An Operational Evaluation of the 2005 Release of Models-3 CMAQ Version 4.5

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1. INTRODUCTION

This evaluation report compares 2001 annual simulations of the 2005 release of the Community Multiscale Air Quality (CMAQ) model version 4.5 with monitoring data from five nationwide networks. The simulations cover a 12km×12km Eastern United States domain and a 36km×36km continental United States domain. While the majority of the report focuses on the performance of the 12-km simulation of CMAQ v4.5, there are also comparisons of the 36-km simulation against the 12-km simulation for v4.5, as well as a comparison of CMAQ v4.5 against the previous year's release of CMAQ version 4.4 for the 12-km horizontal grid domain.

Simulated ambient air concentrations of O_3, $PM_{2.5}$ and various aerosol species are examined, including: sulfate (SO_4^{2-}), nitrate (NO_3^-), ammonium ($NH4^+$), elemental carbon (EC) and organic carbon (OC) with measurement data collected by four networks: Interagency Monitoring of PROtected Visual Environments (IMPROVE) network, Speciated Trends Network (STN), Clean Air Status and Trends Network (CASTNet) and the Air Quality System (AQS). There is also a comparison of simulated wet deposition values and concentrations for several species including SO_4^{2-}, NO_3^- and $NH4^+$ against observations from the National Atmospheric Deposition Program (NADP) network.

When comparing the model results to these observational networks, model results are evaluated separately for each season and/or month to consider temporal biases and uncertainty, since the seasonal variability is particularly important for aerosol species which are influenced by seasonal changes in emissions and meteorology. Additionally, spatial assessment of model performance is also considered for each species. This report provides a comprehensive record of the operational evaluation of the new CMAQ version 4.5. Further analyses will be included in future publications on the evaluation of this model release.

2. CMAQ v4.5 MODEL DESCRIPTION

Significant modifications have been made to the chemistry and aerosol processing capabilities in CMAQ v4.5. The gas/particle partitioning module, ISORROPIA, was updated to the latest available version including better representation of the aerosol liquid water content and corrections to a number of existing discontinuities in the phase transitions. CMAQ's aerosol module was upgraded (version AE4) including the model's first consideration of sea salt aerosols emitted from wind and wave action over ocean areas. The sea salt aerosols can interact with nitric acid and hydrochloric acid within the phase partitioning module for an equilibrium balance of accumulation mode aerosols. The aerosol dry deposition algorithm was also updated to include a new impaction term and a revised equation for combining turbulent deposition fluxes and gravitational settling. Also, a new routine has been added to the aerosol module that provides a more rigorous definition of aerosols contained within the 2.5 µm diameter cutoff for $PM_{2.5}$.

Within the gas-phase chemistry modules, a chlorine chemical mechanism was added to the existing Carbon Bond IV (CB-IV) chemical kinetics mechanism, along with an efficient Euler Backward Iterative numerical solver for the combined chemistry. In areas with relatively high chlorine gas emissions, ozone photochemistry can be enhanced. Also, twenty gas-phase Hazardous Air Pollutants (HAPS), or air toxics species, have been added to the CB-IV and SAPRC-99 chemical kinetics mechanisms, as options to simulate their fate and transport by the CMAQ model. Some of these species, such as formaldehyde and acetaldehyde, explicitly participate in active photochemistry, but most undergo only simple atmospheric degradation reaction with OH. CMAQ's emissions processor and associated emissions inventory now allow the incorporation of these new primary source emissions.

Updates to the physical processes within CMAQ have also been made. The pollutant mixing model within convective clouds has been modified based on the Asymmetric Convective Model (ACM) that allows in-cloud transport from a source layer to all other in-cloud layers. This is an improvement upon earlier schemes in that it permits gradual layer-by-layer downward mixing through compensatory subsidence. Pollutant diffusion within the planetary boundary layer has also been modified by permitting higher specified minimum diffusion coefficients for urban areas than non-urban areas. The higher urban coefficients are meant to reflect less nighttime stability resulting from urban heat-island effects. Also, a new mass continuity scheme is introduced in CMAQ v4.5 that is globally mass-conserving and uses a piecewise parabolic numerical method for horizontal advection, deriving a vertical velocity component that satisfies the mass continuity equation. Lastly, the vertical grid structure has been further generalized by allowing users to specify the number of vertical layers in their domain at run-time in a dynamic manner.

New diagnostic tools are also included with CMAQ v4.5, including a carbon source apportionment version of the model that tracks the contributions of elemental and primary organic carbon from up to ten different source categories or source regions. A sulfur tracking version of the model is also available that tracks sulfate production from the gas-phase and aqueous-phase chemistry, as well as contributions from direct emissions and initial and boundary conditions.

Collaborations between EPA research staff and scientists at DOE's Sandia National Laboratory have introduced computational efficiencies into the CMAQ model that allows continental U.S. model applications (36-km grid cell size) or Eastern/Western U.S. domain applications (12-km grid cell size) to be run for full-year simulations within one week of computer time using 8-processor Linux cluster computers.

3. CMAQ SIMULATION CHARACTERISTICS

For this evaluation, the results of an annual CMAQ v4.5 simulation using a 12km×12km horizontal grid cell size and a 14-layer vertical structure will be presented. The domain covers an area from roughly central Texas, north to North Dakota, east to Maine and south to central Florida. Additionally, a comparison of this simulation to a CMAQ v4.4 simulation for the same domain is presented for the winter season (December, January and February 2001) and the summer season (June, July and August 2001). These 12-km simulations were nested within 36km×36km horizontal grid domain which used the same configuration of CMAQ as the nested domain. The same meteorology and emissions have been used for these CMAQ v4.5 and 4.4 simulations to ensure a consistent comparison. The meteorological fields were simulated at both 36-km and 12-km (nested within the 36-km simulation) by MM5, the Fifth-Generation Pennsylvania State University/National Center for Atmospheric Research (NCAR) Mesoscale Model (Grell et al., 1994). The MM5 fields were processed for CMAQ using version 3.0 of the Meteorology-Chemistry Interface Program (MCIP).

The CMAQ v4.5 simulations utilized the CB-IV gas-phase chemistry mechanism, the efficient Euler Backward Interactive (EBI) solver, the AERO4 aerosol module which contains mechanisms dealing with sea salt emissions, the Yamo mass adjustment scheme and the asymmetric convective module (ACM) for cloud treatment in the model. For the simulations using CMAQ v4.4, the model configuration was slightly different, utilizing the Piecewise Parabolic Method (PPM) mass adjustment scheme, the RADM cloud scheme and no method for the treatment of sea salt. All other configuration options were the same between the simulations for the two model versions. Additional details regarding the latest release of CMAQ, including changes associated with Version4.5, can be found at the Atmospheric Sciences Modeling Division laboratory website (http://www.epa.gov/asmdnerl/).

Emissions of sulfur dioxide (SO_2), carbon monoxide (CO), nitrogen oxides (NO_x), ammonia (NH_3) and volatile organic compounds (VOCs) were based on EPA's 2001 National Emission Inventory (NEI) and were processed by the Sparse Matrix Operator Kernel Emission (SMOKE) processor. Since current NEI NH_3 emissions are limited to annual estimates with no intra-annual variation, monthly NH_3 emissions factors developed by Gilliland et al. (2005) were used to allow temporal variability. Biogenic emissions were processed using the Biogenic Emissions Inventory System (BEIS) version 3.13.

4. OBSERVATION NETWORK DESCRIPTIONS

Five monitoring networks were utilized in this evaluation report (AQS, IMPROVE, STN, CASTNet, NADP), each having its own sampling methodology and measurement frequency. Therefore, the evaluation of each network is presented separately, although when applicable, multiple networks are presented on a single plot (with different colors and symbols) in order to conserve space. No adjustments have been made to the observations obtained from the networks to account for measurement uncertainties.

4.1 AQS

Ozone data used in the evaluation were acquired from the U.S. EPA's AQS (previously known as the Aerometric Information Retrieval System (AIRS)). Observations of ozone from the AQS are available on an hourly timeframe and are obtained from numerous Federal, State and local agency run locations across the nation. Over 1000 AQS sites are available nationwide, however only about 775 AQS sites are available within the 12-km domain used in this report. Both hourly concentrations and the daily 8-hr average maximum ozone concentrations are utilized for this report.

4.2. IMPROVE

The IMPROVE network began in 1985 and is a collaborative monitoring effort between Federal, State and local organizations. IMPROVE monitors, the majority of which reside in the western United States, collect 24-hr integrated samples (midnight to midnight, LST) every third day. The network was established to aid in the protection of Federal class I areas (national parks and wilderness areas), and therefore the network is useful in evaluating the performance of the model in extremely rural areas. Since the majority of the IMPROVE sites are located in the west, only 45 sites are located within the 12-km Eastern United States simulation used in this evaluation. Detailed information regarding the IMPROVE network can be found in Malm et al. (2004) or at the IMPROVE website, http://vista.cira.colostate.edu/improve/. IMPROVE species used in this evaluation include SO_4^{2-}, NO_3^-, $PM_{2.5}$, EC and OC (NH_4 was omitted from the analysis due to the sparse number of observations available during 2001 at the IMPROVE sites).

4.3. STN

The STN network has been more recently developed by EPA and follows closely the protocol of the IMPROVE network, with 24-hr integrated samples taken every third day. However, unlike the IMPROVE network, STN sites are located in urban locations, and therefore are useful in evaluating the model's performance in urban areas. The number of STN sites available in 2001 varied as the network was being established, with more sites becoming available as the year progressed. STN species used in this evaluation include SO_4^{2-}, NO_3^-, NH_4^+, $PM_{2.5}$, EC and OC.

4.4 CASTNet

The CASTNet was developed in 1987 from the National Dry Deposition Network (NDDN) with the purpose of providing atmospheric data on the dry deposition portion of total acid deposition. CASTNet is the primary source of dry acidic deposition data, providing weekly average atmospheric concentrations of sulfate, nitrate, ammonium, nitric acid and sulfur dioxide. In 2001, there were 73 active CASTNet sites nationwide (most of which are located in the east), of which approximately 50 are located within the 12-km simulation used in this evaluation. CASTNet species used in this evaluation include SO_4^{2-}, NO_3^-, NH_4^+ and HNO_3. Additional information regarding CASTNet can be found at the network's website: http://www.epa.gov/castnet/.

4.5 NADP

The NADP network is a cooperative effort between many different groups, including the U.S. Department of Agriculture, U.S. Geological Survey, the State Agriculture Experiment Stations and various other governmental and private groups. The network began in 1978 as 22 sites and has grown to over 200 sites across the United States, Alaska, Puerto Rico and the Virgin Islands. The purpose of the network is to collect data on precipitation chemistry, providing aggregated weekly observations of wet deposition SO_4^{2-}, NO_3^-, NH_4^+, as well as precipitation. NADP species used in this evaluation include wet deposition SO_4^{2-}, NO_3^-, NH_4^+ and precipitation. Additional information regarding the NADP network can be found at the network's website: http://nadp.sws.uiuc.edu/.

5. STATISTICAL MEASURES

Due to the different sampling periods among the networks described in the previous section, statistics were calculated separately for each network. It is necessary for the CMAQ output to be post-processed for compatibility with the observation network and species. The Site Compare post-processing program, which is released as a tool along with the 2005 CMAQ version 4.5 model, was used to pair observations and model results in space (no interpolation) and time (hourly, daily or weekly depending on the network). It should, of course, be noted that the observation network measurements are made at specific locations, while each CMAQ concentration represents a grid-cell volume-averaged value. Referred to as incommensurability, this discrepancy in spatial representativeness is an underlying source of uncertainty when evaluating models, particularly in urban areas, where sub-grid variations can be large (Seigneur, 2001).

There is a large number of statistical metrics available for use in model evaluation. For the purposes of this evaluation report, only a select few of the numerous metrics available are presented. For a bias metric, Normalized Mean Bias (NMB) was chosen, and for an error metric, both Root Mean Square Error (RMSE) and Normalized Mean Error (NME) were chosen. RMSE provides an actual (i.e. measured in ppm or µg/m^3), while NMB and NME provide normalized (%) measure of performance. Definitions for each of these metrics are given below.

$$RMSE = \sqrt{\frac{1}{N}\sum_{1}^{N}(C_m - C_o)^2} \qquad NMB = \frac{\sum_{1}^{N}(C_m - C_o)}{\sum_{1}^{N}C_o}\cdot 100\% \qquad NME = \frac{\sum_{1}^{N}\left|(C_m - C_o)\right|}{\sum_{1}^{N}C_o}\cdot 100\%$$

The variables C_m and C_o are modeled and observed concentrations, respectively. NMB and NME have the advantage of avoiding inflated values, since the normalization is achieved by dividing by the sum observed concentrations instead of the individual observations, which can inflate some other metrics when they are applied to low concentrations. Analyses using these same metrics are presented in Eder and Yu (2005) for the CMAQ version 4.4 model release. The RMSE provides a quantitative estimate of the uncertainty in the predictions, as compared to a given set of observational data. The NME and NMB provide a relative comparison of the model predicted bias and error against a given set of observational data.

