Appendix C: Chemical Transport Model Results for Sulfate Source Attribution Studies in the Northeast U.S.

Model description and performance evaluation

Shan He, Emily Savelli, Jung-Hun Woo, John Graham, Gary Kleiman
Northeast States for Coordinated Air Use Management (NESCAUM)
Boston, MA 02114.

ABSTRACT

Regional Scale Air Quality Modeling is being conducted by NESCAUM with two primary modeling systems based on the CMAQ and REMSAD models. As meteorological and emissions datasets are being finalized, preliminary modeling efforts are being migrated to a 12-km Eastern U.S. domain consistent with the RPO projection national domain. CMAQ provides one atmosphere results for multiple pollutants while the REMSAD model is used primarily for attribution of sulfate and mercury species in the Eastern US via the species-tagging scheme included in Version 7.10 and newer versions of the model. Performance evaluations for both models will be refined once final data inputs have been developed, but early indications suggest reasonable performance for the species of interest for each platform.

Appendix C: Chemical Transport Model Results for Sulfate Source Attribution Studies in the Northeast U.S.

C.1. Introduction

Air quality models have been extensively used as important tools within academia, federal and state governments, and other regulatory, policy, and environmental research communities to understand the underlying causes and formation mechanisms of air pollution on the local, regional and global scale. Recent evidence has shown that the Northeast US region has had a significant increased frequency of observed concentrations exceeding EPA standards for criteria pollutants such as Ozone and $PM_{2.5}$ (Ray et al., 1996). To assist states in developing effective solutions to these air pollution issues, NESCAUM has established in-house air quality modeling capabilities that include emission processing, meteorological input analysis, and chemical transport modeling. Preliminary work has been conducted to develop a number of modeling platforms for a variety of applications (e.g. annual runs, episodic simulations, source tagging, etc.) and to evaluate model performance. These efforts form the foundation upon which future modeling studies will be built ranging from SIP modeling for Regional Haze, Ozone, and fine particles to studies of mercury deposition and potential air quality impacts of climate change.

This appendix introduces air quality modeling platforms established by NESCAUM, provides details of several ongoing modeling studies, evaluates model performance with respect to spatial and temporal variations of ozone and PM species and their precursors, and summarizes the current status and future improvements of each platform's development.

C.2. Platforms

Currently two regional-scale air quality models have been evaluated and used by NESCAUM to perform air quality simulations. These are the Community Multi-scale Air Quality modeling system (CMAQ; Byun and Ching, 1999) and the Regional Modeling System for Aerosols and Deposition (REMSAD; SAI, 2002). CMAQ was developed by USEPA, while REMSAD was developed by ICF Consulting/Systems Applications International (ICF/SAI) with USEPA support. CMAQ has undergone extensive community development and peer review (reference) and has been successfully used in a number of regional air quality studies (Bell and Ellis, 2003;Hogrefe et al., 2004; Jimenez and Baldasano, 2004; Mao and Talbot, 2003; Mebust et al. 2003). REMSAD has also has been peer reviewed (Seigneur et al., 1999) and used by EPA for regulatory applications (reference HDD and CSA) to study ambient concentrations and deposition of sulfate and other PM species.

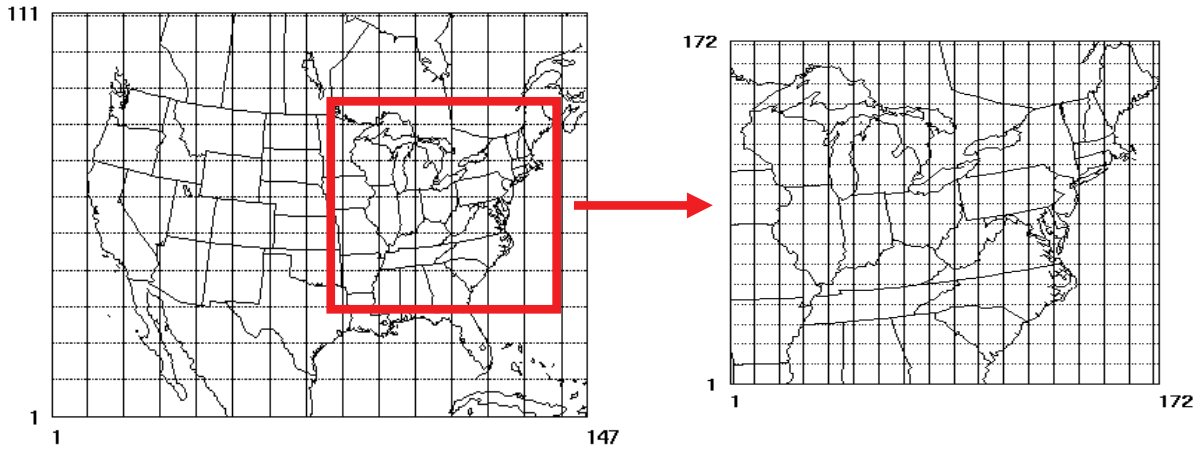
C.2.1. CMAQ

The CMAQ modeling system is a three-dimensional Eulerian model that incorporates output fields from emissions and meteorological modeling systems and several other data sources through special interface processors into the CMAQ Chemical Transport Model (CCTM). The CCTM then performs chemical transport modeling for

multiple pollutants on multiple scales. With this structure, CMAQ retains the flexibility to substitute other emissions processing systems and meteorological models. CMAQ is designed to provide an air quality modeling system with a "one atmosphere" capability containing state-of-science parameterizations of atmospheric processes affecting transport, transformation, and deposition of such pollutants as ozone, particulate matter, airborne toxics, and acidic and nutrient pollutant species (Byun and Ching, 1999).

NESCAUM has primarily run the CMAQ model in two different configurations. The first configuration utilized a national domain covering the continental US and portions of Canada and Mexico with 36km resolution (See Domain 1 in Figure C-1a). The horizontal dimension extends from 58°W~136°W in longitude and 19°N~58°N in latitude, yielding 147X111 grid cells. This domain is being used for a collaborative effort between Georgia Institute of Technology and the Massachusetts Institute of Technology under a USEPA Science to Achieve Results (STAR) grant focused on the air quality impact of climate change within the continental US. The 36km horizontal resolution may be too coarse to effectively characterize the air quality impact on MANE-VU states by the Northeastern US and surrounding RPO regions. Therefore, a finer resolution has been adopted for the purpose of Regional Haze and PM SIP modeling for the MANE-VU region (see Domain 2 in Figure C-1b). This domain covers the Northeast region including northeastern, central and southeastern US as well as Southeastern Canada with 12km resolution. It extends from 66°W~94°W in longitude and 29°N~50°N in latitude with 172X172 grid cells. For both domains, the same Lambert-Conformal map projection is used in MM5 and CMAQ.

Figure C-1: Modeling domains used in NESCAUM air quality modeling studies. (a) Domain 1: 36km National US domain with location of 12km domain highlighted; (b) Domain 2: 12km Northeast US domain. The gridline interval shown represents 10 cells.



Vertically, Domain 1 has 9 layers extending from the ground surface up to ~300hPa, while Domain 2 has 16 vertical layers from the ground surface up to ~200hPa. The vertical structure details of the two domains are given in Table C-1. Domain 1 has 6 layers and Domain 2 has 8 layers below 850hPa to resolve boundary layer processes. Domain 1 has only 2 layers in between 850hPa and 500hPa (near mid-troposphere) and none between 500hPa and 300hPa (near tropopause), whereas Domain 2 has 5 layers and 2 layers in those pressure intervals, respectively. The vertical resolution is selected

depending on the research interest and resolution of the meteorological field. Domain 1 uses a coarse vertical resolution above the boundary layer for modeling efficiency since the study is focused on ground level air quality across the inland US. Domain 2 has a finer vertical resolution within the troposphere so that it can capture complex atmospheric circulations between the east coast of the US and the northern Atlantic Ocean in the boundary layer, the free and upper troposphere, and potentially cross-tropopause transport.

Table C-1: Vertical structures of air quality modeling domains.

Level Index	σ level	Pressure (hPa)	Temperature (K)	Height (m) Full	Height (m) Half
		Domain 1 - 36km resolution			
9	0.0000	275.58	232.05	14590.18	10114.30
8	0.3000	562.85	269.23	7264.53	4838.47
7	0.6500	776.60	284.76	2935.83	2224.34
6	0.8000	881.57	292.07	1566.21	1150.57
5	0.9000	947.78	297.95	751.56	519.70
4	0.9600	980.56	300.81	293.74	219.20
3	0.9800	992.79	301.86	145.77	109.06
2	0.9900	999.92	302.46	72.61	45.32
1	0.9975	1003.99	303.10	18.10	9.05
0	1.0000	1013.20		0.00	
Values of P,T,H are for grid cell (-75°W,40°N) on 16:00 UTC July 1, 2001					
		Domain 2 - 12km resolution			
16	0.0000	195.63	225.65	18780.65	12387.84
15	0.2750	373.25	247.05	8908.85	7934.47
14	0.3750	468.12	259.85	7051.40	6250.92
13	0.4750	562.17	269.29	5512.88	4830.05
12	0.5750	632.59	274.21	4193.49	3887.73
11	0.6250	703.13	278.38	3596.76	3033.85
10	0.7250	771.51	281.33	2503.38	2271.28
9	0.7700	814.17	282.37	2048.45	1827.37
8	0.8150	857.00	283.65	1613.90	1402.32
7	0.8600	897.41	286.85	1196.99	1016.06
6	0.9000	932.90	289.90	839.78	687.58
5	0.9350	961.18	292.37	538.20	432.15
4	0.9600	982.31	294.19	327.67	244.73
3	0.9800	996.37	295.39	162.55	121.61
2	0.9900	1004.51	296.08	80.94	50.92
1	0.9975	1009.18	296.94	20.98	10.48
0	1.0000	1013.20		0.00	
Values of P,T,H are for grid cell (-75°W,40°N) on 16:00 UTC August 6, 2002					

CMAQ V4.2.2 was used to model July 2001 and January 2002 on the 36km national US domain (Domain 1). The SAPRC-99 mechanism with modified Euler backward iterative (MEBI) solver was used to simulate gas phase chemistry. The Regional Acid Deposition Model (RADM) is used for cloud chemistry. The AERO3 and AERO_DEPV2 modules were used for aerosol dynamics and aerosol deposition. The Piecewise parabolic method (PPM) was used for PPM Horizontal and vertical advection,

and Eddy diffusion for vertical mixing. The minimum vertical eddy coefficient is set at 0.3 m^2/sec. The initial concentrations and boundary conditions were generated using the preprocessors ICON and BCON based on a set of default concentration data representing relatively clean conditions in the eastern half of the US. The lookup table of photolysis rates was generated using JPROC with TOMS data.

CMAQ V4.4 was used to model the 11-days period from August 6 to 16, 2002 on the 12km northeastern US domain (Domain2). The model configuration was the same as the modeling setup for the 36km domain, except the Carbon Bond IV mechanism (Gery et al., 1989) was used for gas phase chemistry. While the SAPRC-99 mechanism is supposed to have better correspondence with observations than the CB-IV mechanism because of more updated complex chemistry, the CB-IV mechanism is more time efficient. It is still inconclusive whether the SAPRC-99 mechanism performs better than the CB-IV mechanism. A future modeling study on the same 11-days period on the 12km domain using SAPRC-99 mechanism will be conducted at NESCAUM to identify the more effective and efficient mechanism in our region before proceeding to 2002 annual simulations.

C.2.1.1. Meteorology

All meteorological fields have been simulated using the Fifth-Generation Pennsylvania State University/National Center for Atmospheric Research (NCAR) Mesoscale Model (MM5) system (http://www.mmm.ucar.edu/mm5/). Originally developed by Penn State and NCAR, MM5 is a model with limited-area primitive equations of momentum, thermodynamics, and moisture with the option of hydrostatic and non-hydrostatic physics. It is designed to simulate mesoscale atmospheric circulation. Domains are uniform rectangular grids representing three-dimensional regions of the atmosphere. The horizontal coordinated system is equally spaced geographically and uses the Arakawa-B gridding scheme. The resolution can be as high as 1km. Sigma (σ) is a terrain-following vertical coordinate that is a function of pressure at the point (for hydrostatic) or reference state pressure (non-hydrostatic) (P), the surface pressure (P_{s0}), and the pressure at the top (P_{top}) of the model. $\sigma = (p-p_{top}) / (p_{s0}-p_{top})$

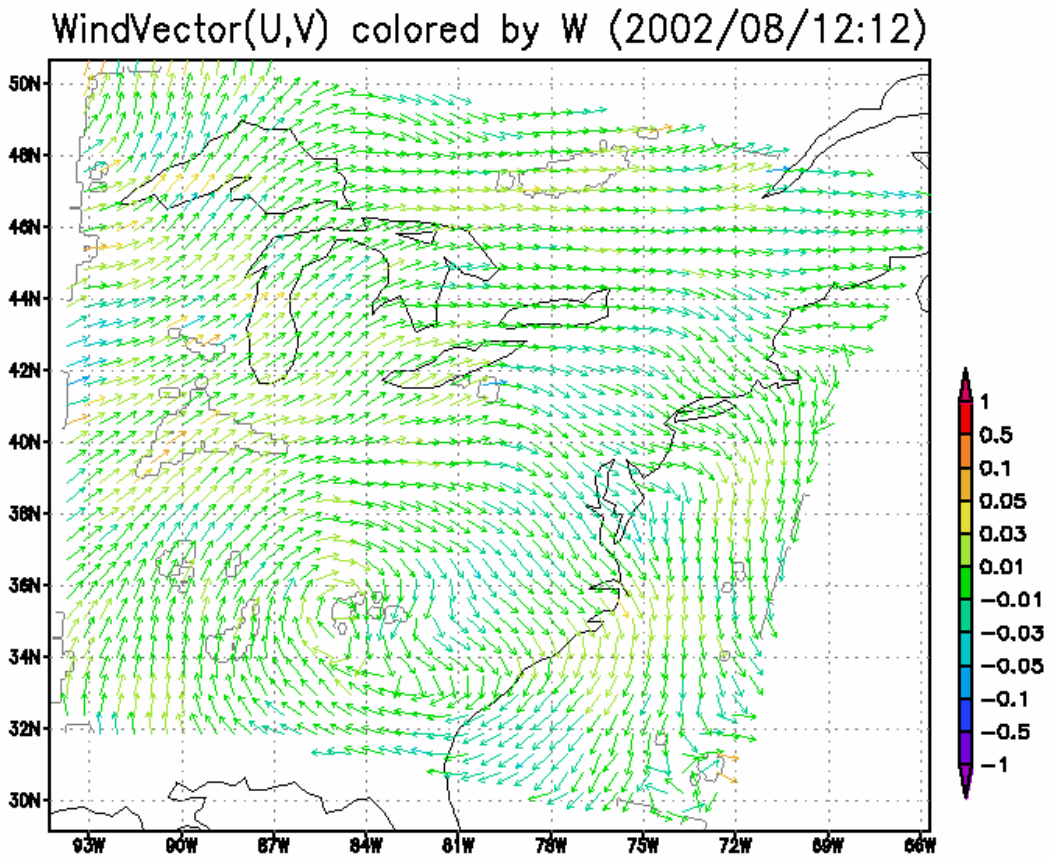
Professor Ted Russell's group from Georgia Institute of Technology (GIT) provided meteorological fields for the 36km national domain (Domain 1). For two month-long periods in July 2001 and January 2002, they ran non-hydrostatic MM5 v3.5.3 with a domain with a grid size of 36 km, and a terrain-following sigma coordinate with 25 layers and a radiative upper-boundary condition at 100hPa. Physics options included simple ice microphysics, the Kain-Fritsch cumulus scheme, rapid radiative transfer model, the Pleim-Chang PBL, the Pleim-Xiu land surface model, and FDDA 3D analysis. The model was initialized with ETA analysis data and evaluated with surface hourly data.

