

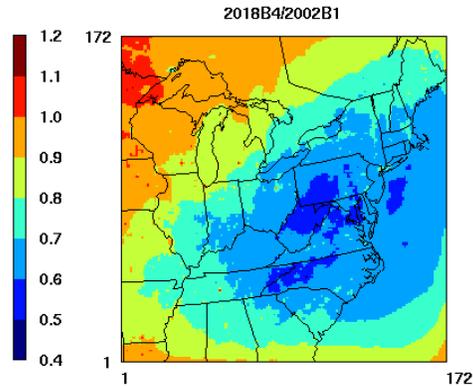
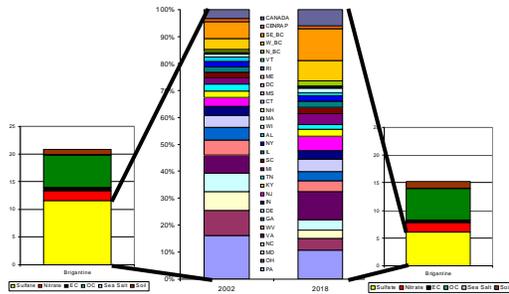
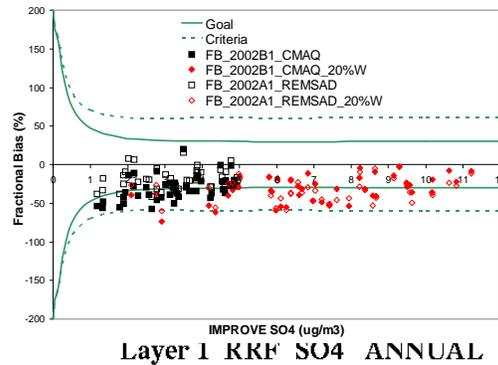
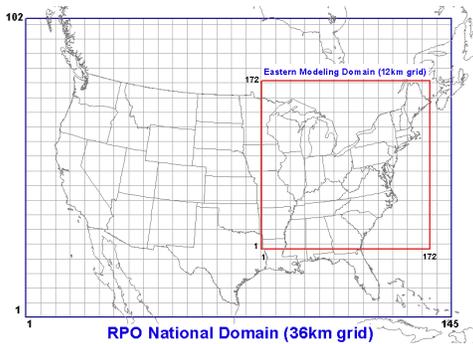
Appendix R

MANE-VU Modeling for Reasonable Progress Goals (February 2008)

THIS PAGE INTENTIONALLY BLANK

MANE-VU Modeling for Reasonable Progress Goals

Model performance evaluation, pollution apportionment, and control measure benefits



Prepared by
NESCAUM
For the
Mid-Atlantic/Northeast Visibility Union Regional Planning Organization

February 7, 2008

Members of Northeast States for Coordinated Air Use Management

Arthur Marin, Executive Director
Northeast States for Coordinated Air Use Management

Anne Gobin, Bureau Chief
Connecticut Department of Environmental Protection, Bureau of Air Management

James P. Brooks, Bureau Director
Maine Department of Environmental Protection, Bureau of Air Quality

Barbara Kwetz, Director
Massachusetts Department of Environmental Protection, Bureau of Waste Prevention

Robert Scott, Director
New Hampshire Department of Environmental Services, Air Resources Division

William O'Sullivan, Director
New Jersey Department of Environmental Protection, Office of Air Quality Management

David Shaw, Director
New York Department of Environmental Conservation, Division of Air Resources

Stephen Majkut, Chief
Rhode Island Department of Environmental Management, Office of Air Resources

Richard A. Valentinetti, Director
Vermont Department of Environmental Conservation, Air Pollution Control Division

MANE-VU Modeling for Reasonable Progress Goals

Model performance evaluation, pollution
apportionment, and control measure benefits

**Prepared by
NESCAUM
for the**

Mid-Atlantic/Northeast Visibility Union Regional Planning Organization

February 7, 2008

**MANE-VU MODELING FOR REASONABLE
PROGRESS GOALS**
MODEL PERFORMANCE EVALUATION,
POLLUTION APPORTIONMENT, AND CONTROL
MEASURE BENEFITS

Project Director

Gary Kleiman, NESCAUM

Editor

Paul Miller, NESCAUM

Administrative Support

Emily Savelli, Iyad Kheirbek, NESCAUM

Principal Contributors

Shan He, Emily Savelli, Jung-Hun Woo, John Graham, NESCAUM

Acknowledgments

NESCAUM could not have completed this work without the preparation of emission inventories by the Mid-Atlantic Regional Air Management Association (MARAMA) and the MANE-VU member states. NESCAUM also acknowledges the funding for this work through USEPA agreement number XA-97318101-0 to the Ozone Transport Commission in support of the MANE-VU Regional Planning Organization. NESCAUM is solely responsible for the content of this report and any errors it may contain.

Printed: February 2008

TABLE OF CONTENTS

Acknowledgments.....	iv
TABLE OF CONTENTS	v
FIGURES	vi
TABLES	vii
Executive Summary	viii
1. Introduction.....	1-1
1.1. Background.....	1-1
1.2. Meteorology.....	1-2
1.3. Emissions Preparations	1-6
1.3.1. Emissions Processing Files	1-8
1.3.2. 2002 Emission Inventory	1-10
1.3.3. 2018 “On the Books/On the Way” (OTB/OTW) Emission Inventory	1-14
1.3.4. 2018 “Beyond on the Way” (BOTW) Emission Inventory	1-18
1.3.5. 2018 Sulfate Tagging (BOTW) Emission Inventory	1-19
1.4. Model Platforms.....	1-20
1.4.1. CMAQ.....	1-20
1.4.2. REMSAD.....	1-21
2. Performance evaluation	2-1
2.1. Meteorological Evaluation.....	2-1
2.2. Model Evaluation.....	2-10
3. 2018 BOTW Projections.....	3-1
4. 2018 Pollution Apportionment	4-1
5. Control Strategy Evaluation.....	5-1
5.1. Reduced sulfur fuel content (S1 and S2)	5-1
5.2. Best Available Retrofit Program (BART)	5-3
5.3. 167 EGU Strategy	5-5
6. Conclusions.....	6-1
7. References.....	7-1

FIGURES

Figure 1-1. Modeling domains used in MANE-VU air quality modeling studies with CMAQ. Outer (blue) domain grid is 36 km and inner (red) domain is 12 km grid. The gridlines are shown at 180 km intervals (5 × 5 36 km cells/15 × 15 12 km cells).	1-2
Figure 1-2. Vertical Structure of Meteorological and Air Quality Modeling Domains ..	1-4
Figure 1-3. MM5 modeled wind field map at 12:00 UTC on August 8, 2002	1-5
Figure 1-4. Observation Network sites within 12km resolution domain.....	1-5
Figure 1-5. Examples of processed model-ready emissions: (a) SO ₂ from Point; (b) NO ₂ from Area; (c) NO ₂ from Onroad; (d) NO ₂ from Nonroad; (e) ISOP from Biogenic; (f) SO ₂ from all source categories	1-7
Figure 2-1. 2002 seasonal average hourly bias of wind speed and direction	2-2
Figure 2-2. 2002 seasonal hourly average index of agreement for wind speed.....	2-3
Figure 2-3. Quarterly correlation coefficient (r) of hourly wind speed between modeling and measurement for each observation site in 2002	2-4
Figure 2-4. Quarterly correlation coefficient (r) of hourly wind direction between modeling and measurement for each observation site in 2002	2-5
Figure 2-5. 2002 Seasonal Hourly Average Bias of Temperature.....	2-7
Figure 2-6. 2002 Seasonal Hourly Average Index of Agreement	2-7
Figure 2-7. Quarterly correlation coefficient (r) of hourly temperature between modeling and measurement for each observation site in 2002	2-8
Figure 2-8. 2002 Seasonal average hourly bias of humidity	2-9
Figure 2-9. 2002 seasonal hourly average index of agreement	2-9
Figure 2-10. Quarterly correlation coefficient (r) of hourly humidity between modeling and measurement for each observation site in 2002	2-10
Figure 2-11. Domain-wide paired comparison of daily average PM _{2.5} species between CMAQ predictions and measurements from IMPROVE networks.....	2-13
Figure 2-12. Spatial distribution of correlation coefficient between PM _{2.5} Sulfate and measurement	2-14
Figure 2-13. Spatial distribution of correlation coefficient between PM _{2.5} and measurement	2-14
Figure 2-14. Mean Fractional Error of PM _{2.5} species within MANE-VU region.....	2-15
Figure 2-15. Mean Fraction Bias of PM _{2.5} species within MANE-VU region.....	2-16
Figure 2-16. Paired comparison of extinction coefficient between CMAQ prediction and IMPROVE measurement	2-17
Figure 2-17. Paired Comparison of Haze Index between CMAQ prediction and IMPROVE measurement at selected Class I sites.....	2-17
Figure 3-1. Projected improvement in visibility at four Northeast sites based on 2009 and 2018 BOTW-1 projections.....	3-2
Figure 3-2. Projected improvement in visibility at three Mid-Atlantic sites based on 2009 and 2018 BOTW-1 projections.....	3-2
Figure 4-1. a. Measured and projected mass contributions in 2002 and 2018 at Acadia National Park on twenty percent worst visibility days.....	4-2
Figure 4-2. a. Measured and projected mass contributions in 2002 and 2018 at Brigantine Wildlife Refuge on twenty percent worst visibility days.....	4-3

Figure 4-3. a. Measured and projected mass contributions in 2002 and 2018 at Lye Brook Wilderness Area on twenty percent worst visibility days.....	4-4
Figure 4-4. a. Measured and projected mass contributions in 2002 and 2018 at Great Gulf Wilderness Area on twenty percent worst visibility days.....	4-5
Figure 4-5. a. Measured and projected mass contributions in 2002 and 2018 at Moosehorn National Wildlife Refuge on twenty percent worst visibility days....	4-6
Figure 5-1. Average change in 24-hr PM _{2.5} due to S1 emission reductions (µg/m ³)	5-2
Figure 5-2. Average change in 24-hr PM _{2.5} due to S2 emission reductions, relative to S1 (µg/m ³)	5-3
Figure 5-3. Potential reductions from BART-eligible sources in the MANE-VU region (tons)	5-4
Figure 5-4. Average change in 24-hr PM _{2.5} due to BART emission reductions (µg/m ³)	5-5
Figure 5-5. Average change in 24-hr PM _{2.5} due to 167 EGU emission reductions (µg/m ³)	5-6
Figure 5-6. Visibility improvement relative to uniform rate of progress at Acadia National Park.....	5-7
Figure 5-7. Visibility improvement relative to uniform rate of progress at Brigantine National Wildlife Refuge.	5-7
Figure 5-8. Visibility improvement relative to uniform rate of progress at Great Gulf Wilderness Area	5-8
Figure 5-9. Visibility improvement relative to uniform rate of progress at Lye Brook Wilderness Area	5-8
Figure 5-10. Visibility improvement relative to uniform rate of progress at Moosehorn National Wildlife Refuge	5-9
Figure 5-11. Visibility improvement relative to uniform rate of progress at Shenandoah National Park.....	5-9
Figure 5-12. Visibility improvement relative to uniform rate of progress at Dolly Sods Wilderness Area	5-10
Figure 5-13. Visibility improvement relative to uniform rate of progress at Presidential Range-Dry River Wilderness Area	5-10
Figure 5-14. Visibility improvement relative to uniform rate of progress at Roosevelt-Campobello International Park	5-11

TABLES

Table 3-1. 2018 twenty percent worst days relative reduction factors.	3-1
Table 5-1. Projected 2018 twenty percent worst day sulfate mass reduction at MANE-VU Class I areas under various control assumptions.....	5-12
Table 5-2. Projected 2018 twenty percent worst day deciview goals for MANE-VU Class I areas under various control assumptions	5-13

Executive Summary

The main purpose of this report is to assist states in developing effective solutions to regional visibility and fine particle problems and comply with requirements under the Regional Haze Rule. NESCAUM has utilized in-house air quality modeling capabilities that include emission processing, meteorological input analysis, and chemical transport modeling to conduct regional air quality simulations for calendar year 2002 and several future periods. This work has been directed at satisfying a number of compliance goals under the Haze State Implementation Plan (SIP), including a contribution assessment, a pollution apportionment for 2018, and the evaluation of visibility benefits of control measures being considered for achieving reasonable progress goals and establishing a long-term emissions management strategy for MANE-VU Class I areas.

The modeling tools utilized for these analyses include MM5, SMOKE, CMAQ and REMSAD, and incorporate tagging features that allow for the tracking of individual source regions or measures. These tools have been evaluated and found to perform adequately relative to USEPA modeling guidance.

Results show that sulfate aerosol – the dominant contributor to visibility impairment in the Northeast’s Class I areas on the 20 percent worst visibility days – has significant contributions from states throughout the eastern U.S. that are projected to continue in future years from all three of the eastern regional planning organizations (RPOs).

An assessment of potential control measures that would address this future contribution has identified a number of promising strategies that would yield significant visibility benefits beyond the uniform rate of progress and, in fact, significantly beyond the projected visibility conditions that would result from “on the books/on the way” air quality protection programs. These “beyond on the way” measures include the adoption of low sulfur heating oil, implementation of Best Available Retrofit Technology (BART) requirements, and additional electric generating unit (EGU) controls on select sources. The combined benefits of adopting all of these programs could lead to an additional benefit of between 0.38 and 1.1 deciviews at MANE-VU Class I areas on the 20 percent worst visibility days by 2018.

1. INTRODUCTION

1.1. Background

This report presents information intended to assist states in developing effective solutions to regional visibility and fine particle problems and comply with requirements under the 1999 U.S. Environmental Protection Agency (USEPA) “Regional Haze Rule” [64 Fed. Reg. 35714 (July 1, 1999)]. NESCAUM has utilized in-house air quality modeling capabilities that include emission processing, meteorological input analysis, and chemical transport modeling to conduct regional air quality simulations for calendar year 2002 and several future periods.

This work has been directed at satisfying a number of compliance goals under the Haze State Implementation Plans (SIPs), including a contribution assessment (*see* NESCAUM, 2006a), a pollution apportionment for 2018, and the evaluation of benefits of control measures being considered for achieving reasonable progress establishing a long-term emissions management strategy for MANE-VU Class I areas.¹ NESCAUM has employed several tools to achieve all of these goals, but the primary tool described and detailed here consists of a regional air quality modeling platform using meteorological fields developed by the University of Maryland using the MM5 platform (Penn State, 2007), emission inventories developed by MANE-VU (MARAMA, 2007a) and processed through the SMOKE emissions processing tool (SMOKE, 2007), and air quality simulations conducted jointly by multiple modeling centers utilizing USEPA’s Community Multi-scale Air Quality (CMAQ) model (Byun and Ching, 1999). Sulfate apportionment was also carried out using the REMSAD model (SAI, 2005) with SO₂ tagging capabilities and control strategy evaluation was conducted utilizing a beta version of CMAQ-PPTM (ICF, 2006).

This report describes these efforts that form the foundation upon which MANE-VU states will base their haze SIP submissions. After the MANE-VU RPO considers the results provided here and consults with neighboring states and federal land managers, we anticipate that a final model simulation will be conducted to serve as a basis for calculating final reasonable progress goals.

This introduction provides a basic description of the modeling platform and the input data that we used for regional air quality simulations. Chapter 2 provides a model performance evaluation for both the meteorological input data as well as the chemical transport model for the base year 2002. Chapters 3 through 5 present results from 2018 simulations with respect to the projected “beyond on the way” scenario that we take as a starting point for the haze program, pollution apportionment for 2018, and haze control strategy evaluation.