6. REFERENCES

Eder, B. and S. Yu, 2005: A performance evaluation of the 2004 release of Models-3 CMAQ, *Atmos. Environ.*, in press

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Seigneur, C., 2001: Current status of air quality models for particulate matter. *J. Air Waste Manage. Assoc*., 51, 1508-1521.

7. DISCLAIMER

The research presented here was performed under the Memorandum of Understanding between the U.S. Environmental Protection Agency (EPA) and the U.S. Department of Commerce's National Oceanic and Atmospheric Administration (NOAA) and under agreement number DW13921548. This work constitutes a contribution to the NOAA Air Quality Program. Although it has been reviewed by EPA and NOAA and approved for publication, it does not necessarily reflect their policies or views.

Evaluation of CMAQ version 4.5: 12km×12km Eastern United States Air Quality System (AQS) 8-hr max Ozone

Available Networks and Species:

AQS – Ozone

Ozone Performance: Introduction

In the following section, we compare the CMAQ version 4.5 simulated ozone to AQS observed values in parts per million (ppmV), utilizing both hourly and daily 8hr-max ozone values. AQS ozone is available as hourly values, as well as daily 1hr-max and 8hr-max values. Since current EPA ozone standards are based on the daily 8hr-max and are no longer based on the daily 1hr-max, the evaluation of ozone performance focuses on the daily maximum 8hr ozone concentrations. The following statistical metrics and plots are provided for ozone performance:

- Model to Observation Scatter plot of 8hr-max ozone
- Diurnal Box Plot using hourly average ozone
- Spatial Plot of NMB (%) and NME (%) of 8hr-max ozone
- Table of select statistical metrics for 8hr-max ozone

While the majority of the above plots and statistics are common evaluation metrics and used throughout this evaluation, the diurnal box plot is applied specifically to hourly ozone performance in this report. Shown on the diurnal box plots are the 25% and 75% quartiles (shaded regions) along with the median value for each hour, for both modeled and observed values. The result is a diurnal curve of observed versus modeled ozone performance to summarize model values and observations across the entire domain. The lines on the scatter plots represent the 1-to-1 and +/- 30% reference lines.

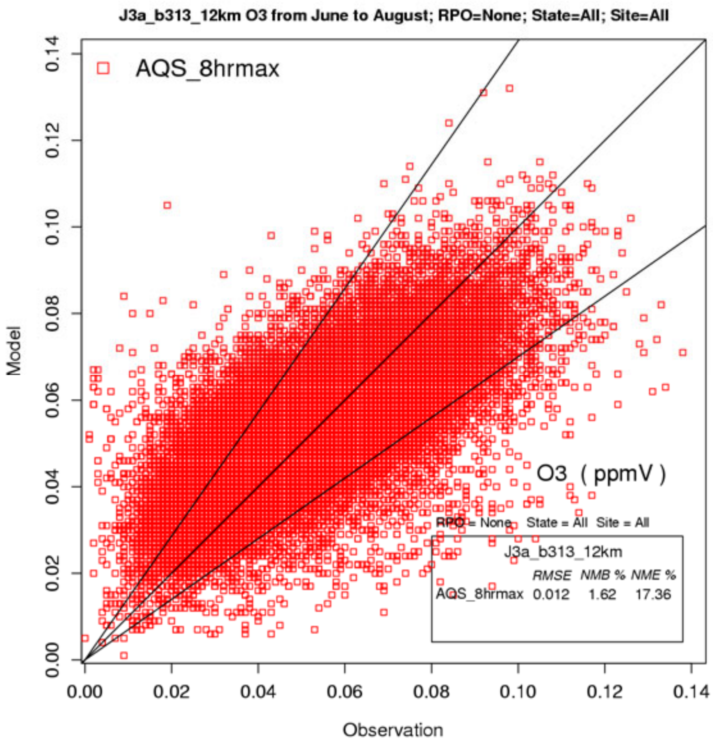
Ozone Performance: Summary

For the summer season consisting of June, July and August, the 8hr-max ozone performance was relatively good, showing a slight positive NMB of 1.62% and a NME of 17.4%. The diurnal box plot shows a consistent over-prediction of ozone, especially during the overnight hours. Nighttime over-predictions in O_3 have been improved over CMAQ 4.4 by modifications to the minimum K_z approximation in CMAQ v4.5, but additional investigations are needed. Ozone predictions during the daytime were much closer to observed values, with a much smaller over-prediction than during the overnight hours. Spatially, ozone performance was good, with the majority of sites having NMB values within +/- 15% and NME values less than 30%. The ozone predictions along the coastal areas (Northeast and Gulf coasts) are poor, with higher NMB and NME than the majority of the domain.

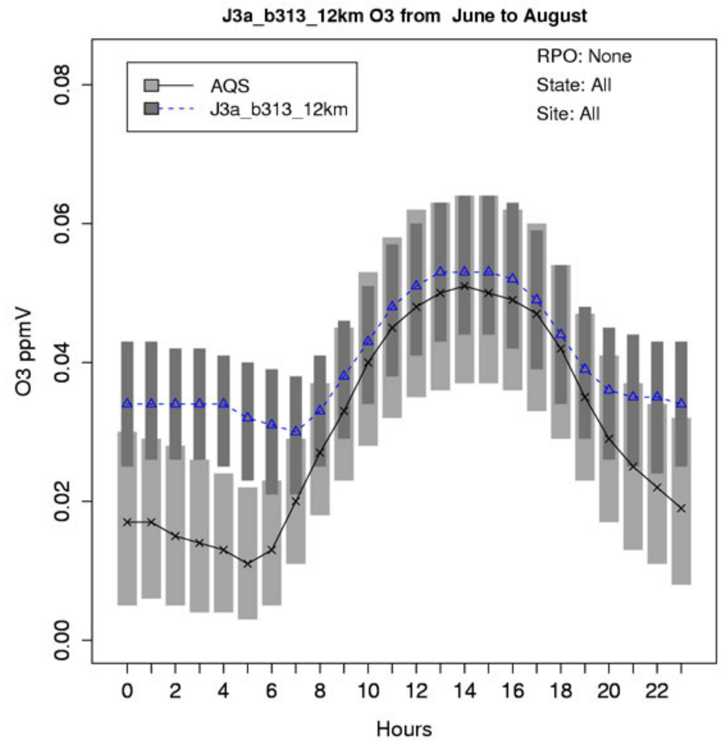
The overall performance of CMAQ to predict ozone is slightly better at 12 km than at 36 km (refer to 36 km vs. 12 km comparison in a following section), although the majority of statistical metrics improve only slightly at the 12 km resolution.

AQS 8-hr max Ozone – Summer (JJA)

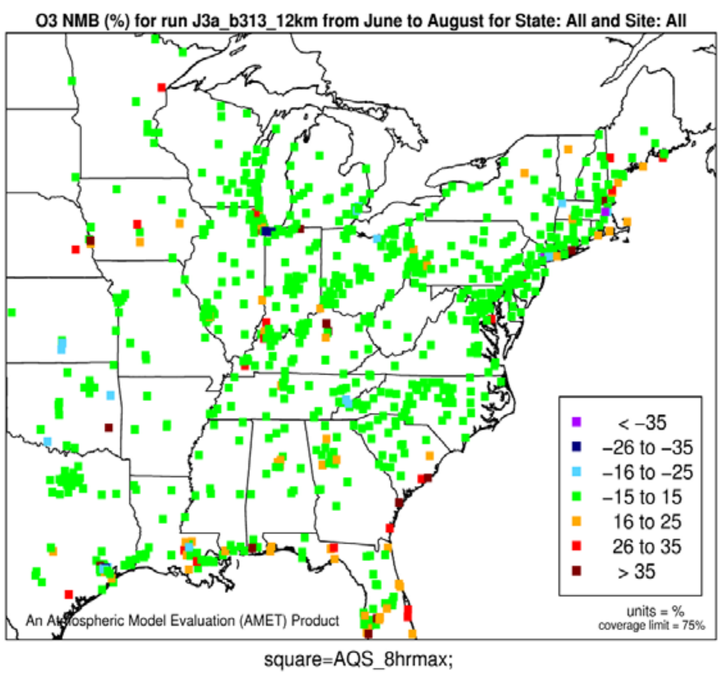
Scatter Plot – 8hr-max Pairs



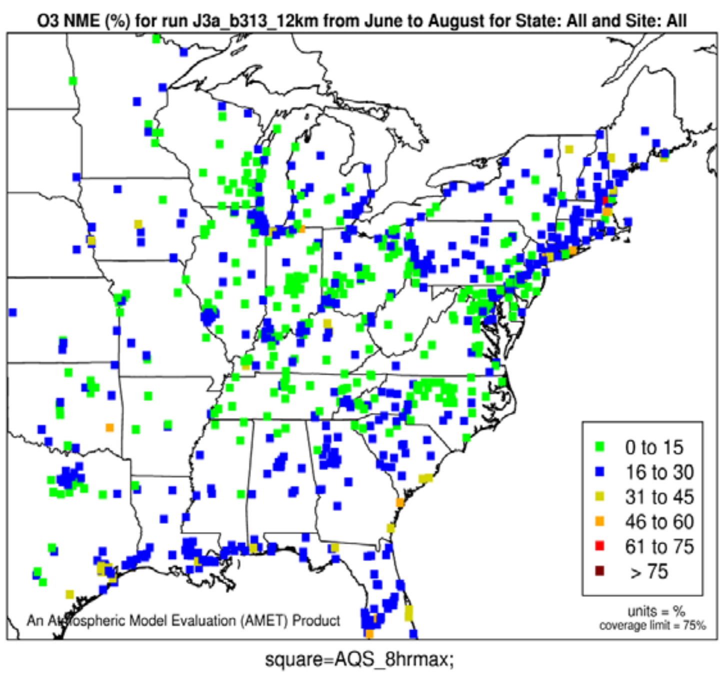
Diurnal Box Plot – All Pairs



Normalized Mean Bias (%) - Summer



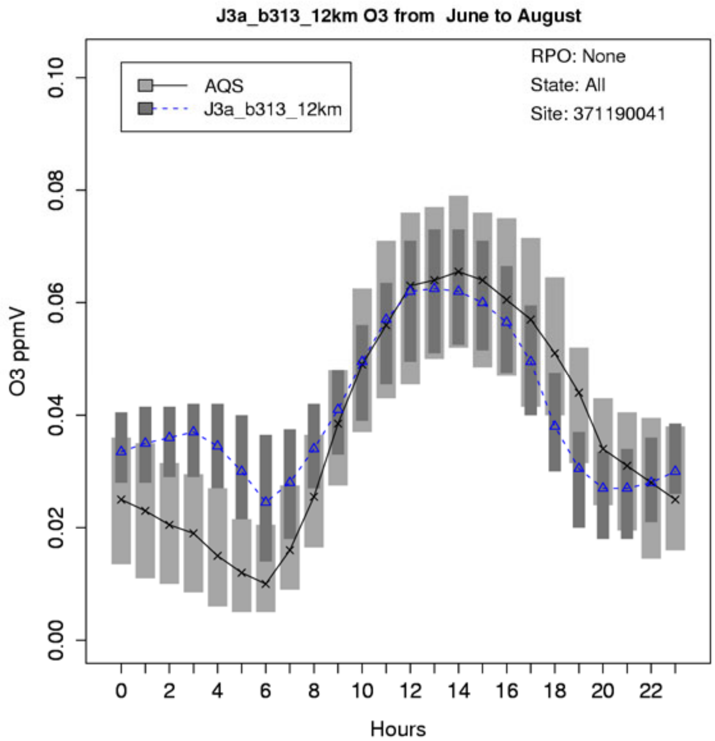
Normalized Mean Error (%) - Summer



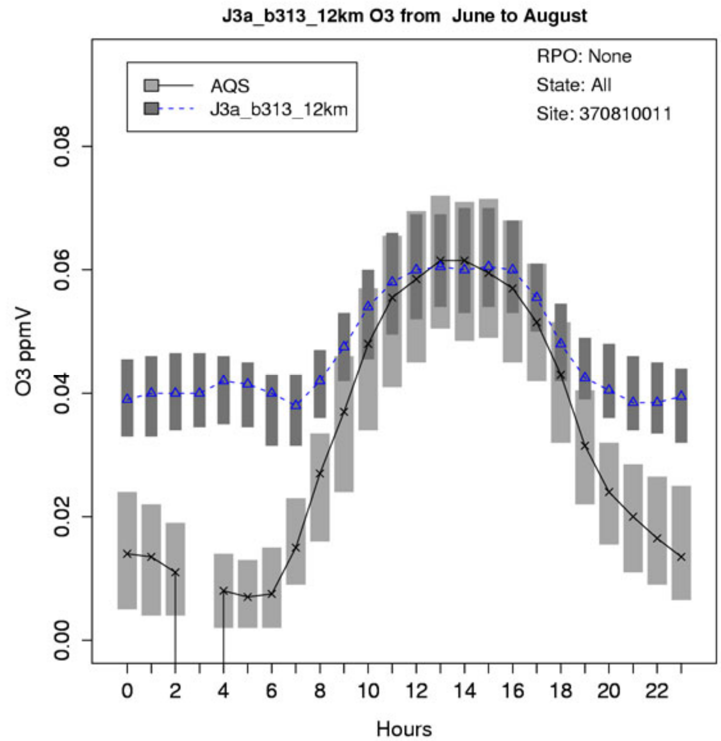
Network	# Obs	Mean Obs	Mean Model	SDEV Obs	SDEV Model	R	RMSE	NMB (%)	NME (%)
AQS 8hr-max	71284	0.052	0.053	0.018	0.013	0.74	0.012	1.62	17.4

