input Option
Emission File:
Matrix_RSMUSA_case1-132.csv
Precursor Factors File:
FactorsInfo_US_Precursor.csv
ShapeLCC File:
JSA_whole_StateShapesLCC_Lamberter.csv
Region File:
US_Multi_region include other.txt

Emission Parameter Settings
All Regions Sampling Number: 20
Each Subregion

Advanced Options
Use the BC Factor
Sectoral Fitting
Sectoral Emission
Sectoral Factors File:
Sectoral Base Case CMAQ File:
Sector Emission Case For Single Region: 16

RSM2.4_US_PM2.5_January_createRSM_T1

Visualization & Analysis QA & Validation Log

Map Receptor Analysis Data

Source Contribution 1 Source Contribution 2 Emissions Control 1 Emissions Control 2

Point Average 1x1
Spatial Average

Control Region (Reduced by)
NE_CR 75%
SE_CR 30%
CEN_CR 30%
Reset all to 30%

NE_CR 75%, SE_CR 30%, CEN_CR 30%, UPMW_CR 30%, OTHER 30%

PM25 Reductions:
NOx\All_MM SO2\All_MM NH3\All_MM
VOC\All_MM PM25\All_MM

NE_CR SE_CR CEN_CR UPMW_CR

Receptor regions

APM25(ug/m3)

NE_CR\PM25\All_MM = 0.93

Individual Contributions of source emissions reduction

Allow to set control % of individual source region

Cancel Back Next

Set New Receptor Regions
Stack Cluster Pie
Receptor: Positive
Output Apply

Receptor Region	NE_CR	SE_CR	CEN_CR	UPMW_CR
APM25(ug/m3)	2.37	2.45	1.86	1.39

RSM-VAT: Receptor Analysis -> Emissions Control

RSM-VAT 2.4

File Experimental Design Visualization & Analysis View

SM2.4_US_PM2.5_January_createRSM_T1

Visualization & Analysis QA & Validation Log / Msg

Map Receptor Analysis Data

Source Contribution 1 Source Contribution 2 Emissions Control 1 Emissions Control 2

PM25 concentrations on selected regions/cities (AL; AR; CT; DE; DC; FL; GA)

25 factors

Region Pollutant Sector

NE_CR\NOx\All_MM 0.75

NE_CR\SO2\All_MM 0.75

NE_CR\NH3\All_MM 0.75

NE_CR\VOC\All_MM 0.75

SE_CR\NOx\All_MM 0.75

Reset All To 1

Select/Combine Factors

Receptor Regions: AL AR CT DE DC FL GA IL IN IA KS KY LA ME

Set New Receptor Regions

Reduction Inverse

Output Apply

Input RSM File (*.rsm):

Create RSM File:

RSM Method Settings

pf-ERSM Low-degree pf-ERSM

Data Input Option

Emission File:

Matrix_RSMUSA_case1-132.csv

Precursor Factors File:

FactorsInfo_US_Precursor.csv

ShapeLCC File:

JSA_whole_StateShapesLCC_Lamberter.csv

Region File:

US_Multi_region include other.txt

Emission Parameter Settings

All Regions Sampling Number: 20

Each Subregion Sampling Number: 20

Advanced Option

Sectoral Base Case CMAQ File:

Sector Emission Case For Single Region: 16

Cancel Back Next

Receptor Region Configuration

Select Region File

US_Multi_Monitor.txt

US_CBSA.txt

US_CBSA_selected_6.txt

US_Multi_region include other

US_STATE.txt

US_Multi_region include other

38 receptors

Id	ShortName	Name
1	AL	Alabama
2	AR	Arkansas
3	CT	Connecticut
4	DE	Delaware
5	DC	District
6	FL	Florida
7	GA	Georgia
8	IL	Illinois
9	IN	Indiana
10	IA	Iowa
11	KS	Kansas
12	KY	Kentucky
13	LA	Louisiana
14	ME	Maine
15	MD	Maryland
16	MA	Massachusetts
17	MI	Michigan
18	MN	Minnesota

0 5

3.77

1.47

2.23

AL AR CT DE DC FL GA

Receptor regions

RSM-VAT: Receptor Analysis -> Emissions Control

RSM-VAT 2.4

File Experimental Design Visualization & Analysis View

Create/Input RSM Option
Model Data Input Option
Validation and QA Option
Visualization Analysis Option