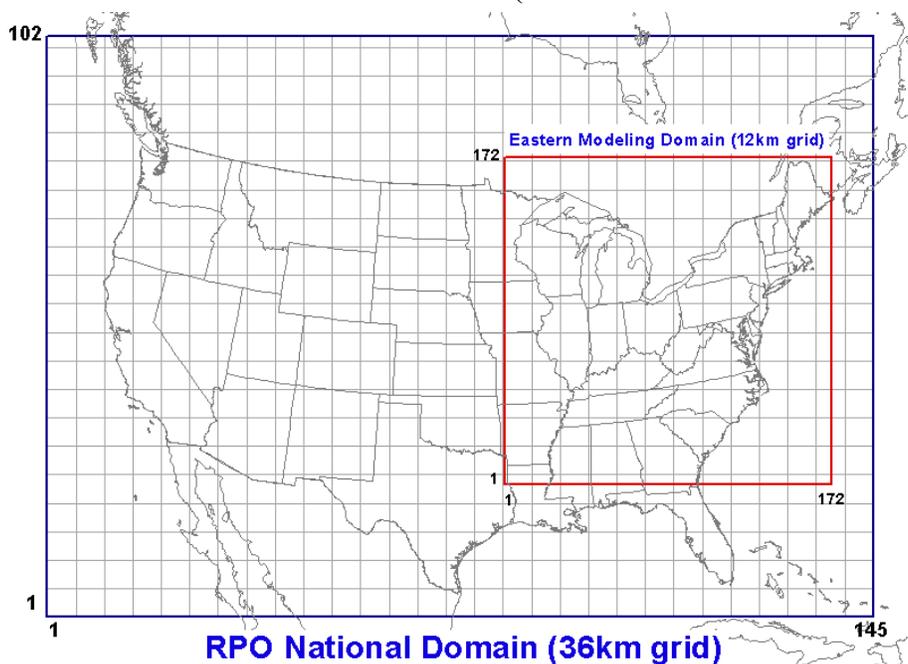
¹ There are seven designated Class I areas in the Northeast and Mid-Atlantic States. They include Acadia National Park and Moosehorn Wilderness Area in Maine; Roosevelt Campobello International Park in New Brunswick and Maine; the Lye Brook Wilderness Area in Vermont; the Great Gulf and Presidential Range-Dry River Wilderness Areas in New Hampshire; and the Brigantine Wilderness Area in New Jersey.

1.2. Meteorology

Professor Dalin Zhang's group from University of Maryland (UMD) provided the 2002 annual meteorological field for air quality modeling. Meteorological inputs for CMAQ are derived from the Fifth-Generation Pennsylvania State University/National Center for Atmospheric Research (NCAR) Mesoscale Model (MM5)² system meteorological fields. 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.

MANE-VU has adopted the Inter-RPO domain description for its modeling runs.³ This 36-km domain covers the continental United States, southern Canada and northern Mexico. The dimensions of this domain are 145 and 102 cells in the east-west and north-south directions, respectively. A 12-km inner domain was selected to better characterize air quality in MANE-VU and surrounding RPO regions. This domain covers the eastern region, which includes the northeastern, central, and southeastern U.S., as well as southeastern Canada. It extends from 66°W~94°W in longitude and 29°N~50°N in latitude with 172 × 172 grid cells (Figure 1-1).

Figure 1-1. Modeling domains used in MANE-VU air quality modeling studies with CMAQ. Outer (blue) domain grid is 36 km and inner (red) domain is 12 km grid. The gridlines are shown at 180 km intervals (5 × 5 36 km cells/15 × 15 12 km cells).



² <http://www.mmm.ucar.edu/mm5/>

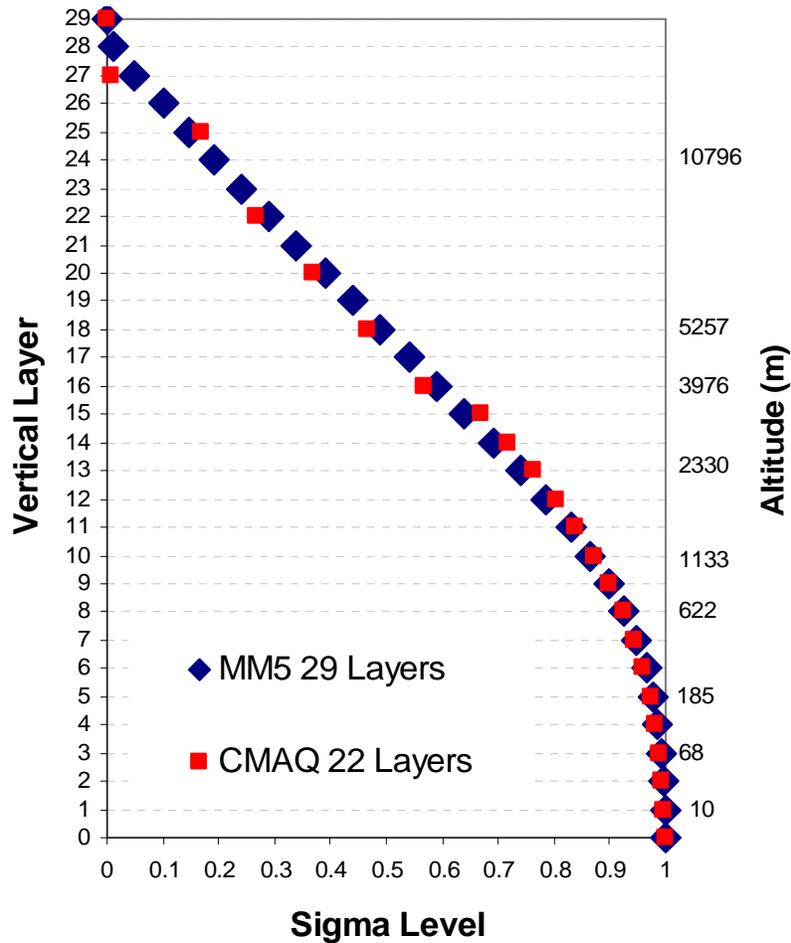
³ The modeling system for 2002 annual simulation is applied with a Lambert Conformal Conic projection with parallels at 33N and 45N. A spherical earth radius of 6370km is used for all elements of the system (MM5/SMOKE/CMAQ).

The UMD MM5 model runs are made on these two nested domains with the inner (12 km) domain using finer resolution terrain data. Initially, we conducted a set of test runs for the period of August 6 to 16, 2002.

The horizontal coordinated system is equally spaced geographically and uses the Arakawa-B gridding scheme. The resolution can be as high as 1 km. Sigma (σ) is a terrain-following vertical coordinate that is a function of pressure at the point (for hydrostatic) or reference (non-hydrostatic) state pressure (P), the surface pressure (P_{s0}), and the pressure at the top (P_{top}) of the model; $\sigma = (P - P_{top}) / (P_{s0} - P_{top})$. The model utilizes a terrain-following sigma coordinate with 29 layers. The first level is at 10 m and a radiative upper-boundary condition is at 50 hPa (Figure 1-2).

Based on test run results, the boundary layer processes were 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. UMD ran the non-hydrostatic MM5 v3.5.3 with three planetary boundary layer (PBL) schemes; (1) modified Blackadar [BL], (2) the Pleim-Xiu scheme with the soil module [P-X], and (3) modified Blackadar with soil module [SSIB]. The model was initialized with the analyses of the National Center for Environmental Prediction (Eta Model). TDL data are used for MM5 nudging. A modeled wind field map (Figure 1-3) shows typical prevailing mesoscale flows from the midwest U.S. to the East Coast.

Figure 1-2. Vertical Structure of Meteorological and Air Quality Modeling Domains



The simulated meteorological fields were compared to the measurements from Techniques Development Laboratory of National Weather Service (TDL NWS) and Clean Air Status and Trends Network (CASTNET). The TDL data are reflective of urban/suburban settings, while the CASTNET sites are more representative of rural areas. There are 48 CASTNET sites and about 800 TDL sites within Domain 2 (as shown in Figure 1-4). Overall, the BL scheme shows a better correspondence to the measured data than the other two schemes, although it poorly captures the 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).

Figure 1-3. MM5 modeled wind field map at 12:00 UTC on August 8, 2002

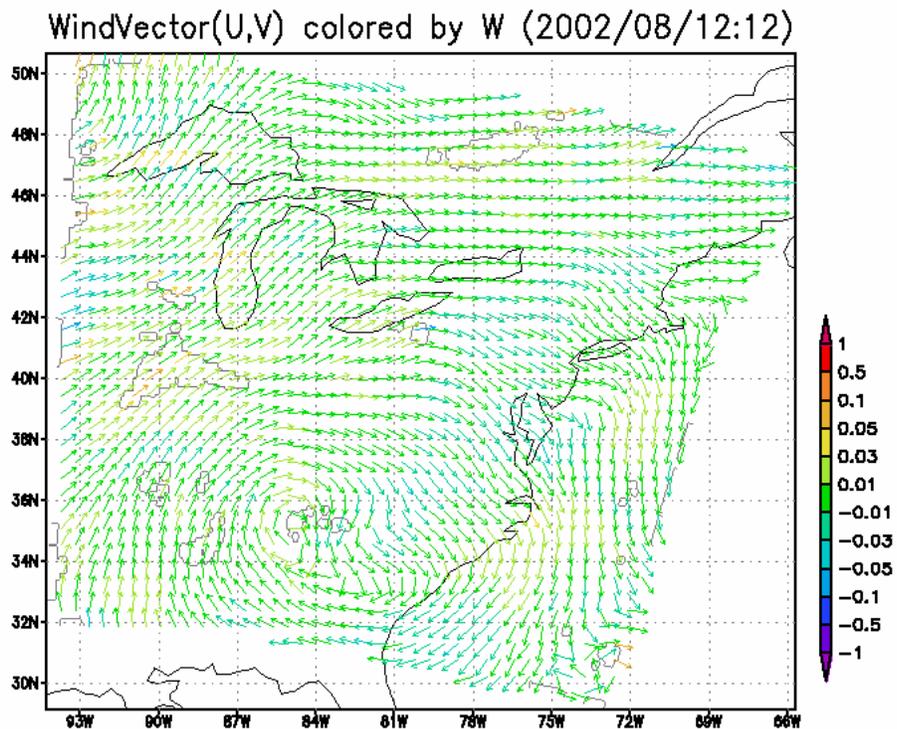
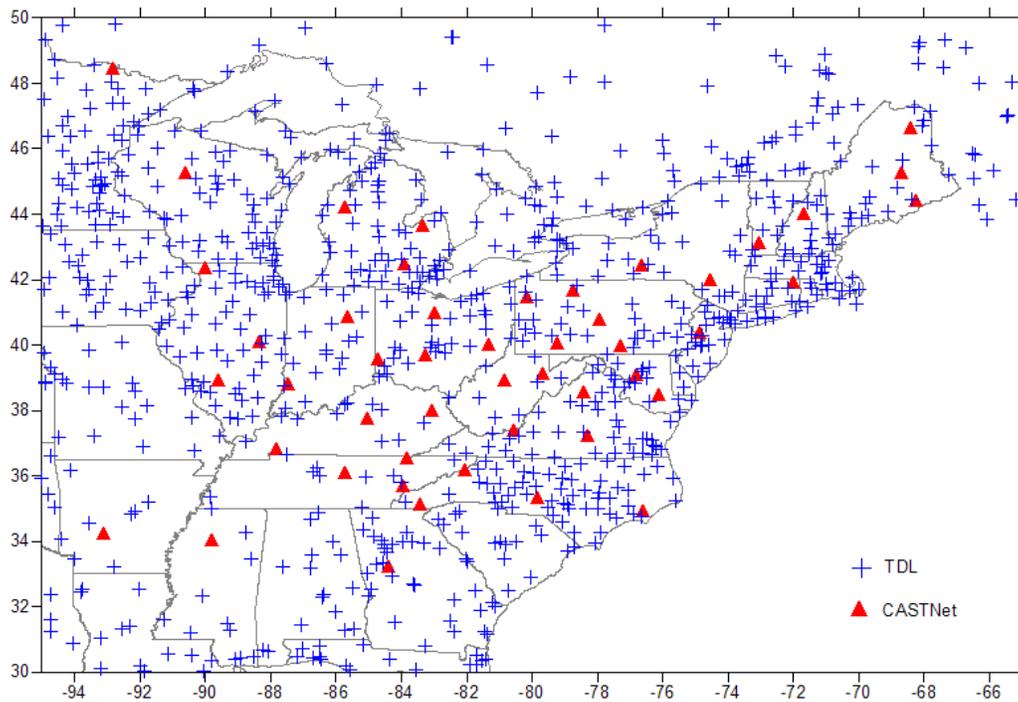


Figure 1-4. Observation Network sites within 12km resolution domain



1.3. Emissions Preparations

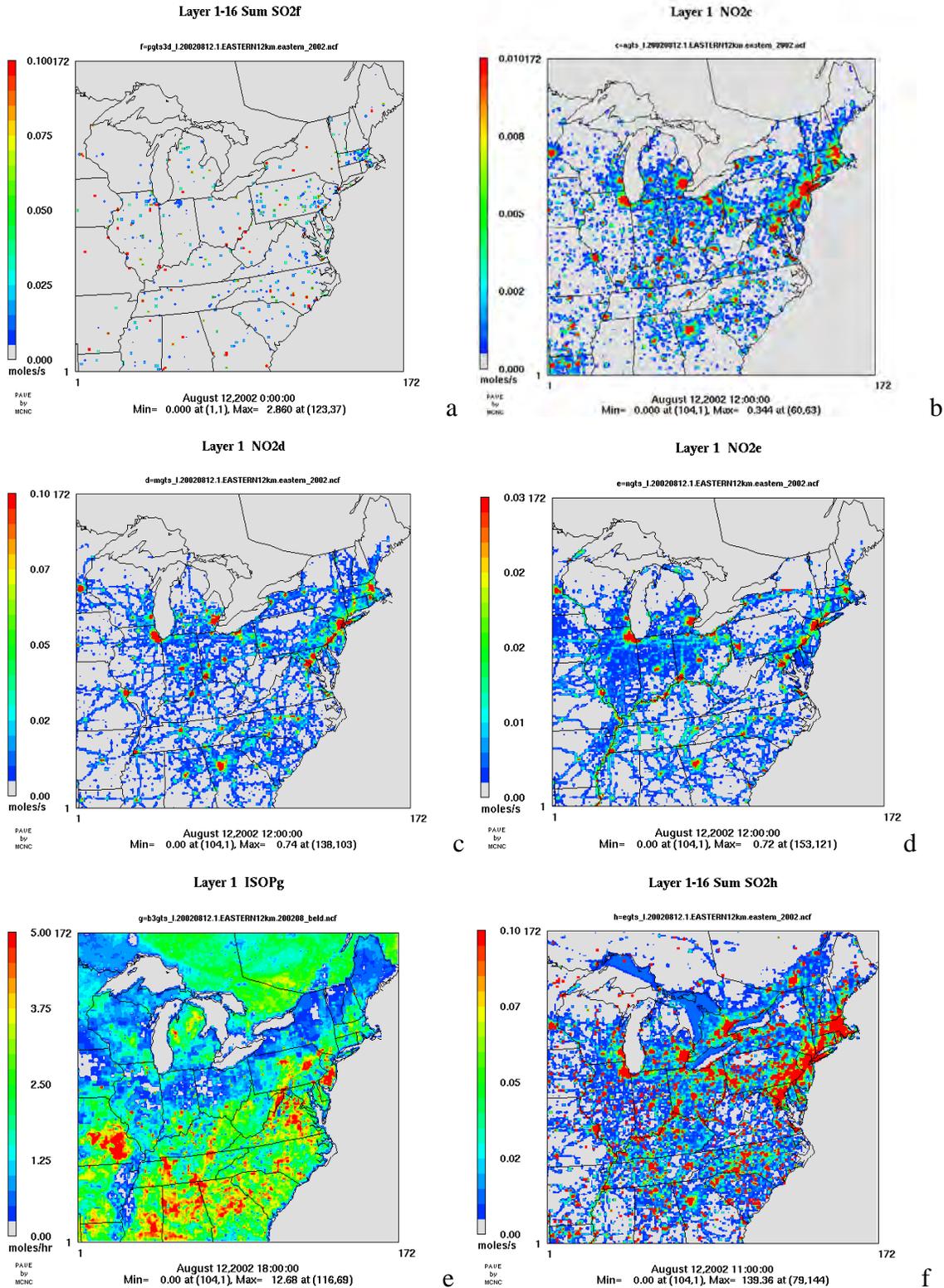
We simulated emission scenarios using the Sparse Matrix Operator Kernel Emissions (SMOKE) Modeling System. SMOKE is primarily an emissions processing system designed to create gridded, speciated, hourly emissions for input into a variety of air quality models, such as CMAQ and REMSAD. SMOKE supports 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 onroad 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 CMAQ for the 36 km national domain and 12 km eastern domain (Domain 2) has been performed by the New York State Department of Environmental Conservation (NYS DEC) (for base year 2002 and future year 2009) and by NESCAUM (for future year 2018) using SMOKE v2.1 compiled on a Red Hat 9.0 Linux operating system with the Portland Group Fortran compiler version 5.1. They use the 2002 static emission inventory, CEM data, and surrogates data based on the 2002 RPO data. Biogenic emissions are calculated using BEIS3 with BELD3 data. Mobile source emissions are processed using MOBILE6. An updated 2000 inventory for Canada and a 1999 inventory for Mexico inventory were used for processing.