AQS Ozone Dirunal Profiles – Urban vs. Rural

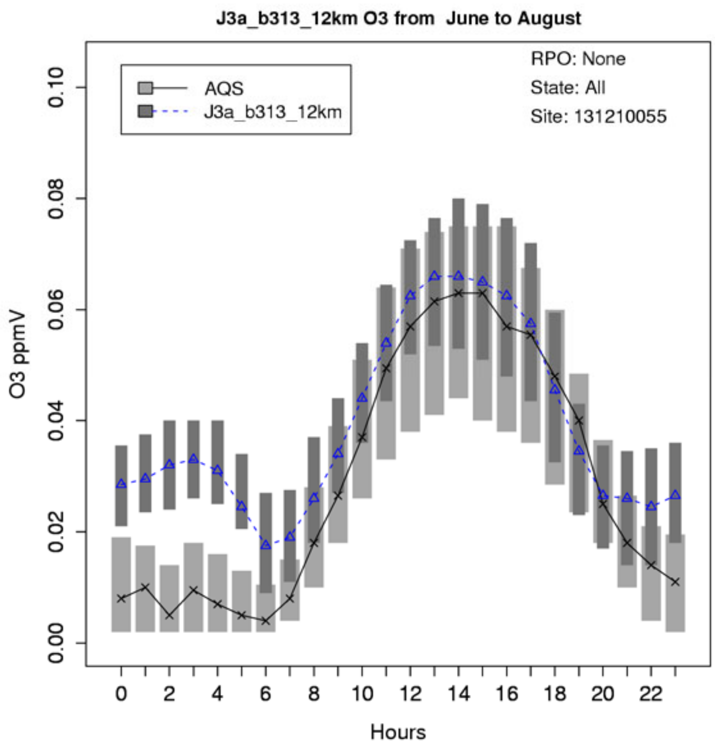
Urban Site (Charlotte, NC)



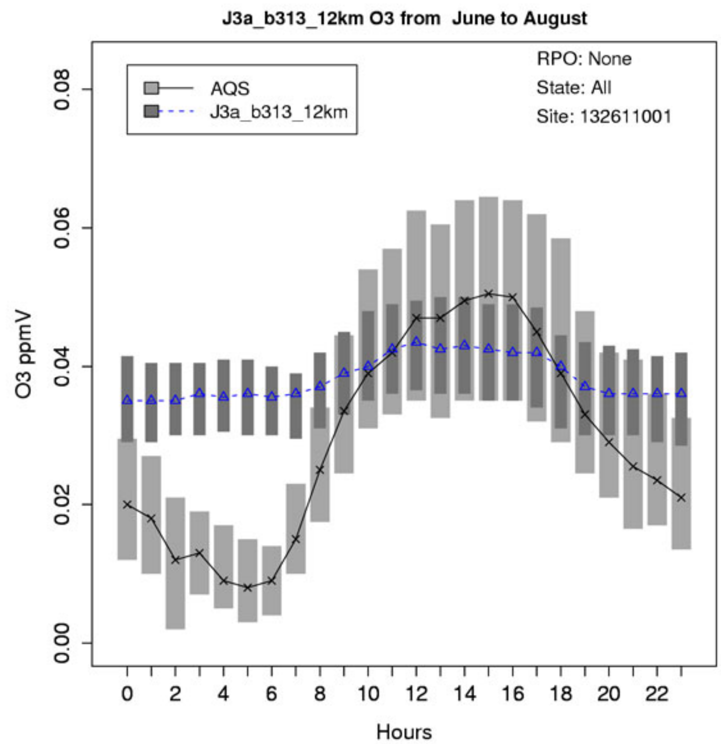
Rural Site (Keely Park, NC)



Sub-urban Site (Atlanta, GA)



Rural Site (Leslie, GA)



Evaluation of CMAQ version 4.5: 12km×12km Eastern United States Inorganic Aerosols: Sulfate (SO_4^{2-}), Nitrate (NO_3^-), Ammonium (NH_4^+), Nitric Acid (HNO_3) and Total Nitrate (TNO_3)

Available Networks and Species:

IMPROVE – Sulfate, Nitrate
STN – Sulfate, Nitrate, Ammonium
CASTNet – Sulfate, Nitrate, Ammonium, Nitric Acid, Total Nitrate

Inorganic Aerosol Performance: Introduction

The list below covers the plots and metrics available for the inorganic aerosol analysis for each of the four seasons (winter, spring, summer, fall):

- Seasonal model to observation scatter plot of various species using all pairs
- Seasonal model to observation scatter plot of various species using monthly averaged pairs
- Seasonal model to observation scatter plot of various species using monthly averaged pairs
- Spatial plots of NMB (%) and NME (%) of various species
- Table of select statistical metrics for various species

Results for the inorganic aerosols sulfate, nitrate, and ammonium as well as related nitric acid and total nitrate (nitric acid and nitrate aerosols) are presented. Where applicable, multiple networks are plotted on each scatter plot and spatial plot. Legends are provided on each plot to help identify each network.

Inorganic Aerosol Performance: Summary

Winter Season (December, January and February)

Sulfate predictions during the winter season are biased low, with NMB values ranging from -28.9 to -1.86%, NME values ranging from 30.7 to 48.0% and correlation values between 0.48 and 0.74. Performance tends to be slightly worse in the Southeast and Great Lakes regions when compared to the rest of the domain. Nitrate is generally over-predicted for the winter season, with NMB values ranging from 2.38 to 17.0%, NME values ranging from 47.2 to 107% and correlation values between 0.65 and 0.76. Nitrate performance tends to be worse in the Northeast and Southeast. Ammonium performance varies between STN and CASTNet, with STN showing a positive NMB of 28.5% (NME = 60.7%) and CASTNet showing a negative NMB of -12.1% (NME = 26.5%). Nitric Acid for the winter season was slightly over-predicted for CASTNet, with a NMB of 11.6% and NME of 46.8%. Total nitrate was slightly over-predicted for CASTNet, with a NMB of 6.38% and NME of 27.2%.

Spring Season (March, April and May)

Sulfate predictions during the spring season are also biased low, with NMB values ranging from -18.4 to 8.21%, NME values ranging from 24.8 to 38.3% and correlation values between 0.63 and 0.85. Sulfate performance tends to be slightly worse in the Northeast region when compared to the rest of the domain. Nitrate is slightly over-predicted at STN and CASTNet sites, with a larger over-prediction at IMPROVE sites for the spring season. NMB values range from 4.23 to 22.5%, NME values range from 59.2 to 90.0% and correlation values range from 0.65 to 0.74. Ammonium predictions for the spring season were similar to that of the winter season, with STN showing a positive NMB of 17.8% (NME = 51.6%) and CASTNet showing a small negative NMB of -4.3% (NME = 24.9%). Ammonium performance was slightly worse in the Northeast region when compared to the rest of the domain. Nitric Acid for the spring season was only slightly under-predicted for CASTNet, with a NMB of -2.73% and NME of 36.4%. Total nitrate for the spring season was nearly unbiased for CASTNet, with a NMB of 1.98% and NME of 25.6%. Total nitrate was nearly unbiased due to small compensating biases in nitrate (positive bias) and nitric acid (negative bias) for the spring season.

Summer Season (June, July and August)

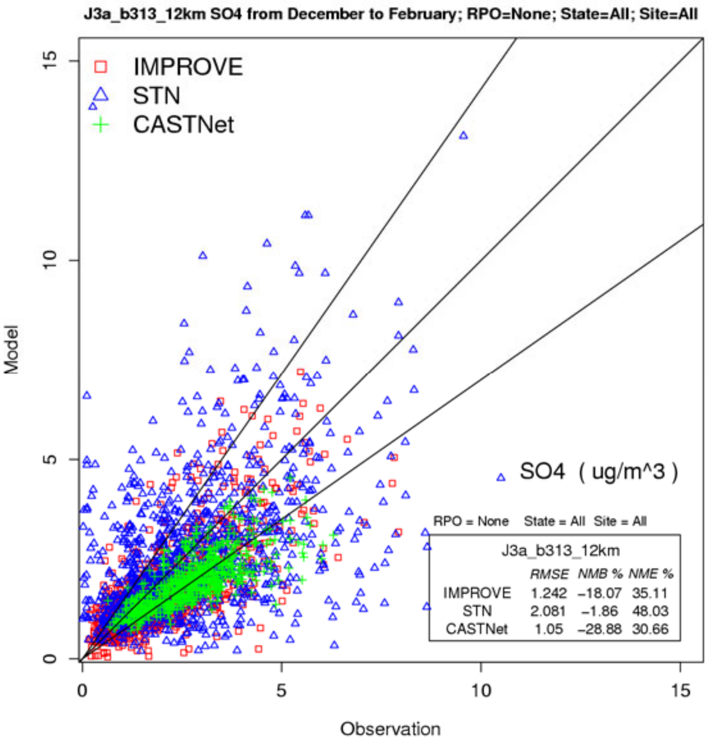
Sulfate predictions during the summer season are nearly unbiased, with NMB values ranging from -0.31 to 12.1%, NME values ranging from 18.9 to 42.2% and correlation values between 0.78 and 0.89. Performance along the Gulf coast tends to be worse when compared to the rest of the domain. Mean nitrate concentrations during the summer season are relatively low when compared to the other seasons. Nitrate concentrations tend to be under-predicted for the summer season, with NMB values ranging from -25.5 to -40.3%, NME values ranging from 83.9 to 95.8% and correlation values between 0.25 and 0.32. Ammonium predictions for the summer season were mixed between STN and CASTNet, with a small positive NMB of 8.02% (NME = 47.5%) at STN sites and a larger negative NMB of 19.0% (NME = 28.2%) at CASTNet sites. Previous studies of the ammonia emission seasonality suggest that the ammonia emissions in the summer are too low, which may be contributing to these differences. Nitric Acid was significantly over-predicted during the summer season, with a NMB of 34.1% and a NME of 43.8%. Total nitrate is over-predicted for the summer season, with a NMB of 25.9% and NME of 34.7%. Over-predictions of total nitrate are dominated by a significant over-prediction in nitric acid for the summer. While nitrate is also over-predicted, the mean concentration of nitrate is much smaller than that of nitric acid.