[Create/Input RSM Option](#)

RSM-VAT Project File (*.rsmproj)
US_PM2.5_January_createRSM_T1.rsmproj

Input RSM File (*.rsm):
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RSM Method Settings
pf-ERSM
Low-degree pf-ERSM

Data Input Option
Emission File:
Matrix_RSMUSA_case1-132.csv
Precursor Factors File:
FactorsInfo_US_Precursor.csv
ShapeLCC File:
JSA_whole_StateShapesLCC_Lamberter.csv
Region File:
US_Multi_region include other.txt

Emission Parameter Settings
All Regions Sampling Number: 20
Each Subregion Sampling Number: 20

Advanced Option
Use the BC Factor
Sectoral Fitting Input Option
Sectoral Emission File:

Visualization & Analysis
QA & Validation
Map
Receptor Analysis
Data

RSM2.4 US_PM2.5_January_createRSM_T1

Source Contribution 1 Source Contribution 2 Emissions Control 1 Emissions Control 2

Point Average 1x1
Spatial Average

Control Region
NE_CR
SE_CR
CEN_CR

Pollutants
NOx
SO2
NH3
VOC
PM25

Sectors
All_MM

Emission reduction(%):
50
75
100

Receptor Regions
A NE CR
B SE CR
C CEN CR
D UPMW CR
E OTHER

PM25 Reductions :
25%, 50%, 75%, 100% emission control

25% 50% 75% 100%

$\Delta PM_{25}(\mu g/m^3)$

Receptor regions

NE_CR SE_CR CEN_CR UPMW_CR OTHER

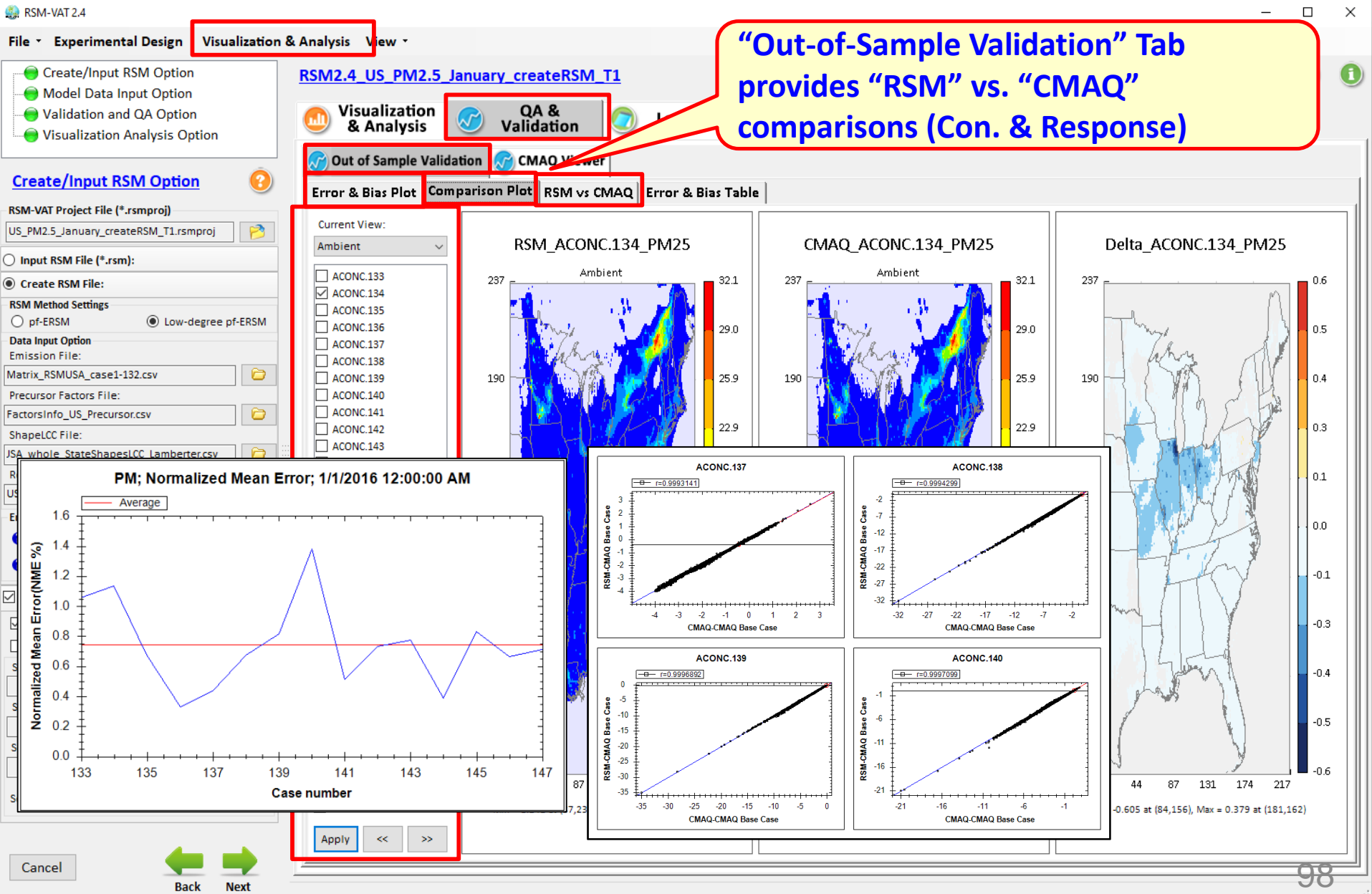
Individual Contributions of source emissions reduction