The meteorological fields for the 12km northeast domain (Domain 2) was developed by Professor Dalin Zhang's group from University of Maryland (UMD). For the August 6 to 16, 2002 test period, they ran a non-hydrostatic MM5 v3.5.3 with 3 PBL schemes (a) modified Blackadar [BL], (b) the Pleim-Xiu scheme with the soil module [P-X], and (c) modified Blackadar with soil module [SSIB]. The simulated meteorological fields were compared to the measurements from TDL (NWS) and CASTNet. The TDL are reflective of urban/suburban settings, while the CASTNet sites are more

representative of rural areas. There are 47 CASTNet and about 600 NWS sites in the TDL data set over the modeling domain. Overall, the BL scheme shows a better correspondence to the measured data than the other two schemes, although it poorly captures diurnal pattern of humidity. While the P-X scheme shows a better correspondence with the observed diurnal pattern for humidity, it fails to perform well for wind speed and temperature (Hao et al., 2004).

The UMD MM5 model runs are made on two nested domains with a grid size of 36 km in the outer domain and a grid size of 12 km in the inner domain. The inner domain uses a finer resolution terrain data. The model utilizes a terrain-following sigma coordinate with 29 layers with the first level at 10 m and a radiative upper-boundary condition at 50hPa. The boundary layer processes are determined using the Blackadar high-resolution planetary boundary layer parameterization. Physics options also included explicit representations of cloud physics with simple ice microphysics (no mixed-phase processes) and the Kain-Fritsch cumulus parameterization. The model was initialized with the analyses of the National Center for Environmental Prediction (Eta Model). A modeled wind field map (Figure C-2) shows a typical prevailing mesoscale flows from midwest US to east coast.

Figure C-2: MM5 modeled wind field map at 12:00 UTC on August 8, 2002



The provided MM5 output meteorological data then serves as input for MCIP2 which NESCAUM uses to generate hourly metrological field required by SMOKE and CMAQ.

C.2.1.2. CMAQ Emissions

Emission scenarios are simulated using the Sparse Matrix Operator Kernel Emissions (SMOKE) Modeling System. SMOKE is primarily an emissions processing system designed to create gridded, speciated, hourly emissions for input into a variety of air quality models such as CMAQ, REMSAD, the Comprehensive Air quality Model with extensions (CAM_X) and the Urban Airshed Model (UAM). SMOKE supports area, biogenic, mobile (both onroad and nonroad), and point source emissions processing for criteria, particulate, and toxic pollutants. For biogenic emissions modeling, SMOKE uses the Biogenic Emission Inventory System, version 2.3 (BEIS2) and version 3.09 and 3.12 (BEIS3). SMOKE is also integrated with the on-road emissions model MOBILE6. The sparse matrix approach used throughout SMOKE permits rapid and flexible processing of emissions data. Flexible processing comes from splitting the processing steps of inventory growth, controls, chemical speciation, temporal allocation, and spatial allocation into independent steps whenever possible. The results from these steps are merged together in the final stage of processing using vector-matrix multiplication. It allows individual steps (such as adding a new control strategy, or processing for a different grid) to be performed and merged without having to redo all of the other processing steps (http://cf.unc.edu/cep/empd/products/smoke/version2.1/html/).

The emission processing for the 36km national domain has been performed by Georgia Tech using SMOKE v1.5. They use the 1999 US national emission inventory, CEM data from EPA, and spatial surrogates data based on the 2000 Census. Biogenic emissions are calculated using BEIS3 with BELD3 data. Mobile source emissions are processed using MOBIL6. Then, 1999 emissions are converted to 2001 and 2002 emissions using EGAS V4.0 with existing control strategies. For the two-month test periods, no emissions from Canada and Mexico were generated. However, emissions from both countries will be used for a planned 2001 annual simulation.

NESCAUM developed emission inputs for the 12km northeast domain using SMOKE V2.0. Specifically, emissions for a 10-day period during the summer of 2002 (August 6 ~ August 16) were formatted for Domain 2 utilizing a variety of emission inventories including EPA's eGRID2002 (year 2000 data), EPA's preliminary 2002 NEI version 1, and EPA's 2002 Continuous Emissions Monitor (CEM) data which contains actual measured emissions on an hourly basis for the years 1999 and 2002, the VISTAS Regional Planning Organization (RPO) 2002 base-case modeling inventory, and a Canadian inventory derived from 1996 EPA Clear Skies Act inventory data to develop a baseline modeling inventory for the August 2002 test period. Specific data sources for individual source categories are listed below.

1) Area Sources
- includes VISTAS 2002 emissions for VISTAS States
- includes WRAP 2002 emissions for WRAP States
- includes specific records of ammonia emissions for CENRAP States
- includes preliminary NEI 2002 emissions for all other states/sources
- excludes all fire emissions from VISTAS and WRAP States
- excludes all PM from fugitive dust sources

2) Non-road Mobile Sources
- includes VISTAS 2002 emissions for VISTAS States
- includes preliminary NEI 2002 emissions for all other States

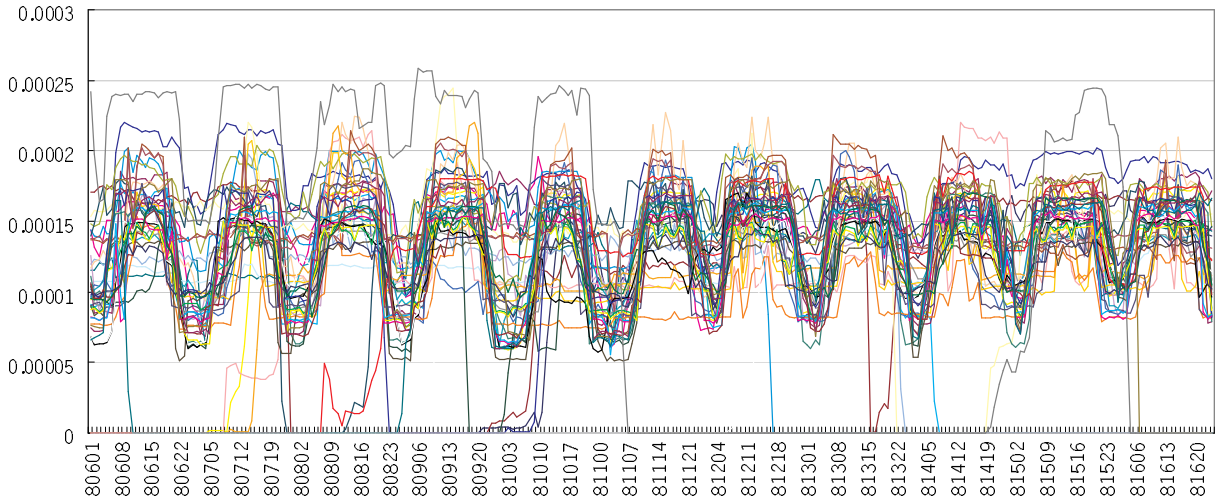
3) On-road Mobile Sources
- includes VISTAS 2002 data on vehicle miles traveled for VISTAS States
- includes preliminary NEI 2002 VMT for all other states

4) Biogenic Sources
- BELD3 land cover data at 4km for national RPO domain

5) Point Sources
- includes both EGU and non-EGU point source emissions
- includes VISTAS 2002 emissions for VISTAS States
- includes WRAP 2002 emissions for WRAP States
- includes EPA 2001 modeling platform emission inputs for all other States/sources

6) Canadian Emissions
- 1996 Nonroad Rule Canadian emissions inventory

Figure C-3: Hourly fraction of heat input from CEM data (X-axis: date/time in MDDHH, Y-Axis: hourly fraction of heat input, dimensionless)



NESCAUM has successfully developed methods to refine point source data representation in models by (1) combining USEPA's 2002 CEM data, which contains actual, measured hourly emissions from large point sources, with annual Inventory Data Analyzer (IDA) format emissions data and (2) developing hourly CEM-based temporal allocation factors which can be applied to criteria pollutants that are not directly measured by CEM (i.e., CO, VOC, NH3, PM10, and PM2.5). The resulting hourly emissions estimates for all pollutants at selected facilities were combined with the annual emissions dataset. Although the CEM-based hourly dataset is highly accurate, its

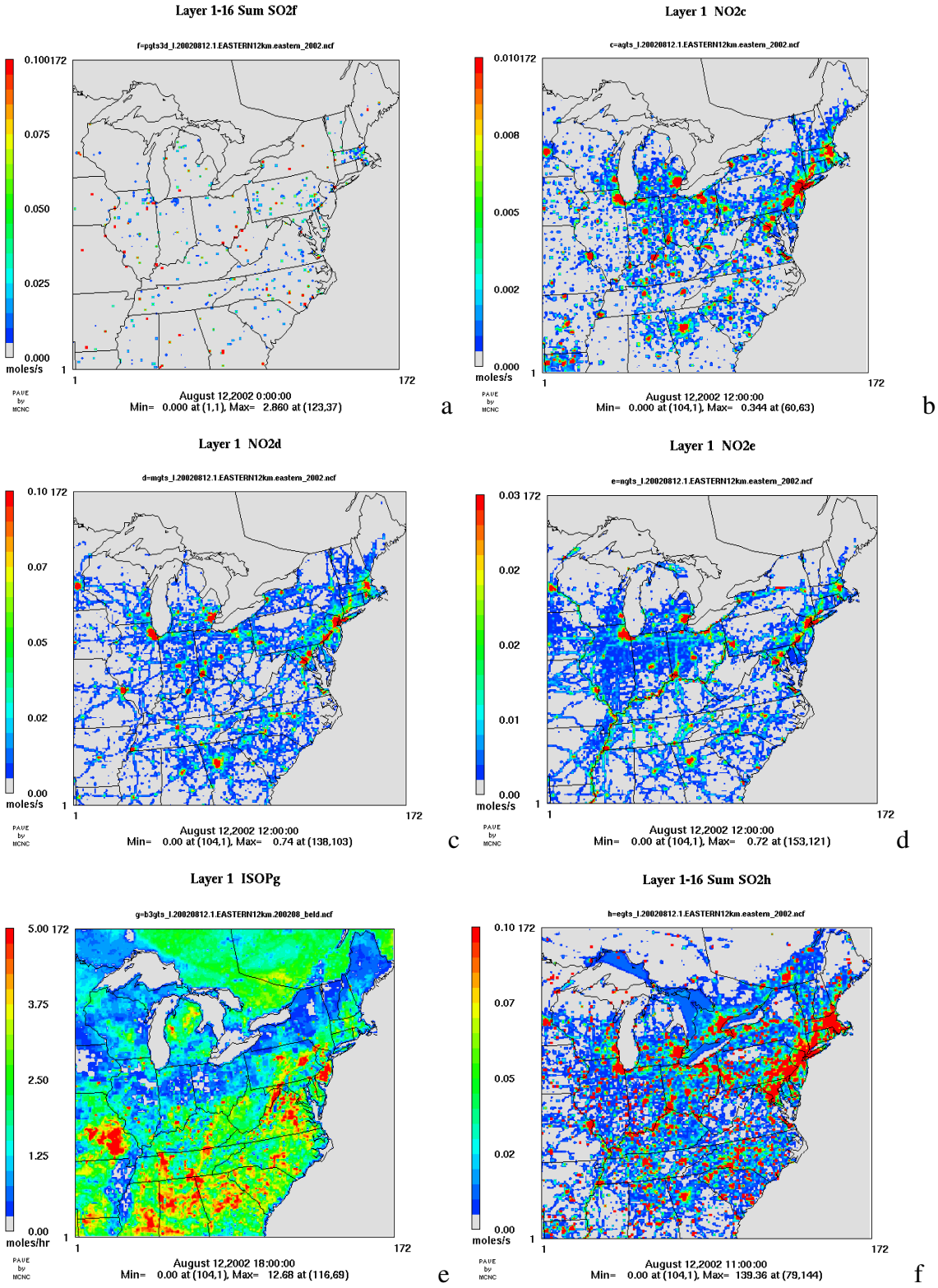
substantial size makes use of this data most appropriate for a subset of sources or for modeling short time periods.

To improve the performance of available air quality models, more comprehensive emission models — specifically, MOBILE 6.2 and BEIS 3 — were used for on-road mobile and biogenic sources, respectively. Activity data (i.e., vehicle miles traveled (VMT) and average vehicle speed) were used to estimate/process on-road mobile source emissions using MOBILE6. BELD3 land cover data and meteorological data were used to estimate/process biogenic emissions data using BEIS3.

To run these models and to process point source emissions data with SMOKE, meteorological data are required. Ten days of detailed MM5 meteorological data provided by UMD for the August 2002 period (see previous section for detailed description) were used to effectively represent meteorological conditions in the eastern United States. Examples of processed emissions outputs are shown in Figure C-4.

Figure C-4: Examples of processed model-ready emissions

(a): SO2 from Point; (b): NO2 from Area; (c): NO2 from On-road; (d): NO2 from Non-Road; (e): ISOP from Biogenic; (f): SO2 from all source categories)



C.2.2. REMSAD

The Regional Modeling System for Aerosols and Deposition (REMSAD) is also a three-dimensional Eulerian model designed to support a better understanding of the distributions, sources, and removal processes relevant to fine particles and other airborne pollutants. It calculates the concentrations of both inert and chemically reactive pollutants by simulating the physical and chemical processes in the atmosphere that affect pollutant concentrations. The basis for the model is the atmospheric diffusion equation representing a mass balance in which all of the relevant emissions, transport, diffusion, chemical reactions, and removal processes are expressed in mathematical terms. REMSAD model performs a four-step solution procedure: emissions, horizontal advection/diffusion, vertical advection/diffusion and deposition, and chemical transformations during one half of each advective time step, and then reverses the order for the following half time step. The maximum advective time step for stability is a function of the grid size and the maximum wind velocity or horizontal diffusion coefficient. Vertical diffusion is solved on fractions of the advective time step to keep their individual numerical schemes stable.