Fall Season (September, October and November)

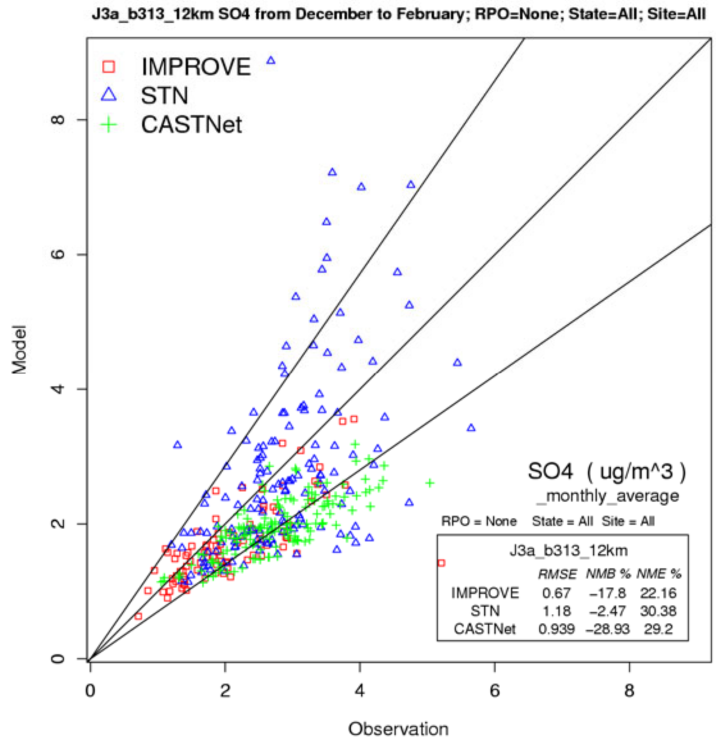
Sulfate predictions during the fall season are biased high, with NMB values ranging from 11.6 to 27.4%, NME values ranging from 20.2 to 50.3% and correlation values between 0.77 and 0.91. Performance along the Mid-Atlantic coast tends to be worse when compared to the rest of the domain. Nitrate concentrations are over-predicted for the fall season, with NMB values between 46.8 and 85.7%, NME values between 84.5 and 138% and correlation values between 0.61 and 0.68. Nitrate concentrations at sites along the coast tend to be biased low, while the majority of inland sites are biased high. Ammonium predictions for the fall season were high, with NMB values for STN and CASTNet of 90.1% (NME=109.4%) and 27.2% (NME = 43.1%) respectively. This may be related to ammonia emissions being too high in the fall. Nitric Acid for the fall season was significantly over-predicted, with a NMB of 49.8% and NME of 62.9%. Total nitrate for the fall season is significantly over-predicted, with a NMB of 48.8% and NME of 53.2%. The over-prediction of total nitrate is driven by significant over-predictions in both nitrate and nitric acid for the fall.

SO_4^{2-} - Winter

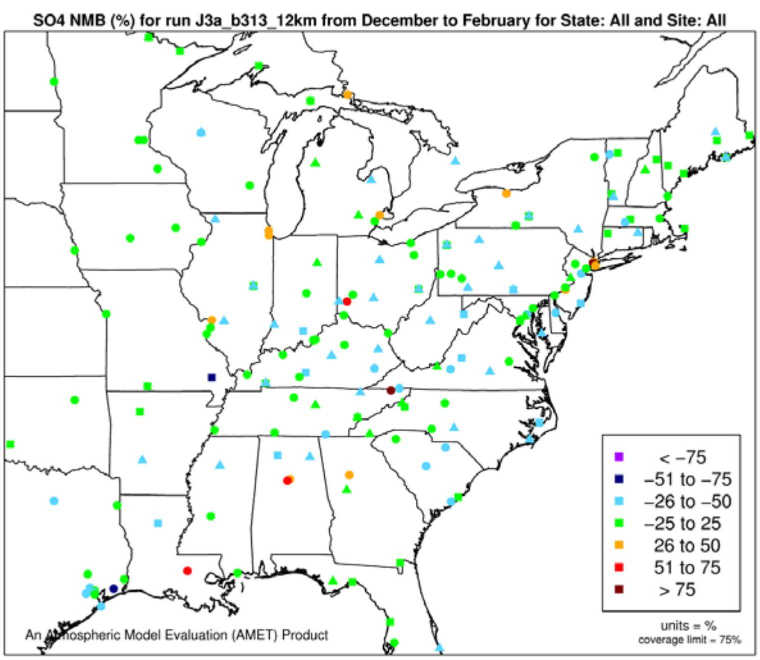
Scatter Plot – All Pairs



Scatter Plot – Monthly Average Pairs

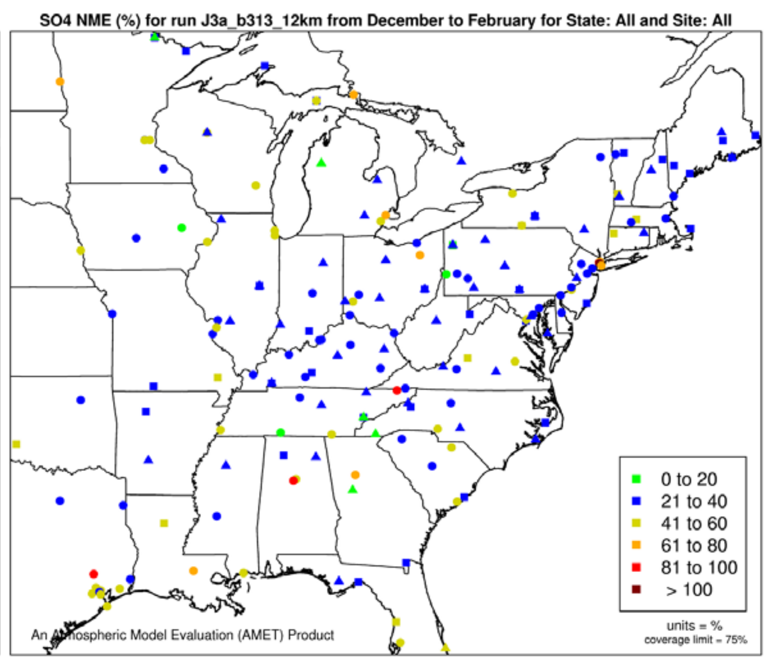


Normalized Mean Bias (%) - Winter



square=IMPROVE; circle=STN; triangle=CASTNet;

Normalized Mean Error (%) - Winter

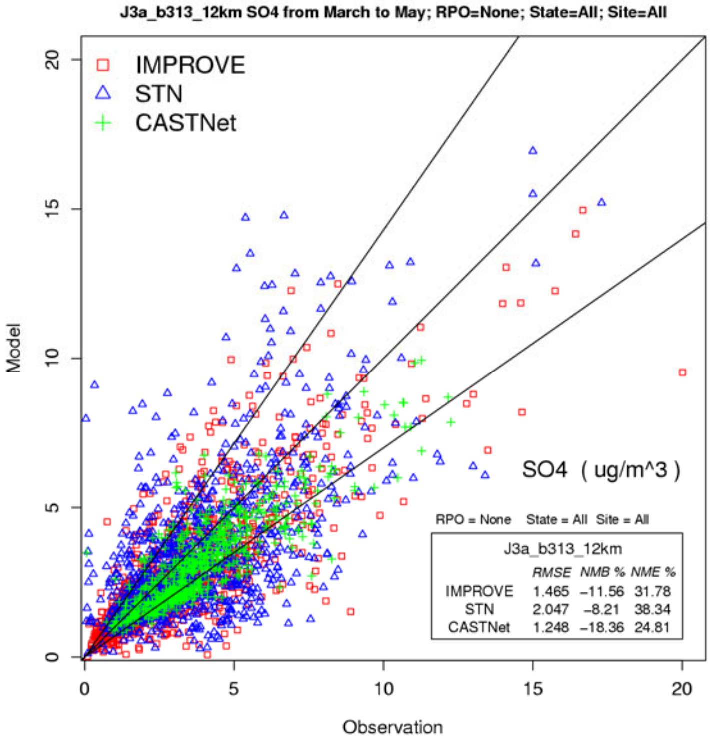


square=IMPROVE; circle=STN; triangle=CASTNet;

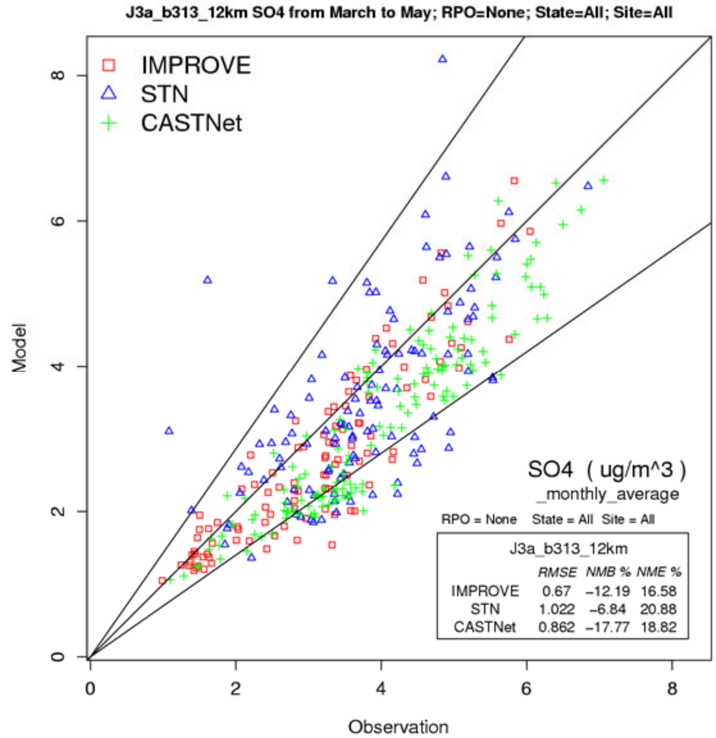
Network	# Obs	Mean Obs	Mean Model	SDEV Obs	SDEV Model	R	RMSE	NMB (%)	NME (%)
IMPROVE	929	2.08	1.70	1.49	1.12	0.62	1.24	-18.1	35.1
STN	1051	2.77	2.72	1.76	2.24	0.48	2.08	-1.86	48.0
CASTNet	589	2.75	1.95	1.01	0.66	0.74	1.05	-28.9	30.7

SO_4^{2-} - Spring

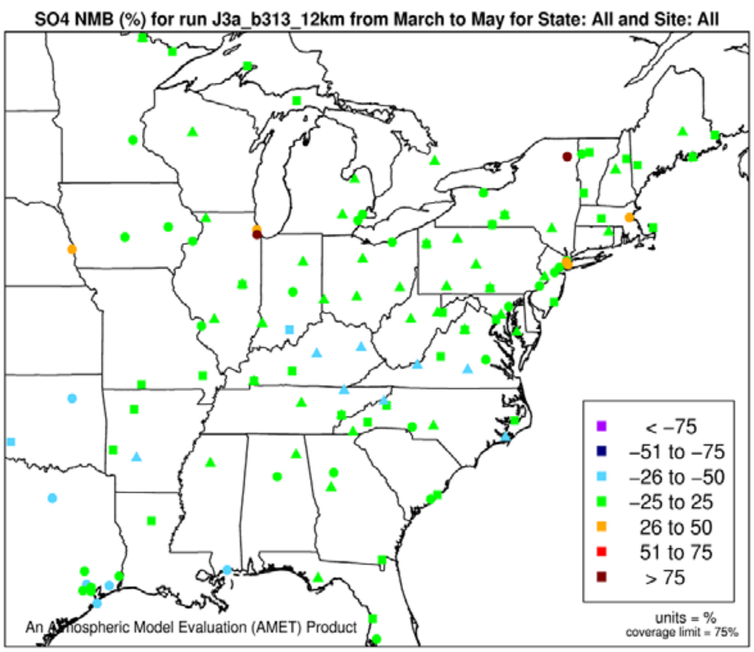
Scatter Plot – All Pairs



Scatter Plot – Monthly Average Pairs



Normalized Mean Bias (%) - Spring



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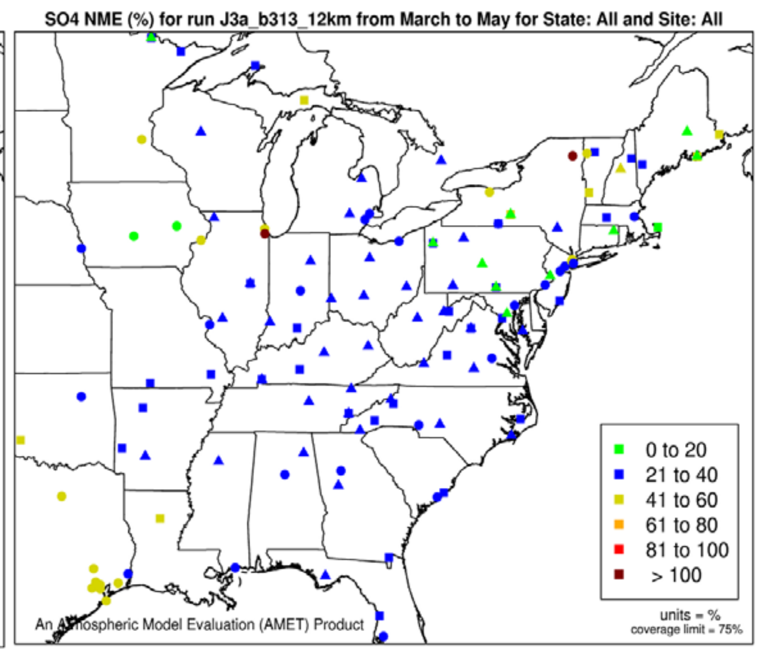
Normalized Mean Error (%) - Spring