The emissions processing was performed on a month-by-month and RPO-by-RPO basis, i.e., SMOKE processing was performed for each of the RPOs (MANE-VU, VISTAS, CENRAP, MRPO, WRAP) individually as well as for Canada and Mexico. Note the processing of WRAP and Mexican emissions was necessary for use with the 36 km grid modeling only. For each month/RPO combination, a separate SMOKE ASSIGNS file was created, and the length of the episode in each of these ASSIGNS files was set to the entire month. Specific data sources for individual source categories are listed below and the examples of processed emissions outputs are shown in Figure 1-5.

Figure 1-5. Examples of processed model-ready emissions:
(a) SO₂ from Point; (b) NO₂ from Area; (c) NO₂ from Onroad; (d) NO₂ from Nonroad; (e) ISOP from Biogenic; (f) SO₂ from all source categories



1.3.1. Emissions Processing Files

The profile and cross reference files listed below are held constant for all modeling years unless stated otherwise.

Temporal Allocation

MANE-VU:

Area and Nonroad sources:

amptpro.m3.us+can.manevu.030205.txt and amptref.m3.manevu.012405.txt

Mobile source: MANEVU_2002_mtpro_02022006_addCT.txt

MANEVU_2002_mtref_02022006_addCT.txt

Point sources: Based on the same files as for the MANE-VU area and nonroad temporal files listed above, but added the VISTAS-generated CEM-based 2002 state-specific temporal profiles and cross-references for EGU sources for the MANE-VU states. No CEM, hour-specific, EGU emissions were used.

CENRAP:

The following temporal profiles and cross-reference files were used for all source categories: amptpro.m3.us_can.cenrap.010605.txt, amptref.m3.cenrap.010605.txt

These files were downloaded from the CENRAP website

www.cenrap.org/emission_document.asp

For point sources, the CEM-based hour-specific EGU emissions described in Section 2.2.4 were utilized to override the annual-total based emissions whenever a match could be established by SMOKE

VISTAS, WRAP and MRPO:

The following month-specific temporal profiles and cross-reference files were used for all source categories:

amptpro_typ_us_can_{MMM}_vistas_27nov04.txt where {MMM} is jan, feb, mar, etc., amptref_2002_us_can_vistas_17dec04.txt

These files were obtained from Greg Stella (Alpine Geophysics)

For point sources (EGU and fires), the hour-specific emission files described in Sections 2.3.4 and 2.5.4 were utilized for the VISTAS and WRAP states to override the annual-total based emissions whenever a match could be established by SMOKE

Canada and Mexico:

The SMOKE2.1 default temporal profiles and cross-reference files (amptpro.m3.us+can.txt and amptref.m3.us+can.txt) were utilized.

Chemical speciation

The same speciation profiles (gspro.cmaq.cb4p25.txt) and cross-references (gsref.cmaq.cb4p25.txt) were utilized for all regions and all source categories. Different versions of these files were obtained (SMOKE2.1 default, USEPA-CAIR modeling, VISTAS, CENRAP and MANE-VU) and compared. After comparing the creation dates and header lines of these files, it was determined that the USEPA-CAIR and MANE-VU files had the most recent updates, and consequently the final speciation profile and cross-reference files used for all regions and source categories was based on the USEPA-CAIR files with the addition of MANE-VU specific updates.

Spatial Allocation

U.S.

The spatial surrogates for the 12 km and 36 km domains were extracted from the national grid 12 km and 36 km U.S. gridding surrogates posted at USEPA's website at www.epa.gov/ttn/chief/emch/spatial/newsurrogate.html. The gridding cross-references were also obtained from this website, but for the processing of MANE-VU area source emissions, MANE-VU specific cross-reference entries posted on the MARAMA ftp site were added.

Canada

The spatial surrogates for Canadian emissions for the 12 km and 36 km domains were extracted from the national grid 12 km and 36 km Canadian gridding surrogates posted at USEPA's website at www.epa.gov/ttn/chief/emch/spatial/newsurrogate.html.

The gridding cross-references were also obtained from this website.

Mexico

The spatial surrogates for Mexican emissions the 36 km domain were extracted from the national 36 km gridding surrogates used by USEPA in the CAIR modeling. These files were obtained from USEPA's CAIR NODA ftp site www.airmodelingftp.com. The gridding cross-references were also obtained from this ftp site.

1.3.2. 2002 Emission Inventory

A 2002 base year emission inventory was developed to assess model performance and to serve as a point of comparison for future year projections in terms of emissions reductions and air quality improvement. In order to assess model performance, actual 2002 emissions (to the extent possible) are incorporated into the inventory and simulated in CMAQ in order to compare with observations. In addition, 2002 simulated values are compared to 2009 or 2018 projections with various emission reductions incorporated to see what degree of air quality improvement can be expected as a result of those reductions.

CANADA:

All source categories except that of point sources were obtained from USEPA's ftp site [ftp.epa.gov/EmisInventory/canada_2000inventory](ftp://ftp.epa.gov/EmisInventory/canada_2000inventory).

No county/province-specific correction factors were available for Canada. Hence, a "divide-by-four" correction for Source Classification Codes (SCCs) listed at www.epa.gov/ttn/chief/emch/invent/index.html#dust were adjusted with FORTRAN prior to running SMOKE.

Area

AS2000_SMOKEready.txt

Nonroad

NONROAD2000_SMOKEready.txt

Onroad

MOBILE2000_SMOKEready.txt

Point

There has long been difficulty in obtaining an up-to-date Canadian criteria emissions inventory for point sources. This is due largely to confidentiality rights afforded to Canadian facilities. Thus far, the most recent inventory of Canadian point sources is rooted in the 1985 NAPAP data. Toward this end, an effort was made to obtain more recent Canadian point source data and incorporate it into an inventory database.

Perhaps the most accurate and publicly accessible source of Canadian pollutant data is now available from the National Pollutant Release Inventory (NPRI) database. The NPRI data are available at Environment Canada's website, www.ec.gc.ca/pdb/npri/npri_home_e.cfm. The page hosts a database available for download as an MS Access or Excel file. The database contains a rather comprehensive list of information. Detailed information is available about each facility, including location, activity and annual emissions. In addition, facilities having stacks with a height of 50 meters or more are required to report stack parameters.

Unfortunately, one of the limitations of the NPRI database for modeling purposes is that the data are only available at the facility level, so in order to

use this data, a few generalizations had to be made. Each facility has a Standard Industrial Classification (SIC) code associated with it; however, emissions models require SCCs. While no direct relationship exists between these two codes, a general albeit subjective association can be made, since SCCs are needed for SMOKE. In most cases, only a SCC3 level code was assigned with confidence.

CENRAP:

All CENRAP BaseB files were downloaded from its ftp site <ftp.cenrap.org>.

County-specific correction factors were applied to take into account fugitive dust for SCCs listed at: www.epa.gov/ttn/chief/emch/invent/index.html#dust; the correction factor file gentl.xportfrac.txt was obtained from USEPA's CAIR NODA ftp site <http://www.airmodelingftp.com> (password protected); this adjustment was performed using the SMOKE programs cntlmat and grwinven to generate an adjusted IDA inventory file used for subsequent SMOKE processing for "other area" and point sources.

Where data sets are month dependant, {MMM} represents JAN, FEB, MAR, etc. Note that for both area and nonroad sources, the annual and monthly inventories were processed in one step. Processed with SMK_AVEDAY_YN set to N such that seasonal profiles were used to apportion the inventories into monthly values.

Area

CENRAP_AREA_MISC_SMOKE_INPUT_ANN_STATE_071905.txt
CENRAP_AREA_BURNING_SMOKE_INPUT_ANN_TX_NELI_071905.txt
CENRAP_AREA_MISC_SMOKE_INPUT_NH3_MONTH_{MMM}_072805.txt
CENRAP_AREA_SMOKE_INPUT_NH3_MONTH_{MMM}_071905.txt
CENRAP_AREA_SMOKE_INPUT_ANN_STATE_081705_xfact.txt
- "_xfact" is the adjusted version for fugitive dust as described above

Nonroad

CENRAP_NONROAD_SMOKE_INPUT_ANN_071305.txt
CENRAP_NONROAD_SMOKE_INPUT_MONTH_{MMM}_071305.txt

Onroad

M6-Input files + VMT - MOBILSMOKE_Inputs.zip (Mar06)
VMT/Speed files: mbinv02_vmt_cenrap_ce.ida,
mbinv02_vmt_cenrap_no.ida, mbinv02_vmt_cenrap_so.ida, and
mbinv02_vmt_cenrap_we.ida

Point

CENRAP_POINT_SMOKE_INPUT_ANNUAL_DAILY_072505_xfact.txt
- "_xfact" is the adjusted version for fugitive dust as described above

MANE-VU:

PECHAN prepared all of the MANE-VUv3.0 inventories for SMOKEv2.1 located at <ftp://ftp.marama.org/2002> [Version 3/](#) (username: mane-vu, password: exchange).

County-specific correction factors were applied to take into account fugitive dust for SCCs listed at: www.epa.gov/ttn/chief/emch/invent/index.html#dust; the correction factor file gcntl.xportfrac.txt was obtained from USEPA's CAIR NODA ftp site <http://www.airmodelingftp.com> (password protected); this adjustment was performed using the SMOKE programs cntlmat and grwinven to generate an adjusted IDA inventory file used for subsequent SMOKE processing for area and point sources.

Area

MANEVU_AREA_SMOKE_INPUT_ANNUAL_SUMMERDAY_040606.txt
MANEVU_AREA_SMOKE_INPUT_ANNUAL_WINTERDAY_040606.txt

Nonroad

MANEVU_NRD2002_SMOKE_030306.ida

Onroad

VMT/Speed: MANEVU_2002_mbinv_02022006_addCT.txt was prepared by PECHAN and NESCAUM; MANEVU_V3_update.tar can be downloaded from http://bronze.nescaum.org/Private/junghun/MANE-VU/onroad_ver3_update/

Point

MANEVU_Point_SMOKE_INPUT_ANNUAL_SUMMERDAY_041006.txt
MANEVU_Point_SMOKE_INPUT_ANNUAL_WINTERDAY_041006.txt

MRPO:

MARAMA contracted Alpine Geophysics to convert MRPO BaseK NIF formatted inventory to IDA, a SMOKE ready inventory format. Files can be found at <ftp.alpinegeophysics.com> – username: marama or on MARAMA's ftp site <ftp.marama.org> – username: mane-vu, password: exchange. Obtained by NESCAUM between April and June 2006.

County-specific correction factors were applied to take into account fugitive dust for SCCs listed at: www.epa.gov/ttn/chief/emch/invent/index.html#dust; the correction factor file gcntl.xportfrac.txt was obtained from USEPA's CAIR NODA ftp site <http://www.airmodelingftp.com> (password protected); this adjustment was performed using the SMOKE programs cntlmat and grwinven to generate an adjusted IDA inventory file used for subsequent SMOKE processing for "other area" and point sources.

Where data sets are month dependant, {MMM} represents jan, feb, mar, etc. and {MM} is 01, 02, 03, etc.

Area

Agricultural Ammonia - arinv_nh3_2002_mrpok_{MMM}_3may2006.txt
Wind Erosion Fug-Dust - dustinv_2002_mrpok_{MMM}_23may2006.txt
- The month-specific files were processed separately from the annual runs and SMK_AVEDAY_YN was set to Y so that no seasonal profiles would be applied and the inventory numbers in the 'average day' column would be used.
Other Area Sources - arinv_other_mrpok_2002_20jun2006_xfact.txt

- Adjusted for fugitive dust as described above
- SMK_AVEDAY_YN was set to N, so seasonal profiles were used to apportion the annual inventory numbers by month.
- To save SMOKE processing, the annual “marine” inventory was processed together with other area sources.

Nonroad

NMIM Generated Sources - nrinv_2002_mrpok_{MMM}_3may2006.txt
MAR (Marine/Air/Rail) - arinv_mar_mrpok_2002_27apr2006.txt
- MAR inventory was SMOKE processed with annual other area sources.

Onroad

M6-Input files & VMT – mobile_inventory_mrpobasek.tar.gz
M6-Ancillary – mobile_m6files_mrpobasek.tar.gz
VMT/Speed file: mbinv_mrpo_02f_vmt_02may06.txt
- VMT is based on VISTAS Phase II modeling which was verified and updated for MRPOs BaseK May 2006 provided by Greg Stella (Alpine Geophysics)

Point

EGU - ptinv_egu_2002_mrpok_1may2006.txt
Non-EGU - ptinv_negu_2002_mrpok_1may2006.txt
- Christian Hogrefe (NYSDEC) merged the two inventories and adjusted for fugitive dust, ptinv_egu_negu_2002_mrpok_1may2006_xfact.txt

VISTAS:

All VISTAS emission files were obtained from Greg Stella (Alpine Geophysics) via ftp.alpinegeophysics.com – username: vistasei They reflect version BaseG of the VISTAS inventory with the exception of fire emissions, which reflect BaseF for Lo-Fires and BaseD for Hi-Fires. Files were obtained between February and August, 2006.

The header lines of these files indicate that the fugitive dust correction was already applied, so no further correction was performed. Where data sets are month dependant, {MMM} represents jan, feb, mar, etc. and {MM} is 01, 02, 03, etc.

Area

arinv_vistas_2002g_2453922_w_pmfac.txt – Base G
ida_ar_fire_2002_vistaonly_basef.ida – Base F low fires

Nonroad

NMIM Generated Sources - nrinv_vistas_2002g_2453908.txt
MAR (Marine/Air/Rail) - marinv_vistas_2002g_2453908.txt

Onroad

M6-Input files – vistas_baseg02_m6_inputs_20Jul06.tar
VMT/Speed – mbinv_vistas_02g_vmt_12jun06.txt Base G generated by C. Loomis (Alpine Geophysics) July 2006 for VISTAS states

Point

Annual EGU - egu_ptinv_vistas_2002typ_baseg_2453909.txt

Annual Non-EGU - negu_ptinv_vistas_2002typ_baseg_2453909.txt
Hour-specific - pthour_2002typ_baseg_{MMM}_28jun2006.ems
Month Dependant Hi-Fire - ptinv_fires_{MM}_typ.vistas.ida (vr.BaseD)
Hour-specific plume-rise - pthour_fires_{MM}_typ.vistas.ida (vr.Jan05)

1.3.3. 2018 “On the Books/On the Way” (OTB/OTW) Emission Inventory

The emissions processing was conducted in a very similar manner for future projection years relative to the 2002 base year, but with the projected inventories. The future years “on the books/on the way” (OTB/OTW) emissions inventories account for emission control regulations already in place as well as emission control regulations that are final but have not yet been fully implemented and are likely to achieve additional reductions by 2009. Processing occurred during January of 2007.