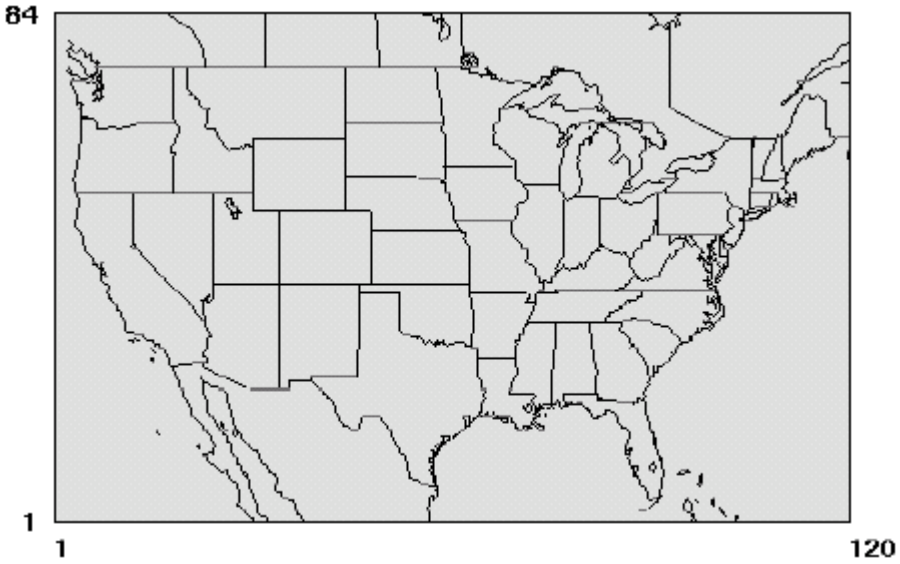
REMSAD uses a flexible horizontal and vertical coordinate system with nested-grid capabilities and user-defined vertical layers. It accepts a geodetic (latitude/longitude) horizontal coordinate system or a Cartesian horizontal coordinate system measured in kilometers. REMSAD uses a simplified version of CB-IV chemistry mechanism which is based on a reduction in the number of different organic compound species and also includes radical-radical termination reactions. The organic portion of the chemistry is based on three primary organic compound species and one carbonyl species. The model parameterizes aerosol chemistry and dynamics for PM and calculates SOA yields from emitted hydrocarbons. REMSAD V7.10 and newer versions have capabilities that allow model tags of sulfur species (up to 11 tags), nitrogen (up to 2 tags), mercury (up to 24 tags), and cadmium (up to 10 tags) to identify the impact of specific tagged species.

Unlike CMAQ, REMSAD provides no choice of chemical and physical mechanisms. The modeling configuration for future work with REMSAD will be similar to the CMAQ modeling setup. The initial concentrations and boundary conditions will be generated using the same concentration profile used by CMAQ. The approach is to use similar model inputs to allow comparison of REMSAD with CMAQ to better understand differences between the two models. Due to the simplified chemistry mechanism, REMSAD may not simulate atmospheric processes as well as CMAQ. However, advantages such as the tagging feature, more efficient modeling, and reasonable correspondence with measurements for many species, make REMSAD an important tool for MANE-VU.

While the two domains presented in the previous section are the target domains for future CMAQ and REMSAD modeling, another domain has been used for preliminary REMSAD regional haze modeling. Domain 3, as shown in Figure C-5, is very similar to Domain 1, with 36km resolution covering the continental US, Southern Canada and Northern Mexico. The horizontal dimension is 120X84 from 66°W to 126°W

in longitude and 24°N to 52°N in latitude. Vertically it divides the region from the ground surface up to 100hPa (~16km in altitude) into 12 levels.

Figure C-5: National USEPA REMSAD domain with 36km resolution.



This domain has been used primarily because it served as the modeling domain for several USEPA regulatory and legislative initiatives including the Heavy Duty Diesel rule and proposed Clear Skies Act of 2003. As a result, model inputs for this domain were readily available to NESCAUM and served as an ideal starting point for analysis of national programs.

C.2.2.1. REMSAD Meteorology

For the preliminary regional haze modeling study, a whole year of MM5 generated meteorological data for 1996 was provided by US EPA and used to drive annual REMSAD tagging modeling.[1] Details for the previous EPA regulatory analyses as well as information on the development of the 1996 meteorological dataset can be found on EPA websites dedicated to these programs (http://www.epa.gov/air/clearskies/). This data was obtained in a model ready format and the reader is referred to the EPA references for details on the development and performance evaluation for these data.

While results are not yet available, REMSAD is also being run on the 12km northeast domain (Domain 2) described earlier. Meteorological inputs for these runs have been developed by applying a simple translation script (MM52REMSAD) provided by the University of Maryland (Jeff Stehr, personal communication) to generate hourly meteorological field required by REMSAD.

[1] Ideally, emissions and meteorology would be from matching years to allow for performance evaluation versus ambient data. However, 2001 meteorological inputs were not available for this exercise.

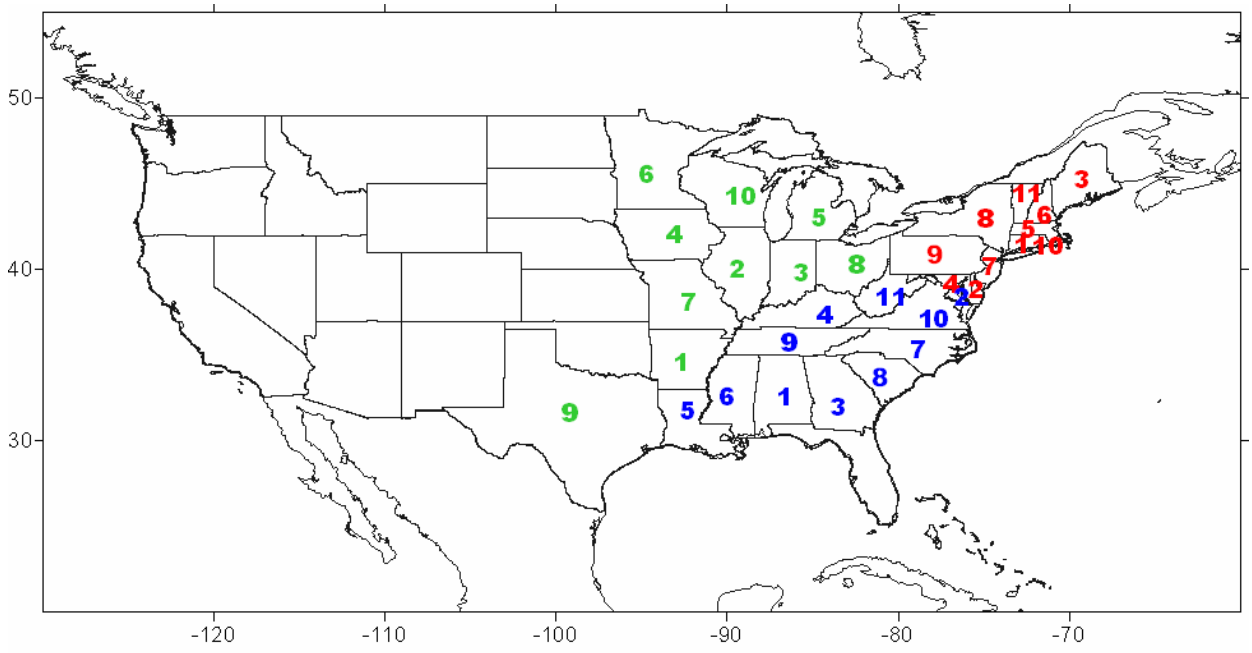
C.2.2.2. REMSAD Emissions

NESCAUM has developed emissions tagging techniques for application in air quality impact analyses using the REMSAD tagging scheme incorporated in REMSAD version 7.10 and higher. In general, these emissions tagging schemes can be used to assess source contributions in various ways including: (1) by size and susceptibility to transport (e.g., as between large elevated sources vs. small, low-level sources); (2) by sectors/types (e.g. by SCCs or by point, area, or mobile source categories); (3) by regions (e.g. by country/state/county); or (4) by combinations (e.g. largest electricity generating unit (EGU) in a specific state). Practical application of this tagging capability to MANE-VU modeling has been delayed until the Mid-Atlantic/Northeast Visibility Union (MANE-VU) 2002 emission inventory is finalized. NESCAUM has, however, successfully applied this newly-developed technique to both mercury and sulfur (using preliminary inventories).

For preliminary results reported here, USEPA REMSAD-ready emission input files were obtained for the Clear Skies Act of 2003 analysis (http://www.epa.gov/air/clearskies/) to be used with the 1996 meteorological inputs described above. Using these data NESCAUM is able to essentially "reproduce" USEPA modeling results for the CSA 2003 analysis. The emissions inventory developed by USEPA was a 2001 "proxy" inventory which is not likely to be completely representative of the year 2001 and the meteorology which was used was for the year 1996, preventing a true comparison of model results with observations for any year (i.e. 1996 or 2001). Nonetheless, as EPA considers this platform useful for policy analysis, MANE-VU has conducted some preliminary runs to inform the early stages of the regional haze planning effort while final quality assured meteorological and emissions inputs are developed for 2002 on the northeast domain.

A significant difference between the two sets of results, however, is that NESCAUM has taken the additional step of reprocessing the elevated point source emission files such that the model input is formatted to take advantage of REMSAD's tagging capabilities. Thus, each of the elevated point sources in over 30 eastern states have been tagged according to state of origin, providing a rough estimate of the contribution that elevated point sources in each state make toward simulated sulfate concentrations at Eastern receptor sites. The tagging scheme employed for this analysis is shown in Figure C-6. Using CSA 2001Proxy emission and 1996 EPA CSA base year meteorology, REMSAD was used for an annual simulation to evaluate the impact of each state on $PM_{2.5}$ over the Northeast US.

Figure C-6: Tagging map for REMSAD modeling. Sulfur species from elevated emission sources are tagged by states with 3 tag groups each including 12 tags.



Tag	SO_2 _1	SO_2 _2	SO_2 _3	SO_2 _4	SO_2 _5	SO_2 _6	SO_2 _7	SO_2 _8	SO_2 _9	SO_2 _10	SO_2 _11	SO_2
1	CT	DE	ME	MD	MA	NH	NJ	NY	PA	RI	VT	All Other Emission
2	AL	DC	GA	KY	LA	MS	NC	SC	TN	VA	WV	All Other Emission
3	AR	IL	IN	IA	MI	MN	MO	OH	TX	WI	Other US States Elevated Emission	All US Surface Emission + All Canada & Mexico Emission

C.2.3. Next Steps for NESCAUM Chemical Transport Model Platforms

Emissions processing work to date has focused on generating model-ready data inputs using SMOKE. The final version of the 1999 NEI and the preliminary version of the 2002 NEI have been processed to use with the CMAQ and REMSAD models. Point, stationary area, non-road mobile, on-road mobile, and biogenic sources all have been processed through SMOKE v. 2.0 to support the use of air quality models in assessing visibility impacts.

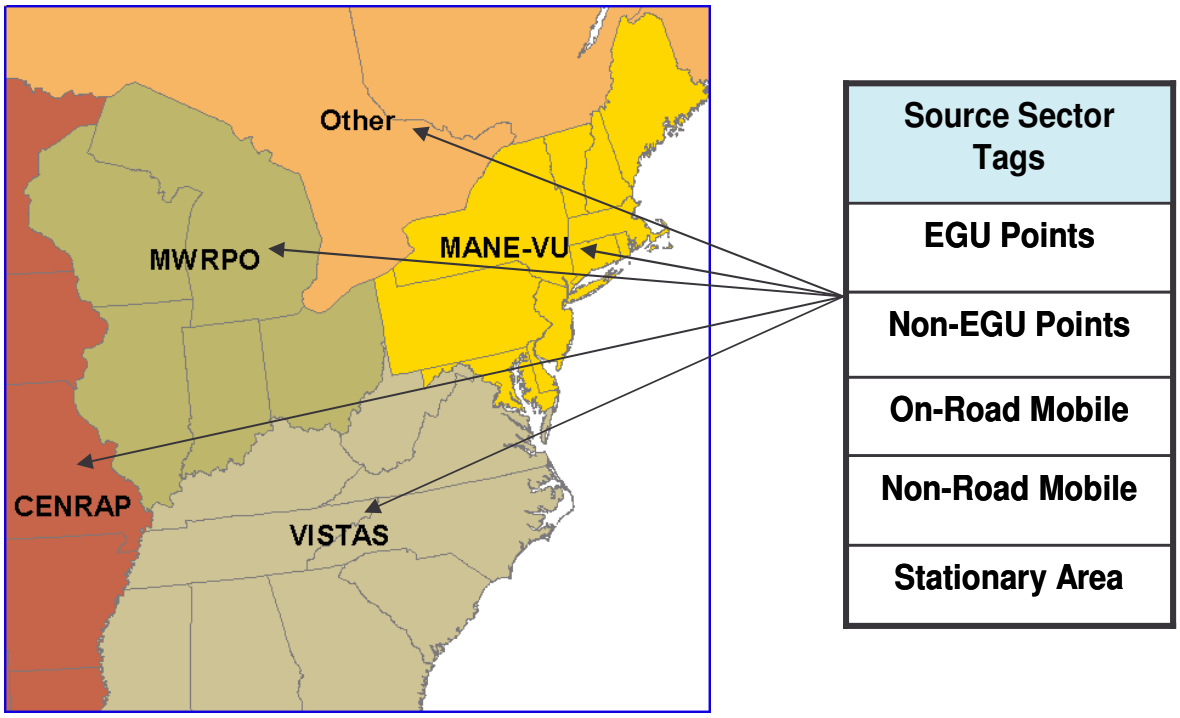
A final version of the MANE-VU emissions inventory will be available by spring 2005. NESCAUM will integrate other Regional Planning Organizations' (RPO) inventories with MANE-VU's inventory and then tag them for further emissions processing through SMOKE. The tagging-friendly version of SMOKE that NESCAUM has been developing will produce REMSAD model-ready outputs to support tagged air quality model runs. In addition to the overall emissions inventory, processing surrogates are being reviewed and revised for the MANE-VU region. NESCAUM has been testing these surrogates using SMOKE to ensure that final inventory data are working correctly for emissions processing.

The description of the CMAQ platform being utilized on Domain 2 presented here, fairly portrays the platform anticipated to be used for a full annual run later this year for the base year (2002) as well as projection years (2010 and 2018).

As the full annual meteorological dataset for 2002 and the RPO's 2002 base year inventories become available and processed through MM52REMSAD and SMOKE, the REMSAD platform will be migrated to Domain 2 as well. Emissions processed for REMSAD will take advantage of the SO_2 tagging capabilities, whereas CMAQ will treat all SO_2 as a single species.

An example of the groupings that will be used in a future MANE-VU tagged modeling exercise is shown in Figure C-7. Regions to be tagged include (1) MANE-VU, (2) Midwest Regional Planning Organization (MWRPO), (3) The Visibility Improvement State and Tribal Association of the Southeast (VISTAS), (4) the Central States Regional Air Partnership (CENRAP), and (5) other. Potential source-sector tags to be used for this exercise include: (1) EGUs, (2) non-EGU point sources, (3) on-road mobile sources, (4) non-road mobile sources, and (5) stationary area sources (e.g., residential and commercial heating).

Figure C-7: Example of a tagging scheme



The design and development of several "policy scenarios" for MANE-VU regional haze modeling will be decided through consultations with the MANE-VU Policy Advisory Group. Several control strategy screening runs will be simulated to provide information on various source sectors and regions in the inventory and to assess their relative contribution to visibility impairment at various receptor sites.