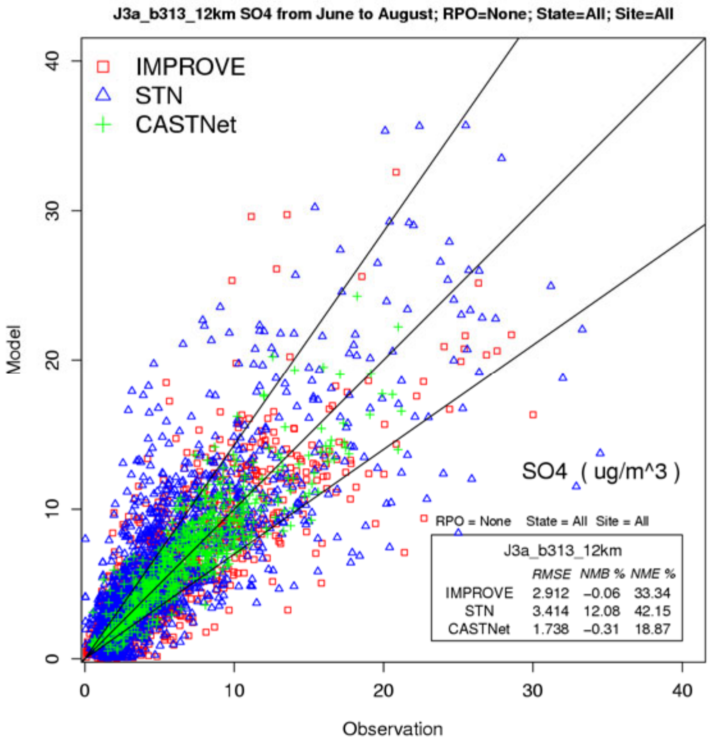


square=IMPROVE; circle=STN; triangle=CASTNet;

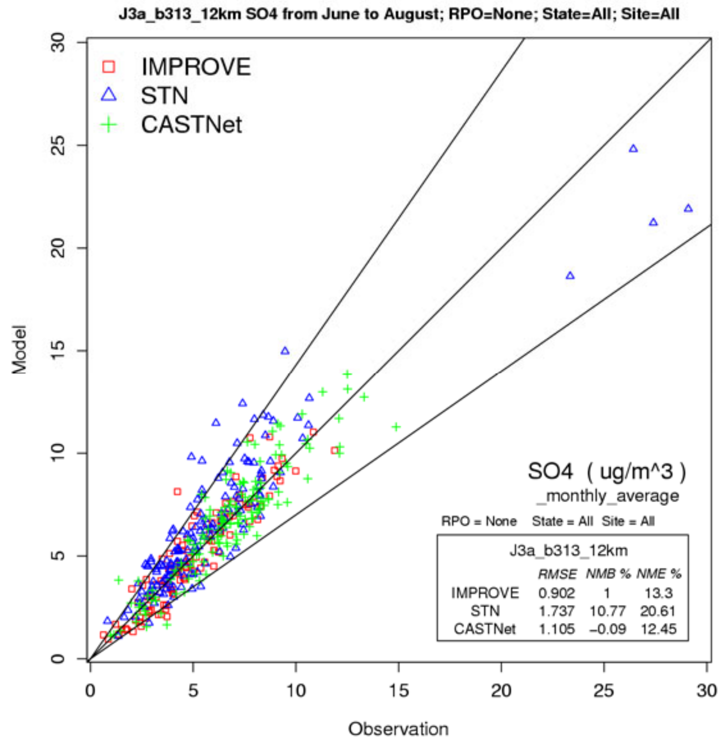
Network	# Obs	Mean Obs	Mean Model	SDEV Obs	SDEV Model	R	RMSE	NMB (%)	NME (%)
IMPROVE	1134	3.12	2.76	2.36	2.10	0.80	1.47	-11.6	31.8
STN	984	3.83	3.52	2.28	2.42	0.63	2.05	-8.21	38.3
CASTNet	623	3.87	3.16	1.91	1.55	0.85	1.25	-18.4	24.8

SO_4^{2-} - Summer

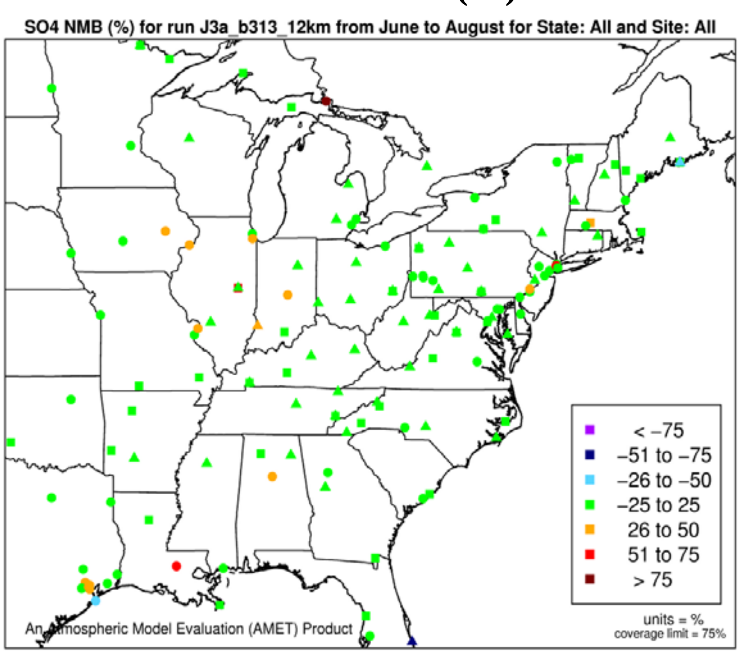
Scatter Plot – All Pairs



Scatter Plot – Monthly Average Pairs

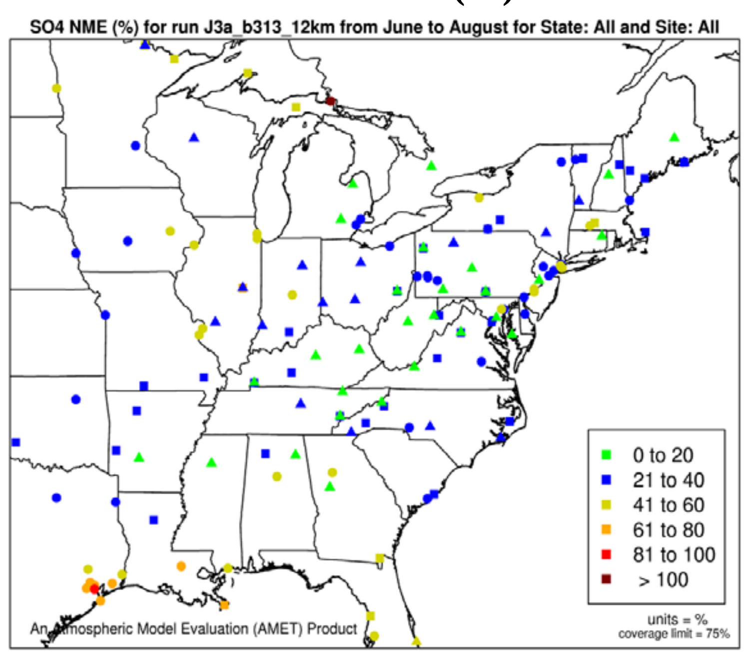


Normalized Mean Bias (%) - Summer



square=IMPROVE; circle=STN; triangle=CASTNet;

Normalized Mean Error (%) - Summer

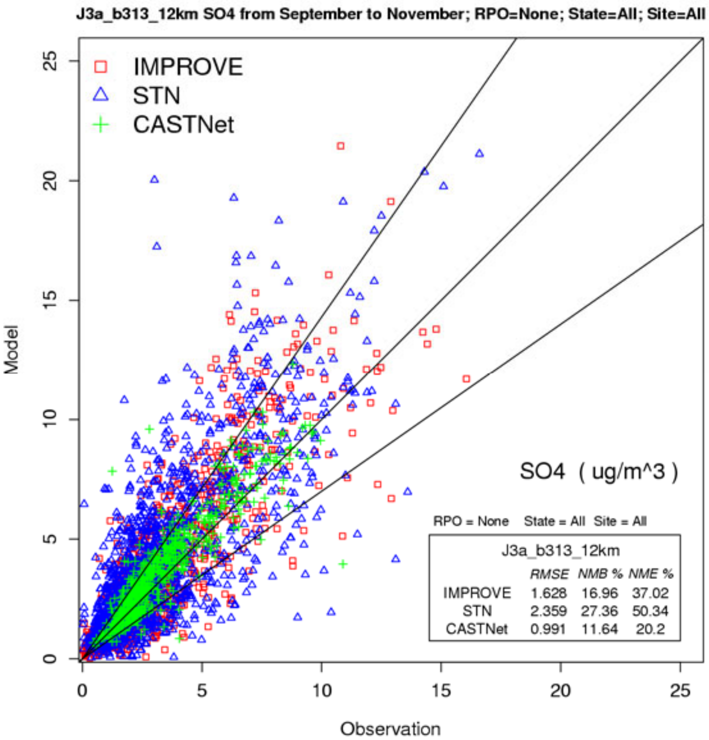


square=IMPROVE; circle=STN; triangle=CASTNet;

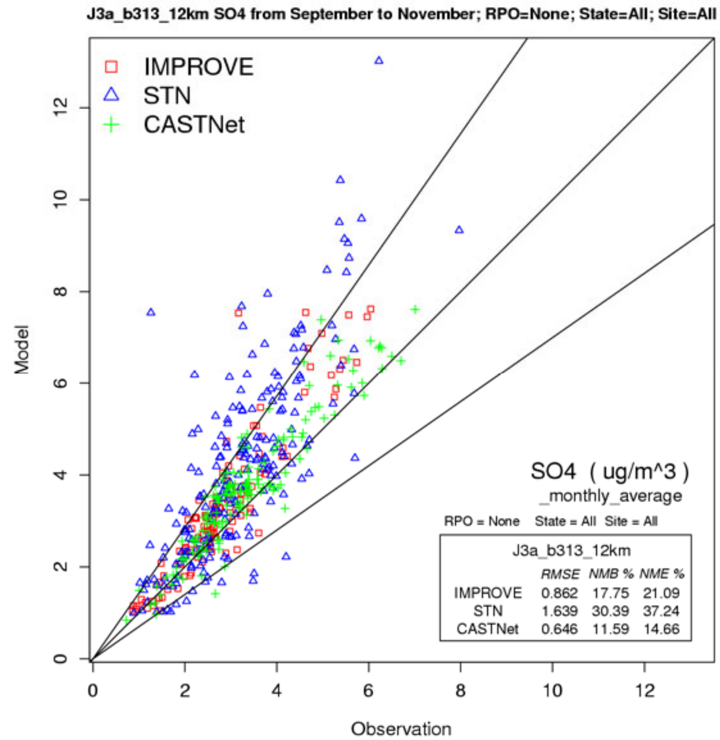
Network	# Obs	Mean Obs	Mean Model	SDEV Obs	SDEV Model	R	RMSE	NMB (%)	NME (%)
IMPROVE	1216	5.23	5.23	4.85	4.60	0.81	2.91	-0.06	33.3
STN	1632	5.46	6.12	4.91	5.20	0.78	3.41	12.1	42.2
CASTNet	652	6.70	6.68	3.74	3.67	0.89	1.74	-0.31	18.9

