

**Technical Support Document for the
Proposed PM NAAQS Rule**

Response Surface Modeling

**U.S. Environmental Protection Agency
Office of Air Quality Planning and Standards
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I. Introduction

This Technical Support Document (TSD) describes the emissions inventories and air quality modeling performed by EPA for the development of the Response Surface Model (RSM) in support of the Regulatory Impact Assessment (RIA) for the proposed National Ambient Air Quality Standards (NAAQS) for PM_{2.5}. Included is information on (1) the emissions inventories and development of projections, (2) the air quality modeling and development of model inputs, (3) development and experimental design of the RSM, and (4) the performance and validation of the RSM as compared to the air quality modeling.

The RSM is based on a new approach known as air quality *metamodeling* that aggregates numerous pre-specified individual air quality modeling simulations into a multi-dimensional air quality “response surface”. Simply, this metamodeling technique is a “model of the model” and can be shown to reproduce the results from an individual modeling simulation with little bias or error. The RSM incorporates statistical relationships between model inputs and outputs to provide real-time estimate of these air quality changes. The RSM provides a wide breadth of model outputs, which we utilize to develop emissions control scenarios. The RSM approach informs the selection and evaluation of various control scenarios. This approach allows for the rapid assessment of air quality impacts of different combinations of emissions reductions and was used to estimate air quality changes for various control scenarios for the proposed PM_{2.5} NAAQS.

II. Emissions Inventories and Projections

Emission inventories were developed for the 48 contiguous States, the District of Columbia, and portions of Canada and Mexico for the purposes of modeling particulate matter (PM) to support the air quality modeling analyses for the RSM development and the proposed PM NAAQS. The model required hourly emissions for the entire year of 2001 and future years on a 36-km national grid of the following pollutants: carbon monoxide (CO), nitrogen oxides (NOx), volatile organic compounds (VOC), sulfur dioxide (SO₂), ammonia (NH₃), particulate matter less than or equal to 10 microns (PM10), and particulate matter less than or equal to 2.5 microns (PM2.5).

The emission sources and the basis for current and future-year emission inventories for the Clean Air Interstate Rule (CAIR), and the PM NAAQS proposal are listed in Table II-1. Readers interested in additional technical detail describing how EPA developed and projected this inventory to 2010 and 2015 can reference the CAIR Emissions Inventory TSD.¹ Section 3 in the CAIR TSD details the 2001 baseline emissions used in each of the inventory sectors in Table II-1. Section 4 in the CAIR TSD details the growth and control methodology used in the 2010 and 2015 CAIR control strategy inventories.

¹ See: <http://www.epa.gov/interstateairquality/pdfs/finaltech01.pdf>. Additional information may be found in Appendix H of the Clean Air Interstate Rule Emissions Inventory TSD, March 2005.

Table II-2 provides summaries for 2001, 2010 CAIR baseline and control, and 2015 CAIR baseline and control emissions by pollutant and inventory sector, as defined in Table II-1, for states in the continental U.S. Appendix B and Appendix H in the CAIR TSD include more detailed summaries that expand the 2001 baseline and 2015 CAIR control strategy (respectively) emissions in Table II-2 to include totals by state, sector and pollutant. Except for the future CAIR control strategy EGU emissions; this information is also available electronically in the CAIR docket (item number OAR-2003-0053-1705) and the CAIR website:

<http://www.epa.gov/cleanairinterstaterule/technical.html>, as a Microsoft® Excel® file, named Emissions_summary_state_sector_2001-2010-2015.xls. Also available are annual total emissions by state and sector (except for CAIR control strategy EGU emissions) after application of chemical speciation factors for 2001, 2010, and 2015, which includes differences among the years. It can be found as a Microsoft® Excel® file Emissions_summary_state_sector_speciation_2001-2010-2015.xls in the CAIR docket (item number OAR-2003-0053-1706) and the CAIR website.

Table II-1. Emissions Sources and Basis for Current and Future-Year Inventories^{a,b}

Sector or Source	Emissions Source	2001 Base Year	Future-Year Base Case Projections
EGU	Power industry EGUs	Point-sources facilities that were matched to facilities in the 2003 National Electric Energy Database System (NEEDS)	Integrated Planning Model (IPM)
Non-EGU, including Point Fugitive Dust (pf dust)	Non-Utility Point, including point source fugitive dust	2001 National Emission Inventory (NEI)	Baseline including CAIR control case: (1) Department of Energy (DOE) fuel use projections, (2) Regional Economic Model, Inc. (REMI) Policy Insight® model, (3) decreases to REMI results based on trade associations, Bureau of Labor Statistics (BLS) projections and Bureau of Economic Analysis (BEA) historical growth from 1987 to 2002, (4) various control strategies outlined in Section 4.3, Table 12 in the CAIR emissions TSD
Average Fire	Wildfire, prescribed burning	Same as future year	Average fires from 1996 through 2002 (based on state total acres burned), with the same emissions rates and country distributions of emissions as in the 2001 NEI
Average Fire	Agricultural burning, open burning	2001 NEI	2001 NEI
Agriculture	Livestock NH ₃	2002 Preliminary NEI ^c	2015 emissions estimated with the same approach as was used for the 2002 preliminary NEI ^c
Agriculture	Fertilizer NH ₃	2001 NEI	2001 NEI

(continued)

Table II-1. Emissions Sources and Basis for Current and Future-Year Inventories^{a,b}
 (continued)

Sector or Source	Emissions Source	2001 Base Year	Future-Year Base Case Projections
Other Area, including Area Fugitive Dust (afdust)	All other stationary area sources, including area-source fugitive dust	1999 NEI, version 3 grown to 2001	(1) DOE fuel use projections, (2) REMI Policy Insight Model, (3) decreases to REMI results based on trade associations, BLS projections and BEA historical growth from 1987 – 2002, (4) various control strategies outlined in Section 4.3, Table 13 in the CAIR emissions TSD
On-road	Highway vehicles	Except for California, the National Mobile Inventory Model (NMIM) using the Mobile6.2 model. California used their own on-road mobile source estimation model (EMFAC2002), which were assigned pollutant-specific monthly variation from NMIM.	Except for California, projected vehicle miles traveled same as CAIR proposed and final rule, emissions from MOBILE6.2 model. For California, 2001 emissions were grown by county and SCC using NMIM 2001 to future year ratios.
Nonroad	Locomotives, commercial marine vessels, and aircraft	2001 NEI; CMV adjusted to new national totals from Office of Transportation Air Quality (OTAQ)	Grown based on national totals from OTAQ, using state/county distribution of emissions from the 2001 NEI
Nonroad	All other nonroad vehicles	NONROAD 2004 model	NONROAD 2004 model

^a This table documents only the sources of data for the U.S. inventory. The sources of data used for Canada and Mexico are explained in the CAIR emissions inventory technical support document.

^b All fugitive dust emissions were adjusted downward using county-specific transportable fractions needed as part of the current state of the art in air quality modeling.

^c ftp://ftp.epa.gov/EmisInventory/prelim2002nei/nonpoint/documentation/nh3inventorydraft_jan2004.pdf.

Table II-2: Sector and pollutant emissions totals for 2001 baseline, 2010 CAIR baseline, 2010 CAIR control, 2015 CAIR baseline, and 2015 CAIR control for all states in the continental U.S.

Year	Sectors	[tons/yr] VOC	[tons/yr] NOX	[tons/yr] CO	[tons/yr] SO2	[tons/yr] PM10	[tons/yr] PM2.5	[tons/yr] NH3
2001 Base	afdust	0	0	0	0	10,117,152	1,735,883	0
	Agriculture	0	0	0	0	0	0	3,140,563
	Average fire	653,544	238,931	10,767,438	49,108	1,103,540	979,607	38,237
	EGU	52,737	4,937,398	452,092	10,901,127	721,415	598,937	7,918
	NonEGU	1,537,208	2,942,618	3,963,754	2,958,692	914,250	701,381	82,550
	Nonroad	2,584,513	4,050,655	22,789,871	433,249	320,999	307,520	1,753
	on-road	4,709,818	8,064,067	61,057,851	271,032	216,924	161,373	277,379
	Other area	7,326,991	1,462,276	3,712,654	1,295,146	875,944	764,395	141,193
	Pfdust	0	0	0	0	12,752	3,915	0
2001 Base Total		16,864,812	21,695,944	102,743,660	15,908,354	14,282,977	5,253,010	3,689,593
2010 CAIR Base	Afdust	0	0	0	0	10,428,325	1,784,758	0
	Agriculture	0	0	0	0	0	0	3,220,011
	Average fire	653,544	238,931	10,767,438	49,108	1,103,540	979,607	38,237
	EGU	41,391	3,672,929	578,358	9,903,882	796,300	668,487	928
	NonEGU	1,363,530	2,931,360	4,421,697	3,189,864	957,490	739,036	93,078
	Nonroad	1,903,516	3,282,339	26,195,189	219,032	262,247	250,607	2,069
	on-road	2,593,430	4,683,086	37,718,382	27,439	151,876	91,721	341,564
	Other area	6,777,802	1,630,411	2,959,763	1,408,990	833,547	710,557	153,569
	Pfdust	0	0	0	0	14,727	4,405	0
2010 CAIR Base Total		13,333,213	16,439,056	82,640,827	14,798,315	14,548,052	5,229,178	3,849,456
2010 CAIR Control	Afdust	0	0	0	0	10,428,325	1,784,758	0
	Agriculture	0	0	0	0	0	0	3,220,011
	Average fire	653,544	238,931	10,767,438	49,108	1,103,540	979,607	38,237
	EGU	41,160	2,427,892	583,089	6,283,602	648,643	522,951	905
	NonEGU	1,363,530	2,931,360	4,421,697	3,189,864	957,490	739,036	93,078
	Nonroad	1,903,516	3,282,339	26,195,189	219,032	262,247	250,607	2,069
	on-road	2,593,430	4,683,086	37,718,382	27,439	151,876	91,721	341,564
	Other area	6,777,802	1,630,411	2,959,763	1,408,990	833,547	710,557	153,569
	Pfdust	0	0	0	0	14,727	4,405	0
2010 CAIR Control Total		13,332,982	15,194,019	82,645,558	11,178,035	14,400,395	5,083,642	3,849,433
2015 CAIR Base	Afdust	0	0	0	0	10,564,873	1,803,965	0
	Agriculture	0	0	0	0	0	0	3,299,775
	Average fire	653,544	238,931	10,767,438	49,108	1,103,540	979,607	38,237
	EGU	40,129	3,540,893	563,434	9,425,988	765,282	642,055	917
	NonEGU	1,553,429	3,183,499	4,971,592	3,422,915	1,080,189	833,372	102,627
	Nonroad	1,648,402	2,912,387	27,364,911	232,628	228,217	217,762	2,264
	on-road	2,031,739	3,152,563	34,182,190	30,823	134,202	70,697	379,401
	Other area	7,132,086	1,702,154	2,810,041	1,480,348	839,500	709,230	166,326
	Pfdust	0	0	0	0	16,517	4,959	0
2015 CAIR Base Total		13,059,329	14,730,427	80,659,606	14,641,810	14,732,320	5,261,647	3,989,547
2015 CAIR Control	Afdust	0	0	0	0	10,564,873	1,803,965	0
	Agriculture	0	0	0	0	0	0	3,299,775
	Average fire	653,544	238,931	10,767,438	49,108	1,103,540	979,607	38,237

EGU	42,782	2,172,837	652,215	5,111,436	603,800	476,350	717
NonEGU	1,553,429	3,183,499	4,971,592	3,422,915	1,080,189	833,372	102,627
Nonroad	1,648,402	2,912,387	27,364,911	232,628	228,217	217,762	2,264
on-road	2,031,739	3,152,563	34,182,190	30,823	134,202	70,697	379,401
Other area	7,132,086	1,702,154	2,810,041	1,480,348	839,500	709,230	166,326
pf dust	0	0	0	0	16,517	4,959	0
2015 CAIR Control Total	13,061,982	13,362,371	80,748,387	10,327,258	14,570,838	5,095,942	3,989,347

III. Development of the Response Surface Model

U.S. EPA has devoted significant efforts to developing air quality models for the assessment of regulatory impacts and designs of effective emissions control strategies. Air quality models use mathematical and numerical techniques to simulate the physical and chemical processes that affect air pollutants as they disperse and react in the atmosphere. These models are designed to characterize primary pollutants that are emitted directly into the atmosphere and, in some cases, secondary pollutants that are formed as a result of complex chemical reactions within the atmosphere, based on inputs of meteorological data and source information like emission rates and stack height. From ozone and particulate matter control strategies assessment to evaluation of acid deposition and air toxics, photochemical air quality models are widely used to support policy analysis as part of the decision-making process. These photochemical models are large-scale air quality models that simulate the changes of pollutant concentrations in the atmosphere using a set of governing equations characterizing the chemical and physical processes in the atmosphere. These models are applied at multiple spatial scales from local, regional, national, and global.