The period from August 6 to August 16, 2002 was selected for detailed analysis of a summer peak ozone and PM episode (see detailed analysis of this episode in

NESCAUM, 2004). UMD is in the process of developing a full annual run of MM5 for MANE-VU and a one-week period in January 2002 will be treated as a test data set to evaluate a winter peak PM episode and ensure optimal performance of the MM5 model. Inter-comparison tests between actual meteorological measurements and alternative simulated MM5 outputs (GIT) will verify the validity of the meteorological models and parameters selected.

C.3. Model Performance Evaluation

C.3.1. CMAQ performance for Ozone

For ozone, CMAQ simulations on the 12km northeast US domain over the August 6~16, 2002 period are used to compare with AIRS surface ozone hourly concentration by location and time. To minimize the influence of the initial condition concentration field on modeling predictions, only simulation results from August 9 to 16 were used in the evaluation. AIRS sites within NESCAUM states (106 sites out of 601 sites as shown in Figure C-8) were located at corresponding grid cells of the 12km domain. Hourly ozone observations were extracted and paired with CMAQ hourly surface ozone concentrations. In addition, ozone observed values were manipulated to generate diurnal maximum, daytime (8AM~6PM) average, and daily average and paired with modeling predictions for analysis.

Figure C-8: AIRS stations within 12km Northeast US domain. Total number of sites is 601, while 106 sites located within NESCAUM states as red triangles, 76 sites located within PA, MD, DC, and DE as blue triangles, 81 sites located within VA, WV, and NC as green triangles.

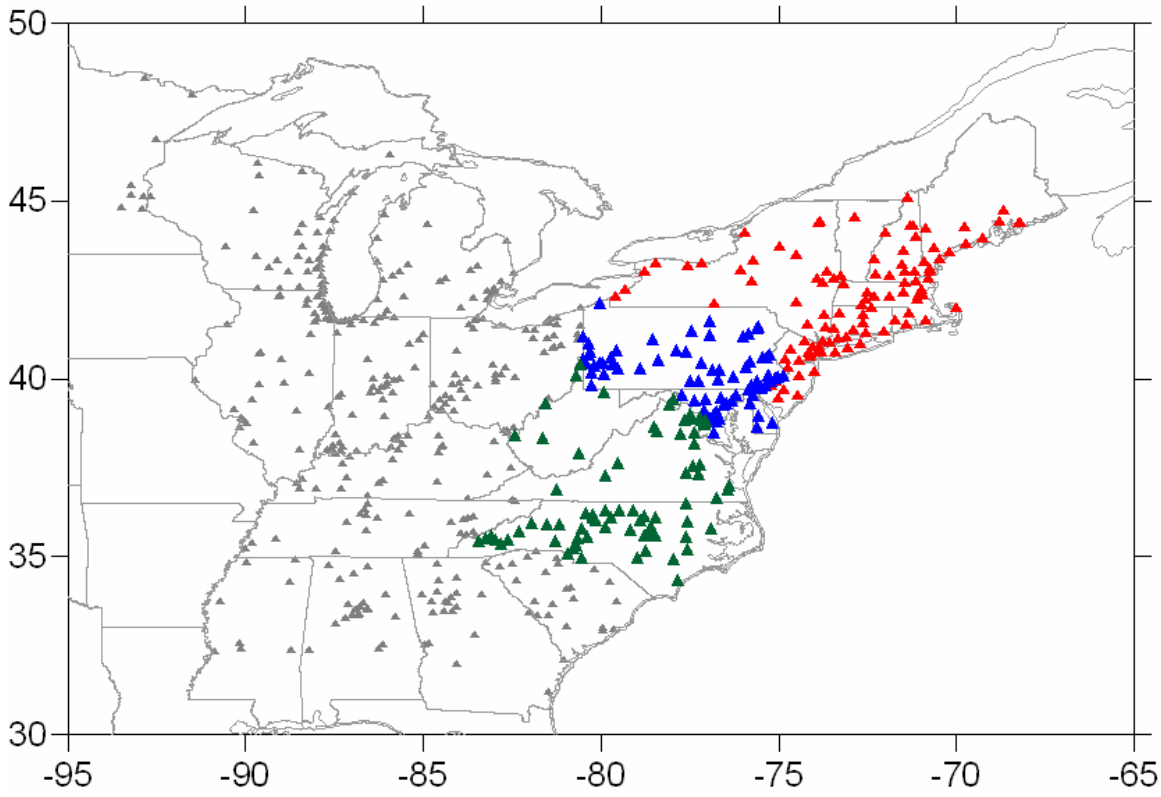
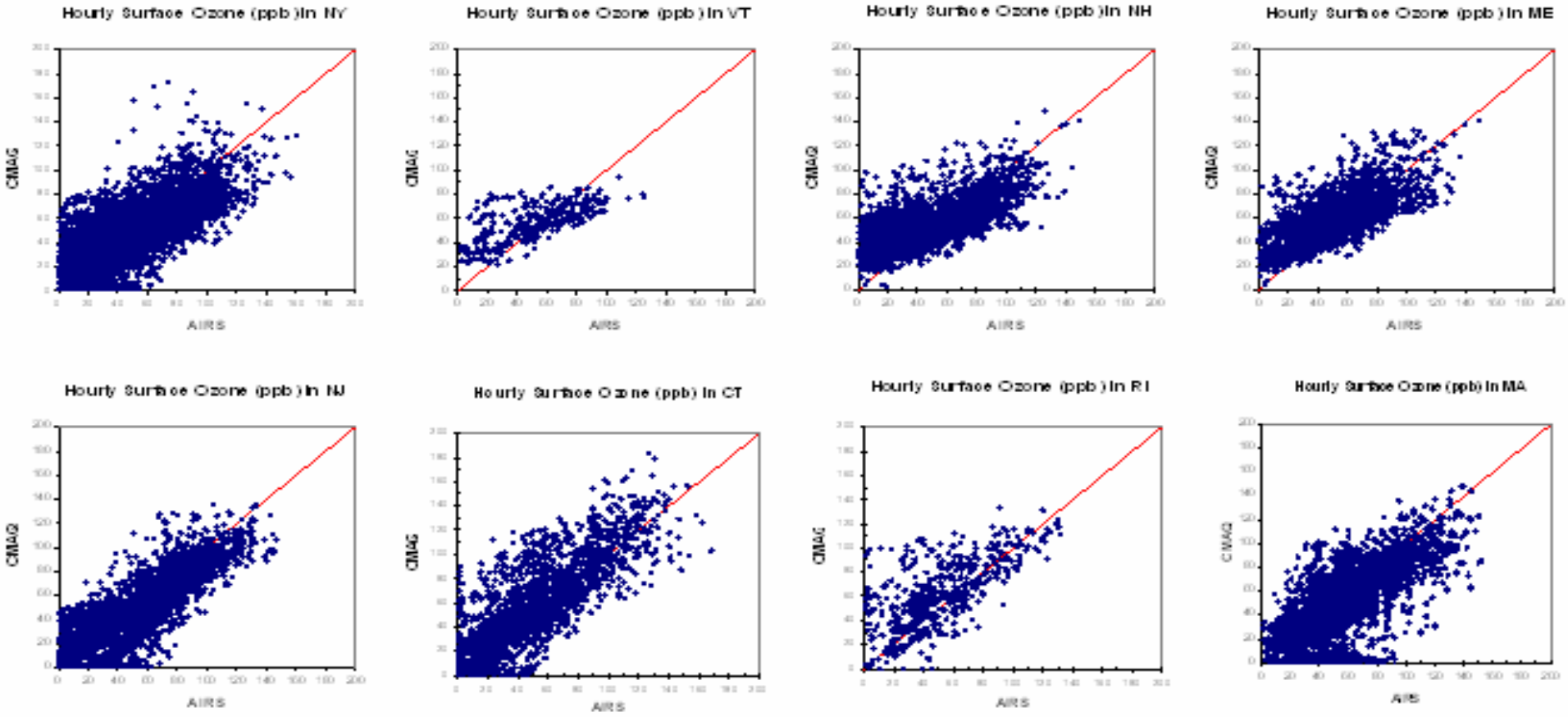


Figure C-9: shows the comparison of paired hourly surface ozone concentrations between CMAQ modeling and AIRS measurements for the eight NESCAUM states during the evaluation period. In every state, the majority of data points are concentrated along the 1:1 line indicating good agreement between the model and observations. In VT and RI, CMAQ overestimates at low ozone levels (<40ppbv), while it underestimates a small portion of total data points in MA. VT and RI have the lowest correlation coefficients (~0.68) whereas NJ has the highest correlation coefficient of 0.827. In general, the observed CMAQ performance is very good.

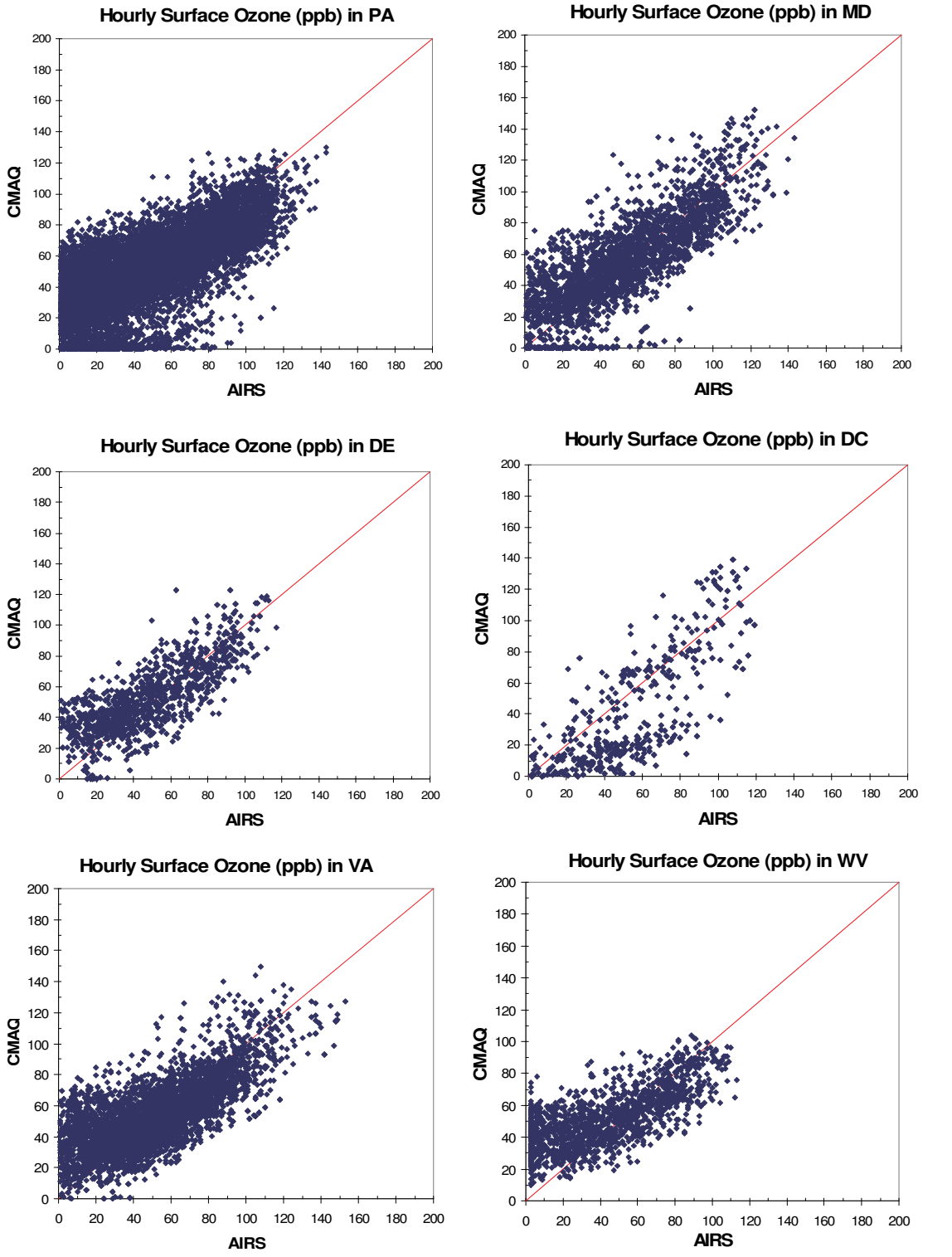
Similar performance is observed for the Mid-Atlantic states as shown in Figure C-10. The comparison of paired hourly surface ozone concentrations between CMAQ modeling and AIRS measurements for the six MARAMA states during the evaluation period indicates, again, that in every state the majority of data points are concentrated along the 1:1 line. Several states (including Virginia and West Virginia show some tendency for the model to overestimate concentrations at low ozone levels. Pennsylvania shows some small portion of the observed data is significantly underestimated. Correlations range from 0.71 to 0.79. In general, the observed CMAQ performance is very good in this region as well.

Figure C-9: Comparison of hourly surface ozone between CMAQ modeled values and AIRS observed values for each NESCAUM state for the August 9~16, 2002 simulation.



AIRS vs. CMAQ	CT	MA	ME	NH	NJ	NY	RI	VT
Correlation Coefficient	0.798	0.734	0.731	0.706	0.827	0.742	0.684	0.676

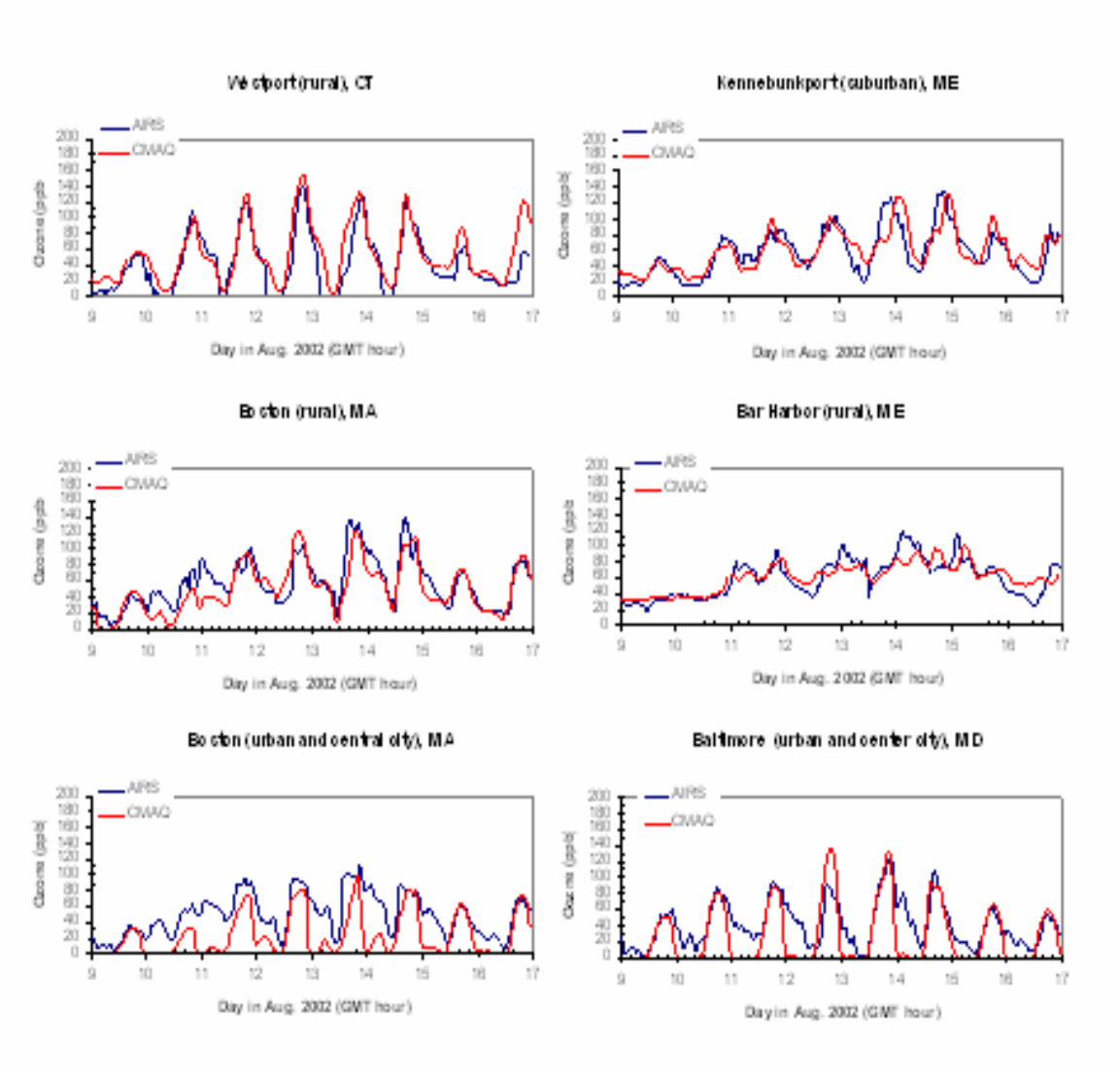
Figure C-10: Comparison of hourly surface ozone between CMAQ modeled values and AIRS observed values for each MARAMA state for the August 9~16, 2002 simulation.



