An Annual Evaluation of Models-3 CMAQ Using a 2001 Simulation

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1.0 INTRODUCTION

The Clean Air Act and its Amendments require that EPA establish National Ambient Air Quality Standards for Particulate Matter (PM) and assess current and future air quality regulations designed to protect human health and welfare. Air quality models, such as EPA's Models-3 Community Multiscale Air Quality (CMAQ) model, provide one of the most reliable tools for performing such assessments. CMAQ simulates air concentrations and deposition of various pollutants including PM. These simulations, which can be conducted on a myriad of spatial and temporal scales, support both regulatory assessment as well as scientific studies conducted by research institutions.

In order characterize its performance and to build confidence in the air quality regulatory community, CMAQ, like any model, needs to be evaluated using observational data. Accordingly, this evaluation compares PM concentrations simulated by CMAQ with data collected by the Interagency Monitoring of PROtected Visual Environments (IMPROVE) network, the Clean Air Status and Trends Network (CASTNet) and the Speciated Trends Network (STN).

1.1 CMAQ General Description

CMAQ is an Eulerian model that simulates the atmospheric and surface processes affecting the transport, transformation and deposition of air pollutants and their precursors (*Byun and Ching*, 1999). CMAQ follows first principles and employs a "one atmosphere" philosophy that tackles the complex interactions among multiple atmospheric pollutants and between regional and urban scales. Pollutants considered within CMAQ include tropospheric ozone, PM, airborne toxics, as well as acidic and nutrient species. The model also calculates visibility parameters.

1.2 CMAQ Aerosol Module Description

The aerosol component within CMAQ, described in *Binkowski and Roselle* (2003), was derived from the Regional Particulate Model (RPM). Particle size distributions are represented as the superposition of three lognormal modes. $PM_{2.5}$ particles are represented by two modes, the Aitken and accumulation modes, each having variable standard deviations. Aitken mode particles are those with diameters smaller than about 0.1 µm. Accumulation mode particle diameters range between 0.1 and 2.5 µm. Each mode receives primary emitted material, is subject to wet and dry deposition, and may form through condensation of gaseous precursors. The two modes interact through coagulation, and the Aitken mode may grow into the accumulation mode and partially merge with it. $PM_{2.5}$ species considered within CMAQ include: SO_4, NO_3, NH_4, water, primary organic aerosols, secondary organic aerosols from anthropogenic and biogenic origin, elemental and organic carbon, and primary aerosol material not otherwise specified. The coarse particle mode within CMAQ, representing particles having aerodynamic diameters between 2.5 and 10 µm, consists of wind-blown dust and other large particles of unspecified origin. Coarse mode particles in the model also undergo wet and dry deposition.

1.3 CMAQ Simulation Attributes

An annual simulation (2001) using the latest release of CMAQ was used in this evaluation. The modeling domain covers the contiguous U.S. with a 36 km grid resolution. The vertical resolution consists of 14 layers that are set on a sigma coordinate. The simulation used the CB-IV gas-phase chemistry mechanism. The meteorological fields were derived from MM5, the Fifth-Generation Pennsylvania State University/National Center for Atmospheric Research (NCAR) Mesoscale Model. Emissions of gas-phase SO_2, CO, NO, NO_2, NH_3, and VOC were based on EPA's 2001 National Emissions Inventory. Primary anthropogenic $PM_{2.5}$ emissions were separated into different species including particle SO_4, NO_3, OC, EC. Emissions of HC, CO, NOx, and PM from cars, trucks, and motorcycles under various conditions are based on MOBILE6, while biogenic emissions were obtained from BEIS 3.12.

2.0 OBSERVATIONAL DATA

2.1 IMPROVE

IMPROVE is a collaborative monitoring effort governed by a steering committee comprised of Federal, regional and State organizations (*Pitchford and Scruggs*, 2000). The network was designed to: (1) establish current visibility and aerosol conditions; (2) identify the chemical species and emission sources responsible for visibility degradation; and (3) document long-term visibility trends at over 100 **remote** locations nationwide – with a majority of sites located in the **western** United States. IMPROVE monitors collect 24-hr integrated samples every third day (midnight to midnight LST). Given CMAQ's one year simulation and IMPROVE's sampling schedule we had 115 days available for comparison. IMPROVE species used in this evaluation include: $PM_{2.5}$, SO_4, NO_3, EC and OC.

2.2 CASTNet

The Clean Air Status and Trends Network evolved from EPA's National Dry Deposition Network (NDDN) in 1990. The concentration data are collected at predominately **rural** sites, the majority of which are in the **eastern** United States, using an open-faced, 3-stage filter pack. The filter packs, which are exposed for 1-week intervals (i.e., Tuesday to Tuesday) at a flow rate of 1.5 liters per minute (3.0 liters per minute for western sites), utilize a Teflon filter for collection of the particulate species. Again, given CMAQ's one year simulation period and CASTNet's weekly sampling schedule, we had 51 weekly observations available. As seen in Figure 1a,b., 73 sites were available for use in this study. CASTNet species used in this evaluation include: SO_4, NO_3, NH_4.

2.3 STN

The more recently established Speciated Trends Network, developed by EPA, follows the protocol of the IMPROVE network (i.e. every third day collection) with the exception that most of the sites are found in **urban** areas. The objectives of the STN are to: provide annual and seasonal spatial characterization of aerosols; provide air quality trends analysis; and track the progress of control programs. The number of STN sites available during 2001 varied – as the network was ramping up. STN species used in this evaluation include: SO_4, NO_3, NH_4 and $PM_{2.5}$.

3.0 STATISTICS

Because of the noted differences in sampling protocols, evaluation statistics were calculated separately for each network. In addition to general summary statistics (not shown), two measures of model bias: the Mean Bias (MB) and the Normalized Mean Bias (NMB) and two measures of model error: the Root Mean Square Error (RMSE) and Normalized Mean Error (NME) were calculated as seen below:

$$\mathrm{MB} = \frac{1}{N}\sum_{1}^{N}(\mathrm{Model} - \mathrm{Obs}) \quad (1)$$

$$\mathrm{NMB} = \frac{\sum_{1}^{N}(\mathrm{Model} - \mathrm{Obs})}{\sum_{1}^{N}(\mathrm{Obs})} \cdot 100\% \quad (2)$$

$$\mathrm{NME} = \frac{\sum_{1}^{N}\left|\mathrm{Model} - \mathrm{Obs}\right|}{\sum_{1}^{N}(\mathrm{Obs})} \cdot 100\% \quad (3)$$

$$\mathrm{RMSE} = \left(\frac{1}{N}\sum_{1}^{N}(\mathrm{Model} - \mathrm{Obs})^2\right)^{0.5} \quad (4)$$

Scatter plots of monthly aggregated concentrations of CMAQ and observations are also provided for each network and specie, with two-to-one reference lines. In order to highlight potential regional differences in specie concentration and model performance, the scatter plots were segregated into east (color symbols) *versus* west (black symbols) with the divide being 100^o West Latitude. Similarly, the measures of NMB and NME are also presented spatially, to highlight potential regional differences in model performance.