Air quality models can be a powerful regulatory tool for comparing the efficacy of various emissions control strategies and policy decisions. However, due to the often enormous computational costs and the complication of the required emission inputs and processing, using complex air quality models to generate outputs to meet time-pressing requirements of policy analysis always presents a challenge and is typically inefficient, if not ineffective. A promising tool for addressing this issue, Response Surface Modeling (RSM), has been developed by utilizing advanced statistical techniques to characterize the relationship between model outputs and input parameters in a highly economical manner. The RSM is a metamodel of a model (i.e., air quality model); it is a reduced-form prediction model using statistical correlation structures to approximate model functions through the design of complex multi-dimension experiments. The RSM technique has been successfully tested and evaluated for PM_{2.5} and ozone, respectively.² In this section, we describe the development of the multi-pollutant RSM application using the Community Multi-Scale Air Quality (CMAQ) Modeling System developed at EPA. The processes involved in developing the multi-pollutant RSM application using CMAQ will be discussed, including the selection of modeling domain and configuration, development of multi-dimension experimental design for control strategies, and implementation and validation of the RSM technique (Figure III-1). Within the section describing implementation and validation of the RSM technique we will discuss the generation of air quality model simulations, statistical

² U.S. Environmental Protection Agency, 2006. Technical Support Document for the Proposed Mobile Source Air Toxics Rule: Ozone Modeling, Office of Air Quality Planning and Standards, Research Triangle Park, NC.

modeling and construction of representative surfaces, model validation, and development of the Visual Policy Analyzer, a standalone software tool for viewing and manipulating the response surface.

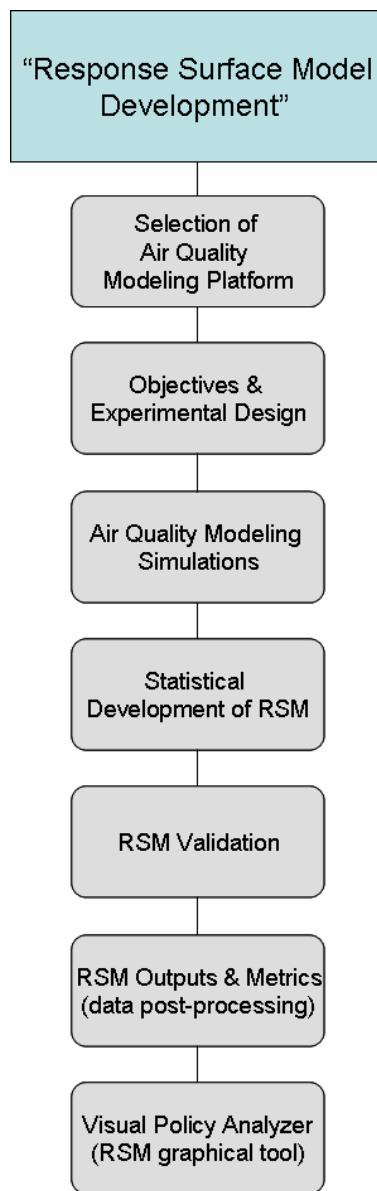


Figure III-1. Flow diagram identifying key steps within the development of Response Surface Modeling.

A. Use of RSM

The RSM is intended to provide a modeling surrogate tool that can effectively simulate real-time PM impacts for a variety of regulatory alternatives for use in Regulatory Impact Analyses. For

example, generating estimates of the health benefits of reductions in PM precursors and providing screening level estimates of the impacts of control strategies on NAAQS design values are functions the RSM supports. While the RSM may not provide a complete picture of all changes necessary to reach various alternative standards nationwide, it is highly useful in the context of providing illustrative control scenarios for selected areas, and understanding the contribution of different source categories, source regions and pollutant emissions to air quality across the U.S. The RSM can be used in a variety of ways: (1) strategy design and assessment (e.g. comparison of urban vs. regional controls; comparison across sectors; comparison across pollutants); (2) optimization (develop optimal combinations of controls to attain standards at minimum cost); (3) model sensitivity (systematically evaluate the relative sensitivity of modeled ozone and PM levels to changes in emissions inputs).

B. Technical Approaches and Experimental Design of RSM

B.1 CMAQ Modeling Platform for RSM

Multi-pollutant (particulate matter (PM_{2.5}) and ozone) air quality modeling was performed using the Community Multi-scale Air Quality (CMAQ) model for the development of an integrated PM_{2.5} and ozone Response Surface Model (RSM). Precursors of both PM_{2.5} and ozone and their transformations and transport were modeled. For the purpose of the PM_{2.5} NAAQS RIA, model evaluation and control strategy assessment will focus exclusively on PM_{2.5}, its constituents and precursors. Currently, the RSM is used as the foundation to conceptualize control strategy scenarios and resulting outcomes. Likewise, the use of RSM will be extended to investigate and better inform sector based control scenarios based on a multi-pollutant approach (i.e., ozone and PM analyses).

CMAQ is a three-dimensional regional grid-based air quality model designed to simulate particulate matter and ozone concentrations and deposition over large spatial scales (e.g., over the contiguous U.S.) over an extended period of time (e.g., up to a year).³ The CMAQ model includes state-of-the-science capabilities for conducting urban to regional scale simulations of multiple air quality issues, including tropospheric ozone, fine particles, toxics, acid deposition, and visibility degradation. The CMAQ model is a publicly available (supported by the Community Modeling and Analysis System (CMAS) Center; <http://www.cmascenter.org/>), peer reviewed, state-of-the-science model consisting of a number of science attributes that are critical for simulating the oxidant precursors and non-linear organic and inorganic chemical relationships associated with the formation of sulfate, nitrate, and organic aerosols. CMAQ also

³ Dennis, R.L., Byun, D.W., Novak, J.H., Galluppi, K.J., Coats, C.J., and Vouk, M.A., 1996. The next generation of integrated air quality modeling: EPA's Models-3, *Atmospheric Environment*, 30, 1925-1938.

Byun, D.W., and Ching, J.K.S., Eds, 1999. Science algorithms of EPA Models-3 Community Multiscale Air Quality (CMAQ) modeling system, EPA/600/R-99/030, Office of Research and Development, U.S. Environmental Protection Agency.

Byun, D.W., and Schere, K.L., 2006. Review of the Governing Equations, Computational Algorithms, and Other Components of the Models-3 community Multiscale Air Quality (CMAQ) Modeling System. *J. Applied Mechanics Reviews*, Accepted.

simulates the transport and removal of directly emitted particles which are speciated as elemental carbon, crustal material, nitrate, sulfate, and organic aerosols.

The RSM is based on air quality modeling using CMAQ version 4.4 with a 36 km horizontal domain (148 x 112 grid cells) and 14 vertical layers. The modeling domain encompasses the contiguous U.S. and extends from 126 degrees to 66 degrees west longitude and from 24 degrees north latitude to 52 degrees north latitude (Figure III-2).

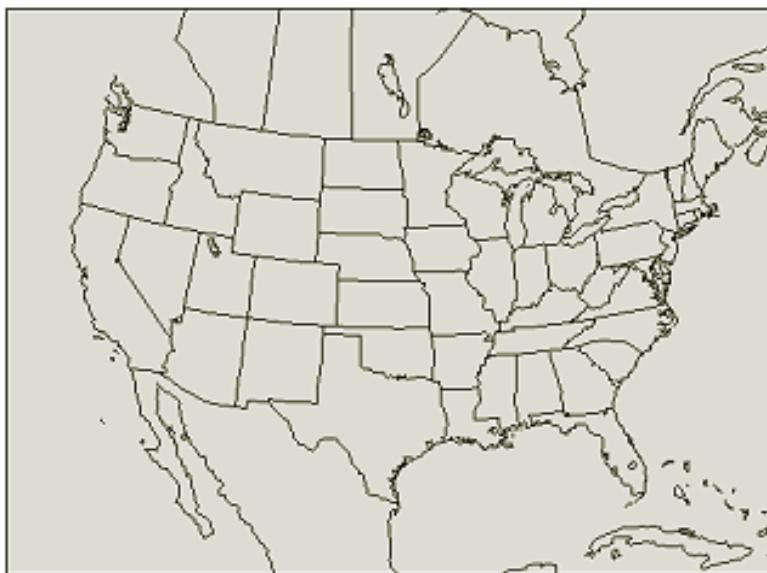


Figure III-2. Map of the CMAQ and RSM modeling domain used for PM_{2.5} NAAQS Review

This CMAQ version 4.4 reflects updates to earlier versions in a number of areas to improve the underlying science and address comments from the peer review. The improvements in version 4.4 compared to earlier versions include (1) use of a state-of-the-science inorganic nitrate partitioning module (ISORROPIA) and updated gaseous, heterogeneous chemistry in the calculation of nitrate formation, (2) a state-of-the-science secondary organic aerosol (SOA) module that includes a more comprehensive gas-particle partitioning algorithm from both anthropogenic and biogenic SOA, (3) an in-cloud sulfate chemistry module that accounts for the nonlinear sensitivity of sulfate formation to varying pH, and (4) an updated CB-IV gas-phase chemistry mechanism and aqueous chemistry mechanism that provide a comprehensive simulation of aerosol precursor oxidants.

A complete description of CMAQ, meteorological, emission, and initial and boundary condition inputs used for this analysis are discussed in the CAIR TSD.⁴ Before one can combine multiple CMAQ simulations into a metamodel, one must ensure that the base simulations show adequate model performance. An operational model performance evaluation for PM_{2.5} and its related

⁴ U.S. Environmental Protection Agency, March 2005a. Technical Support Document for the Clean Air Interstate Rule: Air Quality Modeling, Office of Air Quality Planning and Standard, Research Triangle Park, NC. (Docket No. OAR-2005-0053-2151).

speciated components (e.g., sulfate, nitrate, elemental carbon, organic carbon, etc.) as well as deposition of ammonium, nitrate, and sulfate for 2001 was performed in order to estimate the ability of the CMAQ modeling system to replicate base year concentrations.⁵ The purpose of the base year PM air quality modeling was to reproduce the atmospheric processes resulting in formation and transport of fine particulate matter across the U.S.

B.2 Statistical Development of RSM

Response surface models typically use a limited number of complex model runs at a set of statistically selected points in a design space, e.g. mobile NOx emission levels 10 to 120 percent of current levels. By using design of experiments theory, the response surface method can improve the accuracy of model approximations while minimizing costly model runs.⁶ The response-surface method uses statistical techniques to relate a response variable (in this case annual and 98th percentile daily PM_{2.5} at receptor sites throughout the U.S.) to a set of factors that are of interest, e.g. emissions of precursor pollutants from particular sources and locations.

To develop a response surface approximation to CMAQ, a sophisticated interpolation approach (i.e., multidimensional kriging approach) was used, implemented through the MIXED procedure in SAS (2005) software.⁷ This modeling approach is well suited to data generated using a non-stochastic computer model, and can approximate highly nonlinear surfaces as long as they are locally continuous.

The predicted changes in PM_{2.5} in each CMAQ grid cell were modeled as a function of the weighted average of the modeled responses in the experimental design. The weight assigned to a particular modeled output depends on the Euclidean distance between the factor levels defining the policy to be predicted and the factor levels defining the CMAQ experimental run.

We specify a model structure that assumes that the response of CMAQ predicted concentrations to changes in emissions is a Gaussian stochastic process, such that

$$(1) \quad Y(\vec{x}) = \beta_0 + Z(\vec{x})$$

⁵ U.S. Environmental Protection Agency, March 2005b. Updated CMAQ Model Performance Evaluation for the 2001 Annual Simulation, Office of Air Quality Planning and Standard, Research Triangle Park, NC. (Docket No. OAR-2005-0053-2149).