CANADA:

All source categories except that of point sources were obtained from USEPA’s ftp site ftp.epa.gov/EmisInventory/canada_2000inventory.

No county/province-specific correction factors were available for Canada. Hence, for Area, Onroad, and Nonroad, a “divide-by-four” correction for SCCs listed at www.epa.gov/ttn/chief/emch/invent/index.html#dust were adjusted with FORTRAN prior to running SMOKE.

Area

AS2020_SMOKEready.txt

Nonroad

NONROAD2020_SMOKEready.txt

Onroad

MOBILE2020_SMOKEready.txt

Point

Non-EGUs -- ptinv_canada_2002_negu.ida same as 2002 BaseB4

EGUs -- egu062idasum_cp.txt and egu062idawin_cp.txt

- U.S.-Canada 2020 Canadian Base Case -- Scenario #062
- Original IPM parsed file (based on NEEDS 2.1.6)

- Annualized emissions were calculated by combining summer and winter with FORTRAN to create and use ptinv_canada_2020_egu.ida

CENRAP

County-specific correction factors were applied to take into account fugitive dust for SCCs listed at: www.epa.gov/ttn/chief/emch/invent/index.html#dust; the correction factor file gentl.xportfrac.txt was obtained from USEPA’s CAIR NODA ftp site <http://www.airmodelingftp.com> (password protected); this adjustment was performed using the SMOKE programs cntlmat and grwinven to generate an adjusted IDA inventory file used for subsequent SMOKE processing.

Area

arinv_nodust_ref_cenrap2002-2018_081705.ida

fdinv.cenrap2002_2018_wfac.ida

nh3inv.annual.cenrap2002_2018.ida

nh3inv.cenrap2002_2018.ann.ida

nh3inv.misc_annual.cenrap2002_2018.ida

nh3inv.misc.cenrap2002_2018.ann.ida

rdinv.cenrap2002_2018.wfac.ida

- To save SMOKE processing, all area source inventories were processed with area sources from the MWRPO and VISTAS.

Nonroad

cenrap_2018_fnl_nrd_emissions091506.txt

nrinv_cenrap_2018_mod_w_mrpok_15sep2006.txt

nrinv_cenrap_2018_mod_w_mrpok_14sep2006.txt

- To save SMOKE processing, all nonroad source inventories were processed with nonroad sources from the MWRPO and VISTAS.
- “mod_w_mrpok” files include both MRPO and CENRAP sources

Onroad

M6List – BaseG_2018_mobile_m6.tar.gz or in the sub-directory input

VMT – cenrap2018_vmt_072005.ida

- bronze.nescaum.org/Private/junghun/CMV_mobile/
- To save SMOKE processing all mobile source inventories were processed with mobile sources from the MWRPO and VISTAS.

Point

EGU – ptinv_egu_2018_cenrap_11sep2006.txt

Non-EGU – ptinv_negu_cenrap2018_25aug2006_xfact.ida

- “_xfact” version is the adjusted version for fugitive dust as described
- Obtained from Alpine Geophysics contracted by MARAMA
[ftp.alpinegeophysics.com/Work_Order_1/Task_2_BaseK_2018\](ftp://alpinegeophysics.com/Work_Order_1/Task_2_BaseK_2018/)
(12-Sep06) – username: marama, password: emisdata
- Used IPM2.1.9 without adjustments

MANE-VU:

MARAMA developed the future year OTB/OTW emissions inventories for non-EGU point, area, and nonroad sources accounting for the OTB/OTW inventories, based on the MANE-VU 2002 Version 3 inventory. (MARAMA, 2007b).

County-specific correction factors were applied to take into account fugitive dust for SCCs listed at: www.epa.gov/ttn/chief/emch/invent/index.html#dust; the factors were obtained from www.epa.gov/ttn/chief/emch/invent/transportfractions.xls; this adjustment was performed outside of SMOKE with FORTRAN for area and point sources.

Area

MANEVU_OTB2018_Area_IDA3V_2.txt (Nov 2006)

[ftp.marama.org/2009,12,18 OTB Version 3.1/AREA/Area IDA files/](ftp.marama.org/2009,12,18_OTB_Version_3.1/AREA/Area_IDA_files/)

Inventory Development Notes:

- After the release of version 3, Massachusetts revised their inventory for heating oil emissions due to two changes: (1) SO₂ emission factors were adjusted for the sulfur content from 1.0 to 0.03; (2) use of the latest DOE-EIA 2002 fuel use data instead of the previous version from 2001. These two changes significantly altered the 2002 SO₂ emissions for area source heating oil combustion. The revised version was used to do the projections.
- The District of Columbia discovered a gross error in the 2002 residential, non-residential, and roadway construction sources. It requested that for PM10-PRIM and PM25-PRIM for SCCs 23110X0000, different values be used for the 2002 base year and as the basis for the 2009/2012/2018 projections

Nonroad

MANEVU_OTB2018_NR_IDAV3_1.txt (Oct 2006)

[ftp.marama.org/2009,12,18 OTB Version 3.1/NONROAD/NONROAD IDA Files v3.1/](ftp.marama.org/2009,12,18_OTB_Version_3.1/NONROAD/NONROAD_IDA_Files_v3.1/)

- MACTEC utilized the NMIM2005 model to develop projections for nonroad engines included in the NONROAD2005 model. Projected emission estimates were calculated using NMIM default data. Prior to starting the NMIM2005 runs, MACTEC confirmed with USEPA's Office of Transportation and Air Quality (OTAQ) that the database used for fuel sulfur content, gas Reid Vapor Pressure (RVP) values, and reformulated fuel programs was current and up to date for the MANE-VU region.
- Emission calculations were made at the monthly level and consolidated to provide annual values. This enabled monthly temperatures and changes in reformulated gas to be captured by the program.

Onroad

ManevuFutureM6_v2_20051103_wjh.tar.gz

- [bronze.nescaum.org/Private/junghun/CMV mobile/](http://bronze.nescaum.org/Private/junghun/CMV_mobile/)

Point

Non-EGU: MANEVU2018NonEGUV3_0_Point_IDA.txt (Jun 2006)

[ftp.marama.org/2009,12,18 OTB Version 3.1/non-EGU Point/nonEGU IDA Files/](ftp.marama.org/2009,12,18_OTB_Version_3.1/non-EGU_Point/nonEGU_IDA_Files/)

MRPO:

Alpine Geophysics was contracted by MARAMA to convert MRPO BaseK NIF formatted inventory to IDA a SMOKE ready inventory format. Files can be found at ftp.alpinegeophysics.com/Work_Order_1/Task_2_BaseK_2018/ – username: marama or on MARAMA's ftp site <ftp.marama.org> – username: mane-vu, password: exchange. Obtained between April and June 2006.

Where data sets are month dependant, {MMM} represents jan, feb, mar, etc. and {MM} is 01, 02, 03, etc.

Area

Other Area Sources – arinv_other_mrpok_2018_22aug2006.txt
Agricultural Ammonia – arinv_nh3_2018_mrpok_{MMM}_22aug2006.txt
Wind Erosion Fug-Dust Base F – dustinv_mrpo_basef_2018_29jul05.ida
- In order to save time, all area source categories were processed simultaneously for CENRAP, MRPO and VISTAS.

Nonroad

arinv_mar_mrpok_2018_22aug2006.txt
nrinv_2018_mrpok_apr_22aug2006.txt
- To save SMOKE processing all nonroad source inventories were processed with nonroad sources from the MWRPO and VISTAS.

On-road

M6LIST – .in files can be found in the sub-directory input
VMT - mbinv_vistas+mrpo_18g_vmt_12jun06.ida
- bronze.nescaum.org/Private/junghun/CMV_mobile/
- To save SMOKE processing all mobile source inventories were processed with mobile sources from the CENRAP and VISTAS.

Point

EGU: ptinv_egu_2018_mrpok_11sep006.txt
Non-EGU: ptinv_negu_2018_mrpok_23aug2006_xfact.txt
- “_xfact” version is the adjusted version for fugitive dust as described
- Used IPM2.1.9 includes post-IPM adjustments

VISTAS:

The header lines of these files indicate that the fugitive dust correction was already applied, so no further correction was performed. Where data sets are month dependant {MMM} is jan, feb, mar, etc. and {MM} is 1, 2, 3, etc.

Area

arinv_vistas_2018g_2453922_w_pmfac.txt
- To save SMOKE processing, area source inventories were processed with area sources from the MWRPO and CENRAP.
Lo-Fire: area_level_fires_vistas2018_baseg.ida

Nonroad

marinv_vistas_2018g_2453972.txt
nrinv_vistas_2018g_2453908.txt
- To save SMOKE processing, all nonroad source inventories were processed with nonroad sources from the MWRPO and VISTAS.

Onroad

M6LIST – .in files can be found in the sub-directory input
VMT - mbinv_vistas+mrpo_18g_vmt_12jun06.ida
- bronze.nescaum.org/Private/junghun/CMV_mobile/
- Based off Base G inventory BaseG_2018_mobile_m6.tar and Baseg_2018_mv_vmt.tar

- To save SMOKE processing all mobile source inventories where processed with mobile sources from the MWRPO and CENRAP.

Point

EGU: egu_18_vistas_g_2453993.txt
Non-EGU: negu_ptinv_vistas_2018_baseg_2453957_xfact.txt
Hourly: pthour_2018_baseg_{MMM}_2453993.ems
Hi-Fire: ptinv.plume.vistasbaseg18.{MM}.ida
ptday.plume.vistasbaseg18.{MM}.ida
Hi-Fire hourly plume-rise: pthour.plume.vistasbaseg18.{MM}.ida
- Used IPM2.1.9 includes post-IPM adjustments

1.3.4. 2018 “Beyond on the Way” (BOTW) Emission Inventory

The emissions processing for a “beyond on the way” (BOTW) inventory was conducted in a very similar manner to other future projection scenarios relative to the 2002 base year, but with different inventories. These inventories were based on additional control measures that the MANE-VU states are considering for attaining various regional haze, ozone, and PM_{2.5} National Ambient Air Quality Standards (NAAQS) goals. The resulting CMAQ simulation (BOTW) is the same run that has been used by the OTC Modeling Committee for projecting the long-term benefits of regional ozone control programs and was conducted on the Integrated SIP Modeling Platform by the five regional modeling centers.

CANADA:

Same as 2018OTB/OTW

CENRAP:

Same as 2018OTB/OTW

MANE-VU:

MARAMA produced the Nonroad, Area and Non-EGU projections for 2018 under different scenarios (MARAMA, 2007b).

The EGU inventories were developed by ICF Consulting for the RPOS using the Integrated Planning Model (IPM version 2.1.9). Alpine Geophysics processed the results into IDA inventory format for MANE-VU.

Fugitive dust correction was applied as county-specific correction factors for SCCs listed at <http://www.epa.gov/ttn/chief/emch/invent/index.html#dust>; the correction factors were obtained from <http://www.epa.gov/ttn/chief/emch/invent/transportfractions.xls>; this adjustment was performed outside of SMOKE with FORTRAN.

Area

manevu_botw2018_area_IDAV3_2_xfact.txt

- “_xfact” version is the adjusted version for fugitive dust as described
- Nonroad*
nrinv_manevu_18_19oct05.txt
- Onroad*
Same as 2018 OTB/OTW
- Point*
EGU: ptinv_egu_2018_manevu_11sep2006.txt
- bronze.nescaum.org/Private/junghun/POINT_2018BOTW_B4
Non-Fossil 2009: manevu_nonfossil_2009_19sept2006.txt
- Alpines ftp – marama -- Work_Order_1/Task_4_2009_Nonfossil/
Non-EGU: MANEVU_BOTW2018_nonegu_IDAV3_1_xfact.txt
- “_xfact” version is the adjusted version for fugitive dust as described

MRPO:

Same as 2018OTB/OTW

VISTAS:

Same as 2018OTB/OTW

1.3.5. 2018 Sulfate Tagging (BOTW) Emission Inventory

An additional BOTW inventory was prepared specifically to allow for a state-by-state tagging run with REMSAD and a sensitivity run with the CMAQ Particle and Precursor Tagging Methodology (CMAQ-PPTM) system. The inventory used for these runs was essentially the same inventory described for the regular BOTW scenario; however, in order to process this inventory for use with the tagging methodology, various components of the inventory were processed separately and identified as a specific “type” of sulfur dioxide so that it could be tracked through the system.

The state-by-state tagging used the identical inventory to the 2018 BOTW inventory described in the previous section. It was processed such that each state’s SO₂ emissions were separately tagged requiring three separate REMSAD simulations to accommodate 29 eastern states, Canada, and the boundaries.

A separate CMAQ-PPTM simulation was conducted using the same inventory, but modified to reflect additional controls due to a number of strategies to be tested. The specific scenarios that were tracked by this run include:

1. OTB/OTW
2. S-1 fuel oil strategy (500 ppm distillate; 0.5% fuel-sulfur content by weight for No. 6 residual oil; 0.25% fuel-sulfur content by weight for No. 4 residual oil.)
3. S-2 fuel oil strategy (15 ppm distillate; 0.5% fuel-sulfur content by weight for No. 6 residual oil; 0.25% fuel-sulfur content by weight for No. 4 residual oil.)
4. BART (approximately 35,000 tons of SO₂ reductions at specific facilities identified by state survey of permitting staff)

5. “167 Stack” Strategy; (90% control on all EGUs in the 167 stacks identified as having the most significant impact on MANE-VU Class I areas)

Two additional tags were required to account for corrections to the assumed baseline fuel sulfur content of distillate and to add EGU emissions reductions back into the system as a result of potential permit trading in response to the 167 stack strategy. These strategies are described in more detail in Chapter 4.

1.4. Model 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 (Amar et al., 2005) 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 been peer reviewed (Seigneur et al., 1999) and used by USEPA for regulatory applications (www.epa.gov/otaq/regs/hd2007/frm/r00028.pdf and www.epa.gov/clearskies/air_quality_tech.html) to study ambient concentrations and deposition of sulfate and other PM species.

1.4.1. 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).

To date, MANE-VU SIP modeling on both 36 km and 12 km domains used CMAQv4.5.1, IOAPI V2.2 and NETCDF V3.5 libraries. The CMAQ model is configured with the Carbon Bond IV mechanism (Gery et al., 1989) using the EBI solver for gas phase chemistry rather than the SAPRC-99 mechanism due to better computing efficiency with no significant model performance differences for ozone and PM as compared to observations.

NY DEC has completed annual 2002 CMAQ modeling on the 36 km domain to provide dynamic boundary conditions for all simulations performed on the 12 km domain. Three-hourly boundary conditions for the outer domain were derived from an annual model run performed by researchers at Harvard University using the GEOS-

CHEM global chemistry transport model (Park et al., 2004). Model resolution was species dependent at either 4° latitude by 5° longitude or 2° by 2.5°.

Five modeling centers are working collectively to maximize efficiency of computing resources in MANE-VU for SIP modeling. These centers include NY DEC, NJ DEP/Rutgers, VA DEQ, UMD, and NESCAUM. Annual CMAQ modeling on the 12 km domain is divided into five periods. UMD is responsible for the period from January 1 to February 28; NJ DEP/Rutgers are responsible for the period from March 1 to May 14; NY DEC is responsible for the period from May 15 to September 30; VA DEQ is responsible for the period from October 1 to October 31; and NESCAUM is responsible for the period from November 1 to December 31. Each period uses a 15 day spin up run to minimize the impact of the default initial concentration fields. Each group performs CMAQ simulations on its period for a series of scenarios including 2002 Base Case, 2009 Base Case, 2018 Base Case, 2009 Control Case, and 2018 Control Case. All scenarios adopt the same meteorological field (2002) and boundary conditions, varying only emission inputs. To ensure consistency, a benchmark test was conducted by each modeling group.