Allow to flexibly set any control % of source region

Cancel Back Next

97

QA & Validation: “Out-of-Sample” Validation



QA & Validation: “CMAQ Viewer” for QA

RSM-VAT 2.4

File Experimental Design Visualization & Analysis View

Create/Input RSM Option
Model Data Input Option
Validation and QA Option
Visualization Analysis Option

Create/Input RSM Option

RSM-VAT Project File (*.rsmproj)
US_PM2.5_January_createRSM_T1.rsmproj

Input RSM File (*.rsm):
Create RSM File:
RSM Method Settings
pf-ERSM Low-degree pf-ERSM

Data Input Option
Emission File:
Matrix_RSMUSA_case1-132.csv

Precursor Factors File:
FactorsInfo_US_Precursor.csv

ShapeLCC File:
JSA_whole_StateShapesLCC_Lamberter.csv

Region File:
US_Multi_region include other.txt

Emission Parameter Settings
All Regions Sampling Number: 20
Each Subregion Sampling Number: 20

Advanced Option
Use the BC Factor
Sectoral Fitting Input Option
Sectoral Emission File:
Sectoral Factors File:
Sectoral Base Case CMAQ File:
Sector Emission Case For Single Region: 16

Cancel Back Next

RSM2.4 US PM2.5_January_createRSM_T1

Visualization & Analysis QA & Validation

Out of Sample Validation CMAQ Viewer

Pollutant: PM25_TOT

Check All

ACONC.1
ACONC.2
ACONC.3
ACONC.4
ACONC.5
ACONC.6
ACONC.7
ACONC.8
ACONC.9
ACONC.10
ACONC.11
ACONC.12
ACONC.13
ACONC.14
ACONC.15
ACONC.16
ACONC.17
ACONC.18
ACONC.19
ACONC.20
ACONC.21
ACONC.22
ACONC.23
ACONC.24
ACONC.25
ACONC.26
ACONC.27
ACONC.28
ACONC.29
ACONC.30
ACONC.31
ACONC.32

Apply << >>

Concentration Response

PM25_TOT ACONC.2

237 190 143 95 48 1 1 44 87 131 174 217

Min = 1.76E-3 at (1,236), Max = 1.213 at (85,157)

PM25_TOT ACONC.3

237 190 143 95 48 1 1 44 87 131 174 217

Min = 7.91E-3 at (1,236), Max = 4.088 at (85,156)

PM25_TOT ACONC.4

237 190 143 95 48 1 1 44 87 131 174 217

Min = -7.76E-4 at (165,14), Max = 5.373 at (115,165)

PM25_TOT ACONC.5

237 190 143 95 48 1 1 44 87 131 174 217

Min = 6.26E-3 at (1,236), Max = 3.251 at (85,156)

“CMAQ Viewer” allow to QA/check individual CMAQ species (Concentration & Response)

End

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