⁶ The experimental design component consists of the selection of the sets of input variables, $d=(d_1, d_2, \dots, d_k)$, (i.e., selection of the emissions control strategy within the defined experimental region) at which to run the experiment and obtain a response. There are a large number of methods, and a correspondingly large volume of literature, available for designing an experiment (Box, G.E.P., and Draper, N.R. (1987). Empirical Model-Building and Response Surfaces. John Wiley and Sons, New York.; Pukelsheim, F. (1993). Optimal Design of Experiments. John Wiley and Sons, New York. Dean, A.M. and Voss, D. (1999). Design and Analysis of Experiments. Springer-Verlag, New York.)

⁷ SAS Institute, 2005. SAS Online Doc© 9.1.3. Accessed online at <http://support.sas.com/onlinedoc/913/docMainpage.jsp>

where Y is the species output metric, \vec{x} is the vector of emissions factors (defined between 0 and 1.2), β_0 is the mean response (estimated), and $Z(\vec{x})$ is a Gaussian process assumed to have mean 0, variance σ^2 , and a correlation structure defined by

$$(2) \quad R(\vec{x}_i, \vec{x}_j) = \sigma^2 \left(\exp(-\text{dist}^2(\vec{x}_i, \vec{x}_j)) \right) / \theta^2$$

where \vec{x}_i is the vector of factor values associated with run i of the experimental design, $\text{dist}^2(\vec{x}_i, \vec{x}_j)$ is the squared distance between the vectors of factors associated with runs i and j , and θ and σ^2 are parameters to be estimated. The variance (σ^2) and correlation (θ) parameters are fit using maximum likelihood methods.

Based on the estimated parameters and the available CMAQ model results, the predicted value for a given species metric is obtained using the equation

$$(3) \quad \hat{y}(\vec{x}_0) = \hat{\beta}_0 + r'(\vec{x}_0)R^{-1}(\vec{y} - \hat{\beta}_0)$$

where \vec{x}_0 is the vector of factor values for which we want a predicted species response, $\hat{y}(\vec{x}_0)$ is the prediction at \vec{x}_0 , $\hat{\beta}_0$ is the estimate of β_0 , R is the matrix of all design points correlated with each other based on equation (2) (with $\hat{\theta}$ as the estimate of θ), R^{-1} is the inverse of R , $r'(\vec{x}_0)$ is the transpose of the vector of correlations, between \vec{x}_0 and each of the design points, namely, $r'(\vec{x}_0) = (R(\vec{x}_0, \vec{x}_1), \dots, R(\vec{x}_0, \vec{x}_n))^T$, and \vec{y} is the vector of the particular species response metrics associated with the design points.

In this specific application, the design points are the 180 \vec{x} vectors, each of length 12, consisting of the selected 12 emission control factors defined below in *Section B.5*. The vector \vec{x}_0 consists of the values of the 12 factors for which the predicted species metric is desired. \vec{y} is the vector of CMAQ modeled species metric values and has 180 elements. The matrix R is formed as a 180x180 matrix with a row and column for each design point. The value in each cell of R is determined by equation (2).

The RSM experimental design covers a change in the baseline emissions of zero to 120 percent, utilizing a staged Latin Hypercube statistical method. This statistical method follows a space filling design within the policy area and policy controls in order to accurately capture the linear and nonlinear interactions among pollutants. The Latin hypercube design retains flexibility, which accommodates the number of runs selected based on limitations (computer resources). A total of 180 CMAQ model runs were conducted (a base case run plus 179 control runs). The model runs were broken into two stages, 120 runs in the first stage and 60 runs each in stage two. This allowed for faster development of preliminary surfaces and allowed testing of additional predictive power for additional model runs. The set of CMAQ simulations provide inputs to the statistical response surface modeling. The complete list of model runs and corresponding control scenarios (selection of policy factor controls) are provided in Appendix A. The CMAQ model

was applied for the 2010 CAIR projection baseline in order to provide annual PM_{2.5} concentrations, visibility, and deposition estimates. The CMAQ model was run for 4 months, one month from each season, February, April, July, October, in order to reduce computational time for such a large number of annual model runs. These months were chosen based on greatest predictability of the quarterly mean. Each quarterly run included a 5-day ramp-up (i.e., "spin-up") period designed to minimize the influence of the initial concentration fields (i.e., initial conditions) used at the start of the model run. The development of initial condition concentrations is described in the CAIR TSD. The ramp-up periods used for the RSM CMAQ applications are as follows:

- First quarter ramp-up period is January 27 - 31, 2001
- Second quarter ramp-up period is March 27 - 31, 2001
- Third quarter ramp-up period is June 26 - 30, 2001
- Fourth quarter ramp-up period is September 26 - 30, 2001

Model predictions from these ramp-up periods were discarded and not used in analyses of the modeling results.

Once the response surface model has been generated, it can be used to simulate the functions of the more computationally expensive atmospheric chemistry model. The RSM can be used to derive analytical representations of model sensitivities to changes in model inputs. For example, the RSM is designed to show how CMAQ (air quality model) predicts the atmosphere would respond to emission reductions for selected sources and pollutants, though it does not provide how those reductions in pollutants can be accomplished (i.e. specific control technologies). The RSM allows for comparison on an equal footing of controls for different source/pollutant combinations, and between local and regional sources. It should be noted that because RSM is built from CMAQ air quality model runs, it therefore has the same strengths and limitations of the underlying model and its inputs.

B.3 Modeling Scenarios and Emission Inventories and Sectors

The PM NAAQS RIA modeled relative changes in air quality for the entire U.S. using the Response Surface Model (RSM) applied to the 2010 regulatory Base Case developed by EPA as part of the analysis for the Clean Air Interstate Rule (CAIR). While CAIR targets controls of SO₂ and NO_x in the Eastern United States, the other rules/programs in the 2010 baseline include Clean Air Non-Road Diesel Rule, Heavy Duty Diesel Rule, Tier 2, and the NO_x SIP Call. Because our base year of analysis is 2015, we extrapolate the baseline year from 2010 to 2015 and to include CAIR controls.⁸ 2015 serves as a logical base year for analysis because it is a reasonable estimate of the date by which States would begin to implement controls to attain the revised standard; assuming promulgation in 2006, designations would require 3 years, and States would then have 5 years to attain. The RSM control strategy outputs are based on projected

⁸ We developed the RSM with a 2010 baseline so that it could serve the analytical needs of both the final PM NAAQS implementation rule (due in late 2006) for the current standard as well as the PM NAAQS RIA for the revised standard.

2015 post-CAIR emissions inventories and therefore reflect any uncertainties in those inventories. Certain source/pollutant inventories may be more uncertain than others.

B.4 Development of SMOKE/CMAQ Utility Interface Module

A pre-requisite task of the integrated PM_{2.5} and ozone CMAQ RSM effort was to develop an interface utility module within the CMAQ to allow the model to directly read the pre-merged SMOKE emission files (e.g., 3-D point sources, 2-D mobile sources, 2-D area sources, 2-D biogenic, sources, etc.), and more importantly, allow the model to directly control the % emission reduction/increase for the RSM scenarios runs that are needed for constructing the PM_{2.5} and O₃ response surfaces. This tool increased the capacity and functionality of the operational CMAQ RSM models runs while (1) eliminating massive emission inputs for CMAQ RSM modeling (2) leading to highly efficient RSM modeling since the process can be automated to eliminate tedious manual operations. A SMOKE/CMAQ interface module has been developed as part of CMAQ system to facilitate and expedite these CMAQ RSM simulations.

B.5 Selection of Emissions Control Factors and Control Ranges

The main purpose of the RSM is to demonstrate the impact of various reductions in precursor emissions from different combinations of sources on air quality. Therefore, constraints were placed on the experimental design space, i.e. the region over which the response is studied, to a set of variables that parameterize a set of possible emissions control strategies, and evaluate the change in ambient PM_{2.5} levels that result from a change (reduction or increase) in emissions.⁹

Selection of policy factors were based on precursor emission type and source category relevant to policy analysis of interest. The experimental design carefully considered factors that would provide maximum information for use in comparing relative efficacy of different emissions control strategies. Hence, 12 variable emission control factors were selected based on precursor emission type and source category, as well as balancing computational efficiency of model runs and resources available. The selection of factors was based on three fundamental areas:

1. Type of PM and PM precursor emissions (NOx, SOx, NH₃, POC, PEC, or VOC);
2. Emissions source category (EGU point sources, NonEGU point sources, area sources (including agriculture); and
3. Location of urban areas contributing to residual PM_{2.5} (including non-road sources) after implementation of the CAIR/CAMR/CAVR and geographically separated in contribution to downwind PM_{2.5} concentrations.

The RSM can evaluate air quality changes that result from adjusting each of the following 12 emissions control factors on a local or regional basis:

1. NOx EGU = NOx IPM EGU point source emissions

⁹ Hubbell, B.J., Dolwick, P.D., Mooney, D., Morara, M., 2005. Evaluating the relative effectiveness of ozone precursor controls: Design of computer experiments applied to the comprehensive air quality model with extensions (CAMx), Air and Waste Management Association Conference Proceedings.

2. NOx NonEGU Point and Area = NOx IPM Non-EGU point source, area source, and agricultural source emissions
3. NOx Mobile = NOx nonroad source and mobile source emissions
4. SOx EGU = SOx IPM EGU point source emissions
5. SOx NonEGU Point = SOx IPM Non-EGU point source emissions
6. SOx Area = SOx area source and agricultural source emissions
7. NH₃ Area = Ammonia area source and agricultural source emissions
8. NH₃ Mobile = Ammonia non-road source and mobile source sources
9. POC/PEC Point (EGU and NonEGU) = Elemental carbon and organic carbon IPM EGU point source and IPM Non-EGU point source emissions
10. POC/PEC Mobile = Elemental carbon and organic carbon nonroad source and mobile source emissions
11. POC/PEC Area = Elemental carbon and organic carbon area source and agricultural source emissions
12. VOC All = Volatile organic carbon IPM EGU point source, IPM Non-EGU point source, area source, agricultural source, nonroad source, and mobile source emissions¹⁰

Source groupings with small contributions to emissions were grouped with similar larger source groupings for efficiency (Figure III-3). NonEGU Area NOx and SOx sources were primarily smaller industrial combustion sources, such as coal, oil, and natural gas powered boilers and internal combustion engines. Agricultural area sources were only significant contributors to ammonia emissions. VOC sources were lumped together because VOCs are not expected to influence PM levels significantly.

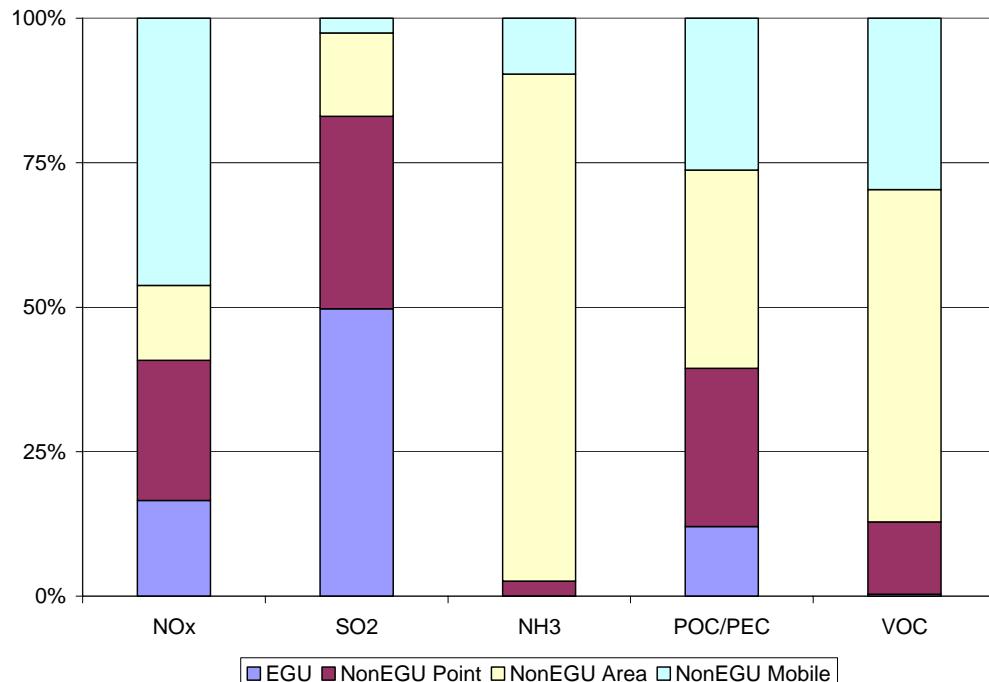


Figure III-3. National analysis of source contributions to emissions sectors.¹¹

¹⁰ This version of the RSM did not address direct emissions of inorganic metallic particles from sources such as steel mills and other industrial processes.