4.0 RESULTS

Examination of the scatter plots and tables reveals that CMAQ varies in its ability to accurately simulate the various species. Simulations of $\mathbf{SO_4}$ are by far the best (Figure 1). Correlations with each data set are high, ranging from 0.78 (STN) to 0.92 (CASTNet) and the vast majority of the aggregated monthly simulations are within a factor of two of the observations. The bias is small, with the NMBs ranging from -4% (CASTNet) to 6% (STN). The errors are relatively small as well, with NMEs ranging from 24% (CASTNet) to 43% (STN). Note that the model generally performs better in eastern locations as opposed to western locations – likely a result of greater experience inherent in CMAQ and its predecessors in simulating eastern locations.

CMAQ simulations of $\mathbf{NO_3}$ (Figure 2) are not nearly as good as those for SO_4. Correlations are lower, ranging from 0.42 (STN) to 0.73 (CASTNet) and the NMBs are larger, ranging from -5% (STN) to 27% (IMPROVE)). The NMEs are much larger, ranging from 76% (CASTNet) to 102% (IMPROVE). When examined over space, the NMEs exhibit little if any difference from one area of the United States to the next. This is not the case for the NMB, however, as CMAQ tends to over predict in the eastern U.S. and underpredict in the western United States (with a few exceptions).

The quality of $\mathbf{NH_4}$ simulations (Figure 3) is similar to, but not quite as good as that of SO_4. Most aggregated monthly simulations are within a factor of two of the observations and the correlations range from 0.58 (STN) to 0.82 (CASTNet). The NMBs are positive and small (7% for CASTNet and 25% for STN), with the majority of overprediction occurring in the eastern U.S. The NMEs range from 34% (CASTNet) to 66% (STN) with the error, for the most part, being equally distributed over the U.S.

The quality of **OC** and **EC** simulations (Figure 4 and 5) are similar and fairly poor, with correlations of 0.46 for EC and 0.34 for OC. Note that many monthly aggregated simulations fall outside the factor of two lines (especially for OC and especially for western stations). For OC the NMB and NME are 34% and 82%, respectively, while for EC they are -2% and 62%. This relatively poor performance is not surprising - given the crude physical representation of organics within the CMAQ aerosol component and the uncertain emission inventories of organics. There is a marked spatial difference with both species in that CMAQ tends to perform considerably better in the eastern U.S. (most NMEs < 50%) when compared to the western U.S. (most NMEs > 50%). OC NMBs are also considerably larger in the western U.S.

The accuracy of the **$PM_{2.5}$** simulations (Figure 6), like $PM_{2.5}$ itself, is a composite of the accuracies of the other species. The majority of the monthly simulations fall within a factor of two of the observations. The correlations range from 0.52 (STN) to 0.68 (IMPROVE). The NMBs are small and similar (7-9%) and the NMEs range from 47-50%. As with the other species, the model does somewhat better in the eastern U.S. as opposed to the western U.S.

Potential sources of the various biases and errors identified in this evaluation include uncertain emissions inventories, erroneous input meteorological data and an incomplete understanding of aerosol dynamics in the CMAQ aerosol component. All are areas of continuing research. Inadequacies in evaluation data sets are also evident.

5.0 REFERENCES

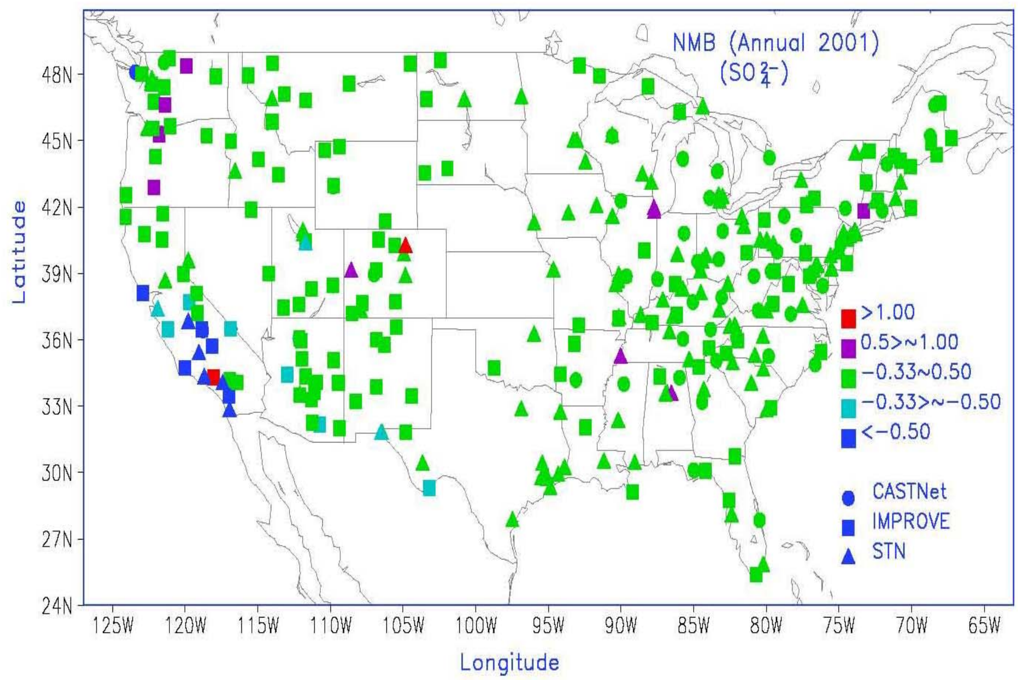
Binkowski, F.S. and S.J. Roselle, Models-3 Community Multiscale Air Quality (CMAQ) model aerosol component. 1. Description, *Journal of Geophysical Research*; Vol. 108 No. D6, 2003.

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, US EPA, US Government Printing Office, Washington D.C., 1999.

Pitchford, M.L. and M. Scruggs, IMPROVE network – Current and future configurations, in: *Spatial and seasonal patterns and temporal variability of haze and its constituents in the United States*, W.C. Malm, principal author, pp. 1-1 – 1-18, Cooperative Institute for Research in the Atmosphere, Colorado State University, ISSN 0737–352–47, 2000.

Figure 1. Annual 2001 sulfate (SO_4) performance at CASTNet, IMPROVE, STN sites: (a) Normalized Mean Bias; (b) Normalized Mean Error.