AIRS vs. CMAQ	DC	DE	MD	PA	VA	WV
Correlation Coefficient	0.776	0.782	0.793	0.710	0.735	0.716

A further analysis of the diurnal variation of surface ozone was conducted. Figure C-11 presents diurnal variations of modeled ozone and observed ozone at a representative group of locations for urban, suburban, and rural sites. It clearly shows that CMAQ captures the diurnal variation of surface ozone at all locations. At rural and suburban areas, the CMAQ ozone curve nearly overlaps with the AIRS ozone curve. In Bar Harbor, ME (second row on right panel), where no obvious diurnal variation occurs, CMAQ also reasonably follows the observations. However, CMAQ does not agree as well with observations in urban areas. In Boston and Baltimore (third row), CMAQ captures the timing of diurnal maximum values. However, the modeled ozone level drops quickly after reaching this peak, which leads to CMAQ underestimation during late afternoon and evening hours. This may be caused by the lack of detailed fine scale meteorology in the complex urban environment, as well as the location of AIRS monitors which could be directly and continuously exposed to pollution sources.

Figure C-11: Diurnal variations of modeled ozone and observed ozone at urban, suburban, and rural locations.



Statistical analysis of hourly surface ozone predictions and observations within NESCAUM states are listed in Table C-2. From August 9 through 16, the mean ozone concentrations of the whole dataset (without cutoff) in the 8-day period are 50.87ppbv observed and 52.14 ppbv predicted. The mean bias is only 1.27ppbv, which indicates CMAQ tends to overestimate ozone. The mean error is 16.31ppbv indicating the average amount of overprediction, while the normalized mean error, the mean normalized error, and fractional error are all high, 32.06%, 101.98%, and 46.08%, respectively. The perspective changes when a 25ppbv level is set to cutoff lower ozone concentration values in the paired analysis. By excluding low ozone values, the mean ozone concentrations are both increased to 62.09ppbv observed and 58.84ppbv predicted. The mean bias changes to -3.25ppbv, again indicating CMAQ is underestimating ozone. The mean error is slightly reduced to 15.17ppbv, while other error parameters such as NME, MNE, and FE are dramatically decreased to 24.44%, 28.26%, and 30.34%, respectively. The changes reflect the effect of low ozone values in the denominator that lead to larger fractional or normalized statistical values; high ozone values in the denominator cause smaller fractional or normalized statistical values. In addition, the mean normalized bias decreases from 73.73% to -0.33%, and the other two values of bias, NMB and MFB, both change from positive to negative, indicating model underestimation. This underestimation may result from the observed CMAQ underprediction in urban areas.

Table C-2: Statistical measures of 12km domain CMAQ hourly ozone modeling evaluation against AIRS hourly ozone observations for NESCAUM states over August 9~16, 2002

Statistical Measure	Whole dataset	Cutoff at 25ppbv
O	50.87	62.09
P	52.14	58.84
MB	1.27	-3.25
MAGE	16.31	15.17
RMSE	21.17	19.85
NMB(%)	2.50	-5.23
NME(%)	32.06	24.44
MNB(%)	73.73	-0.33
MNE(%)	101.98	28.26
MFB(%)	5.02	-8.79
FE(%)	46.08	30.34

*Units are ppbv unless specified. O refers average hourly ozone concentration measurement from AIRS data; P refers average hourly ozone concentration from CMAQ prediction; other statistical parameters are listed in Appendix.

Values of fractional bias and fractional error on paired ozone diurnal maximum values, paired ozone daytime average values, and paired ozone daily average values are presented on a "Soccer Goal" plot in Figures C-12 and C-13 for the NESCAUM and MARAMA regions, respectively. The "Soccer Goal" plot has been widely used in RPO modeling groups for model evaluation analysis. It shows that ozone diurnal maximum, ozone daytime average, and ozone daily average are all located within the red goal which

is considered good model performance, while ozone hourly concentration falls within the orange goal which is considered as acceptable model performance.

Figure C-12: Comparison of fractional error and fractional bias for paired ozone predictions and observations within NESCAUM states

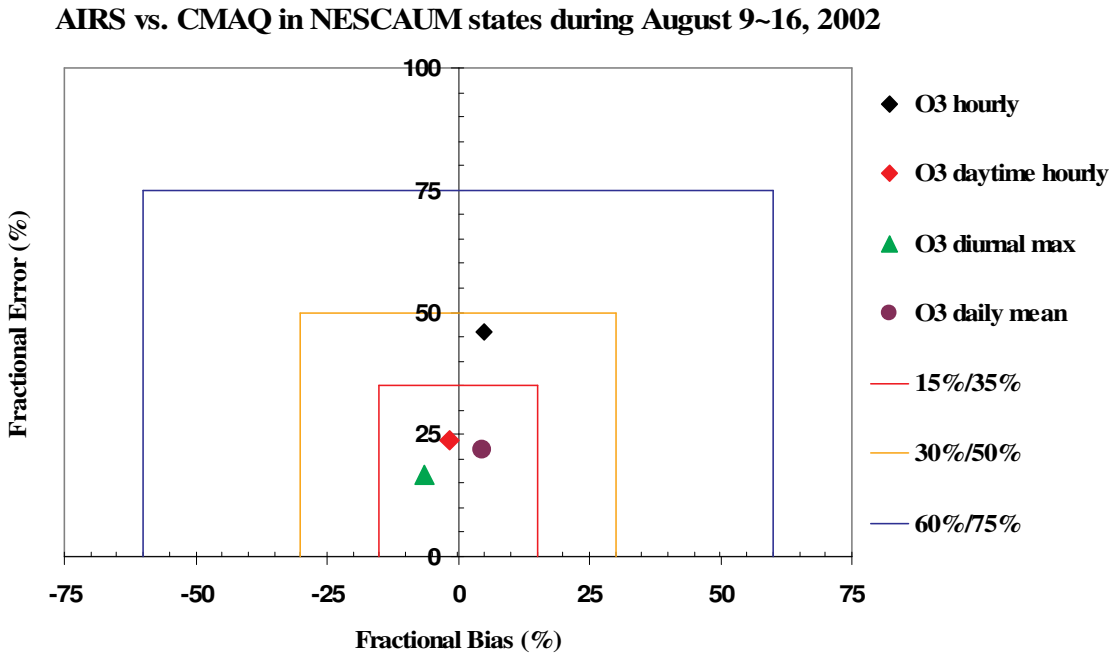
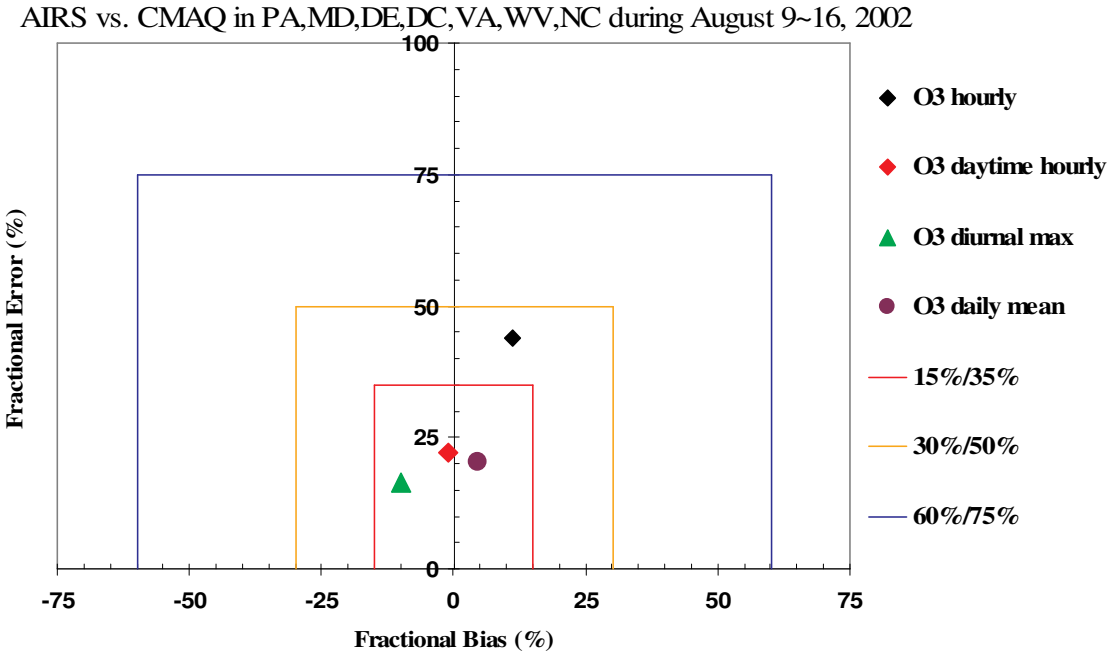


Figure C-13: Comparison of fractional error and fractional bias for paired ozone predictions and observations within MARAMA states



Overall CMAQ performs very well for ozone modeling. It successfully portrays a high ozone episode and its associated diurnal variations within the Northeast US domain. Although CMAQ significantly underestimates surface ozone concentrations during afternoon and night hours in urban areas, it agrees well with observation in rural and suburban areas. CMAQ shows better performance on ozone diurnal maximum, daily mean, and daytime average than on individual hourly ozone metrics.

C.3.2. CMAQ performance on PM2.5 species

For $PM_{2.5}$ species, CMAQ simulations on the 36km national US domain over the months of July 2001 and January 2002 were used to compare with IMPROVE $PM_{2.5}$ species daily concentration by location and time. Figure C-14 presents the spatial distribution of monthly average $PM_{2.5}$ for July 2001 (left column) and January 2002 (right column) from CMAQ modeling (bottom row) and IMPROVE measurements (top row) over the continental US. Observations show that generally the Eastern US and West Coast experience higher $PM_{2.5}$ concentrations than the Mountain Time zone area. CMAQ successfully captures this spatial pattern. For the summertime simulation, CMAQ results agreed well with observations, except for slightly (in the range of $5\mu g/m^3$) underestimating $PM_{2.5}$ in South California and Southwest US, and overestimating in Northern CA, Idaho and Western Montana. As mentioned before, the emission field for 36km domain developed by GIT lacks emissions from Mexico and Canada. No emissions from Mexico may lead to model under-predictions in the Southwest during summer. The over-predictions in the Northwest may be attributable to transport from the high $PM_{2.5}$ level area in Northwest Washington. For the wintertime simulation, CMAQ performed better in the Western US than in the Eastern US. The model systematically overestimates $PM_{2.5}$ over the Eastern US and the West Coast. Previous studies have shown that the version of CMAQ that NESCAUM used in this study tends to overestimate $PM_{2.5}$ in winter[2]. There are several spots in New York and Los Angeles that exhibit significant overestimation (> 10~20$\mu g/m^3$ in the urban areas).

A detailed comparison of $PM_{2.5}$ species between CMAQ predictions and IMPROVE measurements is shown in Figure C-15. For July 2001 (left plot), modeled PM agrees well with observed $PM_{2.5}$ and PM sulfate. Sulfate PM is the dominant species in $PM_{2.5}$, while other species are usually below $10\mu g/m^3$. Taken separately, modeled values of nitrate, ammonium, carbonaceous aerosols, and soil do not agree well with observations, but their concentrations are too small to affect $PM_{2.5}$ accuracy. CMAQ clearly performs better in the summer period than in the winter period. For January 2002, PM nitrate becomes the dominant species in $PM_{2.5}$, which causes dramatic overestimation by CMAQ.

Table C-3 statistically analyzes CMAQ performance for July 2001. A series of statistic parameters were calculated for paired CMAQ results and IMPROVE measurements for both the entire continental US and for the sub-region of NESCAUM states. Based on mean observations, species other than nitrate and soil all have higher averages over the NESCAUM region than averaged over the entire US. CMAQ modeled

[2] The model's nitrate winter chemistry overestimated PM nitrate due to high rate constants and reaction probability for reactions of N_2O_5. CMAQ V4.4 released in October 2004 has fixed this problem.

$PM_{2.5}$ species from the NESCAUM region show better correlation to IMPROVE data than from the entire US, except for nitrate. For example, the correlation coefficient (r) for $PM_{2.5}$ is 0.79 for the continental US but increases to 0.90 for NESCAUM states; r for PM nitrate is 0.50 for the US but only 0.12 for NESCAUM states. Values of mean bias show that CMAQ overpredicts PM sulfate and soil, and underpredicts nitrate, ammonium, and carbonaceous aerosol. According to the values of fractional bias and fraction error, CMAQ modeling of PM sulfate and $PM_{2.5}$ are in the good performance range (as determined by the "Soccer Goal" used in model evaluation on ozone), while ammonium and carbonaceous aerosols are in the acceptable range. PM nitrate is significantly underpredicted, with fractional error larger than 100%, while soil is significantly overpredicted with fractional error around 80~90%. As nitrate chemistry in the model has been modified, such large errors infer that a more accurate emission field for both species would improve CMAQ performance.