In addition to the annual simulations conducted with CMAQ by the five modeling centers, NESCAUM has conducted limited sensitivity analysis of several control measures using the beta version of CMAQ with the particle and precursor tagging methodology (CMAQ-PPTM) (ICF, 2006). These runs and their results are described separately in Chapter 5.

1.4.2. REMSAD

The Regional Modeling System for Aerosols and Deposition (REMSAD) is 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. The 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 that 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 secondary organic aerosol (SOA) yields from emitted hydrocarbons. REMSAD V7.12 and newer versions have capabilities that allow model tags of sulfur species (up to 11 tags), nitrogen (4 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 for sulfur, more efficient modeling, and reasonable correspondence with measurements for many species, make REMSAD an important source apportionment tool for MANE-VU.

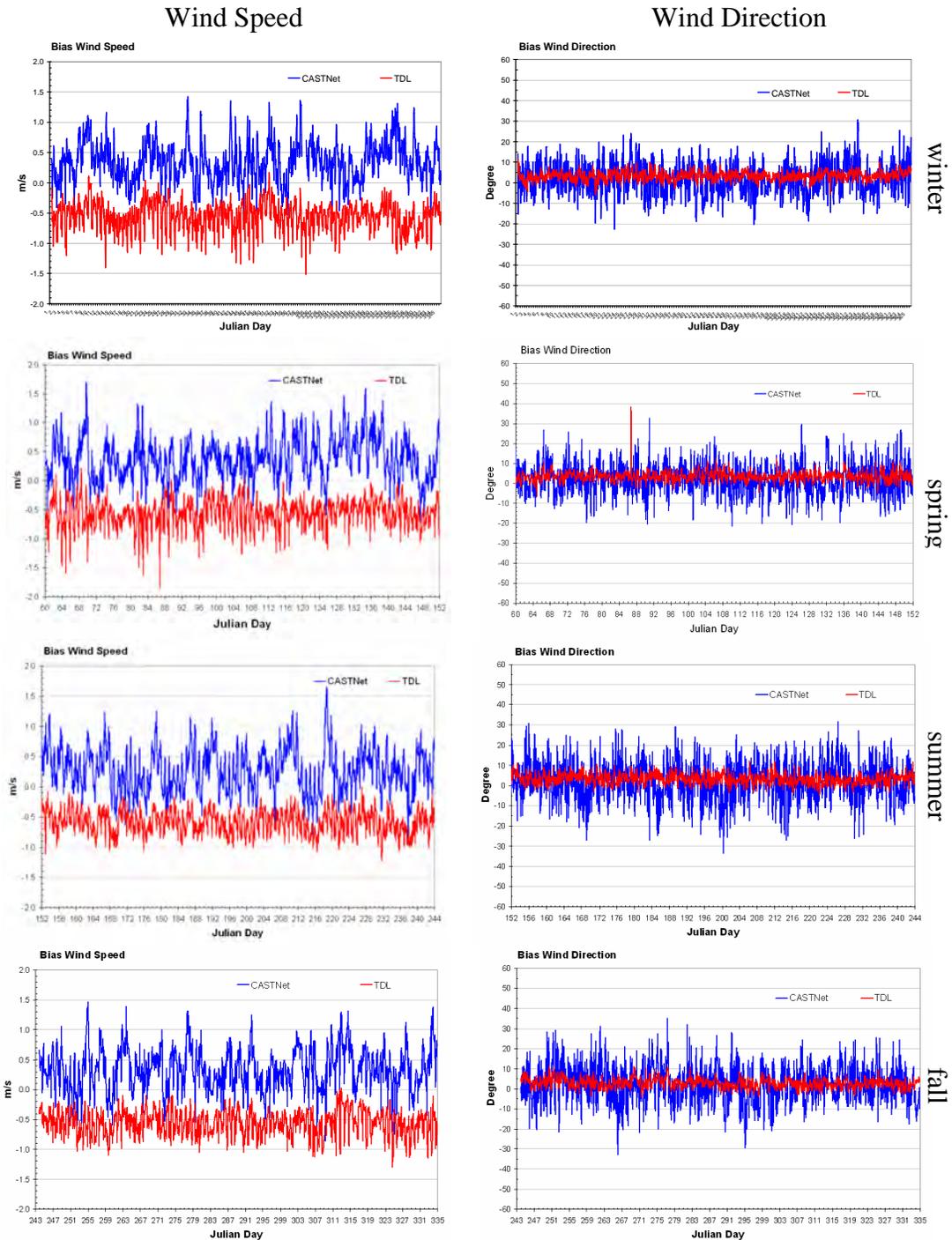
In our present REMSAD modeling, we use the same 12 km domain (i.e., domain2) presented in the previous section for three full annual runs for the base year (2002). Multiple runs are necessary to permit tagging of sulfur emissions for all of the states in the domain, Canada, and the boundary conditions.

2. PERFORMANCE EVALUATION

2.1. Meteorological Evaluation

The 2002 annual 12 km resolution meteorological fields generated by MM5 have been evaluated by NESCAUM using ENVIRON's METSTAT program. Model results of surface wind speed, wind direction, temperature, and humidity are paired with measurements from EPA's Clean Air Status and Trends Network (CASTNET) and National Center for Atmospheric Research's Techniques Data Laboratory (TDL) network by hour and by location and then statistically compared. Figure 2-1 presents domain-wide average hourly bias of wind speed (left panel) and wind direction (right panel) between the MM5 results and two sets of measurement for every season in 2002 (winter includes Jan., Feb., and Dec.; spring includes Mar., Apr., and May; summer includes Jun., Jul., and Aug.; fall includes Sep., Oct., and Nov.). It shows that MM5 capably predicts wind speed with reasonably small bias and equal consistency. Within the domain, MM5 tends to overestimate wind speed (hourly bias up to 1.7 m/s) at CASTNET sites, and underestimate wind speed (hourly bias up to -1.85 m/s) at TDL sites. Seasonal mean bias of MM5 wind speed to CASTNET wind speed is ~0.3 to 0.4 m/s, while seasonal mean bias of MM5 wind speed to TDL wind speed is about ~-0.5 to -0.6 m/s. No significant seasonal variation on this wind speed bias is observed. MM5 prediction of wind direction shows a larger variation with CASTNET wind direction (hourly bias from ~-30 degree to ~30 degree) than with TDL wind direction (hourly bias from ~-5 degree to ~10 degree). However, seasonal mean bias of MM5 wind direction to CASTNET wind direction (~2 degree) is smaller than seasonal mean bias of MM5 wind direction to TDL wind direction (~3 degree) because the large variation of positive and negative bias offset each other.

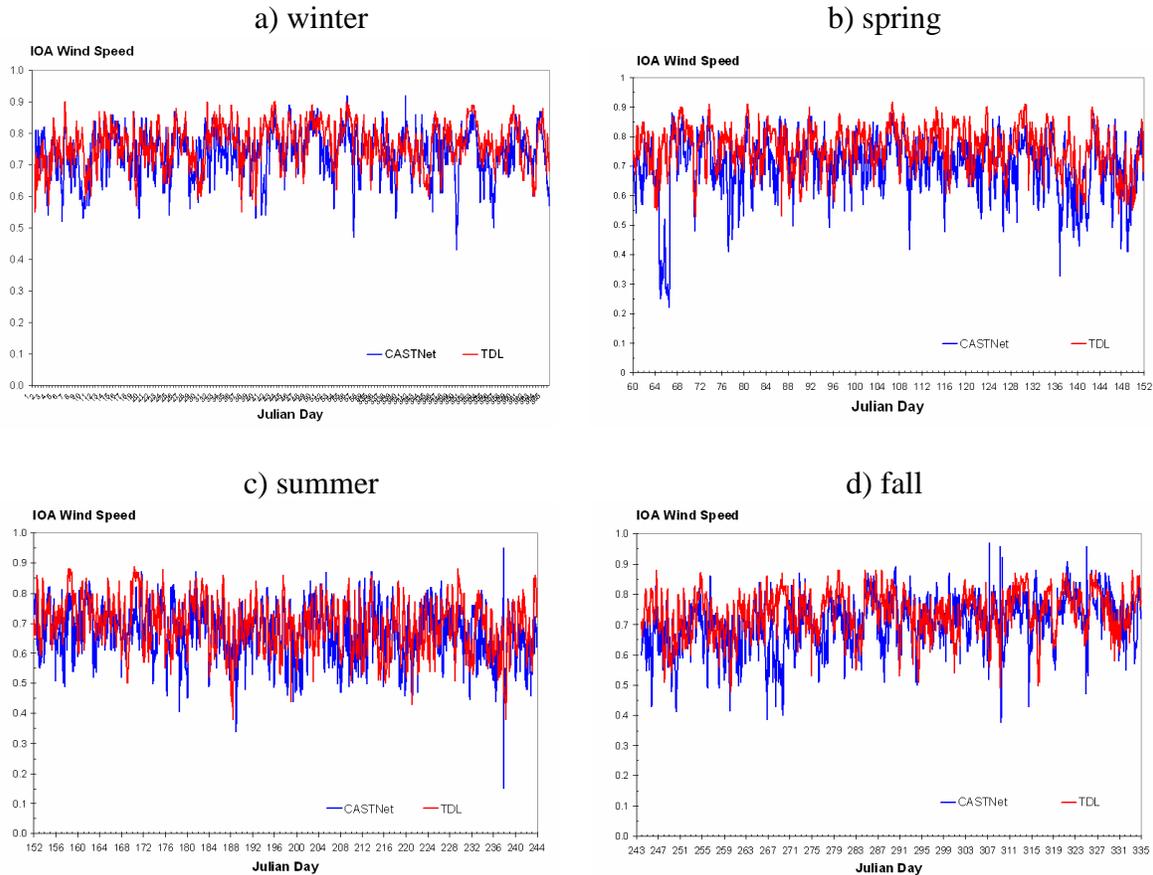
Figure 2-1. 2002 seasonal average hourly bias of wind speed and direction



Index of Agreement (IOA) is a statistical measure of difference between prediction and measurement, calculated as a ratio of Root Mean Square Error to the sum of the difference between prediction and mean observation and difference between observation and mean observation. IOA varies from 0 to 1, with a value of 1 indicating

the perfect agreement between model prediction and observation, and a value larger than 0.5 IOA indicating acceptable model performance. Domain-wide average hourly IOAs of wind speed are presented in Figure 2-2. MM5 predictions of wind speed values are in good agreement (IOA from ~0.5 to ~0.9) to both CASTNET data and TDL data with similar IOA variation. Seasonal mean values of IOA are ~ 0.7. No particular season of the year stands out in terms of its agreement with measurement.

Figure 2-2. 2002 seasonal hourly average index of agreement for wind speed



Quarterly correlation coefficients in Figure 2-3 show good MM5 performance on hourly wind speed for each observation site. MM5 predictions exhibit similar spatial patterns of correlation with CASTNET (left panel) and TDL (right panel) measurements – stronger correlation in north than in south. Over the year, the model has stronger correlation in the 1st quarter (Jan., Feb., Mar., top 1st row), 2nd quarter (Apr., May, Jun., 2nd row) and 4th quarter (Oct., Nov., Dec., bottom row) than it does in the 3rd quarter (Jun., Jul., Aug., 3rd row), with an average of 0.1 correlation coefficient difference. Generally, MM5 predictions and measurements have strongest correlation (0.8~0.9) within the midwestern U.S., strong correlation (0.7~0.8) within the northeastern U.S. and along the coastline, and acceptable correlation (0.5~0.7) within the southern U.S. and interior portions of the U.S. East Coast. MM5 predictions consistently show very similar spatial patterns and temporal variations for wind direction (as shown in Figure 2-4) and

wind speed. There is strong correlation (>0.7) between prediction and measurement for wind direction at most of sites.

Figure 2-3. Quarterly correlation coefficient (r) of hourly wind speed between modeling and measurement for each observation site in 2002

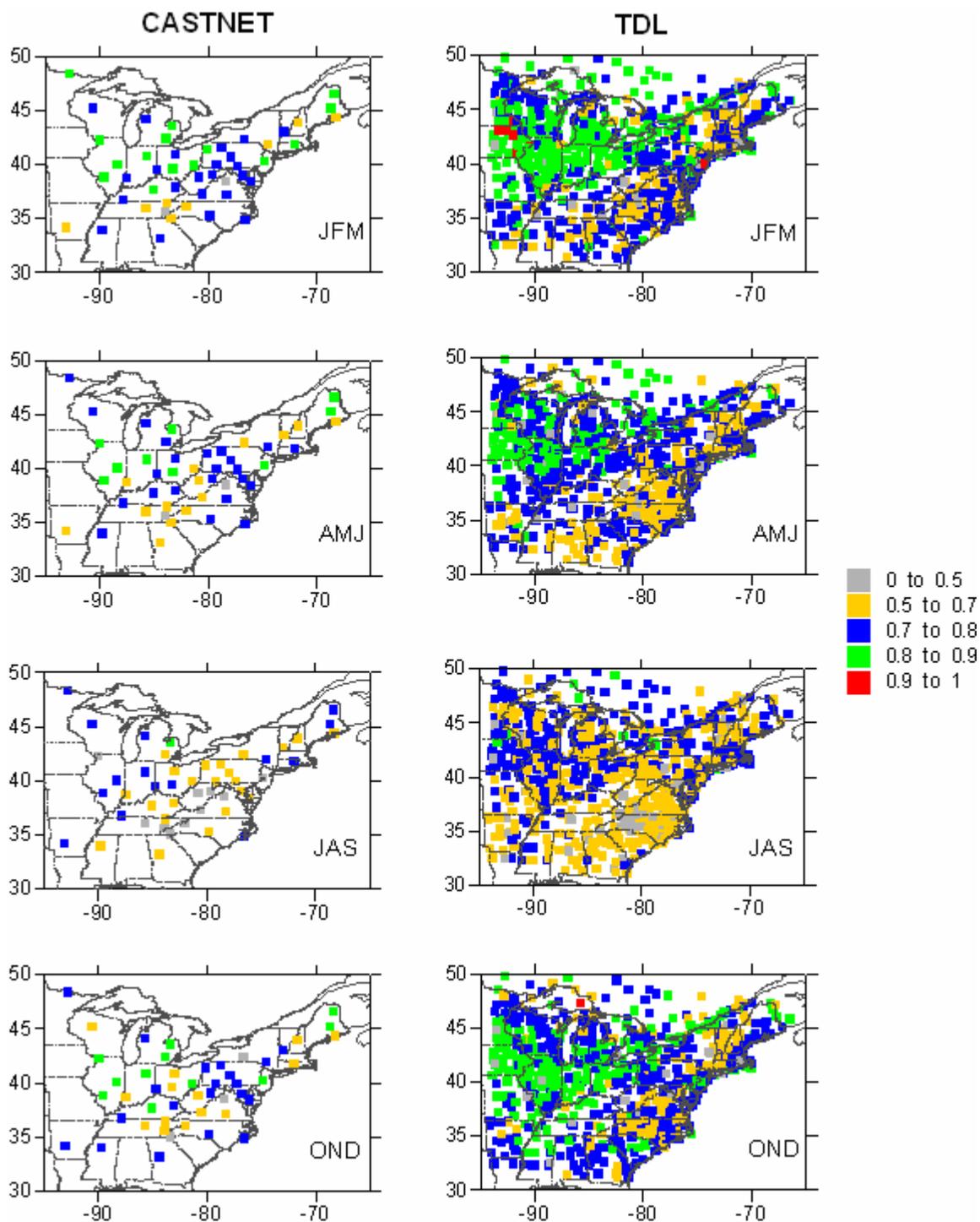


Figure 2-4. Quarterly correlation coefficient (r) of hourly wind direction between modeling and measurement for each observation site in 2002