(a)



(b)

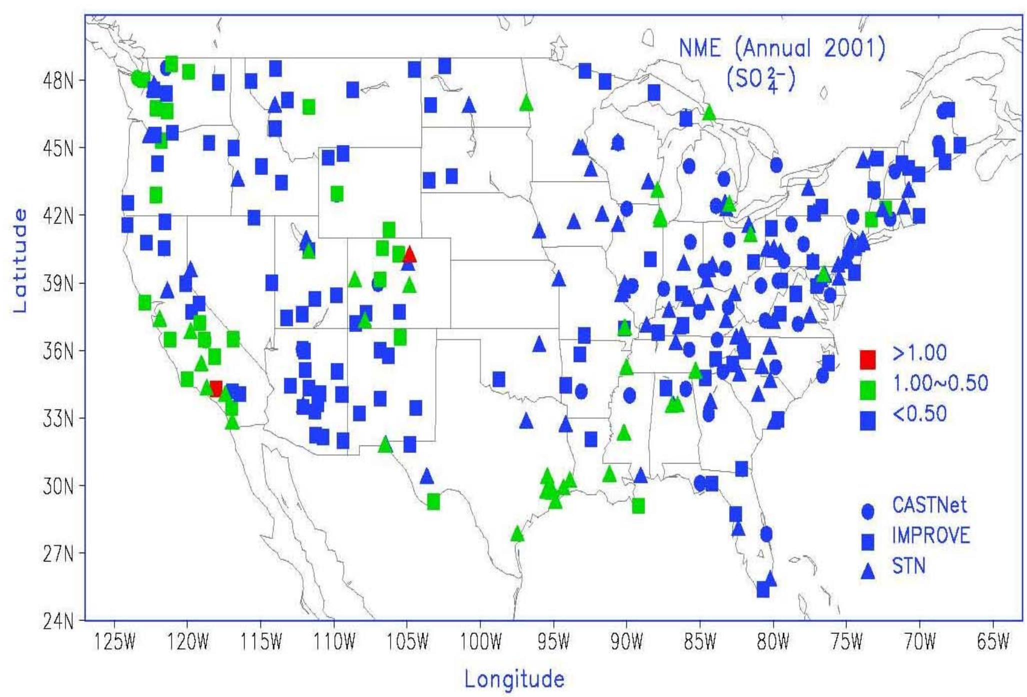
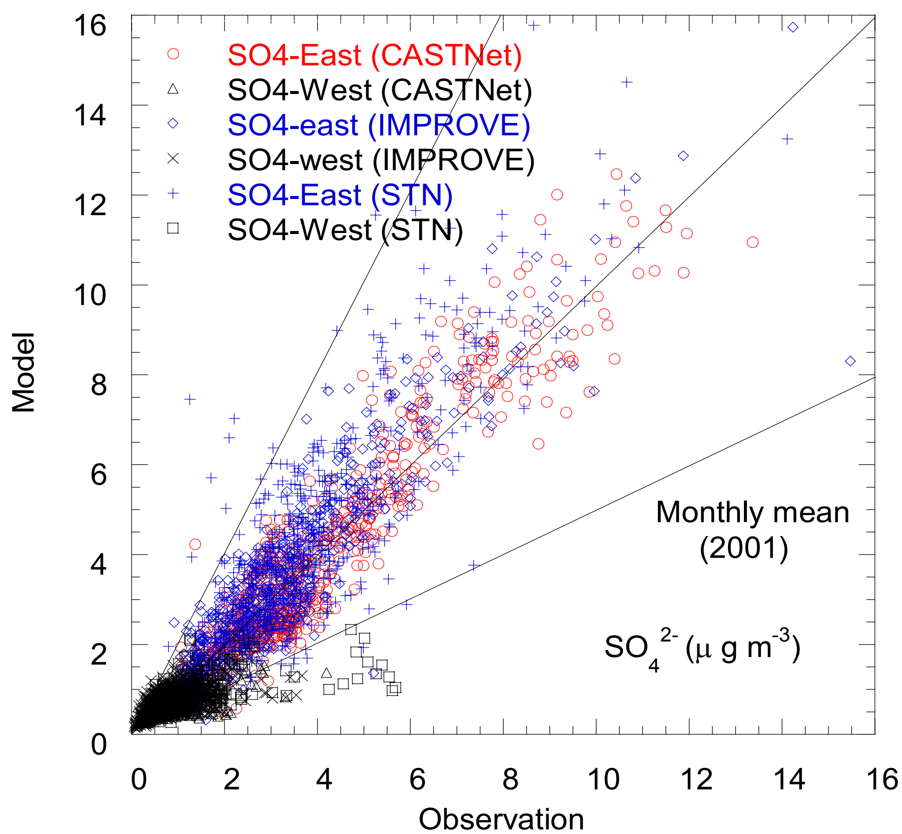


Figure 1. (c) East and west monthly mean sulfate (SO_4) 2001 IMPROVE, CASTNet, and STN observations versus CMAQ predictions; (d) Annual mean SO_4 performance at IMPROVE, CASTNet, and STN sites.

(c)

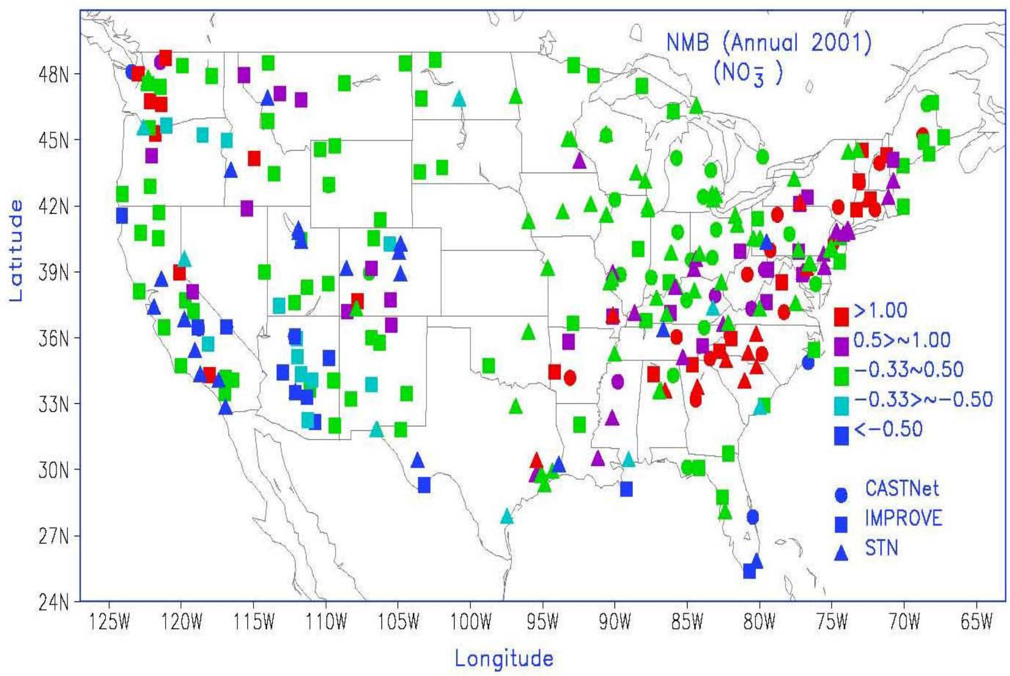


(d)

CASTNet		IMPROVE		STN	
n	3,737	n	13,447	n	6,970
R	0.92	R	0.86	R	0.78
MB	-0.12	MB	0.04	MB	0.22
NMB(%)	-4.0	NMB(%)	2.0	NMB(%)	6.0
RMSE	1.12	RMSE	1.29	RMSE	2.32
NME(%)	24.0	NME(%)	40.0	NME(%)	43.0

Figure 2. Annual 2001 nitrate (NO_3) performance at CASTNet, IMPROVE, STN sites: (a) Normalized Mean Bias; (b) Normalized Mean Error.