SO_4^{2-} - Fall

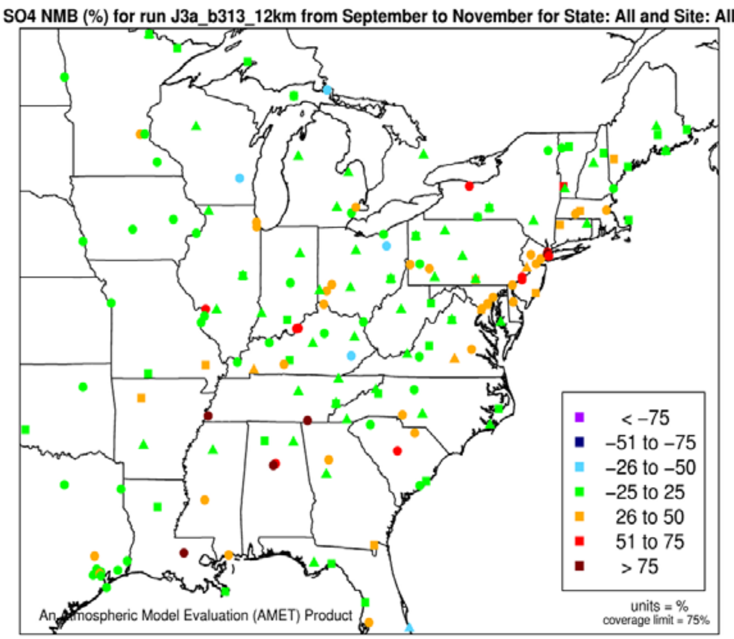
Scatter Plot – All Pairs



Scatter Plot – Monthly Average Pairs

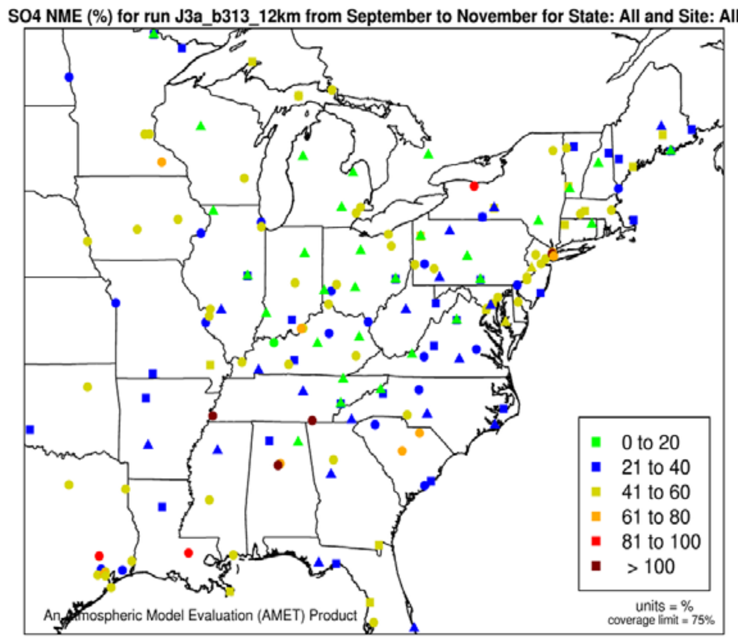


Normalized Mean Bias (%) – Fall



square=IMPROVE; circle=STN; triangle=CASTNet;

Normalized Mean Error (%) - Fall

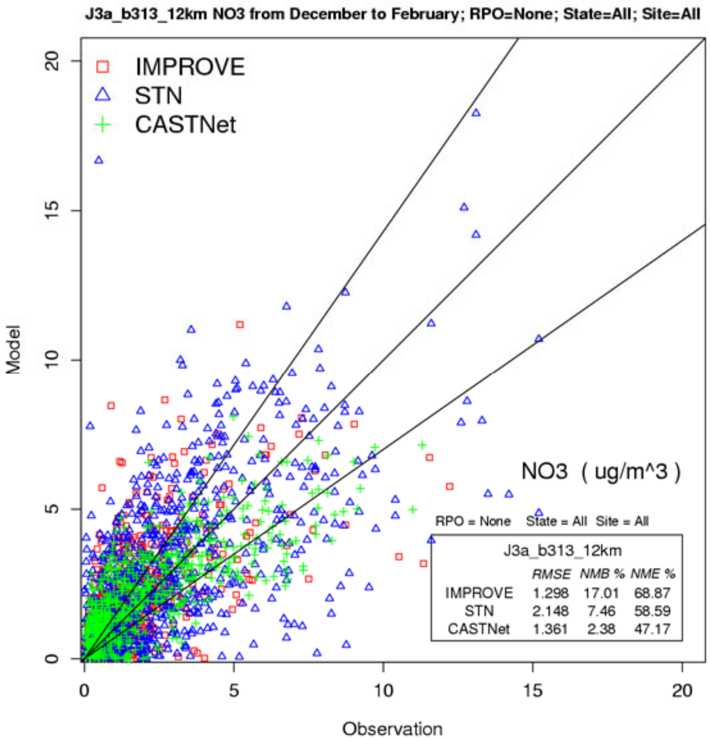


square=IMPROVE; circle=STN; triangle=CASTNet;

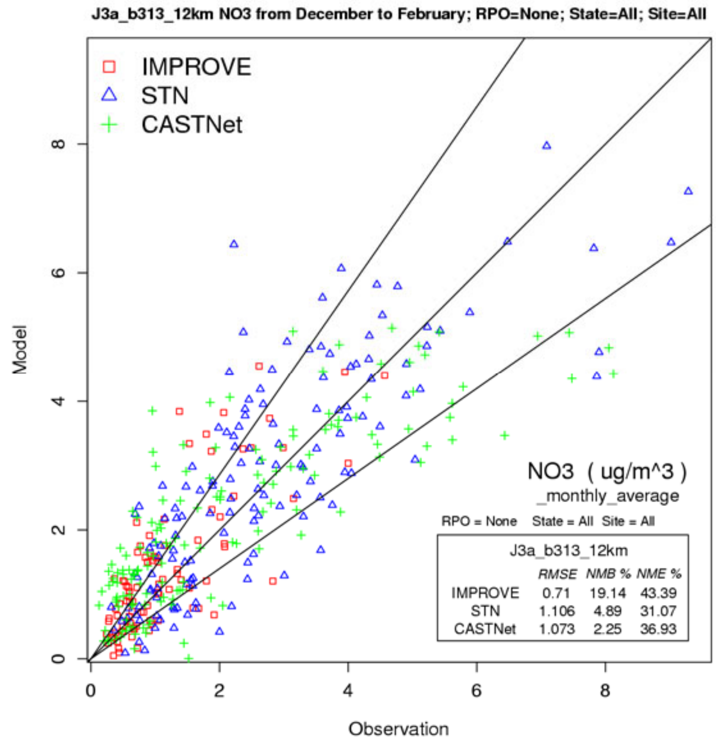
Network	# Obs	Mean Obs	Mean Model	SDEV Obs	SDEV Model	R	RMSE	NMB (%)	NME (%)
IMPROVE	1321	2.83	3.31	2.43	3.08	0.87	1.63	17.0	37.0
STN	1588	3.18	4.05	2.55	3.44	0.77	2.36	27.4	50.3
CASTNet	611	3.39	3.78	1.93	2.16	0.91	0.99	11.6	20.2

NO_3 – Winter

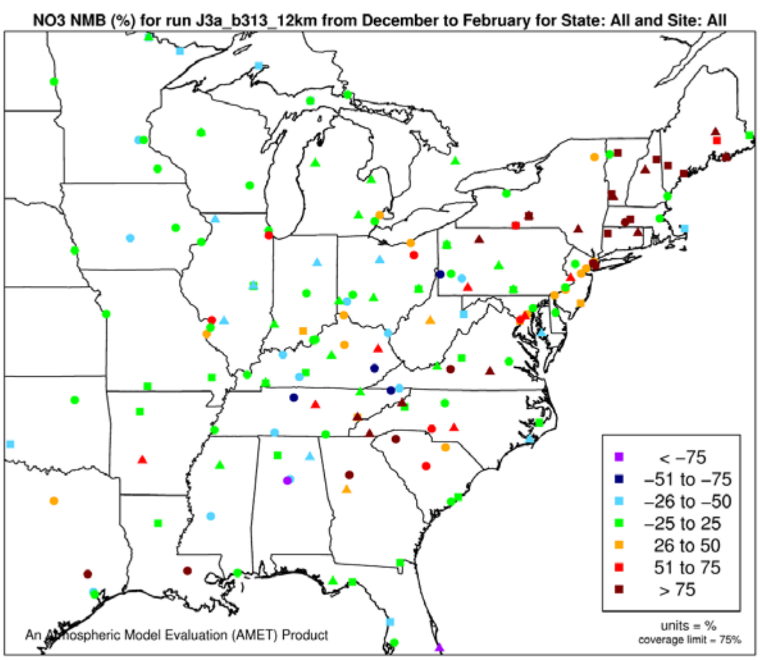
Scatter Plot – All Pairs



Scatter Plot – Monthly Average Pairs

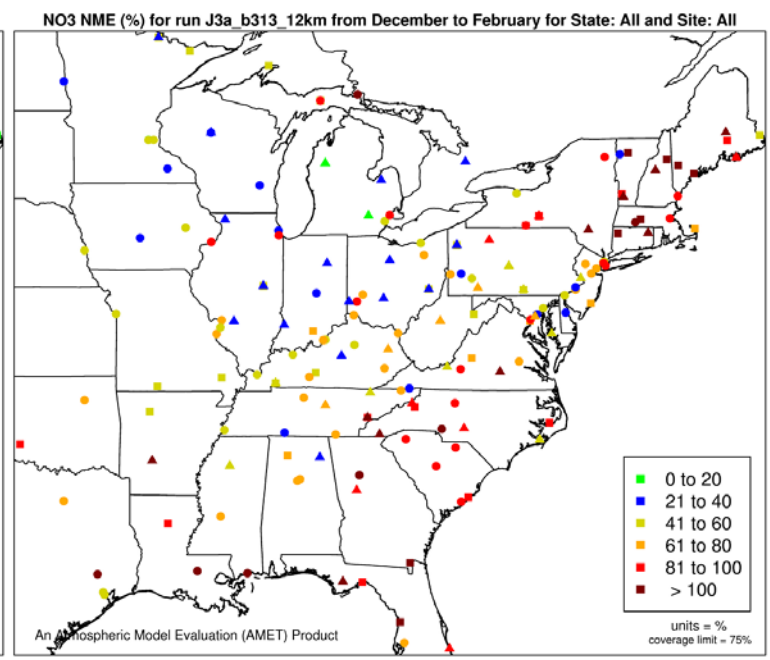


Normalized Mean Bias (%) – Winter



square=IMPROVE; circle=STN; triangle=CASTNet;

Normalized Mean Error (%) - Winter

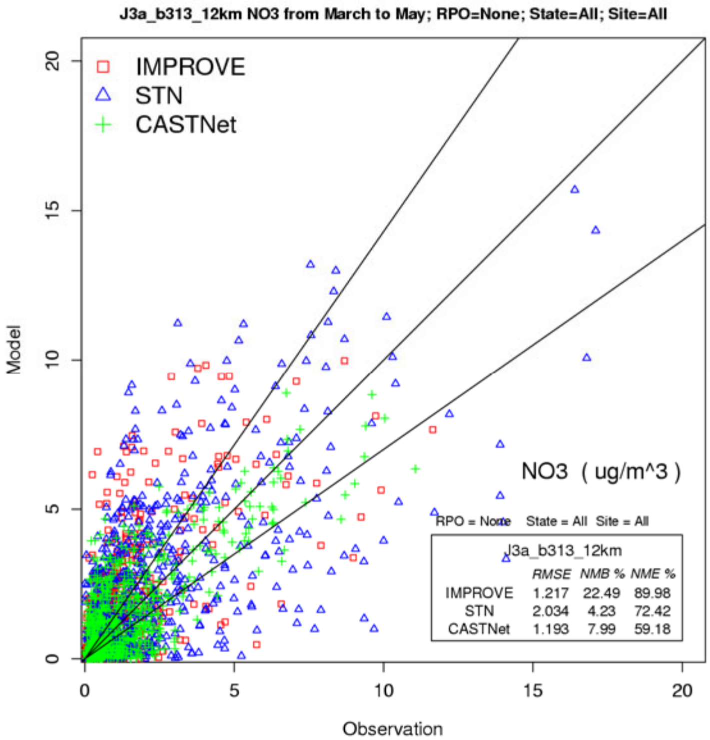


square=IMPROVE; circle=STN; triangle=CASTNet;