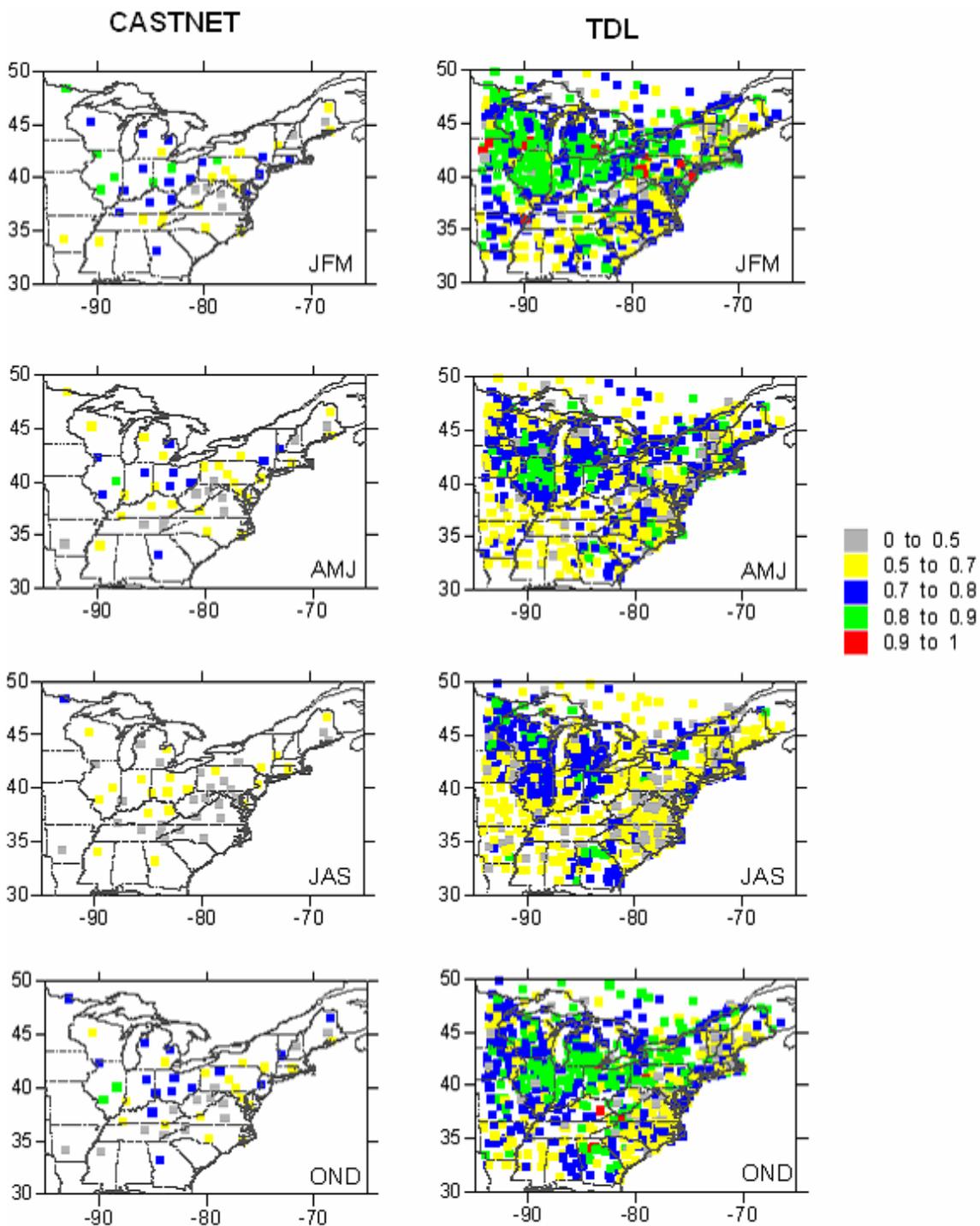


Figure 2-5 presents domain-wide average hourly bias of surface temperature between MM5 results and CASTNET and TDL for every season. MM5 tends to underestimate temperature at TDL sites throughout the year and at CASTNET sites for non-ozone season months. The seasonal mean temperature bias values are from ~ -1 K (winter) to ~ -0.3 K (summer) for TDL sites and ~ -1 K (winter) to ~ 0.5 K (summer) for CASTNET sites. MM5 predictions show significantly larger variations of temperature bias at CASTNET sites (-4 K ~ 9 K) than at TDL sites (-3 K ~ 1 K).

Domain-wide average hourly IOA values of temperature are shown in Figure 2-6. Model predicted temperatures have significantly better agreement with TDL data (average IOA as ~ 0.95) than with CASTNET data (average IOA as ~ 0.85), although both indicate accurate MM5 performance on temperature.

Figure 2-7 shows the spatial distribution of quarterly correlation coefficients between MM5 prediction and measurement of surface temperature. It reveals very strong correlation (>0.95) over most of the domain for TDL data, with strong correlation (>0.8) for the majority of CASTNET sites. No spatial patterns or quarterly variations are apparent. MM5 performs consistently well throughout the year and the domain.

The TDL network also provides humidity measurements. Comparison between MM5 prediction of hourly surface humidity and TDL measurement are presented in Figure 2-8. MM5 captures the general trend of humidity change. It tends to underestimate humidity during the ozone season (seasonal mean bias as ~ 0.35 g/kg), and overestimate it during the rest of year (seasonal mean bias range from ~ 0.17 to ~ 0.4). Domain-wide average hourly humidity bias shows a large diurnal variation, as much as 2g/kg. Domain-wide average hourly IOA in Figure 2-9 shows that MM5 predicted humidity values are in good agreement with TDL data (average IOA as ~ 0.9) throughout year. Spatial distribution of quarterly correlation coefficient in Figure 2-10 shows a distinctive spatial pattern and temporal trend. MM5 results have stronger correlation to TDL data in the northern US than in the Southern US. Through the year, the strongest correlation between MM5 prediction and measurement occurs in the 4th Quarter (>0.95), followed by the 1st and 2nd Quarters, and finally, the 3rd Quarter, which shows the weakest correlation ($0.5\sim 0.9$).

Based on this statistical comparison between model prediction and data from two networks for wind speed, wind direction, temperature, and humidity, MM5 performs well. An acceptable small bias, high index of agreement and strong correlation with CASTNET and TDL data are shown. Since MM5 uses TDL data for nudging, the model predictions are in better agreement with TDL data than with CASTNET data. MM5 performs better in Midwest and Northeast than Southeastern US.

Figure 2-5. 2002 Seasonal Hourly Average Bias of Temperature

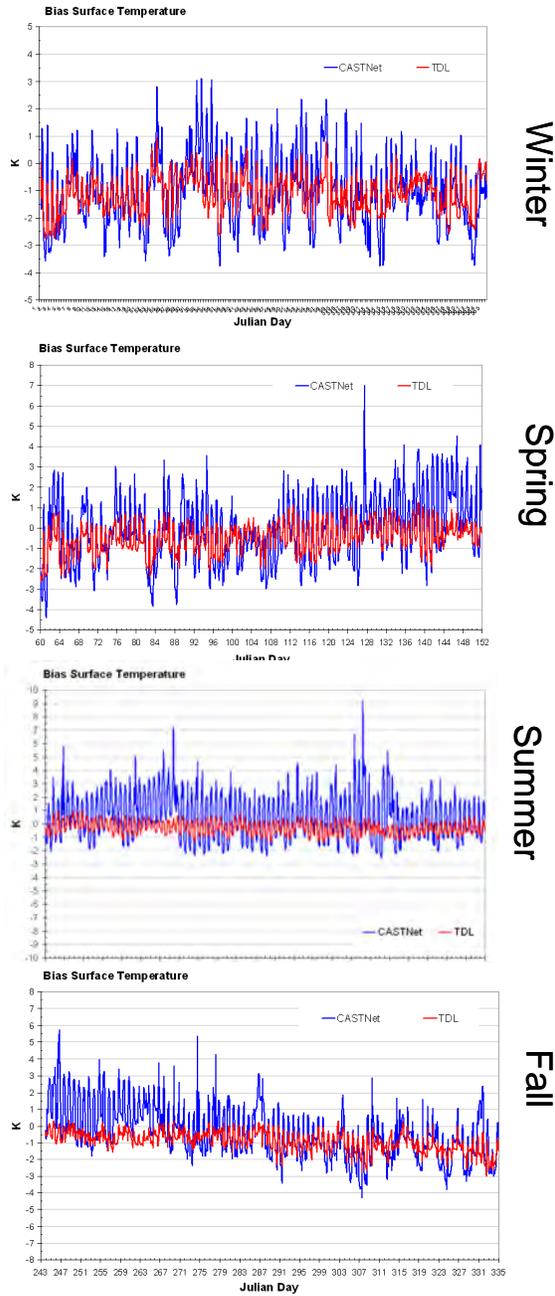


Figure 2-6. 2002 Seasonal Hourly Average Index of Agreement

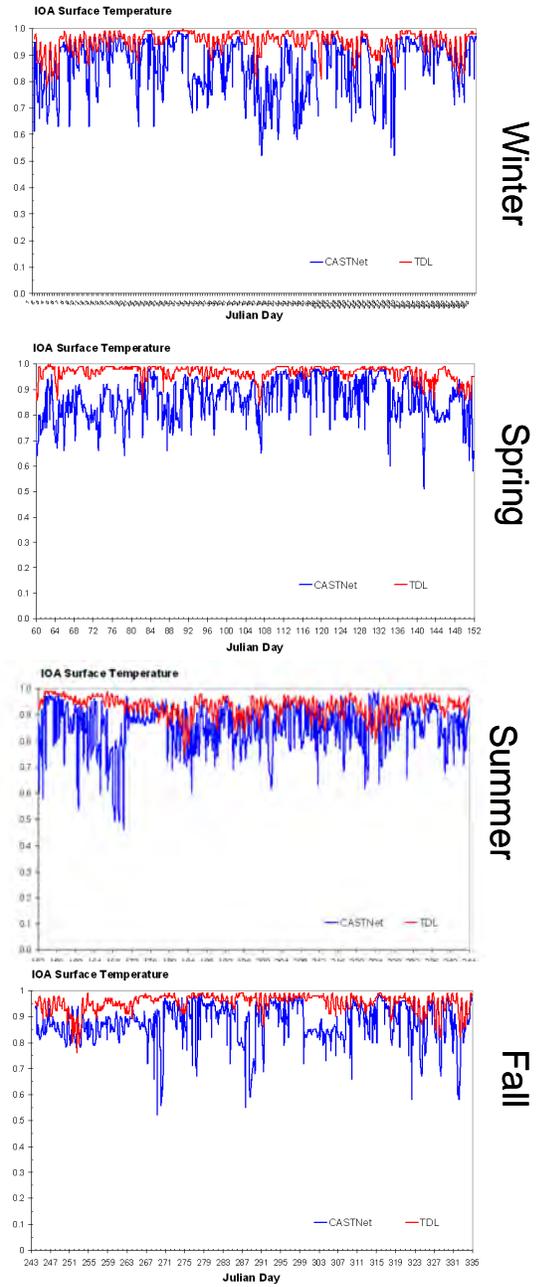


Figure 2-7. Quarterly correlation coefficient (r) of hourly temperature between modeling and measurement for each observation site in 2002