Additional $PM_{2.5}$ evaluations were conducted using CMAQ modeling results from the 12km northeast US domain for the August 9~16, 2002 period and corresponding observation data from the IMPROVE network and EPA AQS database. The analysis is shown in Figure C-16. The left plot shows the paired daily $PM_{2.5}$ comparison, while the right plot shows the paired hourly $PM_{2.5}$ comparison. Both indicate reasonably good agreement between modeled and observed concentrations. The correlation coefficient for CMAQ and IMPROVE daily averages is 0.87, while CMAQ and AQS is 0.77 and 0.61, for daily values and hourly values, respectively. Differences are expected since IMPROVE monitor are primarily located in remote areas whereas AQS data are primarily collected from urban areas. CMAQ tends to over-predict $PM_{2.5}$ concentration in urban areas. The results demonstrate that the 12km domain CMAQ modeling of $PM_{2.5}$ performs as well as the 36km domain modeling. However, since these two studies use different emissions and meteorological fields for different time periods, a direct evaluation of resolution differences cannot be determined (often it is presumed that finer grid resolution should improve model performance). A study using the same emissions and meteorology at different resolutions should provide an answer to effect of different resolutions on model performance.

Overall, NESCAUM CMAQ modeling successfully captures the $PM_{2.5}$ spatial distribution over US, and predicts PM sulfate concentration accurately. Since sulfate dominates $PM_{2.5}$, modeled $PM_{2.5}$ has a strong correlation with measured values. The model performs better for summertime than for wintertime, but the newly release version of CMAQ (V4.4) may correct nitrate overestimation and improve modeling performance. Refined emission inventories should also improve model prediction for other $PM_{2.5}$ species.

At the 2004 RPO modeling meeting, James Boylan from VISTAS collected CMAQ modeling results of PM2.5 species from three RPOs: MANE-VU, VISTAS, and Mid-west RPO, and compared with IMPROVE data at several Class I areas. Note that MANE-VU results are NESCAUM 36km domain CMAQ modeling results. The comparison of every single PM2.5 specie shows (as given in Figure C-17) that although three RPOs used different model setups, emissions, meteorology, and even chemistry mechanisms, no RPOs CMAQ modeling performed significantly better or worse than the others.

Figure C-14: Spatial distribution of monthly average PM2.5 for July 2001 and January 2002 from CMAQ model and IMPROVE measurement

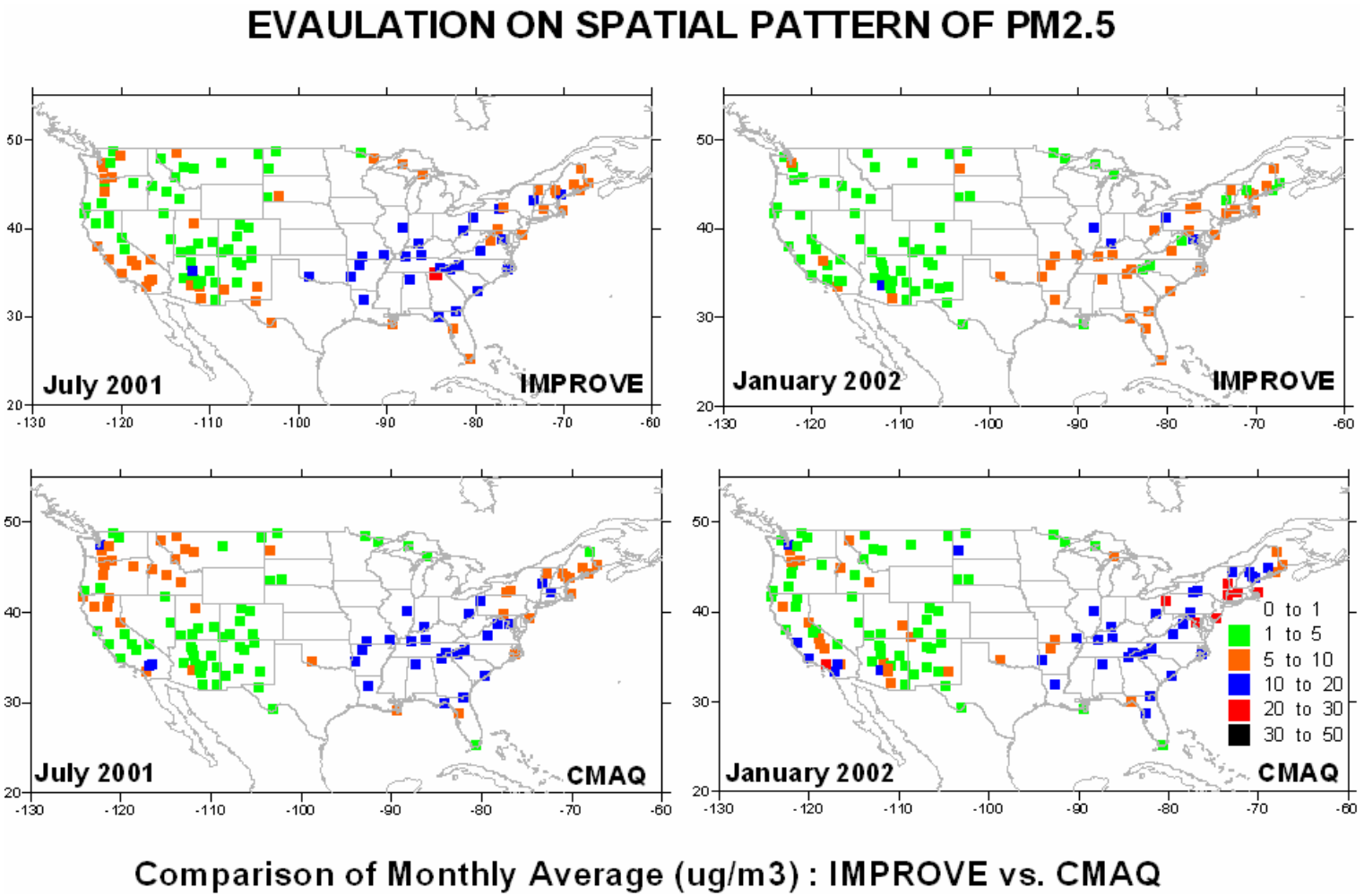


Table C-3: Statistical measures of PM2.5 species for paired daily CMAQ model results and IMPROVE observations in period of July, 2001 over continental US and NESCAUM states

Species	PM	2.5	PM	Sulfate	PM	Nitrate	PM	NH4	PM	OC	PM	EC	PM	Soil
Region	US	NE	US	NE	US	NE	US	NE	US	NE	US	NE	US	NE
Observation	7.37	8.71	2.43	3.18	0.28	0.19	0.99	1.25	1.68	1.92	0.23	0.29	0.84	0.43
Prediction	6.77	7.68	2.87	3.74	0.13	0.06	0.78	0.81	1.67	1.56	0.22	0.28	1.13	1.18
r	0.79	0.90	0.88	0.92	0.50	0.12	0.81	0.86	0.26	0.74	0.54	0.63	-0.06	0.35
MB	-0.61	-1.04	0.43	0.56	-0.15	-0.13	-0.21	-0.44	-0.01	-0.36	-0.01	-0.02	0.28	0.75
ME	2.88	2.57	1.15	1.16	0.22	0.16	0.42	0.58	1.17	0.68	0.13	0.15	0.92	0.83
MNB (%)	5.2	-7.3	31.0	37.4	-59.4	-62.6	39.5	-11.9	47.7	-14.6	33.1	-2.3	189.7	397.0
NMB (%)	-8.2	-11.9	17.7	17.5	-53.0	-67.1	-21.3	-35.5	-0.8	-18.6	-2.4	-6.3	33.4	177.4
MFB(%)	-12.8	-15.6	3.9	17.3	-122.6	-131.9	-22.9	-26.6	-11.2	-27.4	-18.4	-24.4	34.9	79.7
NME (%)	39.1	29.5	47.4	36.6	80.9	84.5	43.1	46.1	69.5	35.4	58.8	52.0	108.6	194.7
FE(%)	46.3	35.0	50.4	42.0	135.3	141.0	52.7	49.0	67.6	44.9	59.4	59.8	81.2	91.9

* US refers continental US regional; NE refers NESCAUM region; O refers mean observation; P refers mean model prediction; r refers correlations coefficient; other statistic parameters defined at the end of the document. Unit s for O, P, MB, ME are $\mu g/m^3$; r is dimensionless.

Figure C-15: Comparison of daily PM2.5 species for July 2001 and January 2002 between CMAQ results and IMPROVE observations

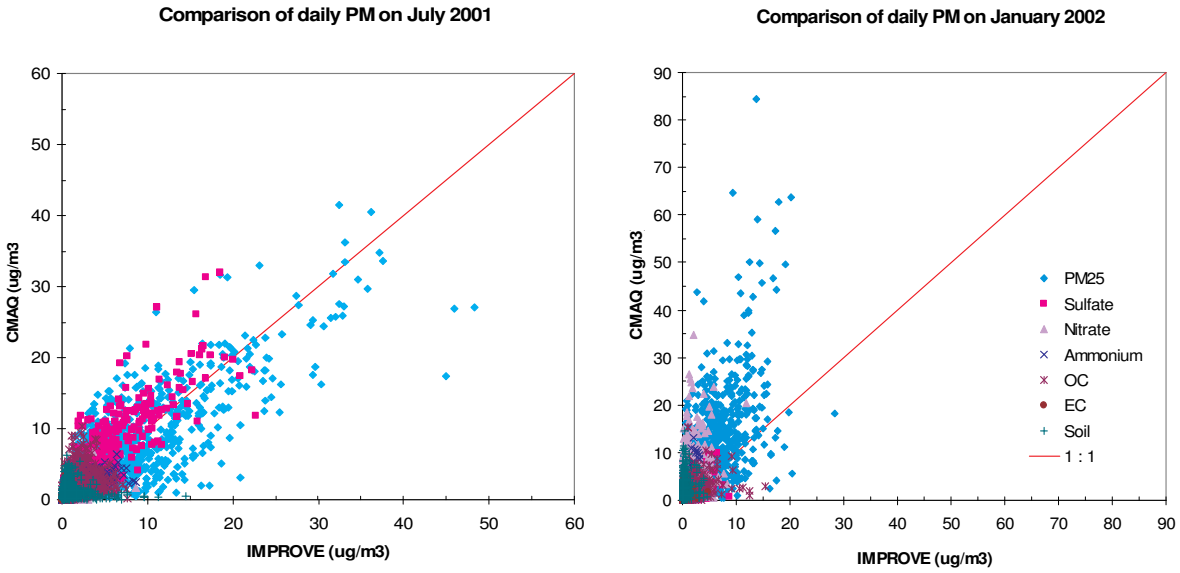


Figure C-16: Comparison of $PM_{2.5}$ between CMAQ results and IMPROVE and AQS data for the 12km domain during the August 2002 period

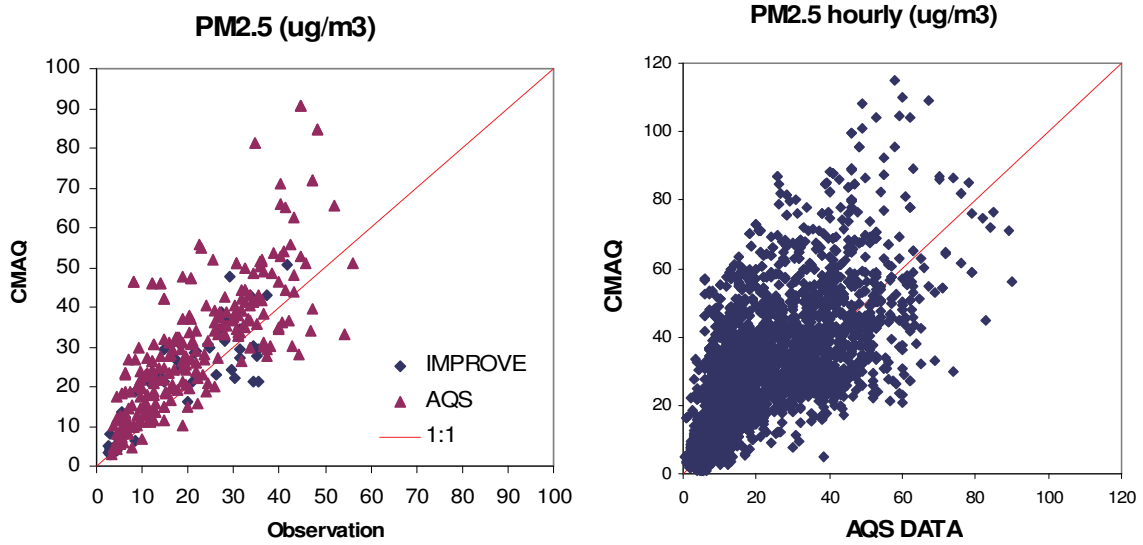
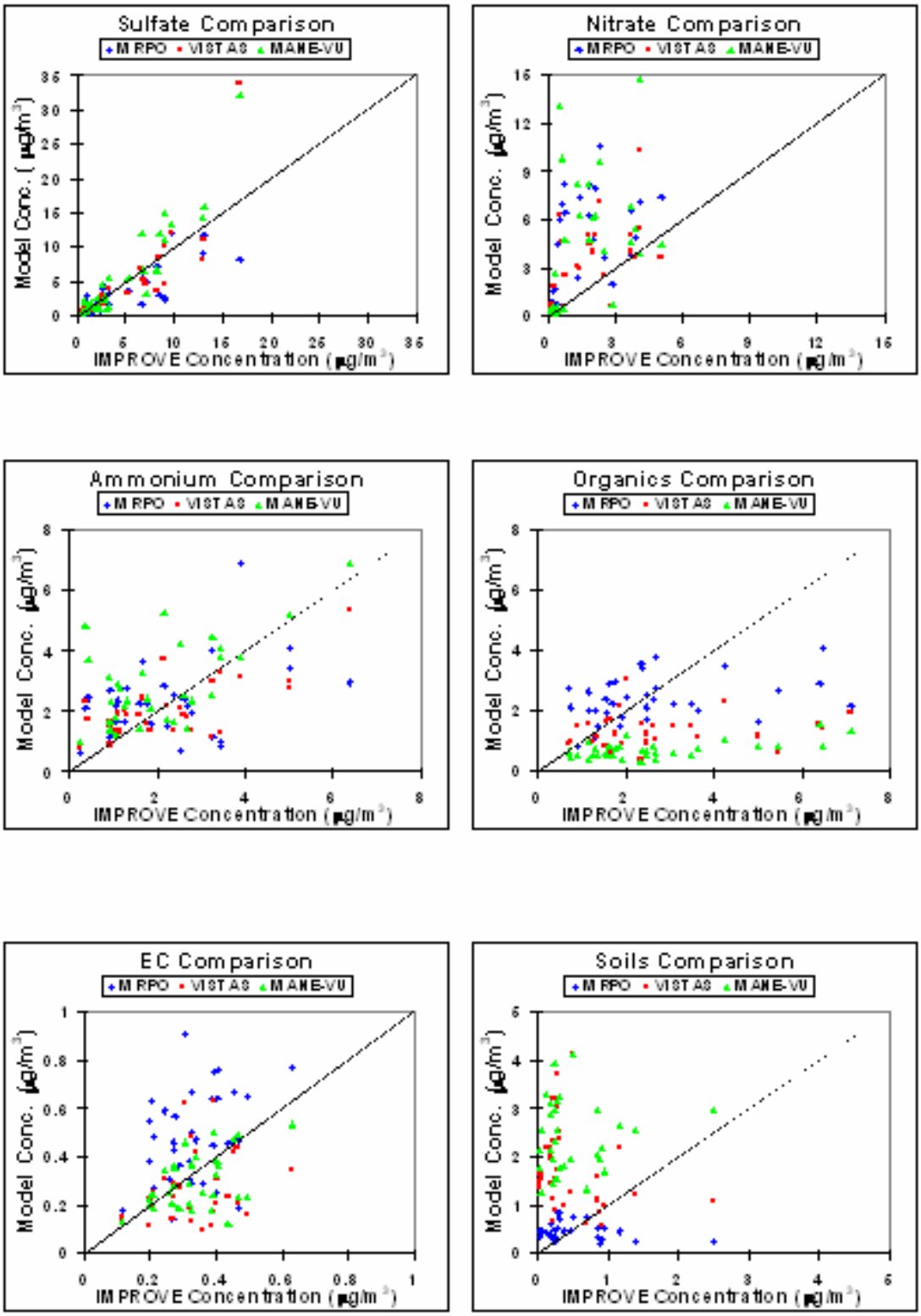


Figure C-17: Comparison of $PM_{2.5}$ species between IMPROVE data and a group of RPO CMAQ modeling on 36km US domain for July 2001 period (after Boylan, 2004)



C.3.3. REMSAD Tagged Species Results

REMSAD has been evaluated by EPA OAQPS for their CSA base case study using 1996 meteorology and 1996 NET Inventory.[3] Modeling results were compared with IMPROVE measurement as summarized in Table C-4. It shows that REMSAD performs better in the Eastern US than in the Western US on PM sulfate and $PM_{2.5}$, although it underestimates ambient levels countrywide. Emissions may contribute to poor performance on soil, carbonaceous aerosols and PM nitrate.