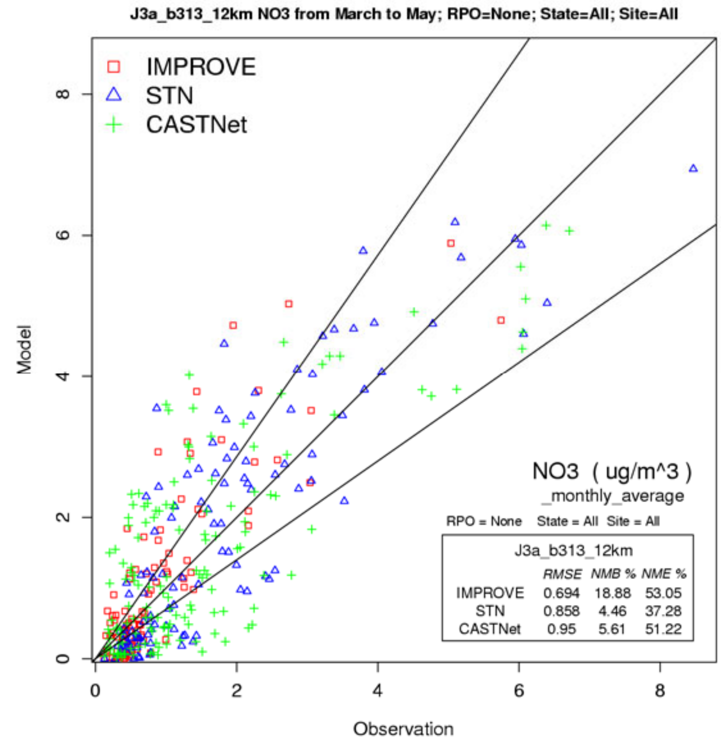
Network	# Obs	Mean Obs	Mean Model	SDEV Obs	SDEV Model	R	RMSE	NMB (%)	NME (%)
IMPROVE	926	1.19	1.39	1.47	1.66	0.67	1.30	17.0	107
STN	962	2.53	2.73	2.47	2.62	0.65	2.15	7.46	58.6
CASTNet	5.88	2.15	2.20	2.08	1.56	0.76	1.36	2.38	47.2

NO_3 – Spring

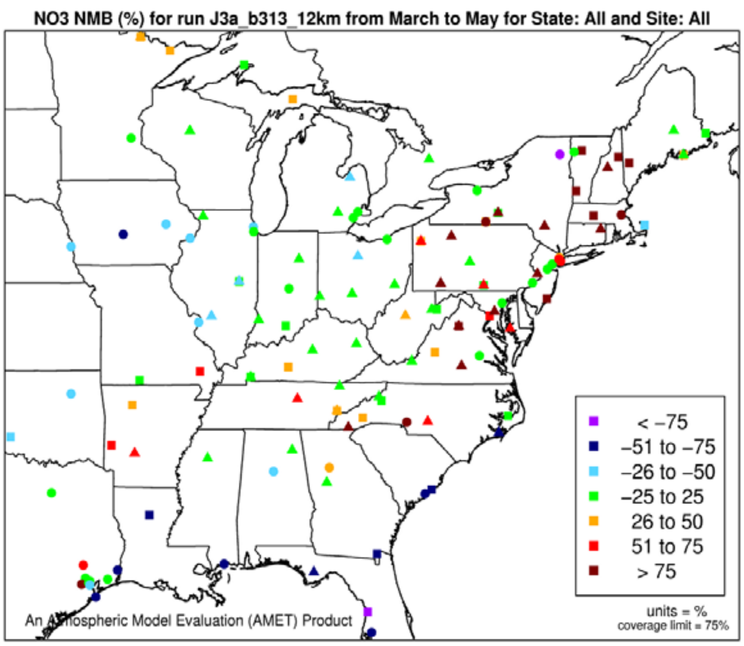
Scatter Plot – All Pairs



Scatter Plot – Monthly Average Pairs

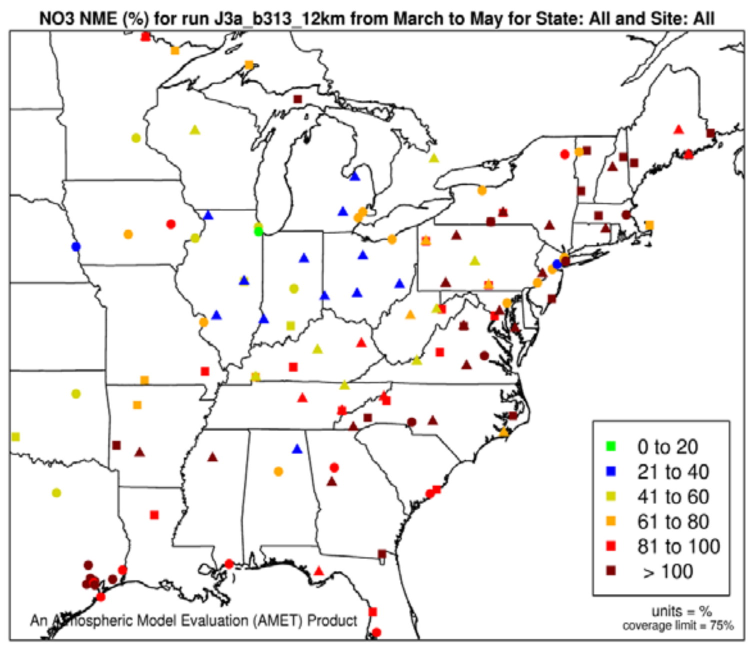


Normalized Mean Bias (%) – Spring



square=IMPROVE; circle=STN; triangle=CASTNet;

Normalized Mean Error (%) - Spring

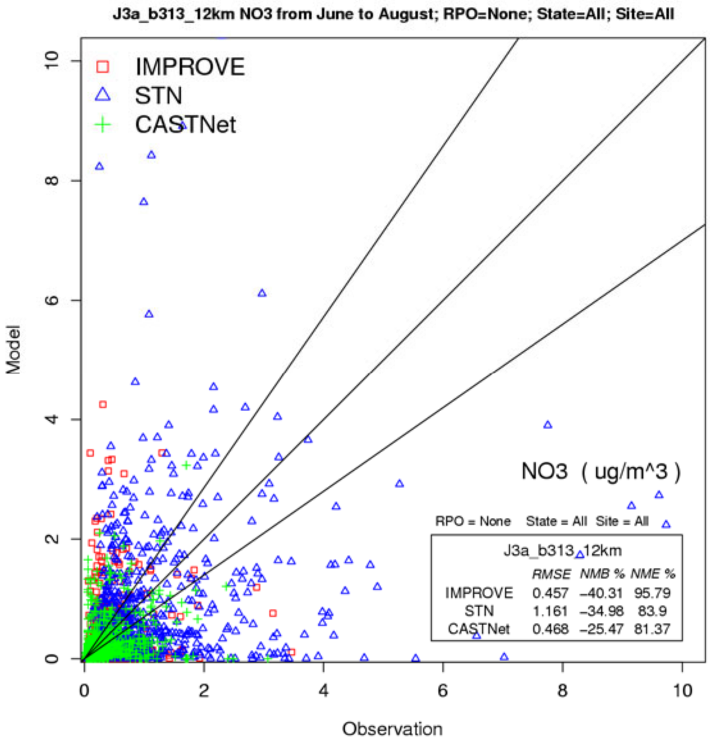


square=IMPROVE; circle=STN; triangle=CASTNet;

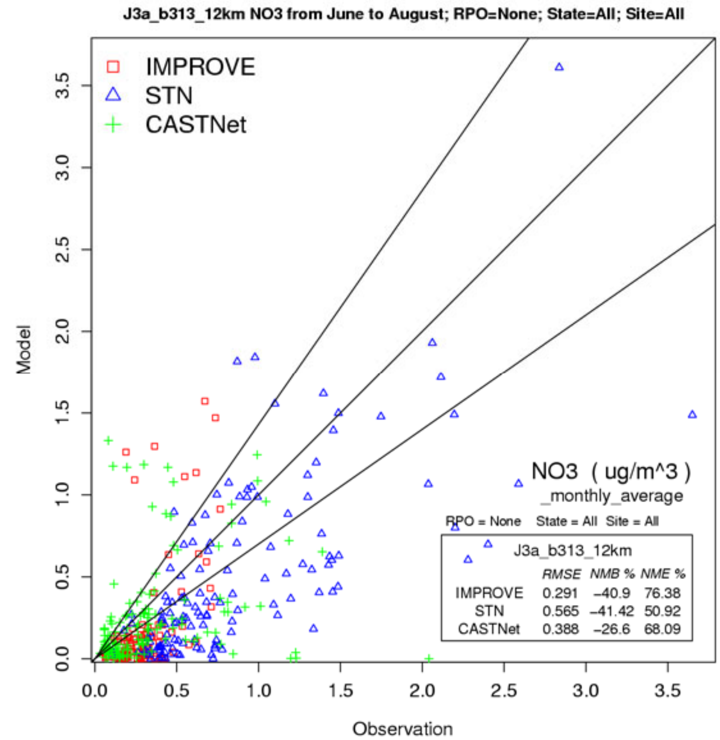
Network	# Obs	Mean Obs	Mean Model	SDEV Obs	SDEV Model	R	RMSE	NMB (%)	NME (%)
IMPROVE	1131	0.81	0.99	1.19	1.64	0.68	1.22	22.5	90.0
STN	983	1.75	1.82	2.42	2.41	0.65	2.03	4.23	72.4
CASTNet	623	1.50	1.62	1.69	1.63	0.74	1.19	7.99	59.2

NO_3 – Summer

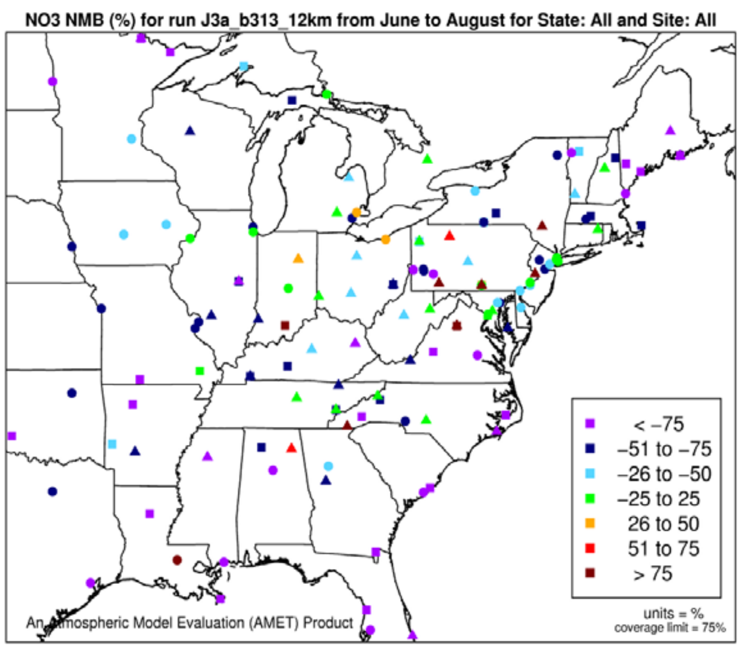
Scatter Plot – All Pairs



Scatter Plot – Monthly Average Pairs

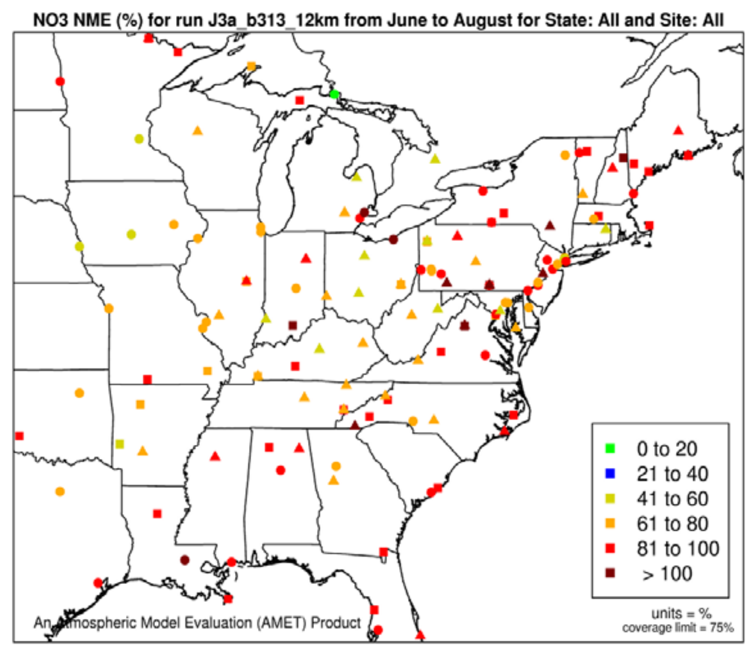


Normalized Mean Bias (%) – Summer



square=IMPROVE; circle=STN; triangle=CASTNet;