(a)



(b)

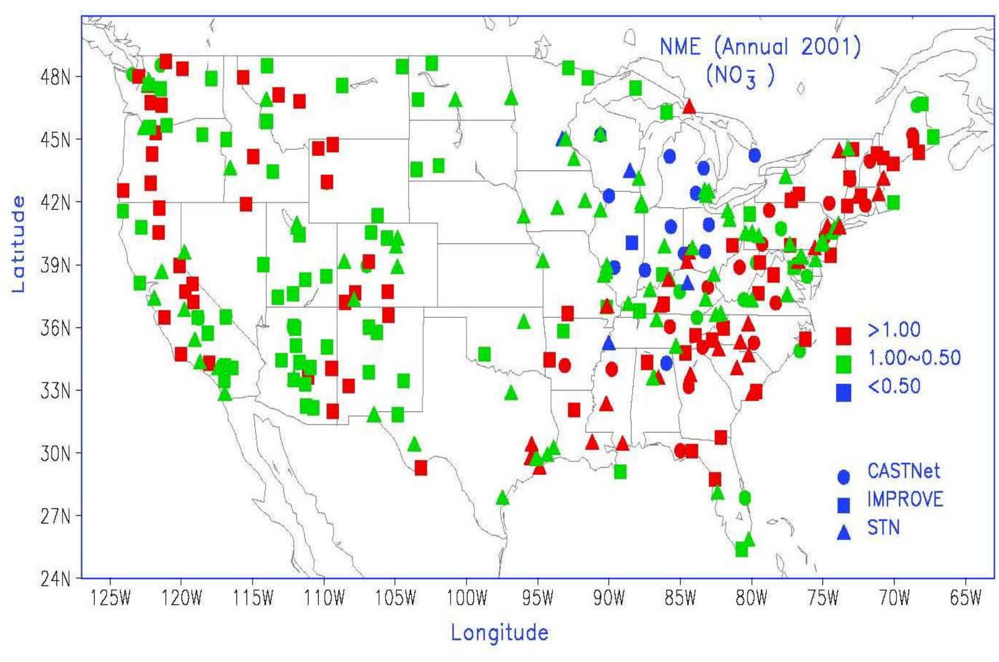
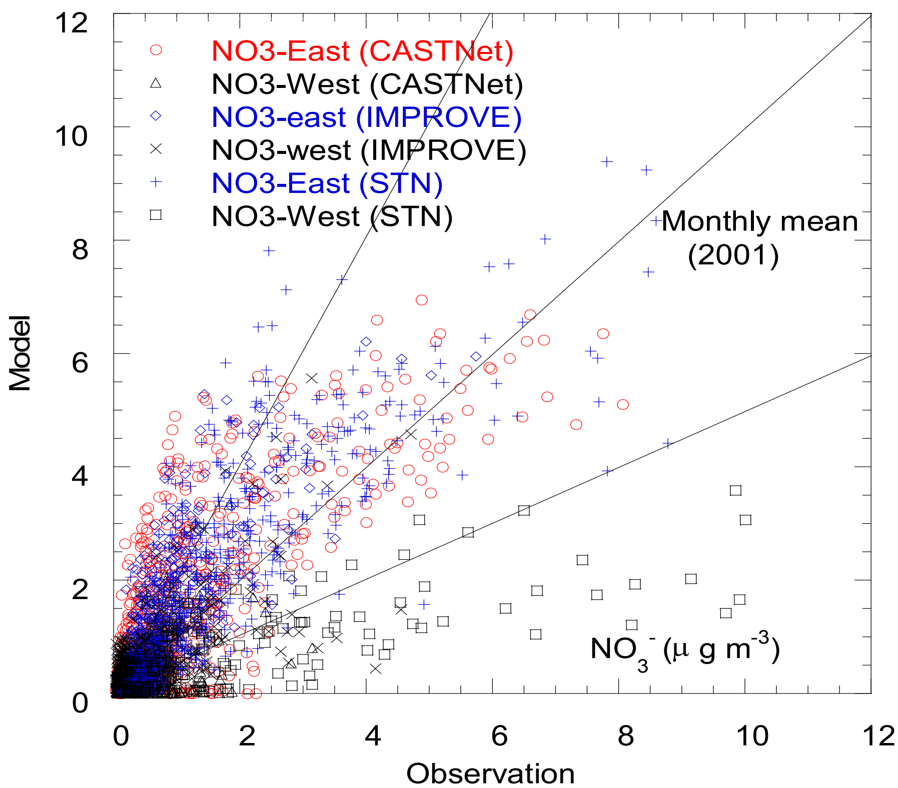


Figure 2. (c) East and west monthly mean nitrate (NO_3) 2001 IMPROVE, CASTNet, and STN observations versus CMAQ predictions; (d) Annual mean NO_3 performance at IMPROVE, CASTNet, and STN sites.

(c)

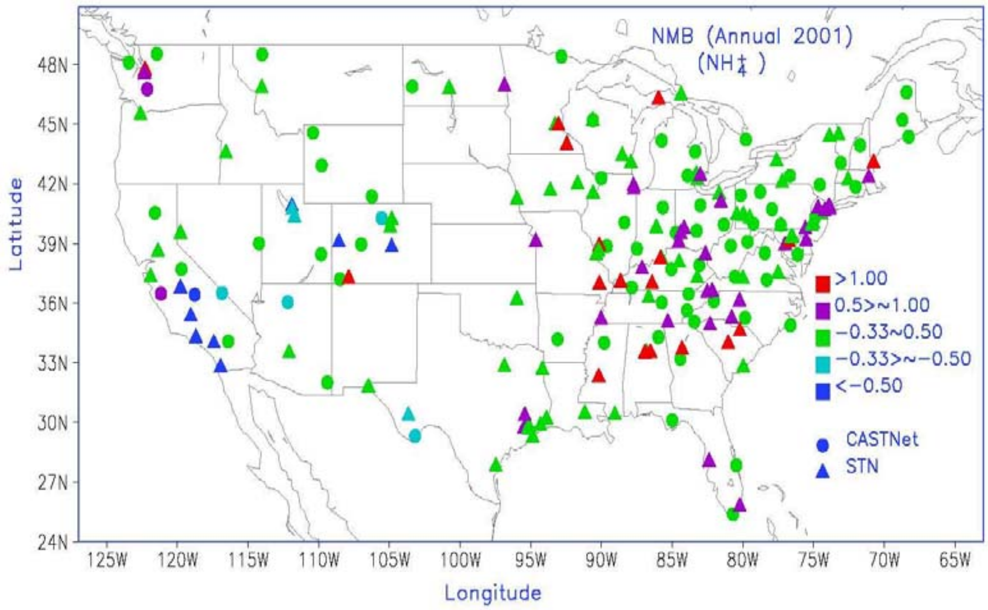


(d)

CASTNet		IMPROVE		STN	
n	3,763	n	13,398	n	6,130
R	0.73	R	0.59	R	0.42
MB	0.26	MB	0.13	MB	-0.08
NMB(%)	26.0	NMB(%)	27.0	NMB(%)	-5.0
RMSE	1.17	RMSE	1.05	RMSE	2.88
NME(%)	76.0	NME(%)	102.0	NME(%)	80.0

Figure 3. Annual 2001 ammonium (NH_4) performance at CASTNet, STN sites: (a) Normalized Mean Bias; (b) Normalized Mean Error.