B.6 Selection of Regional vs. Local Impact

Based on the selection of 12 control factors, the RSM experimental design applied a regional design allowing for development of independent response surfaces for particular urban areas, as well as a generalized response surface (i.e. air quality response) for all other locations (outside of the particular urban areas). A rigorous area-of-influence analysis was conducted for the selection of RSM urban locations to discern the degree of overlap between different urban areas in terms of air quality impacts, and to tease out local versus regional impacts. The area-of-influence analysis incorporated control model runs where emissions were zeroed out in many urban areas. Results of these control runs for the months of February and July are shown in Figures III-4 and III-5. The area-of-influence analysis concluded that ambient PM_{2.5} in each of the 9 urban areas is largely independent of the precursor emissions in all other included urban areas. This conclusion is also supported and clearly seen in Figure III-9 (demonstrating the extent of the air quality influence region), where reductions (represented as spikes in figure display) of PM_{2.5} based on an example of local precursor controls are shown. Thus, selection of these areas allows the RSM to analyze air quality changes in these 9 urban areas and associated counties independent of one another. These 9 urban areas include New York / Philadelphia (combined), Chicago, Atlanta, Dallas, San Joaquin, Salt Lake City, Phoenix, Seattle, and Denver. Figure III-6 displays these 9 urban areas based on the CMAQ model 36-km grids.

¹¹ The data in Figure III-3, which are based on the emissions inventory developed for CAIR, suggest EGUs contribute on the order of 10% of primary organic carbon. More recently, EPA has reviewed data on primary EGU emissions and concluded these estimates are approximately an order of magnitude too high. This suggests that the control costs and reductions associated with any controls for EGU POC are of little relevance. EPA has since corrected this portion of the inventory for future analyses and modeling.

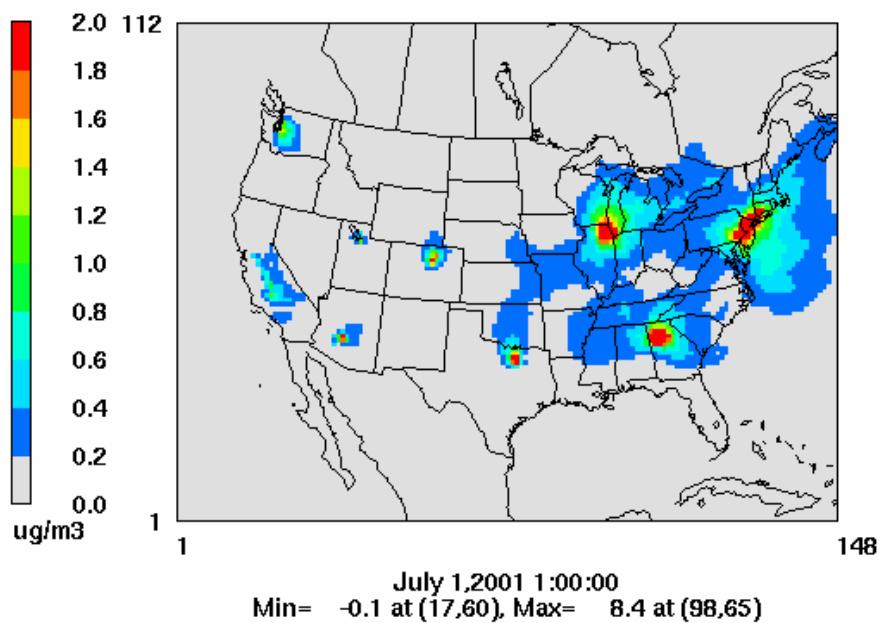


Figure III-4. PM_{2.5}: Areas of influence for nine selected RSM urban locations for the monthly average of July 2001.

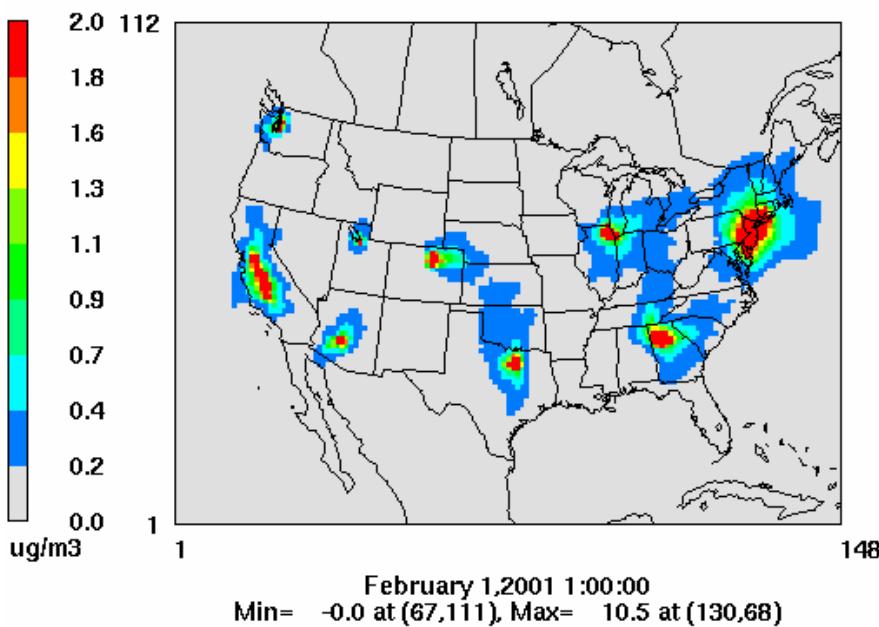


Figure III-5. PM_{2.5}: Areas of influence for nine selected RSM urban locations for the monthly average of February 2001.

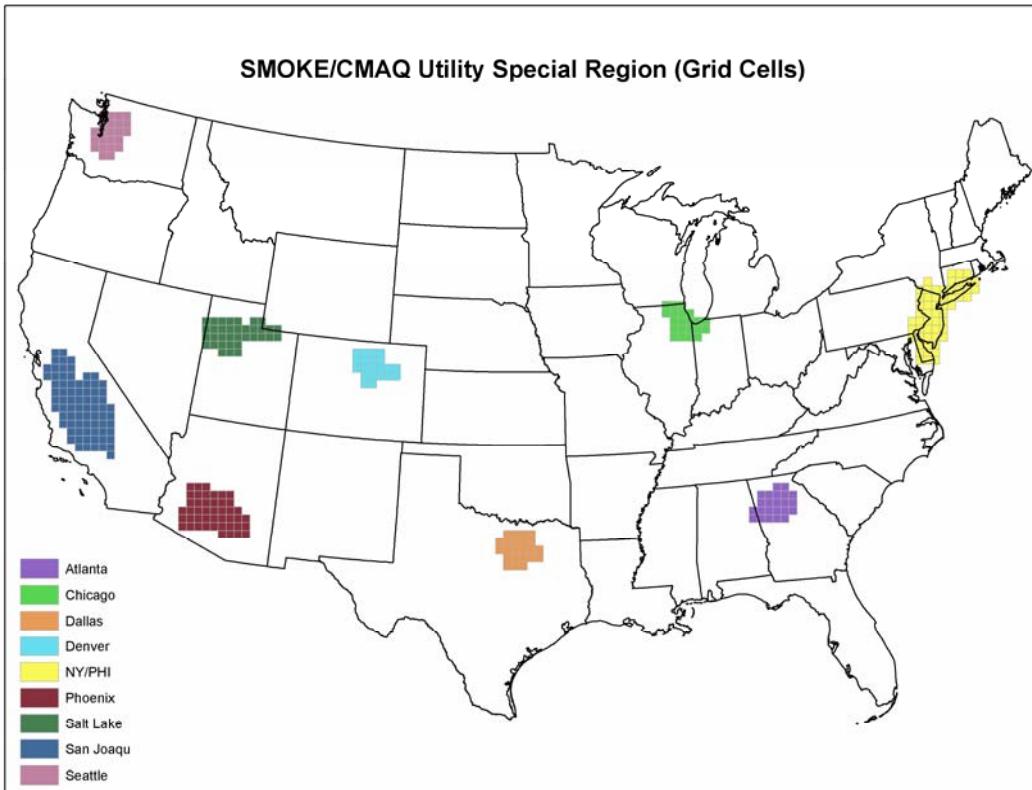


Figure III-6. Map of the CMAQ modeled 36-km grids for nine urban areas modeled.

B.7 Output Metrics for CMAQ RSM PM_{2.5}

Several output measures of PM_{2.5} levels were extracted from the CMAQ model runs which are of particular interest for this PM NAAQS RIA. The quarterly mean and annual 98th percentile daily average of sulfate, nitrate, crustal, elemental carbon, organic carbon, and ammonium concentrations were outputted to influence development of RSM surfaces. Projected PM_{2.5} annual and daily design values at monitored locations were used to assess how the attainment status of an area might be affected by different control strategies.

In general, the procedures for projecting both the annual and daily PM_{2.5} design values are based on using model predictions in a relative sense. In this manner, the 2001 Base Year predictions and the 2015 future predictions are coupled with ambient data to forecast future concentrations. This approach is consistent with the EPA draft guidance documents for modeling PM_{2.5}.¹²

Projected *annual design values* were calculated using the Speciated Modeled Attainment Test (SMAT) approach, the details of which can be found in the report "Procedures for Estimating Future PM_{2.5} Values for the CAIR Final Rule by Application of the (Revised) Speciated Modeled

¹² U.S. Environmental Protection Agency, 2001. Draft Guidance on the Use of Models and Other Analyses in Attainment Demonstrations for the PM_{2.5} NAAQS.

Attainment Test (SMAT)".¹³ Below are the steps we followed for projecting future PM_{2.5} concentrations. These steps were performed to estimate future case concentrations at each FRM monitoring site. The starting point for these projections is the average of the 1999-2001, 2000-2002, and 2001-2003 design values at each monitoring site. By averaging 1999-2001, 2000-2002, and 2001-2003, the value from 2001 is weighted three times, whereas, values for 2000 and 2002 are each weighted twice, and 1999 and 2003 are each weighted once. This approach has the desired benefits of (1) weighting the PM_{2.5} values towards the middle year of the five-year period, which is the 2001 Base Year for our emissions projections, and (2) smoothing out the effects of year-to-year variability in emissions and meteorology that occurs over the full five-year period. This approach provides a robust estimate of current air quality for use as a basis for future year projections.

Step 1: Calculate quarterly mean ambient concentrations for each of the six major components of PM_{2.5} (i.e., sulfate, nitrate, ammonium, elemental carbon, organic carbon, and crustal material) using the component species concentrations estimated for each FRM site and estimate the species fractions at each FRM site, then multiply the average 1999-2003 FRM quarterly mean concentration at each site by the estimated fractional composition of PM_{2.5} species, by quarter (e.g., 20 percent sulfate multiplied by 15.0 µg/m³ of PM_{2.5} equals 3 µg/m³ sulfate).

Step 2: Calculate quarterly average Relative Reduction Factors (RRFs) for sulfate, nitrate, elemental carbon, organic carbon, and crustal material. The species-specific RRFs for the location of each FRM are the ratio of the 2015 CAIR case to 2001 Base Year quarterly average model predicted species concentrations. The species-specific quarterly RRF are then multiplied by the corresponding 1999-2003 quarterly species concentration from Step 1. The result is the future case quarterly average concentration for each of these species.

Step 3: Calculate quarterly average concentrations for ammonium and particle-bound water. The future case concentrations for ammonium are calculated using the future case sulfate and nitrate concentrations determined from Step 2 along with the degree of neutralization of sulfate (held constant from the base year). Concentrations of particle-bound water are calculated using the empirical relationship derived from the AIM model using the future case concentrations of sulfate, nitrate, and ammonium as inputs.