Table C-4: Normalized error of annual mean model prediction to annual mean observation on PM species between IMPROVE measurements and REMSAD 1996 annual simulation (after Timin, B. et al., 2002)

IMPROVE PM Species	National	East	West
PM2.5	-32%	-15%	-49%
Sulfate	-19%	-10%	-39%
Nitrate	5%	82%	-55%
Elemental Carbon	1%	23%	-20%
Organic Aerosols	-45%	-42%	-47%
Soil/Other	38%	225%	-18%

NESCAUM's REMSAD modeling used 1996 meteorology along with the 2001 Proxy emission inventory, thus a direct comparison of modeling results to daily observations cannot be completed. To evaluate REMSAD, NESCAUM first compared its own modeling results with EPA's CSA 2001 case modeling results, which also used 1996 meteorology. As shown in Figure C-18, NESCAUM's results exactly match with EPA's REMSAD modeling on $PM_{2.5}$ and PM sulfate distributions. In addition, NESCAUM compared the long term modeling average (annual mean) of PM species to IMPROVE annual means[4] for three sites. The results are presented in Figure C-19. It shows good agreement on REMSAD modeling of PM sulfate, PM NH_4, OC and EC. Emission inaccuracies may explain the model over-prediction of soil mass, while incomplete chemistry may cause observed differences for PM nitrate.

Given the reassuring results for sulfate, NESCAUM conducted REMSAD tagged sulfur modeling to assess states' impact on PM level over the Northeast US. Figure C-20 shows modeling results of state specific contributions to PM sulfate in the Brigantine, NJ Class I area for over thirty states. Similar plots are shown for Acadia, LyeBrook and Shenandoah (Figures C-21, C-22 and C-23 respectively). Also, the results were used to evaluate contributions to PM sulfate from elevated point sources in each RPO region, as shown in Figure C-24. Such information can help identify pollution source regions, and thus aid in the effect design of control strategies.

[3] Also see Clear Skies Act Air Quality Modeling Technical Support Document at: http://www.epa.gov/air/clearskies/aq_modeling_tsd_csa2003.pdf

[4] Multi-year averages were computed from the measurements to better account for the lack of correspondence between emissions year (2001) and meteorological year (1996).

Figure C-18: Comparison of annual average $PM_{2.5}$ and PM sulfate between NESCAUM REMSAD modeling and EPA REMSAD modeling

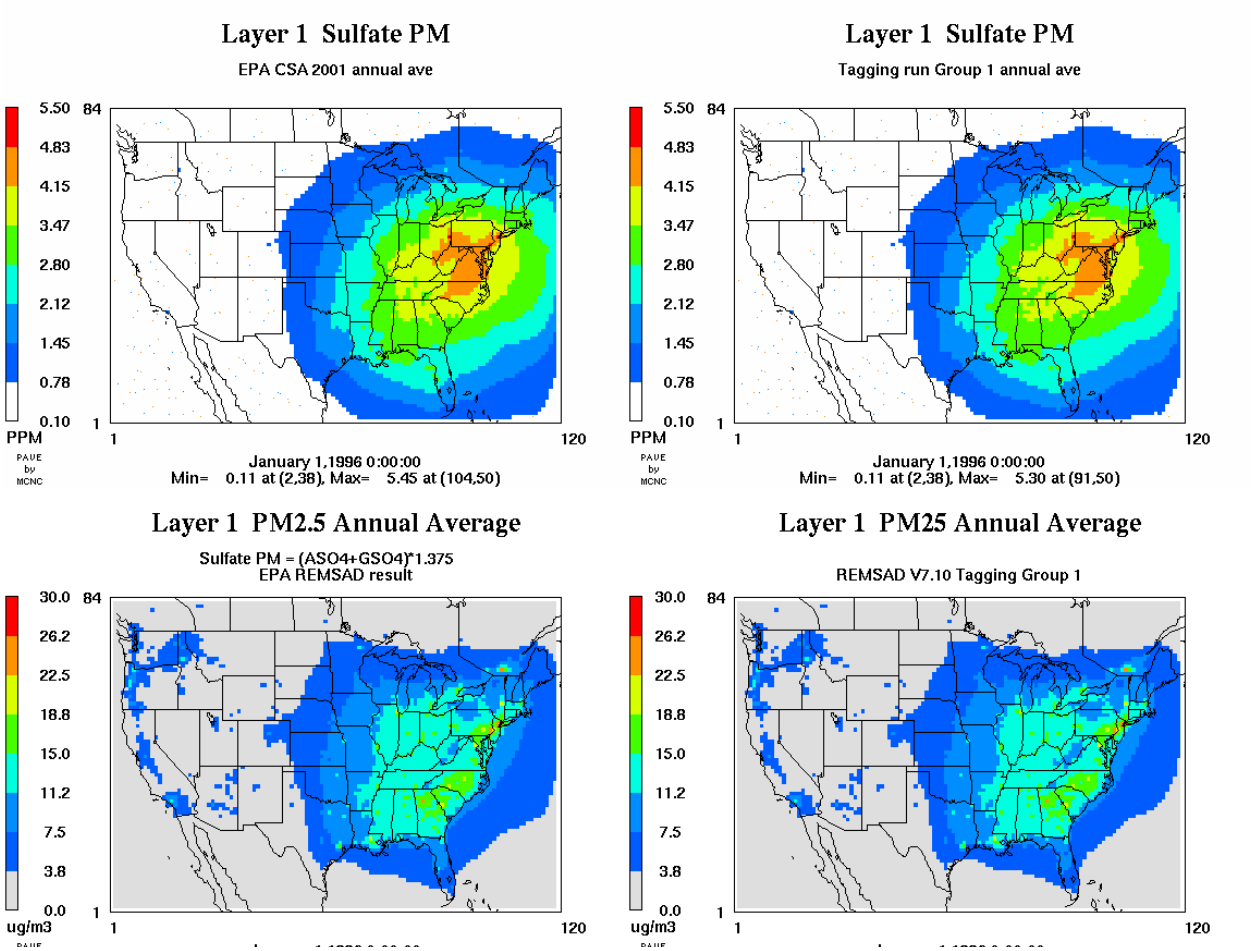


Figure C-19: Comparison of annual average PM species between NESCAUM REMSAD modeling and multi-year average IMPROVE measurements

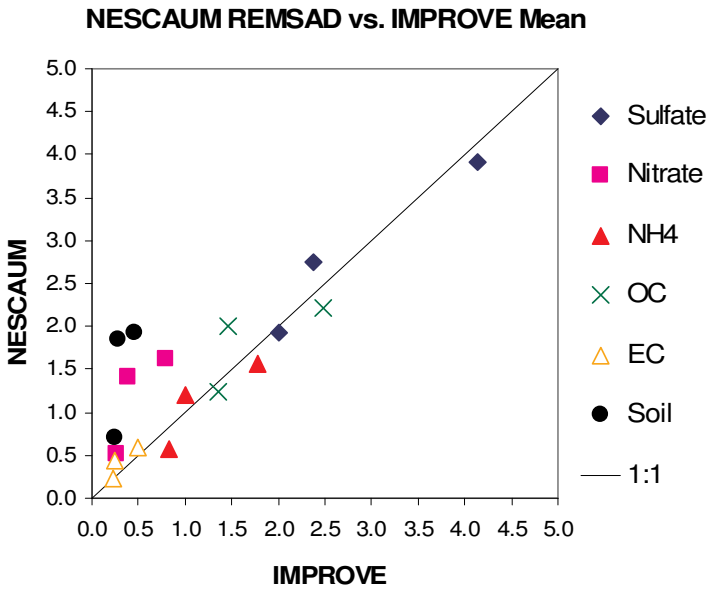


Figure C-20: Contribution to PM sulfate in Brigantine, NJ by states in the Eastern US

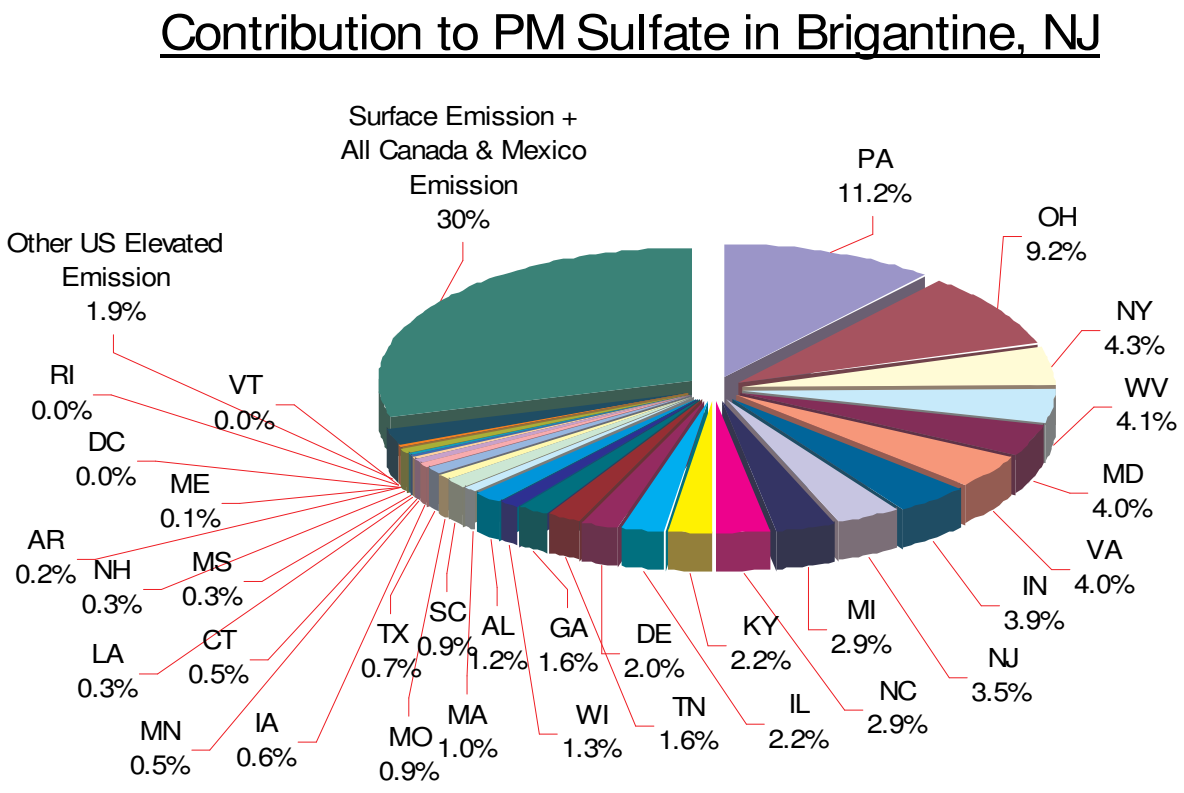


Figure C-21: Contribution to PM sulfate in Acadia, ME by states in the Eastern US

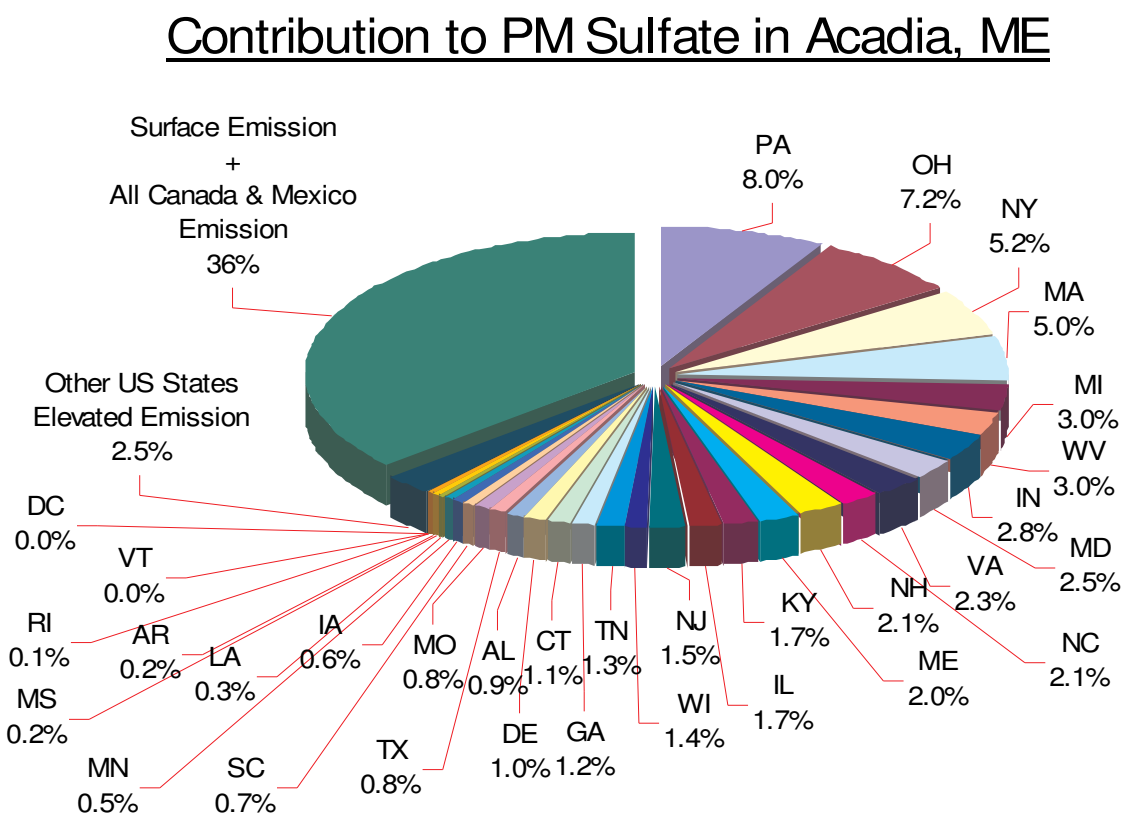


Figure C-22: Contribution to PM sulfate in Lye Brook, VT by states in the Eastern US