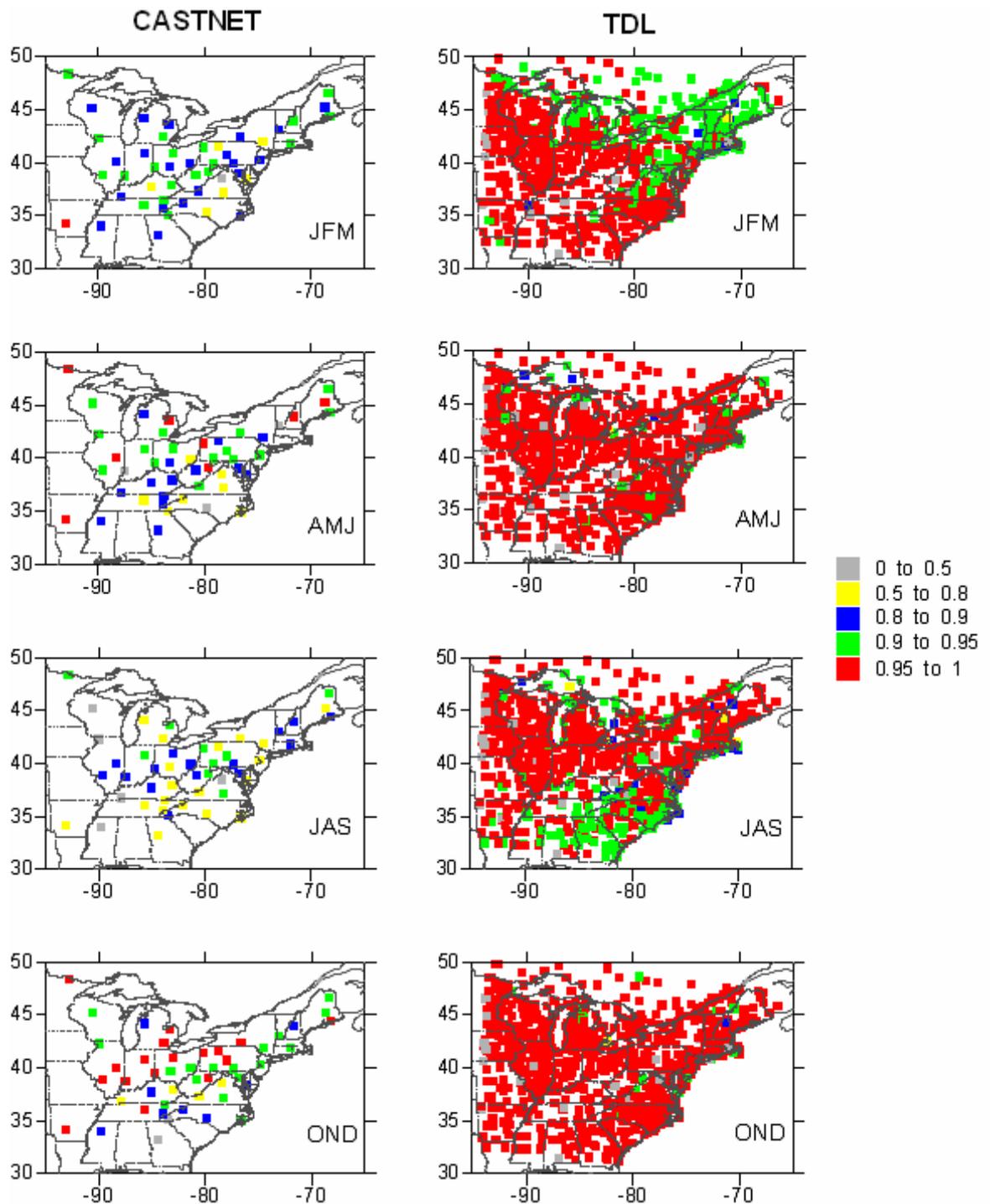


Figure 2-8. 2002 Seasonal average hourly bias of humidity

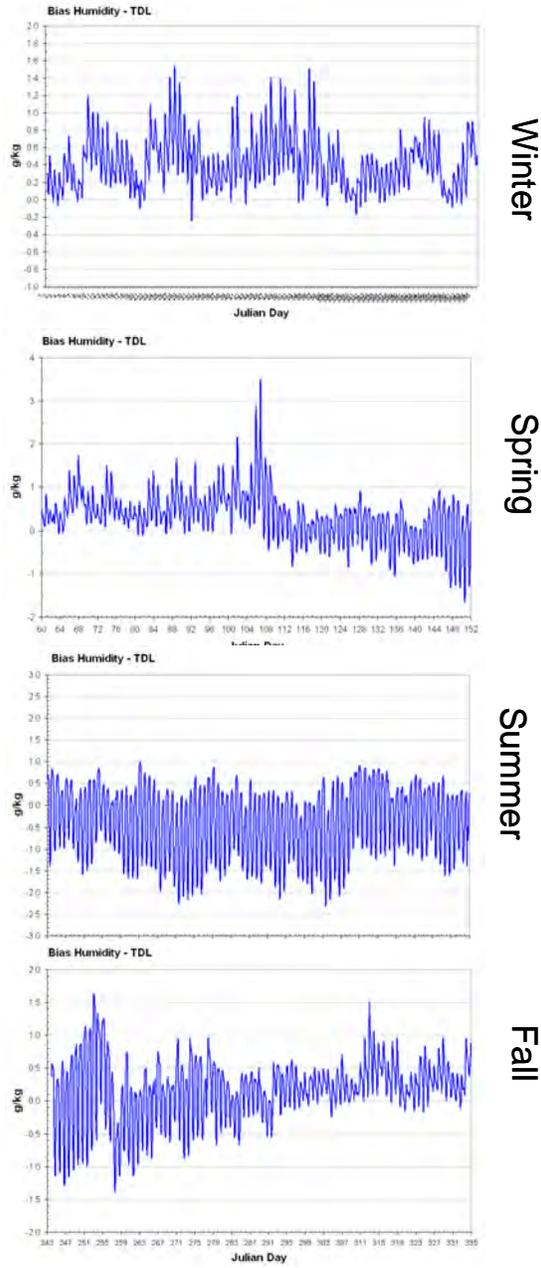


Figure 2-9. 2002 seasonal hourly average index of agreement

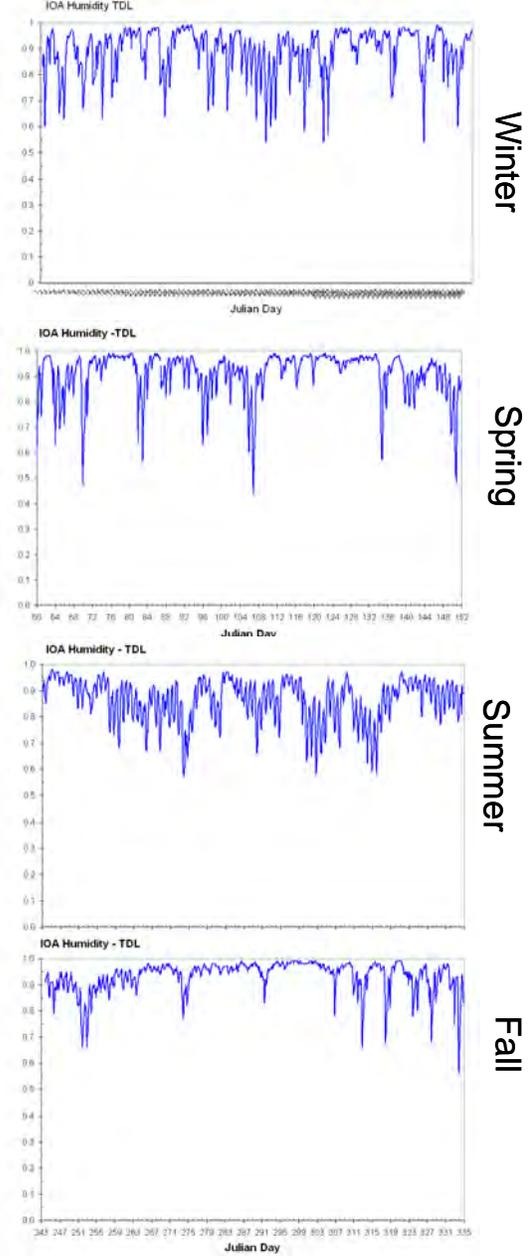
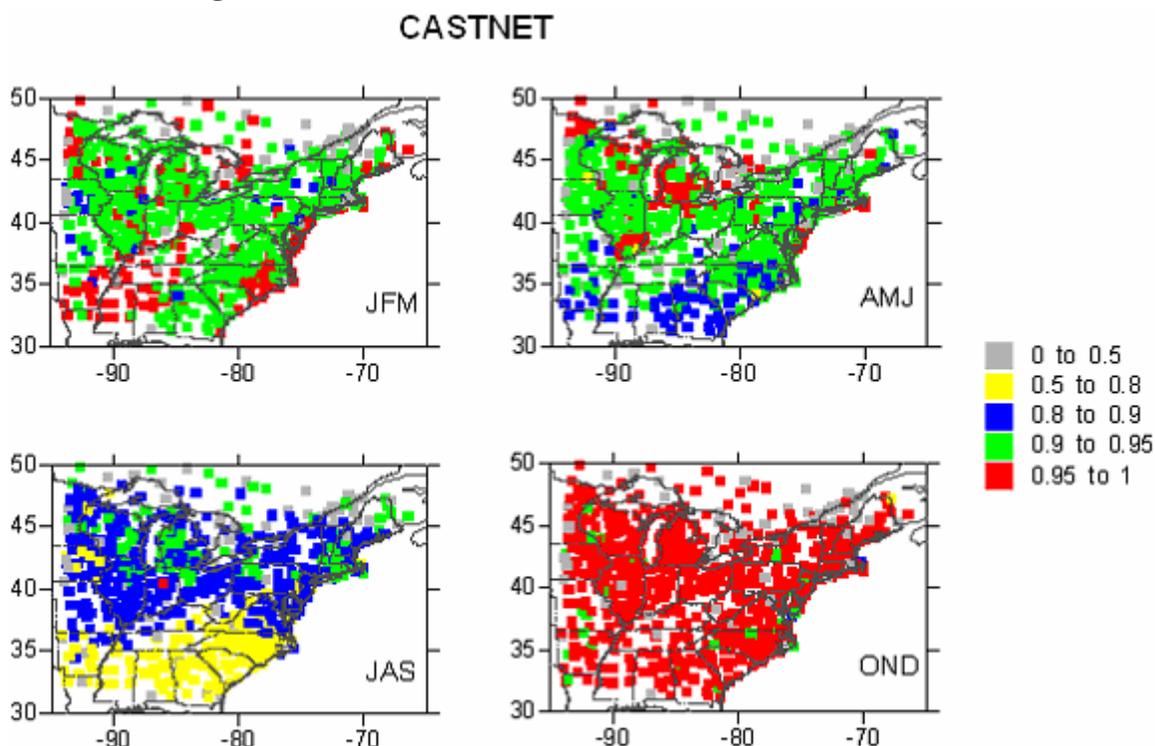


Figure 2-10. Quarterly correlation coefficient (r) of hourly humidity between modeling and measurement for each observation site in 2002



2.2. Model Evaluation

CMAQ modeling has been conducted for the year 2002 (completed by cooperative modeling efforts from NYDEC, UMD, NJDEP, Rutgers, VADEP, and NESCAUM) under the Base B4 emission scenario described in Chapter 1. CMAQ performance for $PM_{2.5}$ species and visibility is examined based on this CMAQ run on a 12 km resolution domain. Measurements from IMPROVE and STN networks are paired with model predictions by location and time for evaluation. Figure 2-11 presents the domain-wide paired comparison of $PM_{2.5}$ species (sulfate, nitrate, OC, EC, fine soil, and $PM_{2.5}$) daily average concentration from the CMAQ simulation and two sets of observations (STN and IMPROVE). It shows that predicted $PM_{2.5}$ sulfate (top row left panel) and measured sulfate are in a good 1:1 linear relationship with r^2 varying from 0.6 to 0.7. $PM_{2.5}$ nitrate (top row right panel) also has close to a 1:1 linear relationship between the model and observations, although the r^2 values are much lower (from ~0.2 to ~0.5) than for sulfate. Paired OC (middle row left panel) concentrations have a scattered distribution with over- and under-estimation and a very weak linear relationship (r^2 of ~0.1). CMAQ tends to overestimate EC (middle row right panel) and fine soil (bottom row left panel) concentrations.

EC and soil are inert species not involved in chemical transformation. Poor emission inventory data may be the main cause for the weak linear relationships between

prediction and measurement. In addition, there are no fire emissions considered in CMAQ modeling. The wild fire in Quebec, Canada in early July of 2002 led to high concentrations of observed OC, EC, and fine soil that are not predicted by CMAQ.

Because sulfate is the dominant PM_{2.5} species, modeled PM_{2.5} (bottom row right panel) shows a relatively strong near 1:1 linear relationship (slope between 0.7–0.8 with r^2 of 0.4–0.5). Figure 2-12 describes the spatial distribution of the correlation coefficient of sulfate between CMAQ prediction and observations (STN data on the top row and IMPROVE data on the bottom row) at network sites. CMAQ predictions show a similar spatial pattern of correlation with both networks.

Generally, the northern region of the domain has stronger correlations than does the southern region. Correlation coefficients within the MANE-VU region are highest (~0.9 on average) compared to other RPO regions. The spatial distribution of correlation coefficient for PM_{2.5} is presented in Figure 2-13. The PM_{2.5} correlation coefficient spatial pattern follows PM_{2.5} sulfate correlation coefficient, although at the same observation site coefficient values are ~0.1 lower than the sulfate coefficient value. Like PM_{2.5} sulfate, CMAQ also performs the best for PM_{2.5} in the MANE-VU region with a ~0.7 annual average for the correlation coefficient.

The goal and the criteria for PM_{2.5} evaluation suggested by Boylan and Baker (2004) have been adopted by every RPO for SIP modeling. The proposed performance goals are: Mean Fractional Error (MFE) $\leq +50\%$, and Mean Fraction Bias (MFB) $\leq \pm 30\%$; while the criteria are proposed as: MFE $\leq +75\%$, and MFB $\leq \pm 60\%$.

CMAQ prediction of PM_{2.5} species from 40 STN sites and 17 IMPROVE sites within MANE-VU region are paired with measurements and statistically analyzed to generate MFE and MFB values. Figure 2-14 presents MFE of PM_{2.5} sulfate, nitrate, OC, EC, fine soil, and PM_{2.5}, and curves of the goal and criteria. MFB values are shown in Figure 2-15. Considering CMAQ performance in terms of MFE and MFB goals, sulfate, nitrate, OC, EC, and PM_{2.5} all have the majority of data points within the goal curve, some are between the goal and acceptable criteria, and only a few are outside the criteria curve. Only fine soil has the majority of points outside the criteria curve, but there are some sites still within the goal. For the MANE-VU region, CMAQ performs best for PM_{2.5} sulfate, followed by PM_{2.5}, EC, nitrate, OC, and then fine soil.

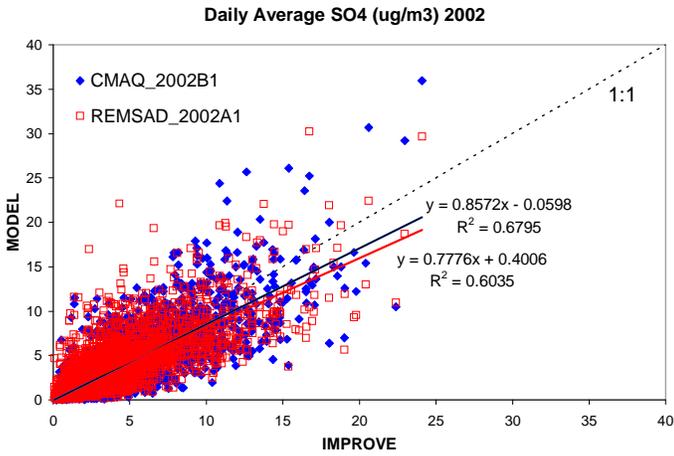
Regional haze modeling also requires a CMAQ performance evaluation for aerosol extinction coefficient (B_{ext}) and the haze index. Modeled daily aerosol extinction at each IMPROVE site is calculated following the IMPROVE formula with modeled daily PM_{2.5} species concentration and relative humidity factors from IMPROVE. The approaches used here and throughout this analysis, have used natural background visibility estimates and the haze index following EPA Guidance.

Figure 2-16 shows the paired comparison between prediction and measurement of daily B_{ext} from seven sites for 2002. The modeled B_{ext} shows a near 1:1 linear relationship (slope of 0.78 and r^2 of 0.46) with IMPROVE observed B_{ext} . The regression excluded three points from July 7, 2002; the monitors were directly impacted by Canadian fires whose emissions were not modeled.

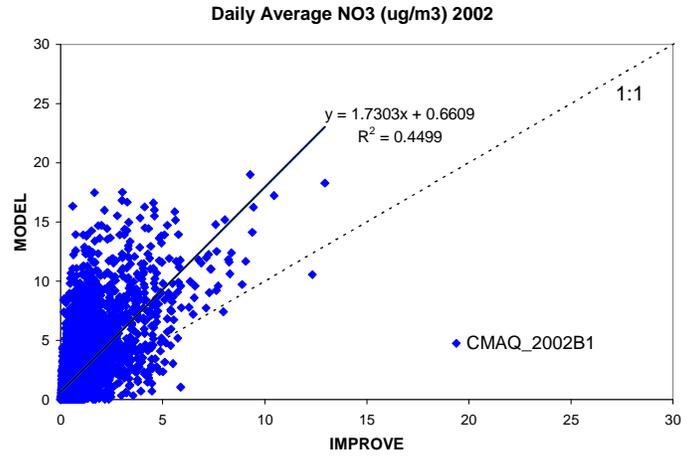
CMAQ prediction of the B_{ext} agrees well with IMPROVE observation because CMAQ performs well on sulfate, which dominates aerosol extinction. Further, the modeled haze index (HI) is calculated based on modeled B_{ext} . Figure 2-17 presents the paired comparison between CMAQ prediction and IMPROVE measurement for 2002 of HI values at seven Class I sites in the eastern U.S.. Acadia and Moosehorn show the best model performance with regression slopes of 0.97 and r^2 of ~ 0.6 . The poorest model performance occurs at Lye Brook and Shenandoah, with regression slopes less than 0.6 and r^2 of ~ 0.3 . Note the regression equations and best fit lines are not plotted.