Step 4: Calculate the mean of the four quarterly average future case concentrations to estimate future annual average concentration for each component specie. The annual average concentrations of the components are added together to obtain the future annual average concentration for PM_{2.5}.

Step 5: For counties with only one monitoring site, the projected value at that site is the future case value for that county. For counties with more than one monitor, the highest value in the county is selected as the concentration for that county.

¹³ U.S. Environmental Protection Agency, 2004. "Procedures for Estimating Future PM2.5 Values for the CAIR Final Rule by Application of the (Revised) Speciated Modeled Attainment Test (SMAT)- Updated 11/8/04".

The *daily design values* are based on applying a similar projection method. As with the annual design value, monitor data for the years 1999 to 2003 are used as the basis for the projection. There are several steps in the projection for each of the base years of monitoring data:

Step 1: The first step in projecting the daily design value is to identify the maximum daily average PM_{2.5} concentration in each quarter that is less than or equal to the annual 98th percentile value over the entire year.

Step 2: These quarterly PM_{2.5} concentrations are then separated into their component species by multiplying the quarterly maximum daily concentration at each site by the estimated fractional composition of PM_{2.5} species, by quarter, based on the observed species fractions from speciation monitors in 2002.

Step 3: The component species are then projected by multiplying each species concentration by the quarterly relative reduction factors for each species derived from the 2015 and 2001 PM2.5 air quality modeling.

Step 4: The projected species components are then summed to obtain a PM_{2.5} concentration for each quarter that represents a potential daily design value.

Step 5: The projected daily design value for each monitor in 2015 is then calculated as the maximum of the projected quarterly values.

This procedure is repeated for each of the years of monitoring data, 1999-2003. A weighted average projected 2015 design value is then calculated by averaging the projections for 3 year intervals (1999-2001, 2000-2002, 2001-2003), and then averaging over the three interval averages. The projected daily design value for a county is then calculated as the maximum weighted average design value (1999 - 2003) across all monitors within a county.

In addition to the aforementioned PM_{2.5} metrics, other outputs were extracted however; they are not currently used for the proposed PM NAAQS RIA. These metrics include: annual and quarterly nitrogen and sulfate deposition, annual mean of visibility (light extinction coefficient of the average 20% worst days, average of 20% best days), daily one-hour ozone maximum, 12-hour daylight average ozone, and daily 24-hour average ozone. The following is the translation of CMAQ output species into PM_{2.5} and related species (units= $\mu\text{g}/\text{m}^3$):

$$\begin{aligned}\text{PM2.5 mass:} \quad & \text{PM2.5} = \text{ASO4I} + \text{ASO4J} + \text{ANH4I} + \text{ANH4J} + \\ & \text{ANO3I} + \text{ANO3J} + \text{AORGAI} + \text{AORG AJ} + \\ & 1.167*\text{AORGPAI} + 1.167*\text{AORGPAJ} + \\ & \text{AORGBI} + \text{AORGBJ} + \text{AECI} + \text{AECJ} + \\ & \text{A25I} + \text{A25J}\end{aligned}$$

$$\begin{aligned}\text{Sulfate PM:} \quad & \text{PM_SULF} = \text{ASO4I} + \text{ASO4J} \\ \text{Nitrate PM:} \quad & \text{PM_NITR} = \text{ANO3I} + \text{ANO3J} \\ \text{Ammonium PM:} \quad & \text{PM_AMM} = \text{ANH4I} + \text{ANH4J} \\ \text{Organic aerosols:} \quad & \text{PM_ORG_TOT} = \text{AORGAI} + \text{AORG AJ} + 1.167*\text{AORGPAI} +\end{aligned}$$

	1.167*AORGPAJ + AORGBI + AORGBC
Elemental Carbon:	PM_EC = AECI + AECJ
Crustal Material (soils):	PM_OTH = A25I +A25J
Coarse PM:	PM_COARS = ASOIL +ACORS + ASEAS

where, PM_SULF is particulate sulfate ion, ASO4J is accumulation mode sulfate mass, ASO4I is aitken mode sulfate mass, PM_NITR is particulate nitrate ion, ANO3J is accumulation mode nitrate mass, ANO3I is aitken mode aerosol nitrate mass, ANH4J is accumulation mode ammonium mass, ANH4I is aitken mode ammonium mass, PM_ORG_TOT is total organic aerosols, AORGAI is accumulation mode anthropogenic secondary organic mass, AORGAI is aitken mode anthropogenic secondary organic mass, AORGPAJ is accumulation mode primary organic mass, AORGPAI is aitken mode primary organic mass, AORGBC is accumulation mode secondary biogenic organic mass, AORGBC is aitken mode biogenic secondary biogenic organic mass, PM_EC is primary elemental carbon, AECJ is accumulation mode elemental carbon mass, AECI is aitken mode elemental carbon mass, PM_OTH is primary fine particles (other unspediated primary PM2.5), A25J is accumulation mode unspecified anthropogenic mass, A25I is aitken mode unspecified anthropogenic mass. PM2.5 is defined as the sum of the individual species. Note that a factor of 1.167 was applied to AORGPAI and AORGPAJ since the CMAQ model assumed the conversion factor between organic carbon to organic mass is 1.2 for primary organic aerosol emission and measurements assumed the conversion factor of 1.4.

B.8 RSM Graphical Tool: Visual Policy Analyzer

The RSM will be part of an integrated suite of 3 distinct tools, the Air Strategy Assessment Program (ASAP) which EPA is creating. ASAP uses a systematic approach for linking data and models for integrated assessments. This suite of tools is intended to facilitate multipollutant screening analyses of multiple air quality control strategies. ASAP serves as a graphical user interface that allows for easy inputs by the user with simultaneous analysis features (graphs and maps). RSM provides information on air quality responses to reductions of pollutants for various sectors. Within the ASAP framework, RSM provides this information in the form of graphical displays: bar charts, pollutant/sector stacked bar charts, and histograms.

The Visual Policy Analyzer (VPA) tool was developed as a graphically based analysis tool for interacting with the RSM. The VPA tool functions outside of the ASAP framework. The VPA allows for simultaneous viewing of inputs of emissions changes on multiple model outputs. For example, the user will be able to change any policy factor (e.g., mobile NOx levels) and see the impact on PM_{2.5} constituents (PM sulfate, PM nitrate, etc.). The future design and advancements of the VPA will be implemented to include real-time interaction with ozone, visibility, and deposition. Figures III-7 – III-9 display example outputs of the VPA.

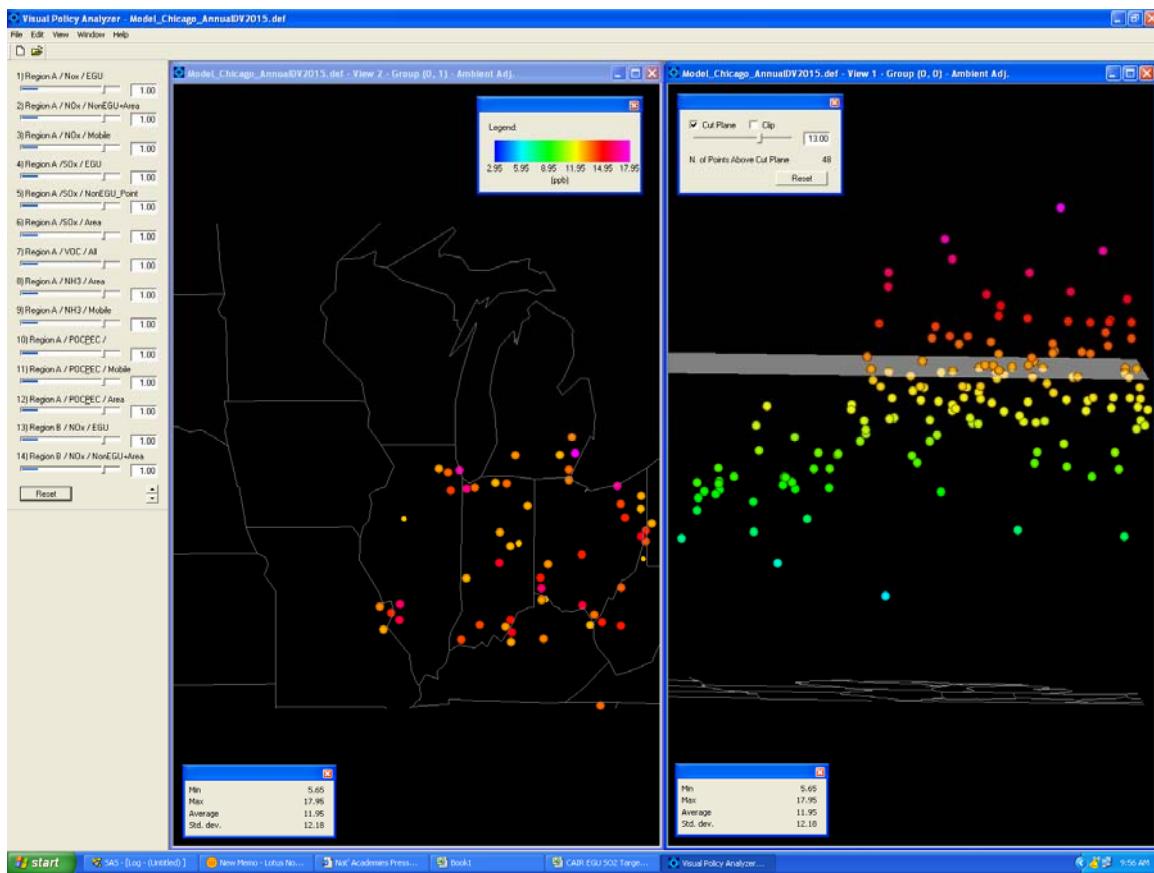


Figure III-7. VPA example: monitors with annual average PM_{2.5} Post CAIR 2015 greater than 13 µg/m³.

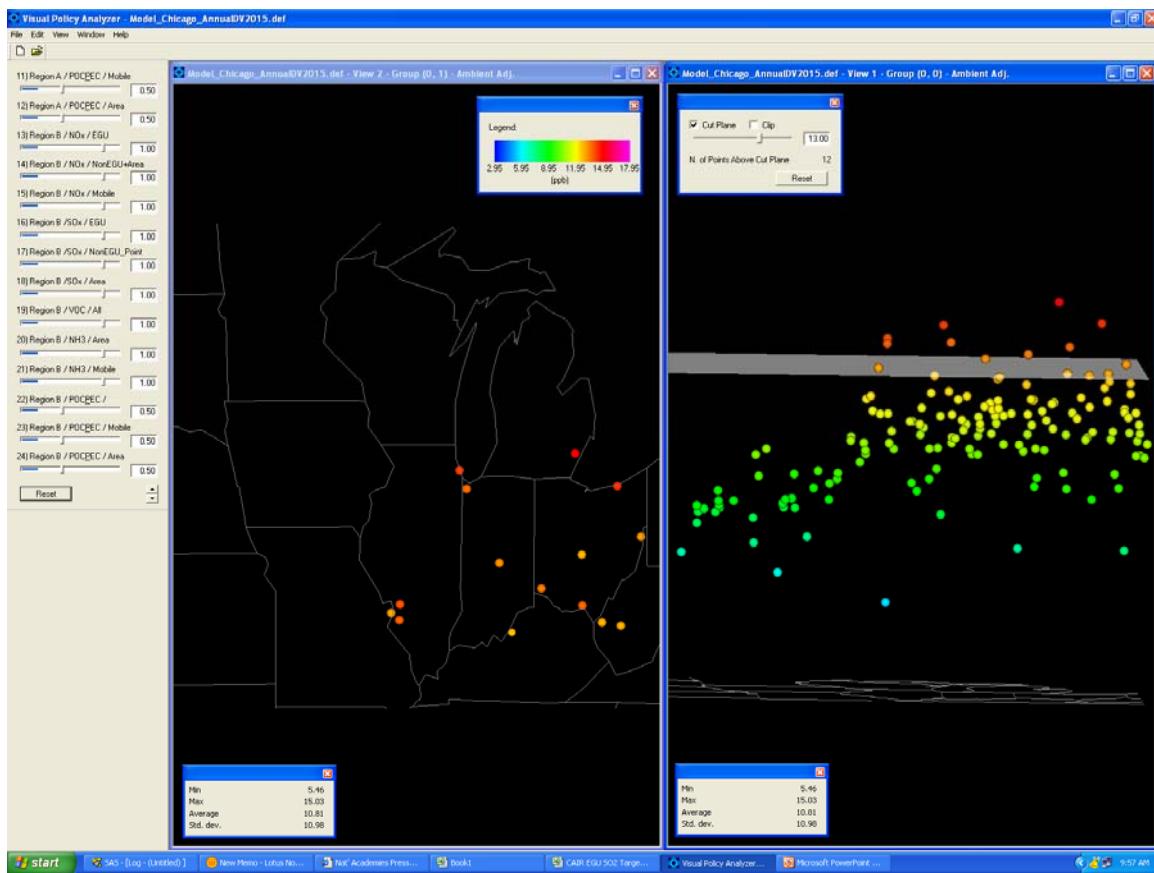


Figure III-8. VPA example: Monitors with annual average PM_{2.5} Post CAIR 2015 greater than 13 $\mu\text{g}/\text{m}^3$ after applying 50 percent reduction in carbon.