(a)



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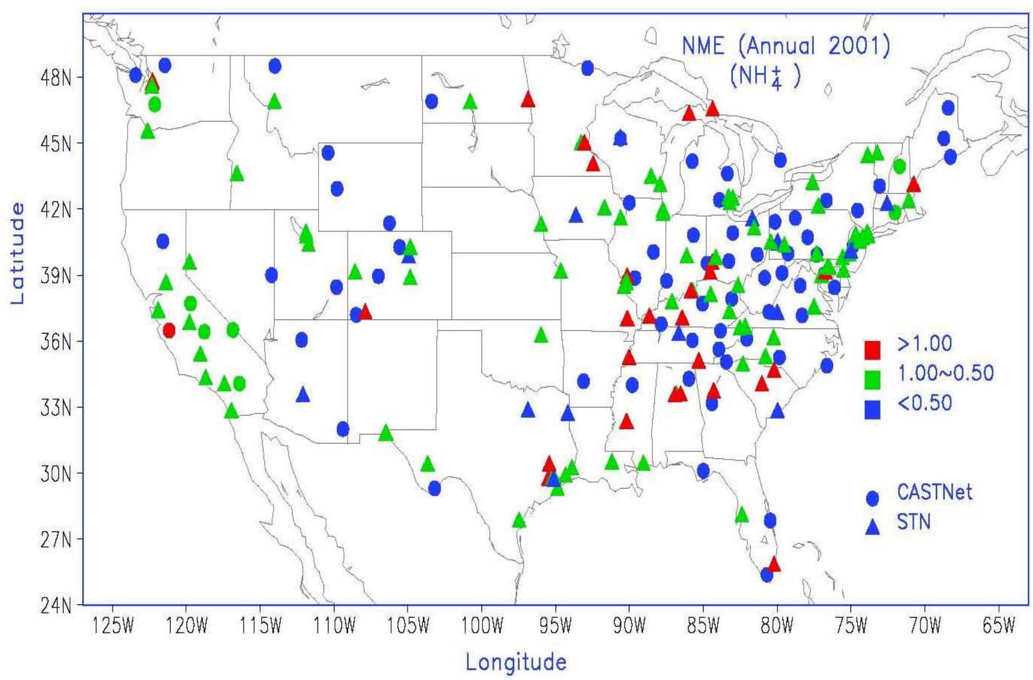
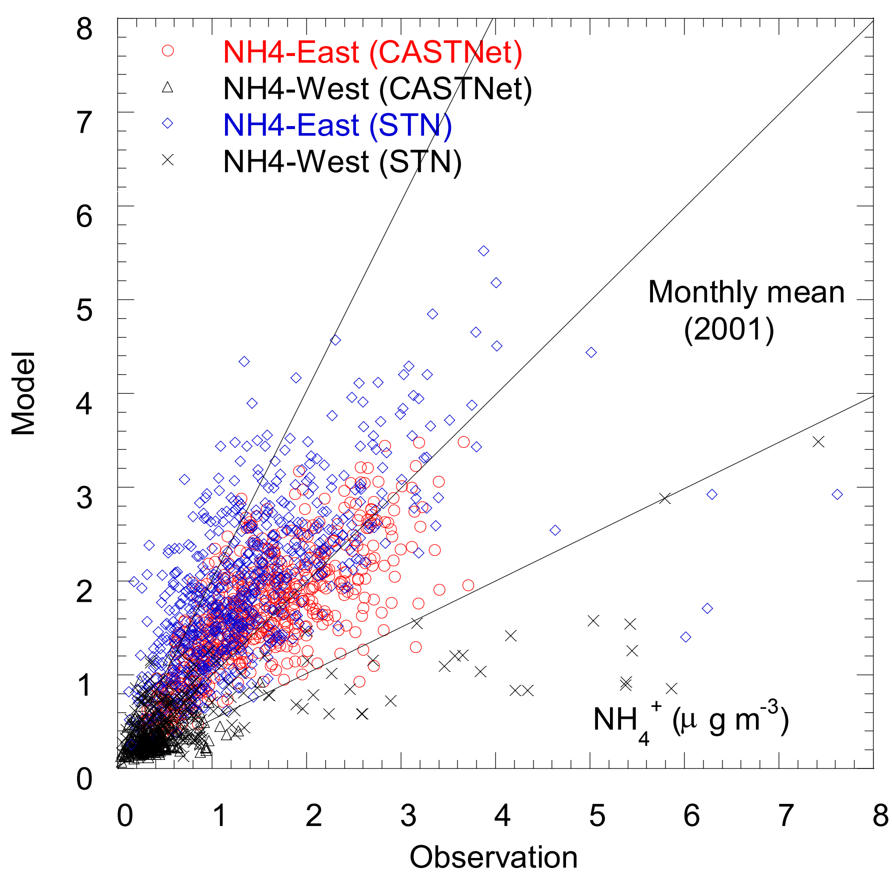


Figure 3. (c) East and west monthly mean ammonium (NH_4) 2001 CASTNet and STN observations versus CMAQ predictions; (d) Annual mean NH_4 performance at CASTNet and STN sites.

(c)

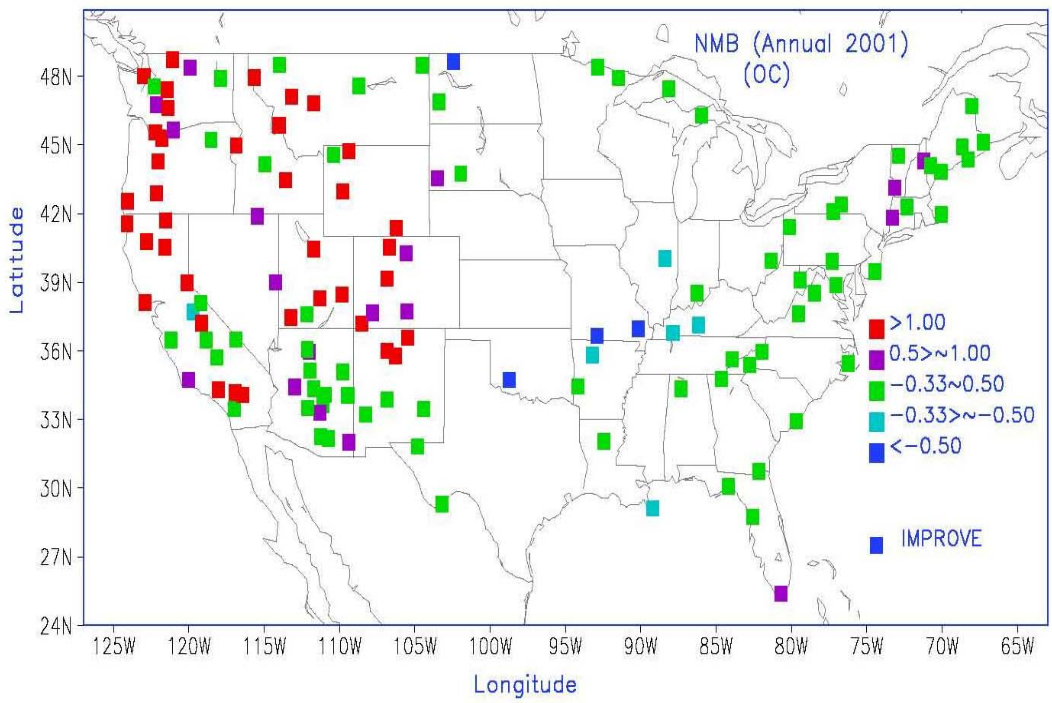


(d)

CASTNet		STN	
n	3,737	n	6,970
R	0.82	R	0.58
MB	0.08	MB	0.32
NMB(%)	7.0	NMB(%)	25.0
RMSE	0.56	RMSE	1.29
NME(%)	34.0	NME(%)	66.0

Figure 4. Annual 2001 organic carbon (OC) performance at IMPROVE sites: (a) Normalized Mean Bias; (b) Normalized Mean Error.