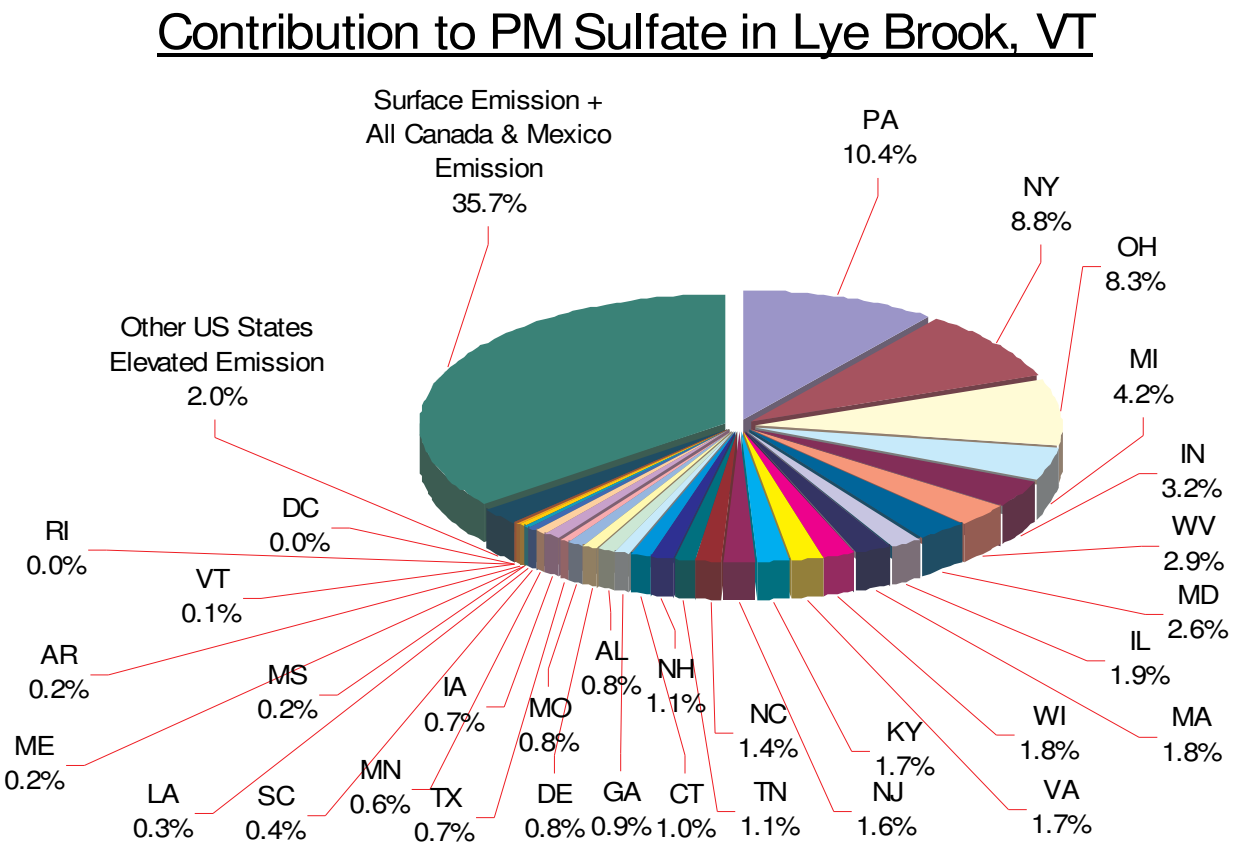


Figure C-23: Contribution to PM sulfate in Shenandoah, VA by states in the Eastern US

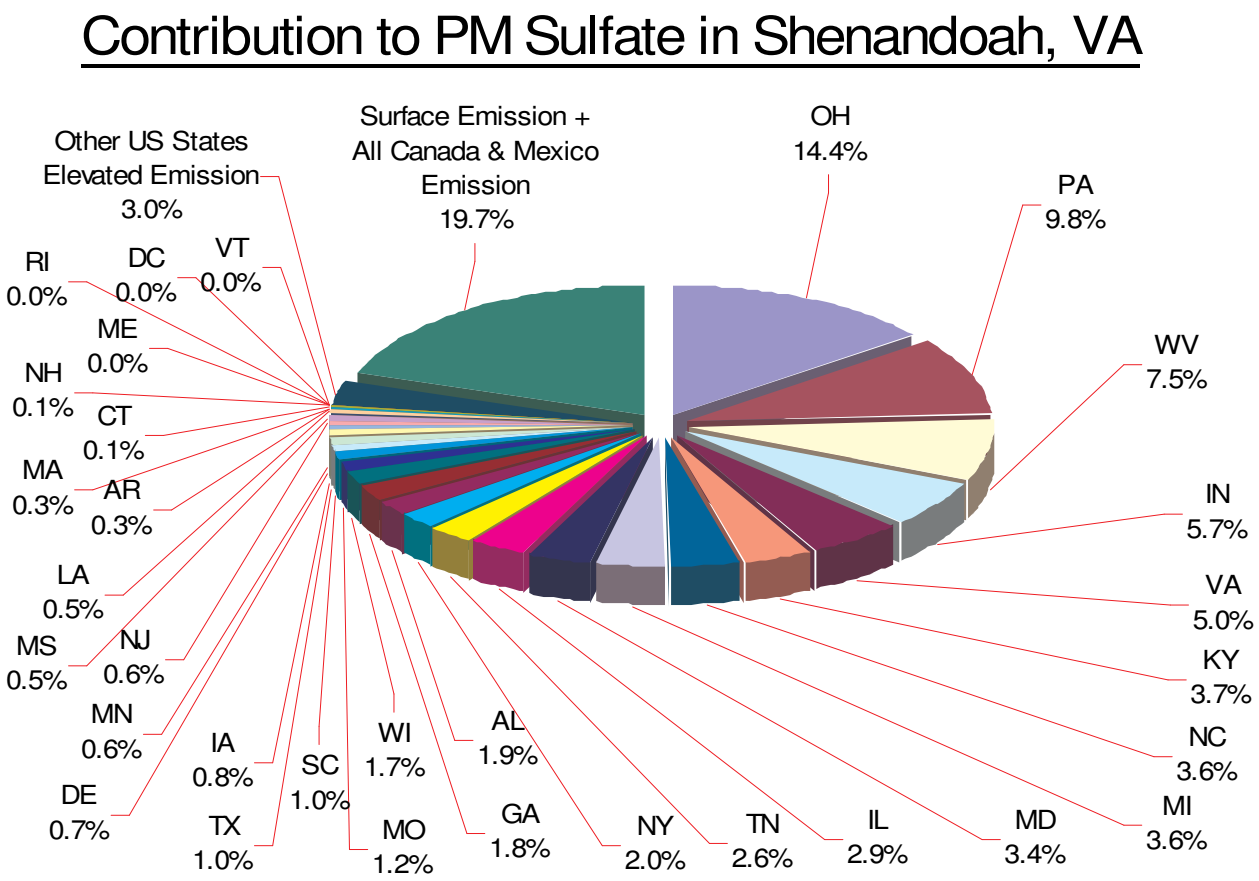
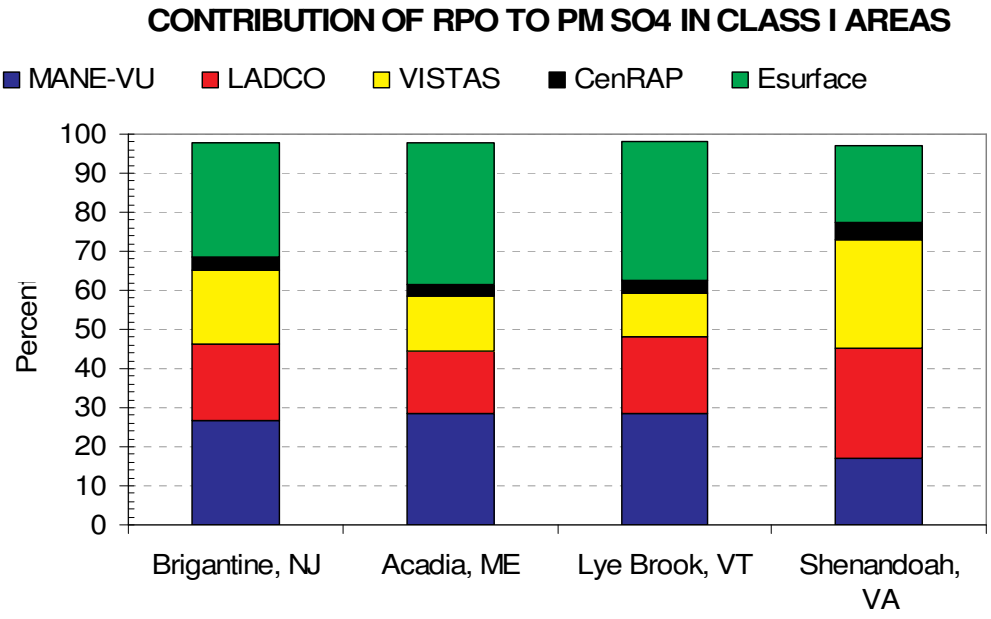


Figure C-24: Contributions to PM sulfate in four Class I areas in the Northeast US by RPO region.



Statistical parameters used in model performance evaluation. P_i and O_i are paired model prediction and observation, respectively. MB, ME, and RMSE are with the same the unit of P_i and O_i, while other parameters with the unit of percent.

Mean Bias (***MB***) $$\frac{1}{N}\sum_{i=1}^{N}(P_i - O_i)$$

Mean Error (***ME***) $$\frac{1}{N}\sum_{i=1}^{N}|P_i - O_i|$$

Root Mean Square Error (***RMSE***) $$\left[\frac{1}{N}\sum_{i=1}^{N}(P_i - O_i)^2\right]^{1/2}$$

Normalized Mean Bias (***NMB***) $$\frac{\sum_{i=1}^{N}(P_i - O_i)}{\sum_{i=1}^{N}O_i}$$

Normalized Mean Error (***NME***) $$\frac{\sum_{i=1}^{N}|P_i - O_i|}{\sum_{i=1}^{N}O_i}$$

Mean Normalized Bias (***MNB***) $$\frac{1}{N}\sum_{i=1}^{N}\frac{(P_i - O_i)}{O_i}$$

Mean Normalized Error (***MNE***) $$\frac{1}{N}\sum_{i=1}^{N}\frac{|P_i - O_i|}{O_i}$$

Fractional Bias (***FB***) $$\frac{2}{N}\sum_{i=1}^{N}\left(\frac{P_i - O_i}{P_i + O_i}\right)$$

Fractional Error (***FE***) $$\frac{2}{N}\sum_{i=1}^{N}\left|\frac{P_i - O_i}{P_i + O_i}\right|$$

References

Bell, M., and H. Ellis. *Comparison of the 1-hr and 8-hr National Ambient Air Quality Standards for ozone using Models-3,* J. Air Waste Manage. Assoc., 53, 1531-1540, 2003.

Boylan, J., and K. Baker. *Photochemical Model Performance and Consistency.* National RPO Modleing Meeting, Denver, CO. May 26, 2004.

Byun D.W., and J.K.S. Ching. *Science Algorithms of the EPA Models-3 Community Multiscale Air Quality (CMAQ) Modeling System*. EPA/600/R-99/030. March 1999.

Gery M.W., G.Z. Whitten, J.P. Killus, and M.C. Dodge. A photochemical kinetics mechanism for urban and regional scale computer modeling. J. Geophys. Res. 94, 12,925-12956, 1989.

Hao, W., M. Ku, and G. Sistla. *Analysis of MM5 Simulations based on three PBL schemes over the eastern US for August 6 to 16, 2002*. NYSDEC-DAR. Albany, NY. March 4, 2004

Hogrefe, C., J. Biswas, B. Lynn, K. Civerolo, J.-Y. Ku, J. Rosenthal, C. Rosenzweig, C. Goldberg, and P.L. Kinney. *Simulating regional-scale ozone climatology over the eastern United States: Model evaluation results.* Atmos. Environ. 38, 2627-2638, 2004.

Jimenez P., and J. M. Baldasano. *Ozone response to precursor controls in very complex terrains: Use of photochemical indicators to assess O3-NOx-VOC sensitivity in the northeastern Iberian Peninsula*. J. Geophys. Res., V109, D20309, 2004.

Mao H., and R. Talbot. *Role of meteorological processes in two New England ozone episodes during summer 2001*. J. Geophys. Res., V109, D20305, 2004.

Mebust, M.R., B.K. Eder, F.S. Binkowski, S.J. Roselle. Models-3 Community Multiscale Air Quality (CMAQ) model aerosol component 2. Model evaluation. *J. Geophys. Res.,* V108, D6*, 4184, 2003*

Ray, J.D., R.L. Heavner, M. Flores, and C.W. Michaelsen. *Surface-level measurements of ozone and precursors at coastal and offshore locations in the Gulf of Maine.* J. Geophys. Res.*,* 101, 29,005-29,011, 1996

SAI. *User's Guide to the Regional Modeling System for Aerosols and Deposition (REMSAD), Version 7.* ICF Consulting/SAI, San Francisco, CA. 2002.

Seigneur C., Hidy G., Tombach I., Vimont J. and P. Amar, "***SCIENTIFIC PEER-REVIEW OF THEREGULATORY MODELING SYSTEM FOR AEROSOLS AND DEPOSITION (REMSAD).***" September 1999*.*

Timin, B., C. Jang, P. Dolwick, N. Possiel, T. Braverman. *Operational Evaluation and Comparison of CMAQ and REMSAD- An Annual Simulation*. CMAS Annual Workshop, RTP, NC. October 22, 2002.

Tonnesen, G., Z. Wang, C.J. Chien, M. Omary, B. Wang, R. Morris, Z. Adelman, T. Tesche, D. Olerud. *Regional Haze Modeling: Recent Modeling Results for VISTAS and WRAP*. CMAS Annual Meeting, RTP, NC. October 27, 2003.

CMAQ Peer Review Report. *Final Report Summary: December 2003 Peer Review of the CMAQ Model* August 2004
http://www.cmascenter.org/html/CMAQ%20peer%20review%20final_CMAS-web.pdf

CMAQ website http://www.cmascenter.org/

CMAQ Manual http://www.epa.gov/asmdnerl/models3/doc/science/science.html

SMOKE website http://cf.unc.edu/cep/empd/products/smoke/index.cfm

SMOKE Manual http://cf.unc.edu/cep/empd/products/smoke/version2.1/html/

MM5 website http://www.mmm.ucar.edu/mm5/

REMSAD website http://www.remsad.com