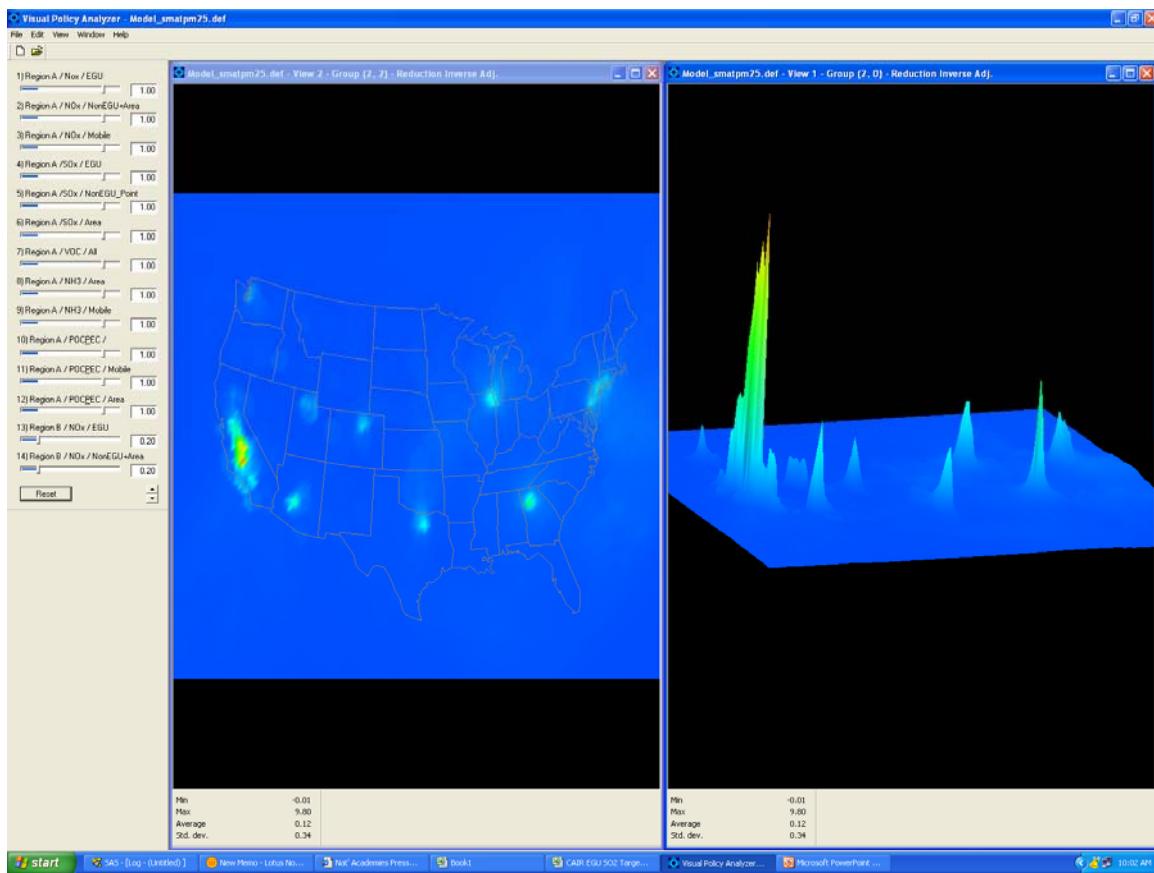


Figure III-9. VPA example: Extent of air quality influence region for the 9 selected urban areas.

IV. Validation of the Response Surface Modeling

To develop a response surface approximation to CMAQ, a multidimensional kriging approach was implemented. The RSM uses a nonlinear 24-dimensional kriging model implemented through SAS (2005)¹⁴ software. Kriging is an interpolation method based on an exponentially weighted sum of the sample data. This modeling approach is appropriate for data generated using a non-stochastic computer model, and can approximate highly nonlinear surfaces as long as they are locally continuous. The predicted changes in PM_{2.5} in each CMAQ grid cell was modeled as a function of the weighted average of the modeled responses in the experimental design. The weight assigned to a particular modeled output depends on the Euclidean distance between the factor levels defining the policy to be predicted and the factor levels defining the CMAQ experimental run.¹⁵

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

Visual inspection of prediction maps was conducted to confirm overall spatial comparability in the predicted versus modeled outputs for each of the CMAQ experimental design runs. Cross-validation was used to evaluate overall response-surface performance. For each iterative run, one of the experimental model runs is left out of the model estimation, and the RSM is then computed and used to predict the omitted run. RSM predicted changes in PM_{2.5} air quality are compared with CMAQ predictions and a standard set of model performance evaluation metrics over all grid cells is computed for the run. These evaluation metrics include: bias, error, normalized bias and error, and fractional bias and error.¹⁶ The performance metrics are defined as follows:

$$(3) \quad BIAS = \hat{y} - Y$$

$$(4) \quad ERROR = |\hat{y} - Y|$$

¹⁴ SAS Institute, 2005. SAS Online Doc© 9.1.3. Accessed online at <http://support.sas.com/onlinedoc/913/docMainpage.jsp>

¹⁵ Hubbell, B.J., Dolwick, P.D., Mooney, D., Morara, M., 2005. Evaluating the relative effectiveness of ozone precursor controls: Design of computer experiments applied to the comprehensive air quality model with extensions (CAMx), Air and Waste Management Association Conference Proceedings.

¹⁶ Boylan, J.W. Evaluation of Model Performance. Presentation for the 3rd Particulate Matter/Regional Haze/Ozone Modeling Workshop, New Orleans, LA, May 19, 2005. Accessed online at: http://cleanairinfo.com/modelingworkshop/presentations/PM_MPE_Boylan.pdf

$$(5) \quad NORMALIZED\ BIAS = \frac{\hat{Y} - Y}{Y}$$

$$(6) \quad NORMALIZED\ ERROR = \left| \frac{\hat{Y} - Y}{Y} \right|$$

$$(7) \quad FRACTIONAL\ BIAS = \frac{\hat{Y} - Y}{\left(\frac{\hat{Y} + Y}{2} \right)} \quad (\text{bounded between } -200\% \text{ and } +200\%)$$

$$(8) \quad FRACTIONAL\ ERROR = \left| \frac{\hat{Y} - Y}{\left(\frac{\hat{Y} + Y}{2} \right)} \right| \quad (\text{bounded between } 0\% \text{ and } +200\%)$$

The process is then repeated for each experimental design model run, and the distributions of the performance metrics are then examined over the total number of model runs to gauge the overall performance of the response surface across the experimental design.

During the beginning stages of the RSM evaluation, an initial cross-validation was performed for selected corresponding CMAQ and RSM grid cells for the months of July and October (Tables IV-1 and IV-2). Comparison of RSM predictions to “true” CMAQ values for July and October total PM_{2.5} show good agreement (Figures IV-1 and IV-2). In addition, comparison of RSM and CMAQ predictions for the July mean total PM_{2.5} for a particular run (run 120) is shown in Figures IV-3 and IV-4. Likewise, Figures IV-5 and IV-6 display a comparison of RSM and CMAQ predictions for October mean total PM_{2.5} for run 120.

Table IV-1. Cross-validation performance metrics for predicted July total PM_{2.5} mass (based on an evenly geographically distributed sub-sample of 700 grid cells, out of ~6,300 in the continental U.S.)

Performance Metric	Cross Validation (n=121)		
	Mean	Minimum	Maximum
Mean Bias ($\mu\text{g}/\text{m}^3$)	0.000	-0.063	0.130
Mean Error ($\mu\text{g}/\text{m}^3$)	0.027	0.006	0.130
Mean Normalized Bias (%)	0.02%	-1.58%	2.96%
Mean Normalized Error (%)	0.71%	0.21%	2.97%
Mean Fractional Bias (%)	0.01%	-1.61%	2.87%
Mean Fractional Error (%)	0.71%	0.22%	2.88%

Table IV-2. Cross-validation performance metrics for predicted October total PM_{2.5} mass (based on an evenly geographically distributed sub-sample of 700 grid cells, out of ~6,300 in the continental U.S.)

Performance Metric	Cross Validation (n=121)		
	Mean	Minimum	Maximum
Mean Bias ($\mu\text{g}/\text{m}^3$)	0.000	-0.100	0.221
Mean Error ($\mu\text{g}/\text{m}^3$)	0.047	0.007	0.221
Mean Normalized Bias (%)	0.03%	-2.70%	6.40%
Mean Normalized Error (%)	1.19%	0.18%	6.73%
Mean Fractional Bias (%)	0.01%	-1.61%	6.40%
Mean Fractional Error (%)	1.19%	0.18%	6.40%

RSM vs CMAQ

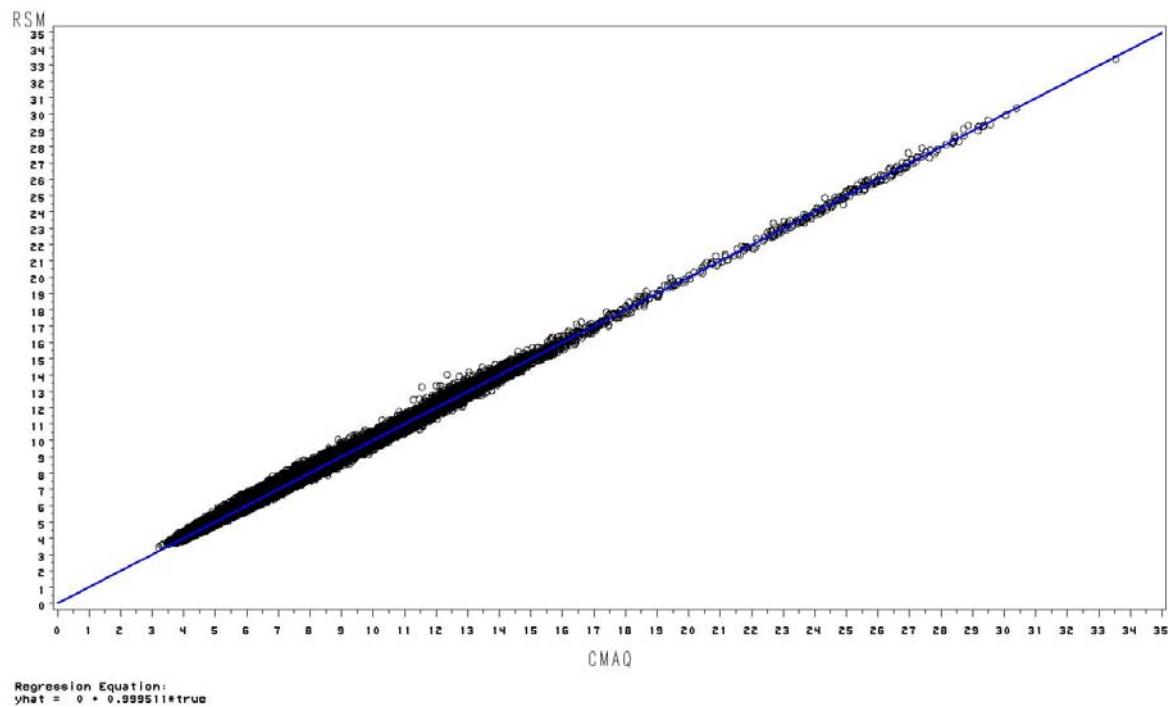


Figure IV-1. Comparison of RSM predictions to “true” CMAQ values for July total PM_{2.5}.