(a)



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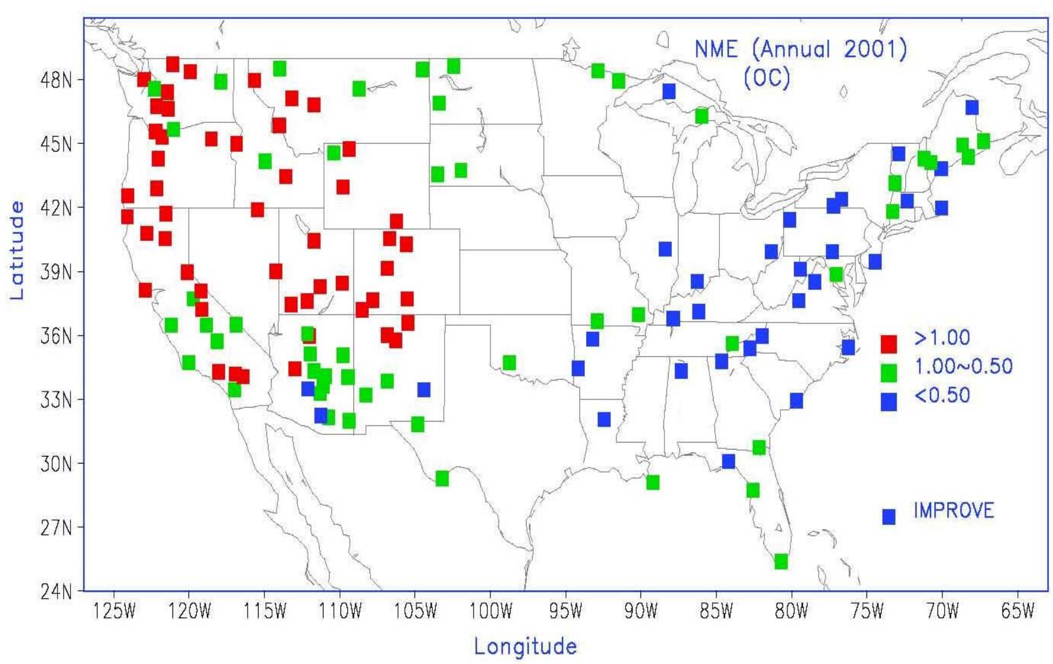
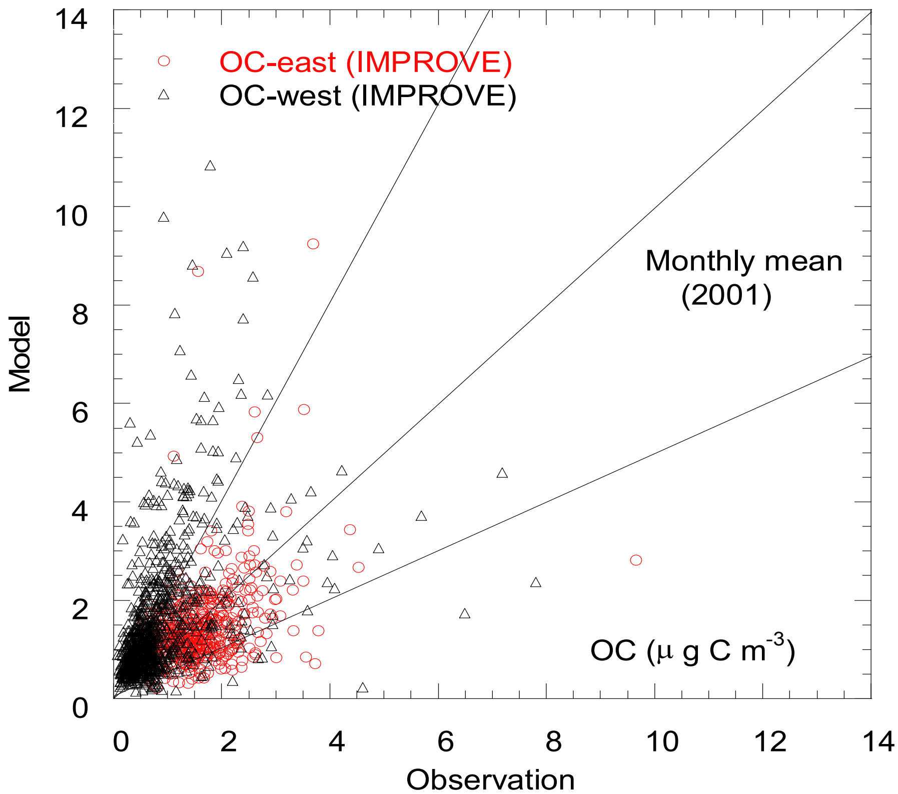


Figure 4. (c) East and west monthly mean organic carbon (OC) 2001 IMPROVE observations versus CMAQ predictions; (d) Annual mean OC performance at IMPROVE sites.

(c)

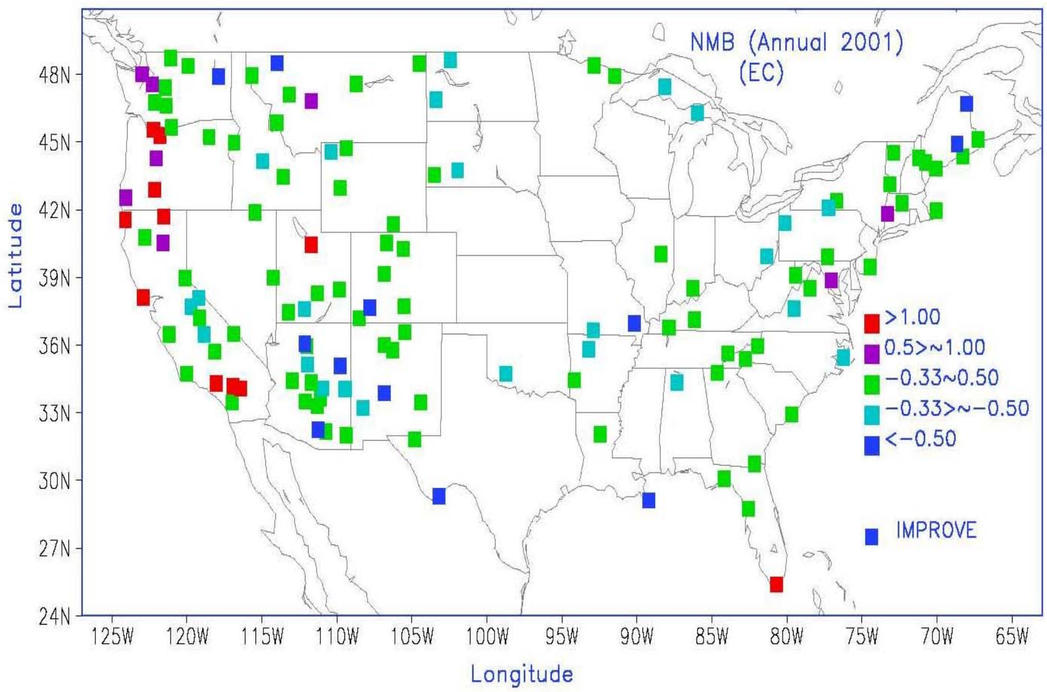


(d)