Figure 2-11. Domain-wide paired comparison of daily average PM_{2.5} species between CMAQ predictions and measurements from IMPROVE networks

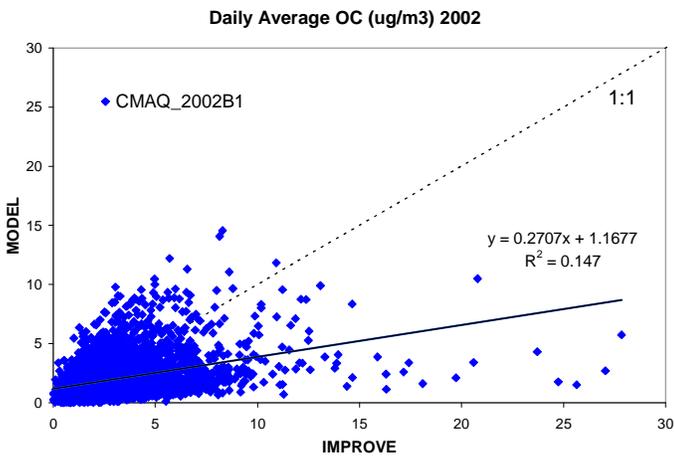
PM_{2.5} Sulfate



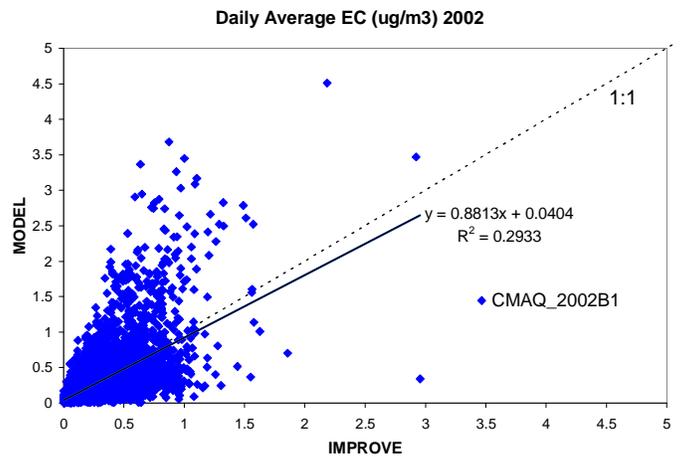
PM_{2.5} Nitrate



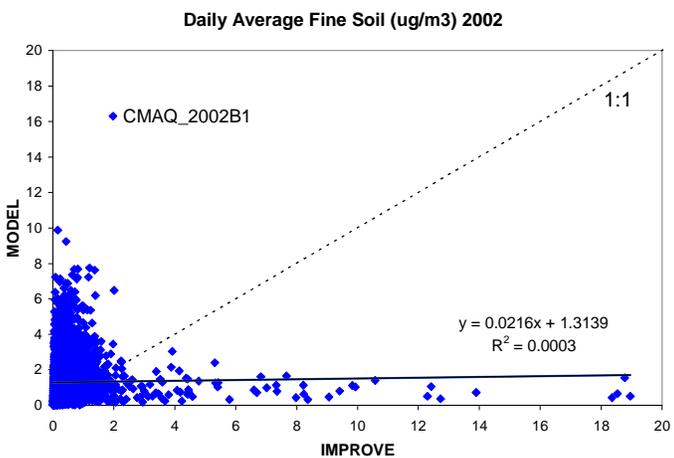
PM_{2.5} Organic Carbon



PM_{2.5} Elemental Carbon



PM_{2.5} Soil



PM_{2.5}

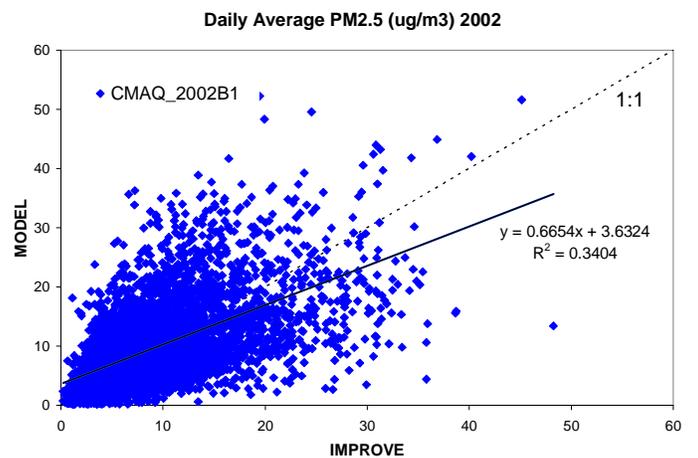


Figure 2-12. Spatial distribution of correlation coefficient between PM_{2.5} Sulfate and measurement

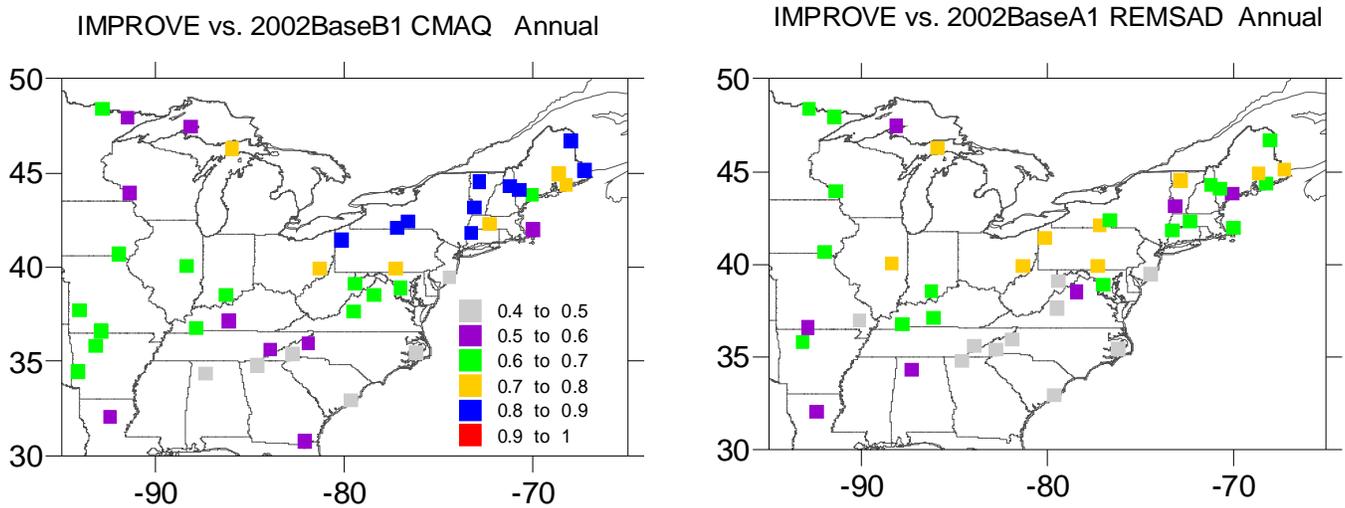


Figure 2-13. Spatial distribution of correlation coefficient between PM_{2.5} and measurement

Correlation Coefficient of Annual PM_{2.5} Species between IMPROVE and CMAQ

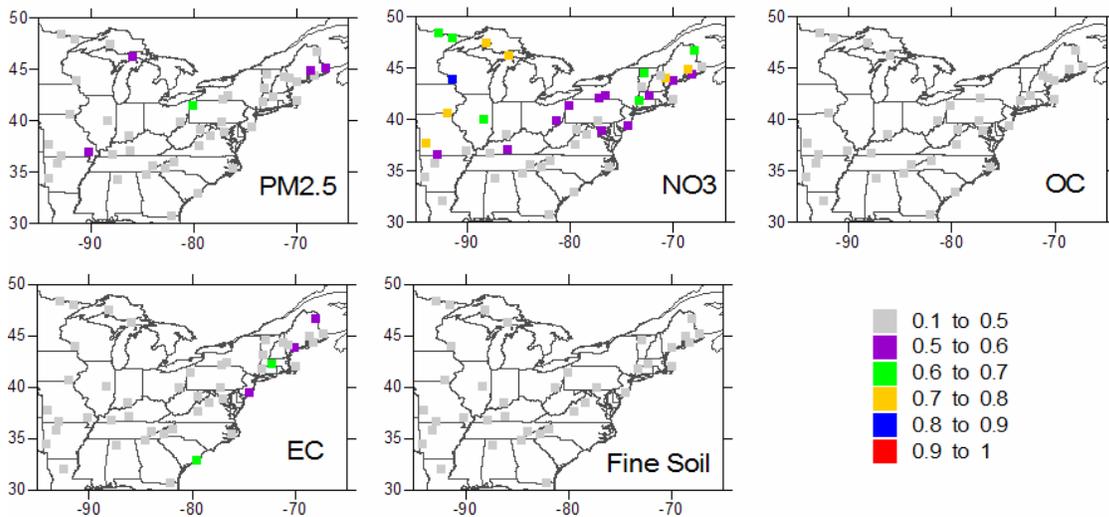


Figure 2-14. Mean Fractional Error of PM_{2.5} species within MANE-VU region

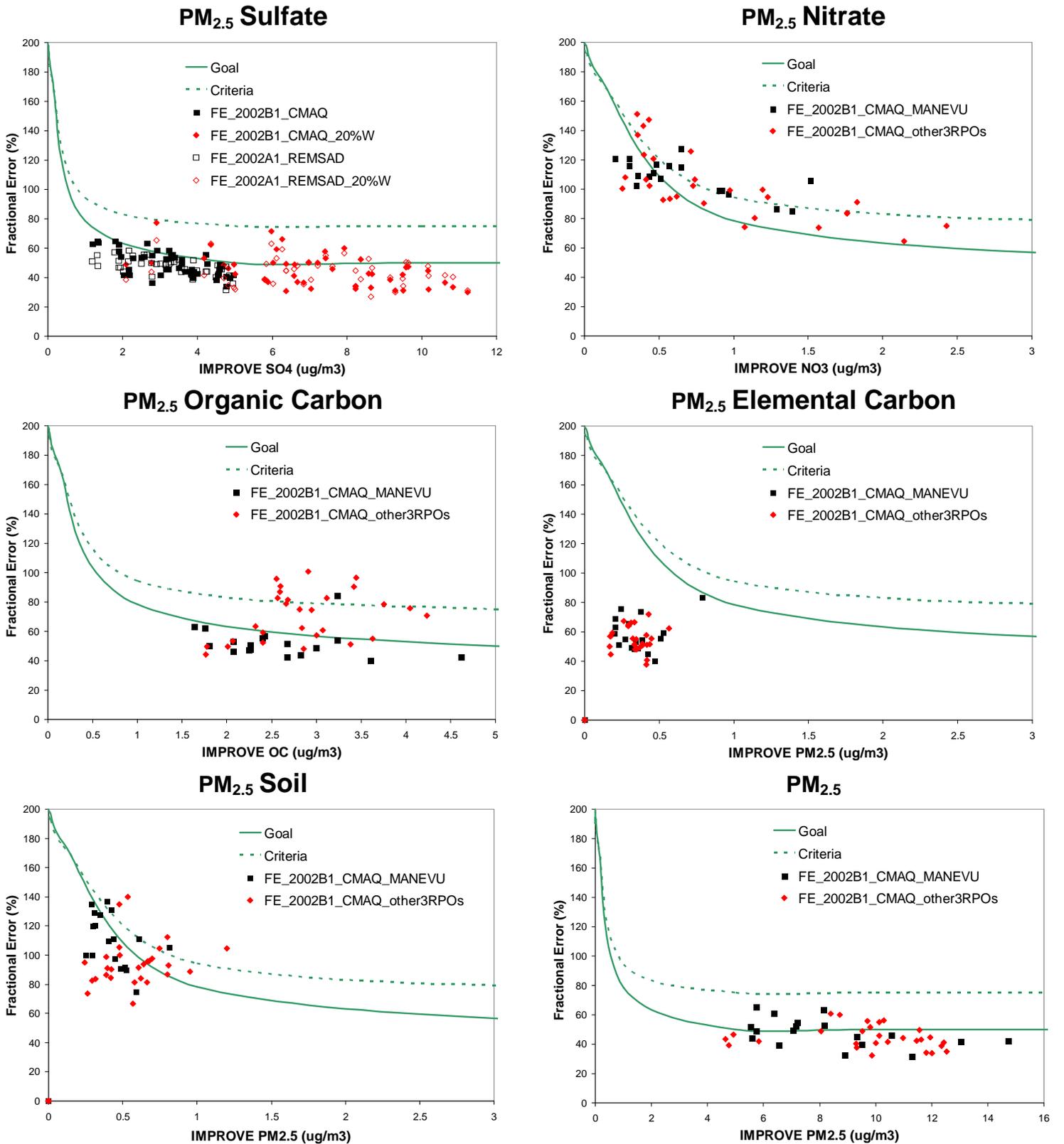


Figure 2-15. Mean Fraction Bias of PM_{2.5} species within MANE-VU region

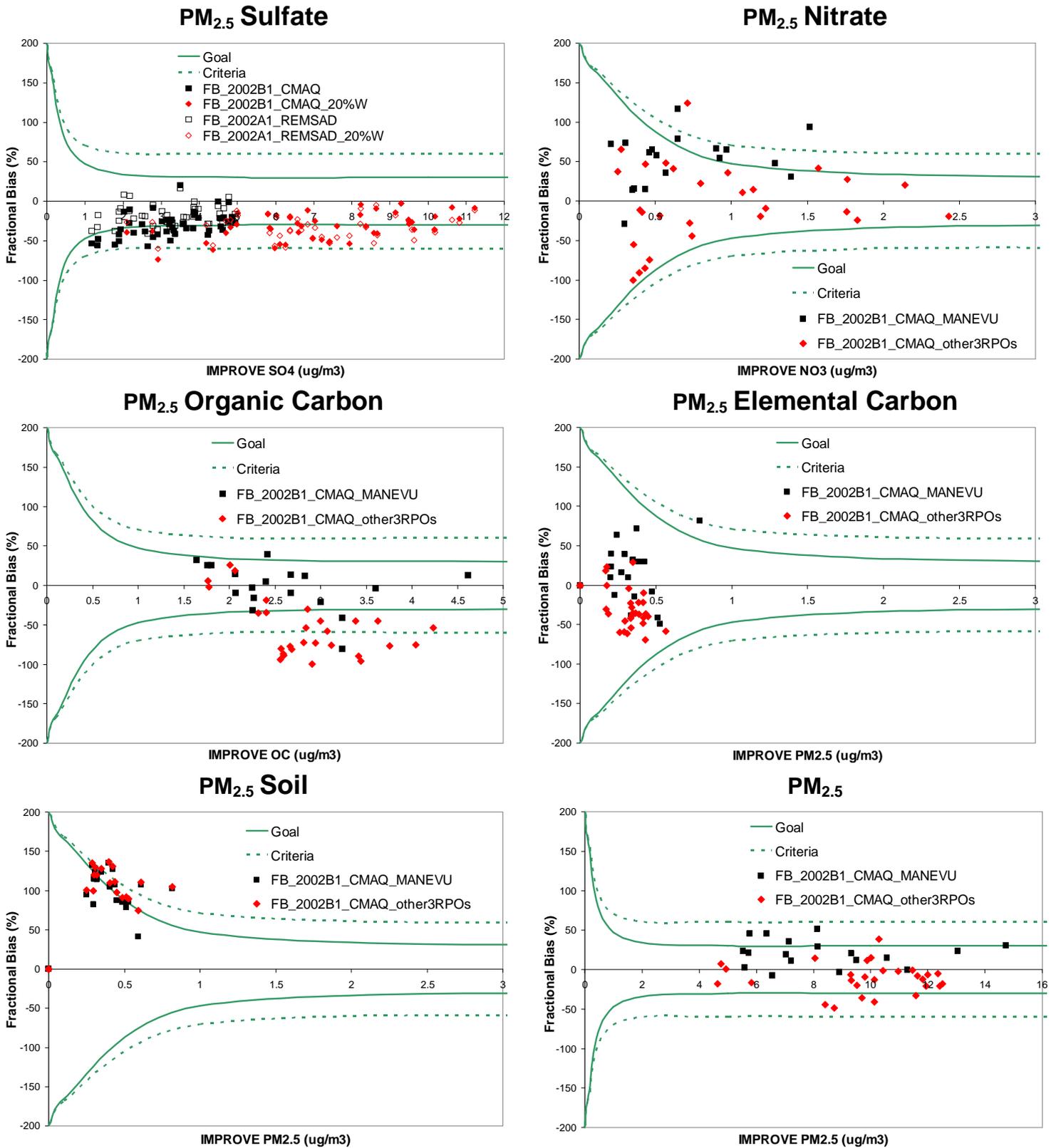


Figure 2-16. Paired comparison of extinction coefficient between CMAQ prediction and IMPROVE measurement

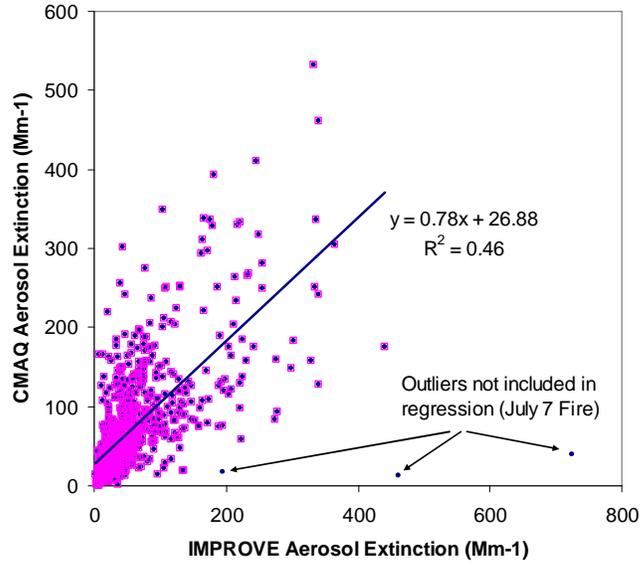


Figure 2-17. Paired Comparison of Haze Index between CMAQ prediction and IMPROVE measurement at selected Class I sites