RSM vs CMAQ

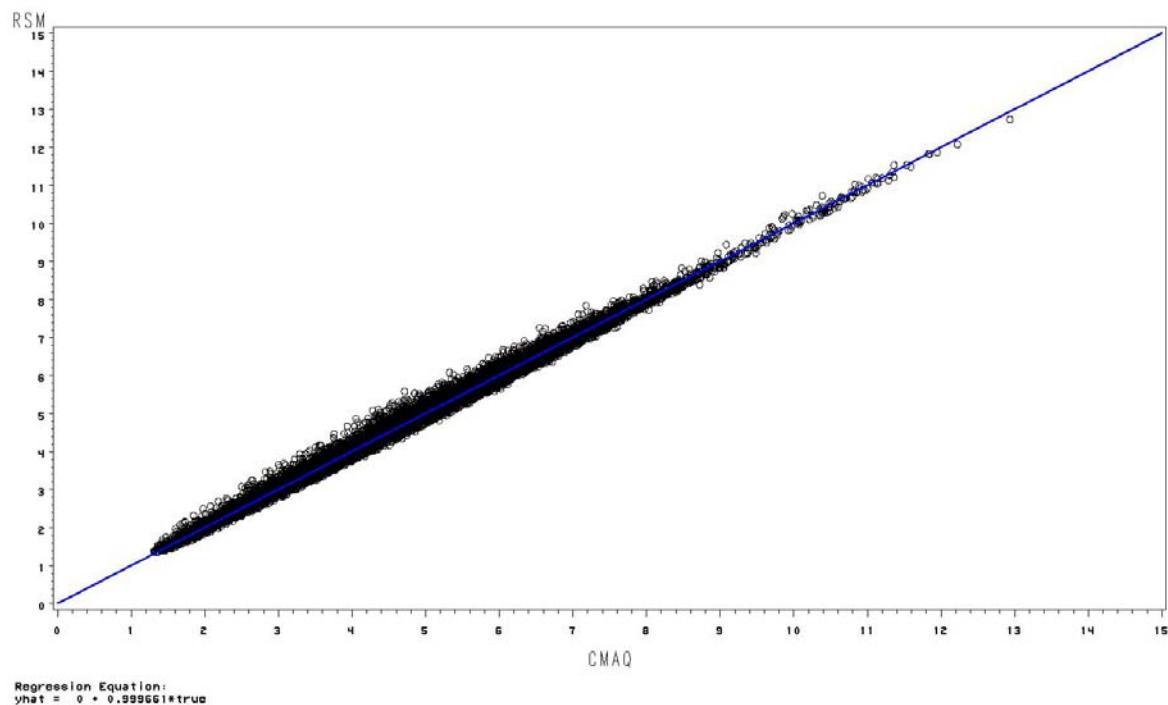
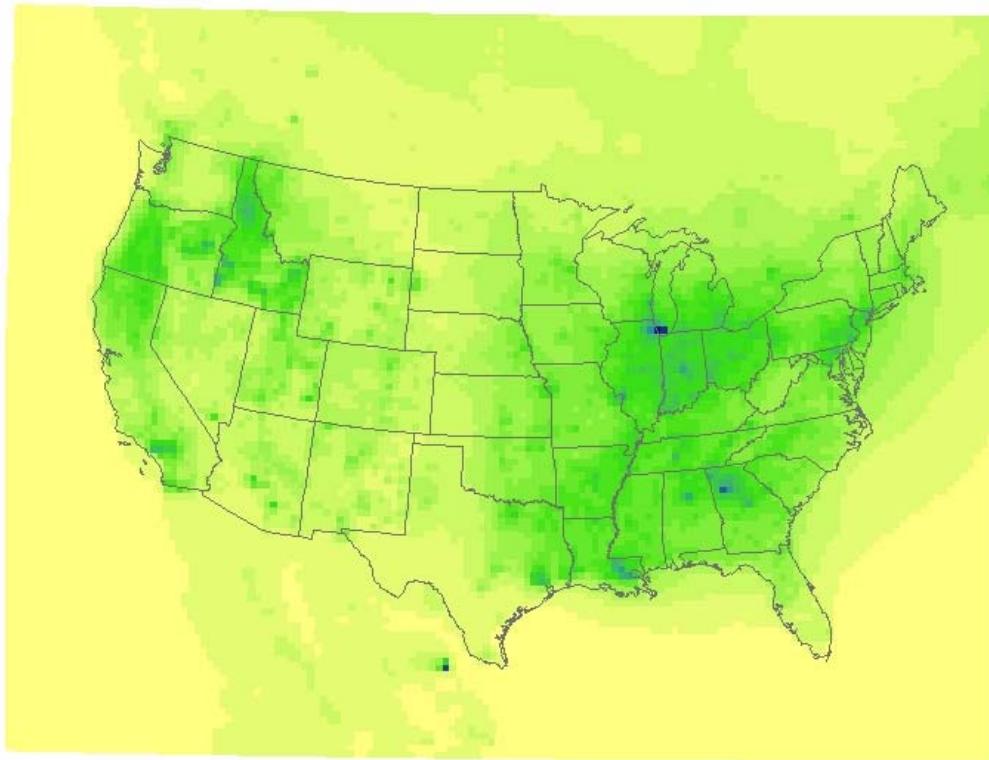


Figure IV-2. Comparison of RSM predictions to “true” CMAQ values for October total PM_{2.5}.



Total PM_{2.5} (ug/m³)

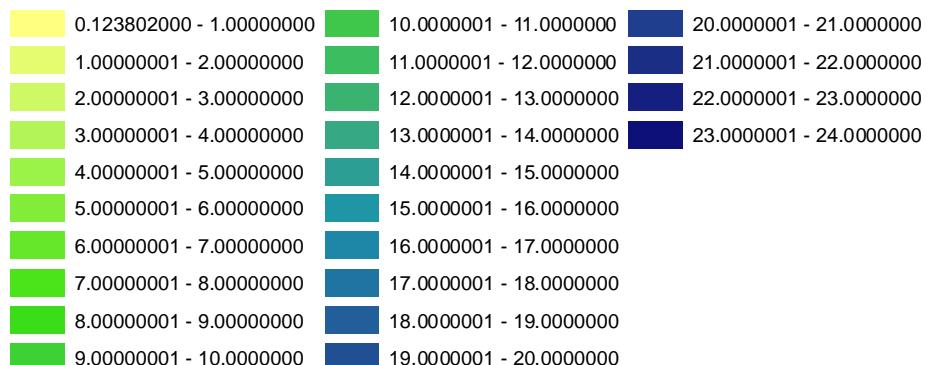


Figure IV-3. PM_{2.5} spatial gradient map for RSM predictions for July mean total PM_{2.5} based on Run 120.

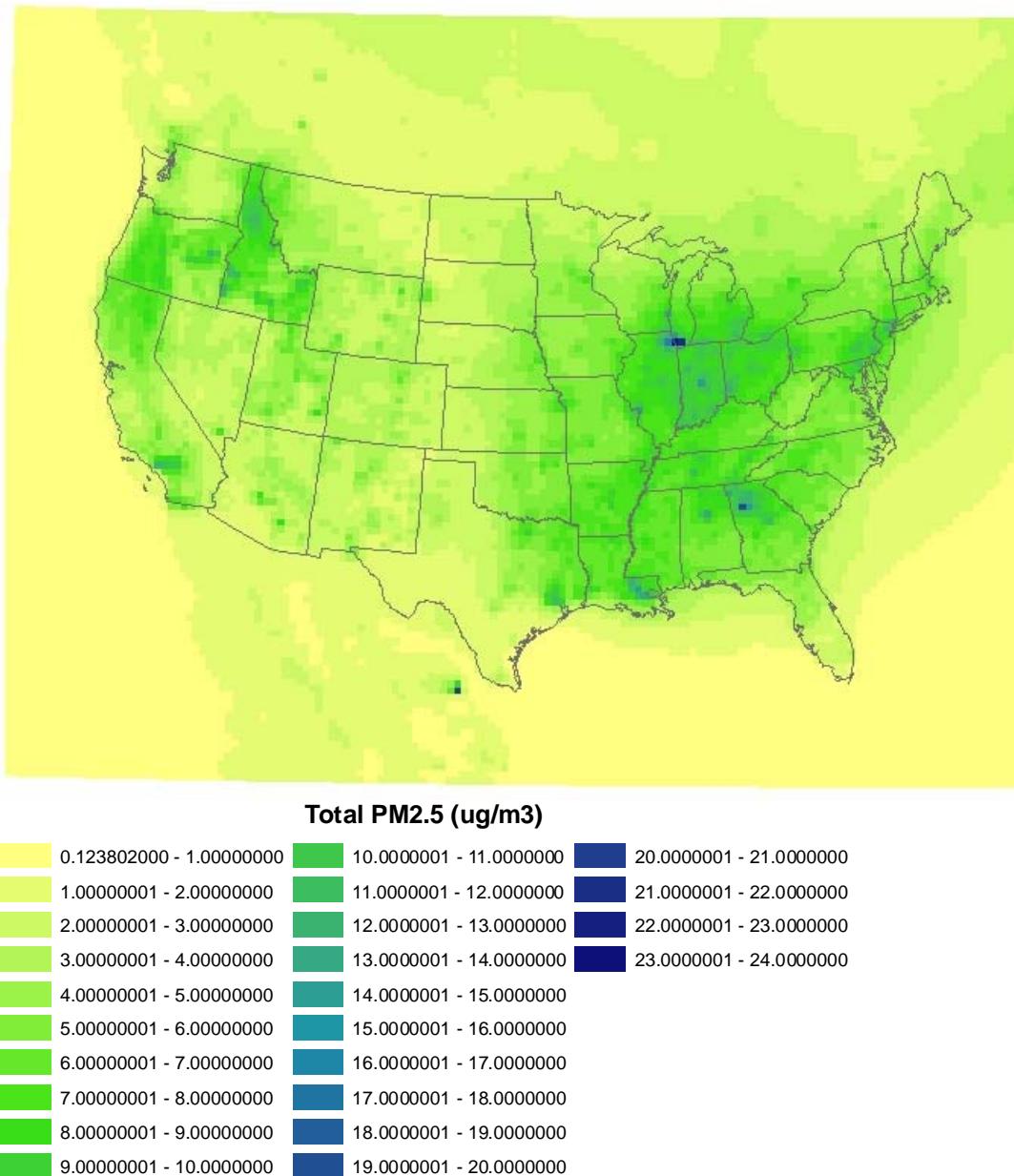


Figure IV-4. PM_{2.5} spatial gradient map for CMAQ simulations for July mean total PM_{2.5} based on Run 120.