IMPROVE	
n	13,427
R	0.34
MB	0.38
NMB(%)	34.5
RMSE	1.77
NME(%)	82.6

Figure 5. Annual 2001 elemental carbon (EC) performance at IMPROVE sites: (a) Normalized Mean Bias; (b) Normalized Mean Error.

(a)



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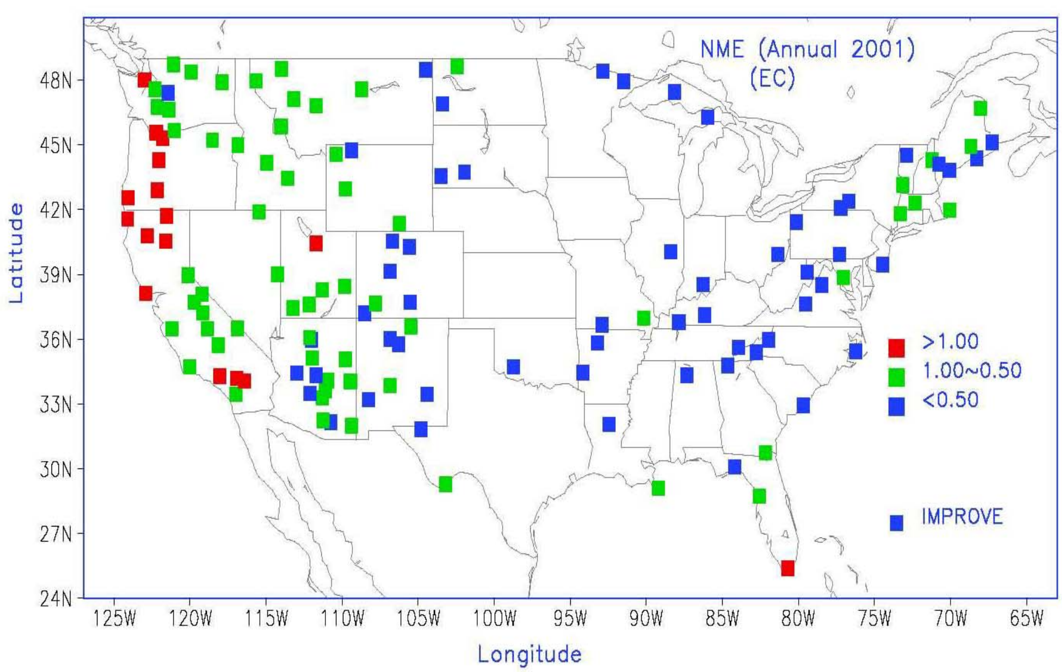
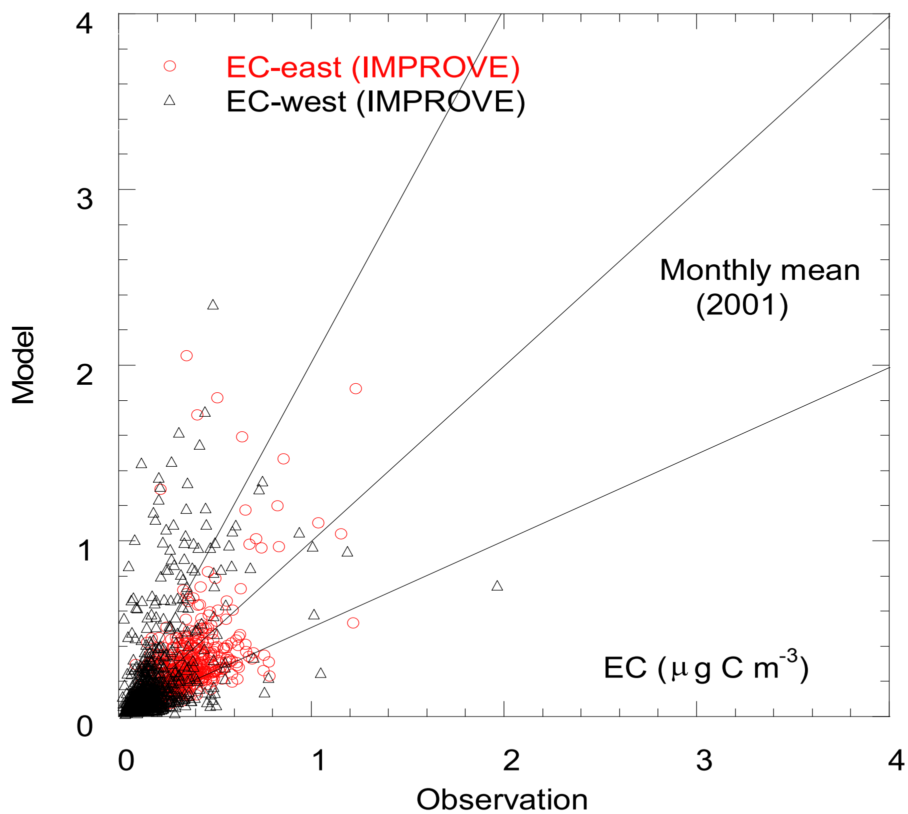


Figure 5. (c) East and west monthly mean elemental carbon (EC) 2001 IMPROVE observations versus CMAQ predictions; (d) Annual mean EC performance at IMPROVE sites.

(c)