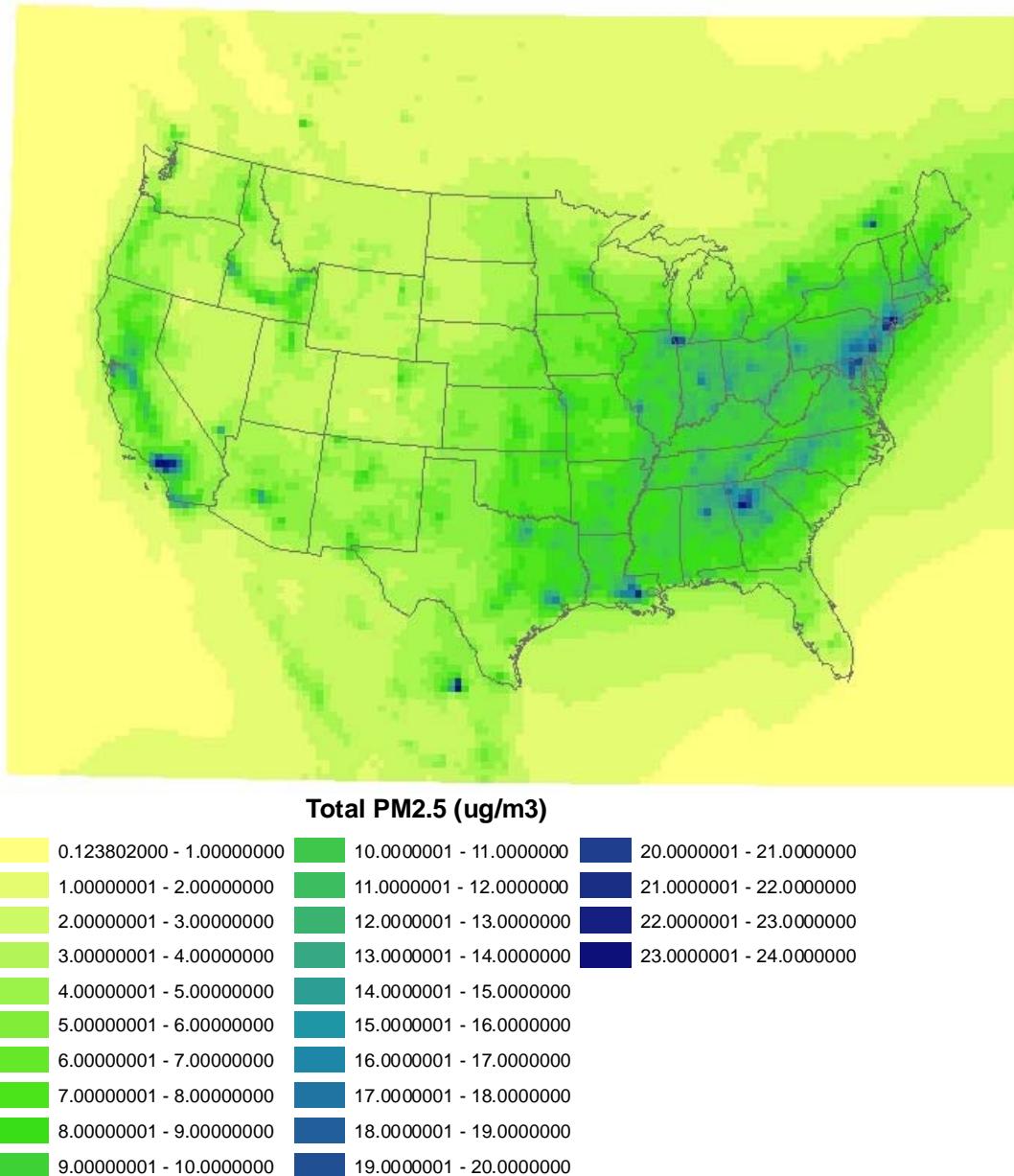


Figure IV-5. PM_{2.5} spatial gradient map for RSM predictions for October mean total PM_{2.5} based on Run 120.

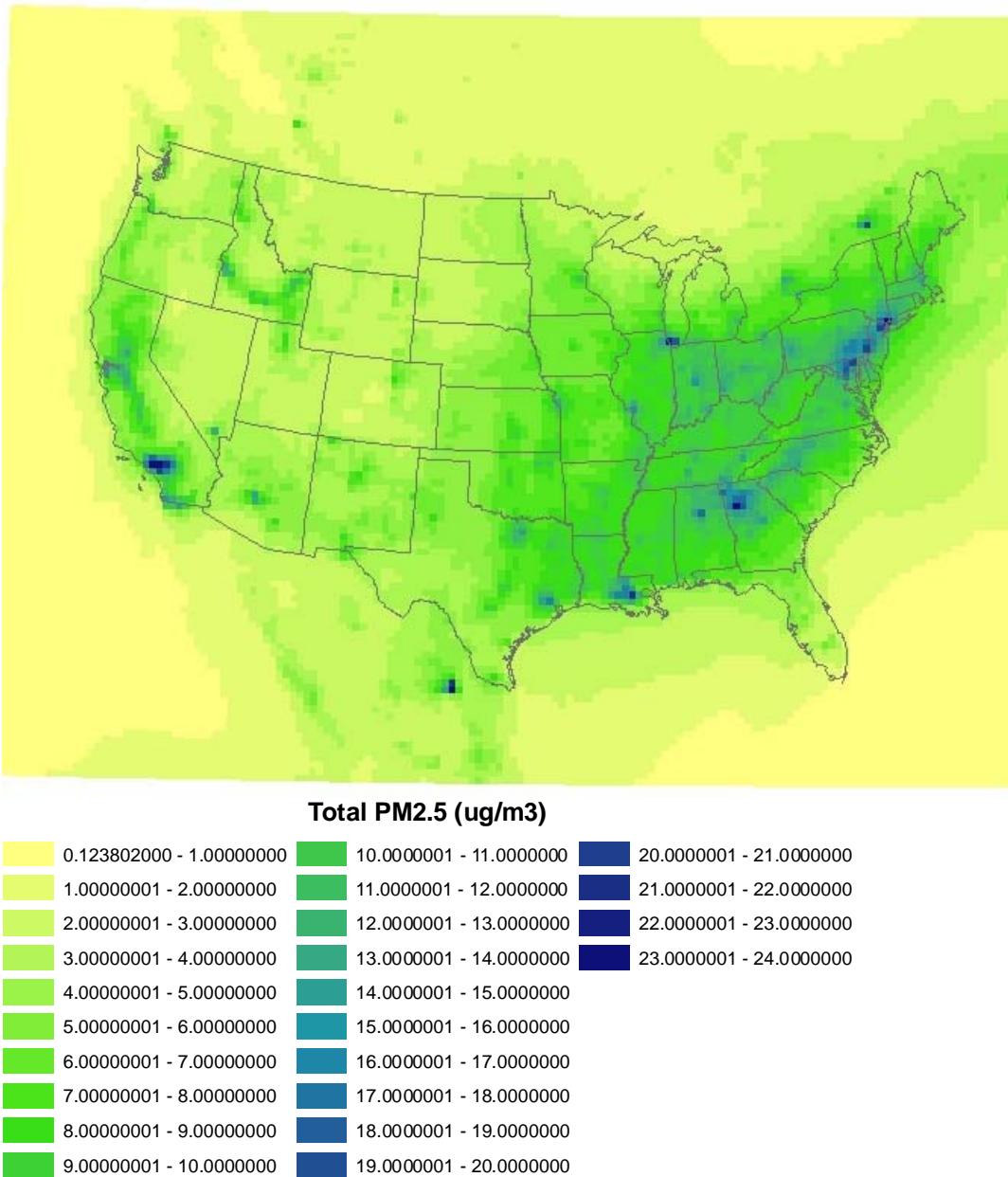


Figure IV-6. PM_{2.5} spatial gradient map for CMAQ simulations for October mean total PM_{2.5} based on Run 120.

An out-of-sample validation was also conducted, by comparing predicted values from the response surface models with actual CMAQ outputs for a set of 60 model runs that are outside of the experimental design and were not used in developing the predictive model. RSM predictions for these model runs are compared with the CMAQ predictions and the performance metrics over all grid cells is computed for each run. These out-of-sample validation runs included 30 boundary condition runs to assess model performance near the edges of the policy space in the outer edge conditions of the RSM. A complete list of model runs (including boundary condition runs) and corresponding control scenarios (selection of policy factor controls) are provided in

Appendix B. The distribution of the performance metrics over the set of 60 runs was then examined.

Cross-validation and out-of-sample performance metrics for the PM_{2.5} design value metric are shown in Table IV-3.

Table IV-3. Cross Validation Performance Metrics for the Predicted PM_{2.5} Design Values

Performance Metric	Daily 98 th Percentile Design Value			Annual Mean Design Value		
	Mean	Minimum	Maximum	Mean	Minimum	Maximum
Mean Bias ($\mu\text{g}/\text{m}^3$)	0.001	-0.646	0.796	0.001	-0.136	0.333
Mean Error ($\mu\text{g}/\text{m}^3$)	0.282	0.147	0.822	0.067	0.021	0.336
Mean Normalized Bias (%)	0.03%	-2.51%	2.81%	0.03%	-1.51%	2.86%
Mean Normalized Error (%)	1.13%	0.57%	3.10%	0.71%	0.21%	2.95%
Mean Fractional Bias (%)	0.02%	-2.62%	2.74%	0.02%	-1.51%	2.86%
Mean Fractional Error (%)	1.14%	0.58%	3.19%	0.71%	0.21%	2.90%

Technical Support Document for the Proposed PM NAAQS Rule

Response Surface Modeling

Appendix A

Control Scenario Model Runs

**U.S. Environmental Protection Agency
Office of Air Quality Planning and Standards
Research Triangle Park, NC 27711
February 2006**

Technical Support Document for the Proposed PM NAAQS Rule

Response Surface Modeling

Appendix B

Out-of-Sample Validation & Boundary Condition Runs

**U.S. Environmental Protection Agency
Office of Air Quality Planning and Standards
Research Triangle Park, NC 27711
February 2006**

RSM Out-of-Sample Validation Runs

RSM Out-of-Sample Validation Runs

Run Number	1) region B / NOx / EGU	2) region B / NOx / NonEGU+Area	3) region B / NOx / Mobile	4) region B / SOx / EGU	5) region B / SOx / NonEGU_Point	6) region B / SOx / Area	7) region B / VOC / All	8) region B / NH3 / Area	9) region B / NH3 / Mobile	10) region B / POC&PEC / EGU+NonEGU	11) region B / POC&PEC / Mobile	12) region B / POC&PEC / Area
	X13	X14	X15	X16	X17	X18	X19	X20	X21	X22	X23	X24
1	0.1519653	0.1961880	1.1554671	0.1013075	0.1326430	0.1994903	0.9914476	0.7454019	0.3534173	0.1516564	0.9159507	0.8955738
2	0.8597807	0.6799551	0.1286710	0.6808934	0.9205714	0.4423814	1.1072527	1.1333337	0.0733681	0.7202979	0.4462096	0.2316762
3	0.9987696	0.4148040	0.0266096	0.2098945	0.3988806	0.2989270	0.1512309	0.4271121	1.1190810	1.1609904	0.0813834	0.10178533
4	0.0004414	0.5102821	0.8369829	0.5344322	0.3457814	0.7869768	0.6874493	0.0644972	0.9204311	0.4979184	0.1466386	0.3949748
5	0.6795360	1.1535434	0.3047290	0.9797036	0.0611852	0.5382001	0.9370773	1.0290124	0.7657021	0.4594554	0.8290758	1.1206523
6	0.5257175	0.0770433	0.9142131	1.1995626	0.6125317	0.6800374	0.7215527	0.9450910	1.0419933	0.2723920	1.0677093	0.2758085
7	1.1036882	0.8345521	1.0130783	0.9019938	0.5545713	0.9829072	0.3254325	0.1674346	0.5144179	0.0867174	0.3465001	0.6617880
8	0.2510849	1.0091329	0.6418123	0.8265405	1.1437687	1.0959518	0.0934004	0.7069583	0.6058423	0.6237262	0.5721935	0.0439104
9	0.4538093	0.3597663	0.5135459	0.4338884	1.0189970	0.0017689	0.5737796	0.3123023	0.1616632	0.9886387	0.6575536	0.5028759
10	0.7990038	0.8722815	0.3603782	0.2402503	0.8124059	0.8514699	0.4413357	0.5349202	0.4797175	0.9565854	1.1366964	0.7694655
11	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000
12	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000
13	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000
14	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000
15	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000
16	0.5000000	0.5000000	0.5000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000
17	1.0000000	1.0000000	1.0000000	0.5000000	0.5000000	0.5000000	0.5000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000
18	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	0.5000000	0.5000000	1.0000000	1.0000000
19	0.5000000	0.5000000	0.5000000	0.5000000	0.5000000	0.5000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000
20	0.5000000	0.5000000	0.5000000	0.5000000	0.5000000	0.5000000	1.0000000	0.5000000	0.5000000	1.0000000	1.0000000	1.0000000
21	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000
22	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000
23	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000
24	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000
25	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000
26	0.1000000	0.1000000	0.1000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000
27	1.0000000	1.0000000	1.0000000	0.1000000	0.1000000	0.1000000	0.1000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000
28	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000	0.1000000	0.1000000	1.0000000	1.0000000
29	0.1000000	0.1000000	0.1000000	0.1000000	0.1000000	0.1000000	0.1000000	1.0000000	1.0000000	1.0000000	1.0000000	1.0000000
30	0.1000000	0.1000000	0.1000000	0.1000000	0.1000000	0.1000000	0.1000000	0.1000000	0.1000000	1.0000000	1.0000000	1.0000000

RSM Boundary Condition Runs

RSM Boundary Condition Runs