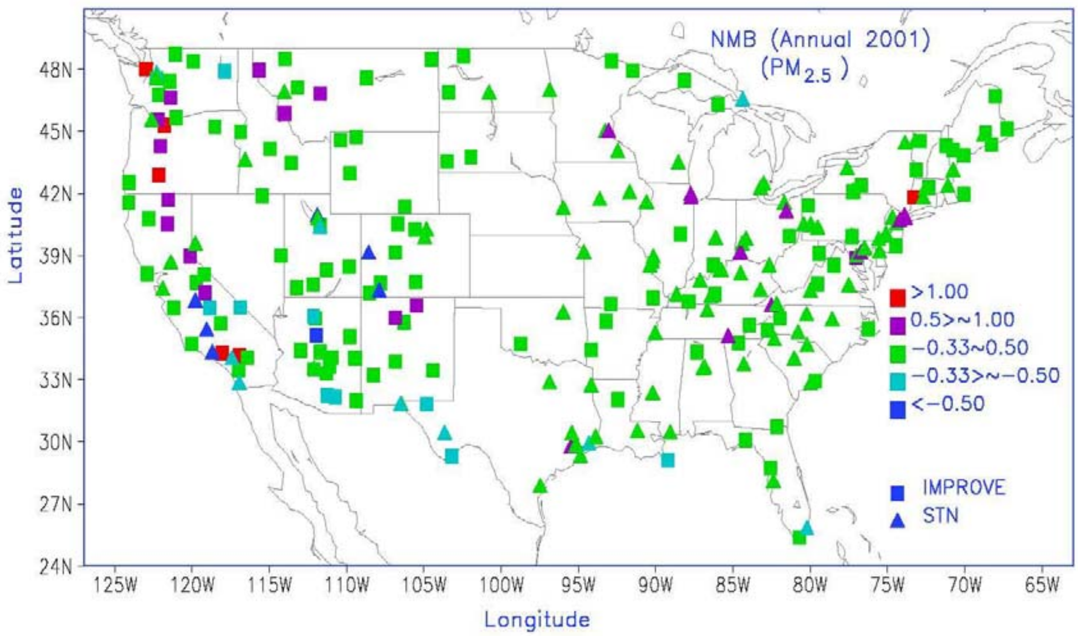


(d)

IMPROVE	
n	13,441
R	0.46
MB	-0.01
NMB(%)	-2.4
RMSE	0.28
NME(%)	61.6

Figure 6. Annual 2001 $PM_{2.5}$ performance at IMPROVE, STN sites: (a) Normalized Mean Bias; (b) Normalized Mean Error.

(a)



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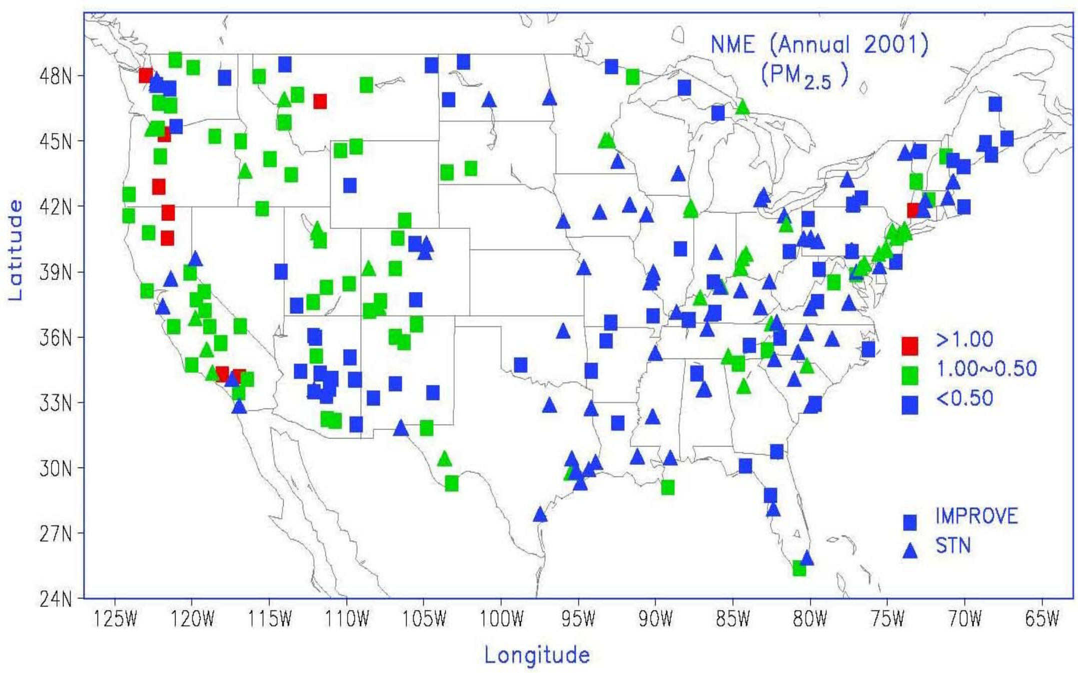
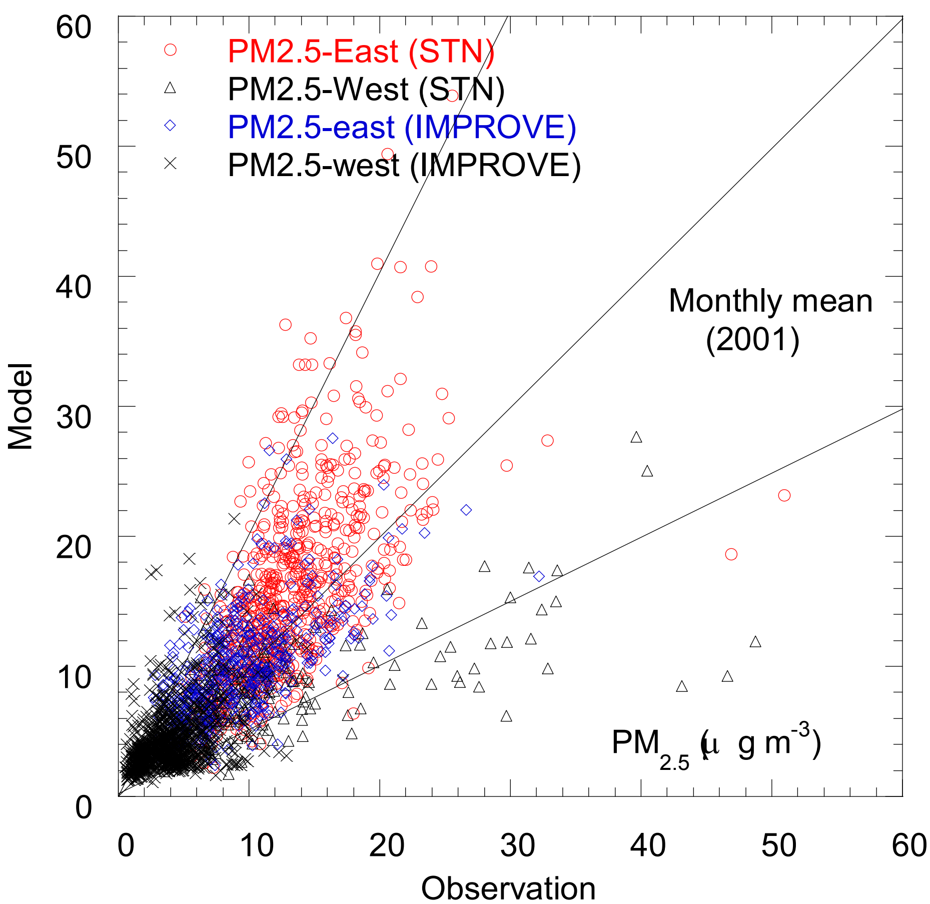


Figure 6. (c) East and west monthly mean $PM_{2.5}$ 2001 IMPROVE and STN observations versus CMAQ predictions; (d) Annual mean $PM_{2.5}$ performance at IMPROVE and STN sites.

(c)



(d)

IMPROVE		STN	
n	13,217	n	6,419
R	0.68	R	0.52
MB	0.54	MB	0.97
NMB(%)	9.0	NMB(%)	7.0
RMSE	4.45	RMSE	9.21
NME(%)	50.0	NME(%)	47.0