Normalized Mean Error (%) - Summer

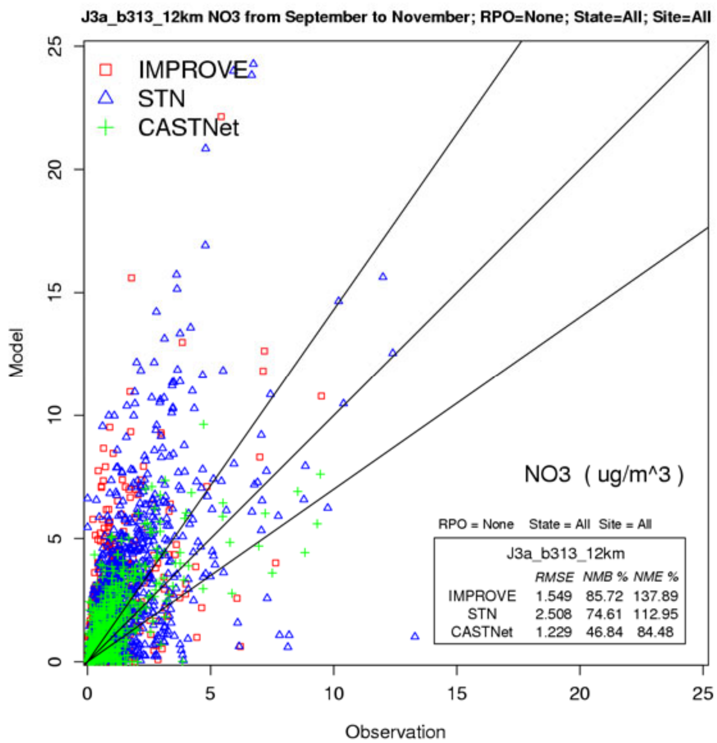


square=IMPROVE; circle=STN; triangle=CASTNet;

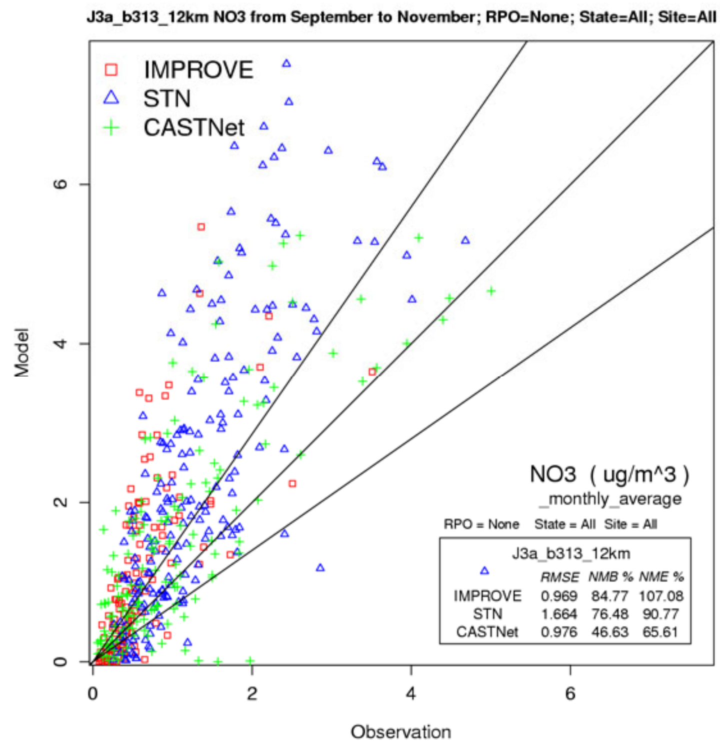
Network	# Obs	Mean Obs	Mean Model	SDEV Obs	SDEV Model	R	RMSE	NMB (%)	NME (%)
IMPROVE	1206	0.30	0.18	0.28	0.42	0.25	0.46	-40.3	95.8
STN	1238	0.80	0.52	0.94	0.98	0.32	1.16	-35.0	83.9
CASTNet	652	0.35	0.26	0.40	0.38	0.28	0.47	-25.5	81.4

NO_3 – Fall

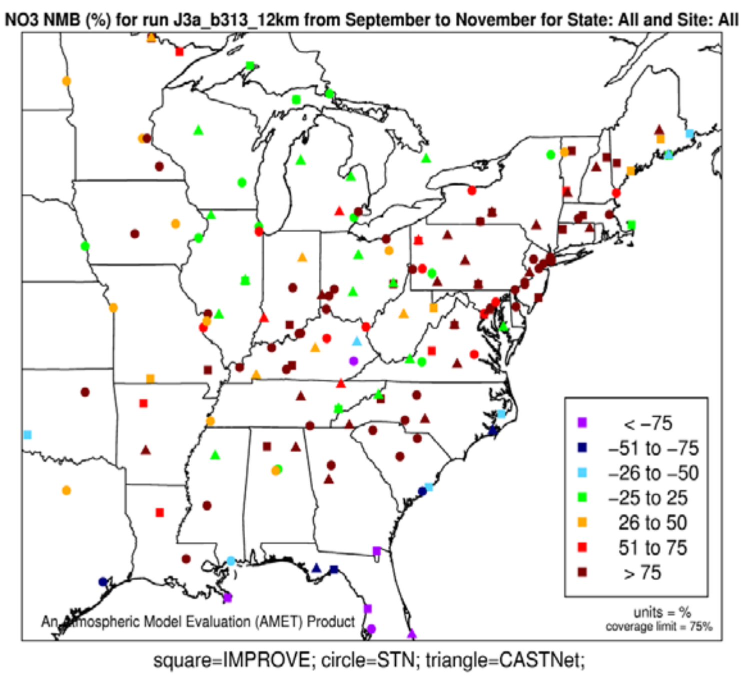
Scatter Plot – All Pairs



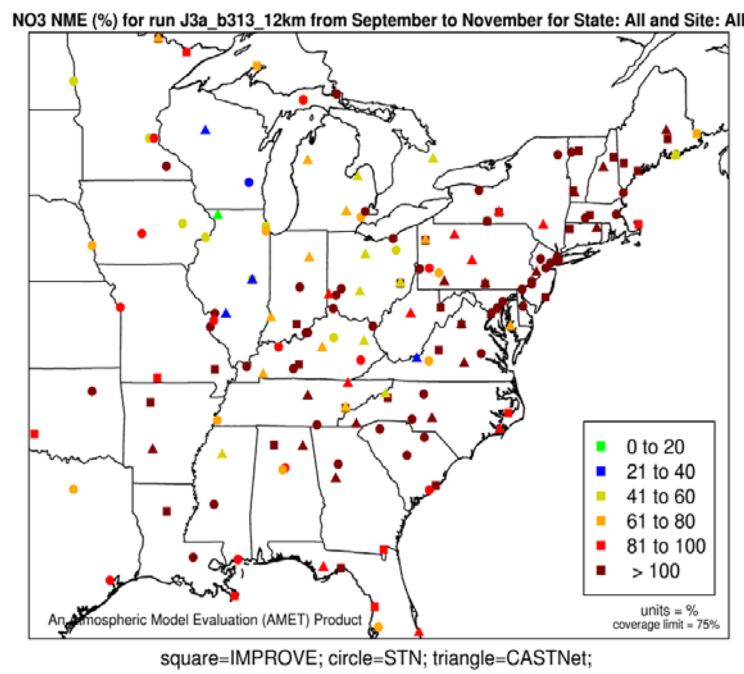
Scatter Plot – Monthly Average Pairs



Normalized Mean Bias (%) – Fall



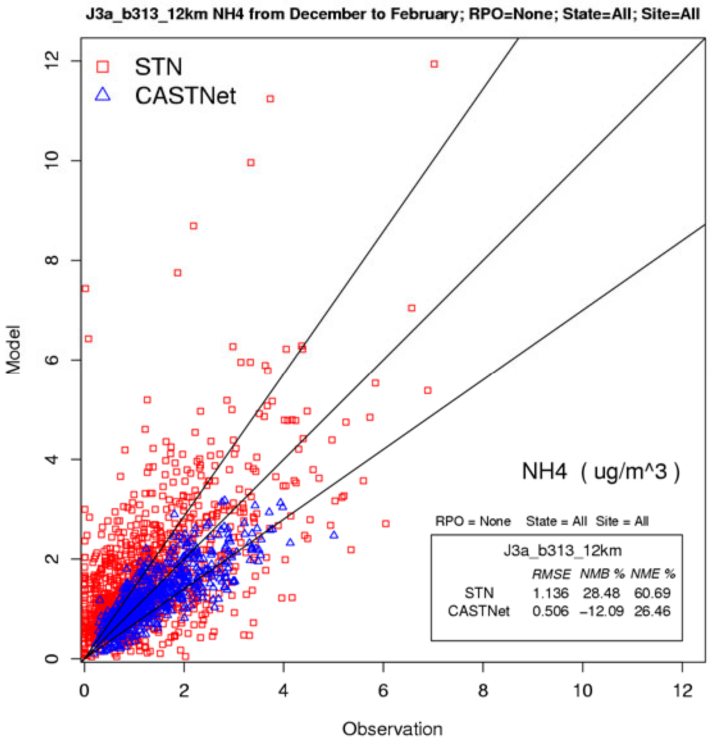
Normalized Mean Error (%) - Fall



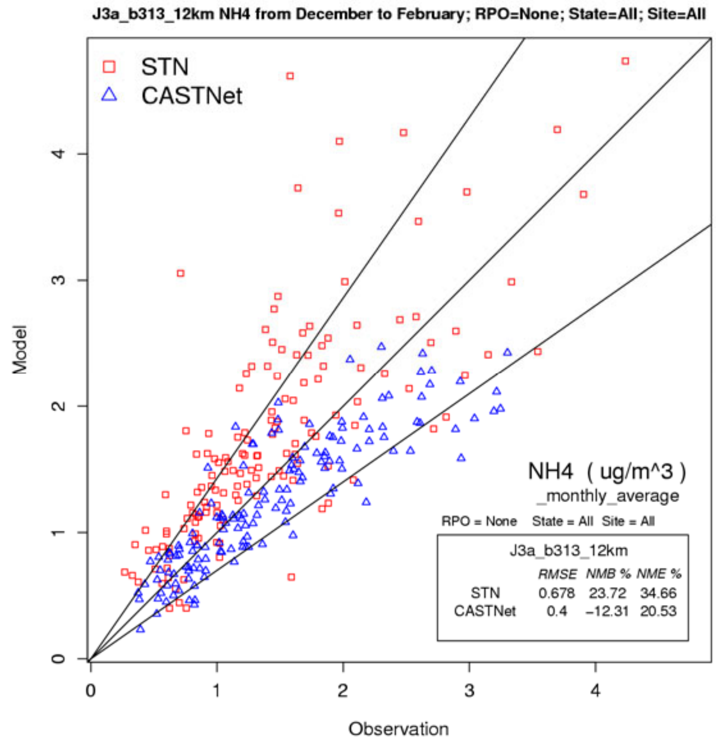
Network	# Obs	Mean Obs	Mean Model	SDEV Obs	SDEV Model	R	RMSE	NMB (%)	NME (%)
IMPROVE	1321	0.57	1.06	0.80	1.82	0.61	1.55	85.7	138
STN	1319	1.33	2.32	1.44	2.90	0.61	2.51	74.6	113
CASTNet	611	1.02	1.49	1.20	1.52	0.68	1.23	46.8	84.5

NH_4 – Winter

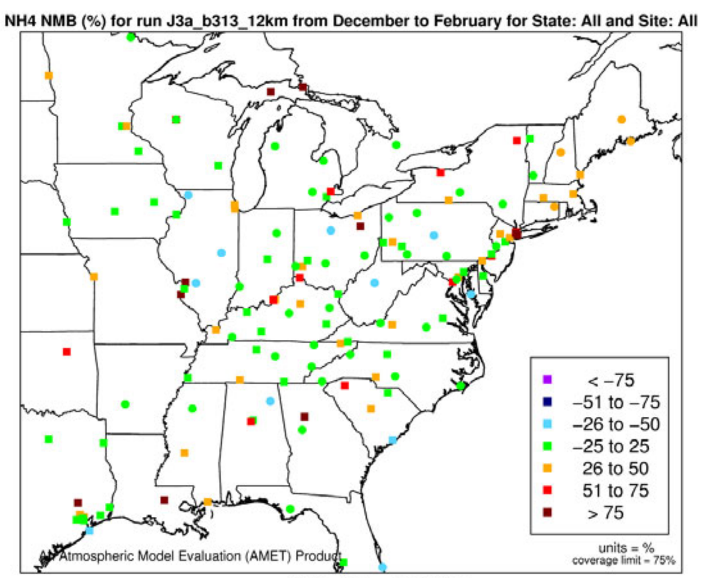
Scatter Plot – All Pairs



Scatter Plot – Monthly Average Pairs

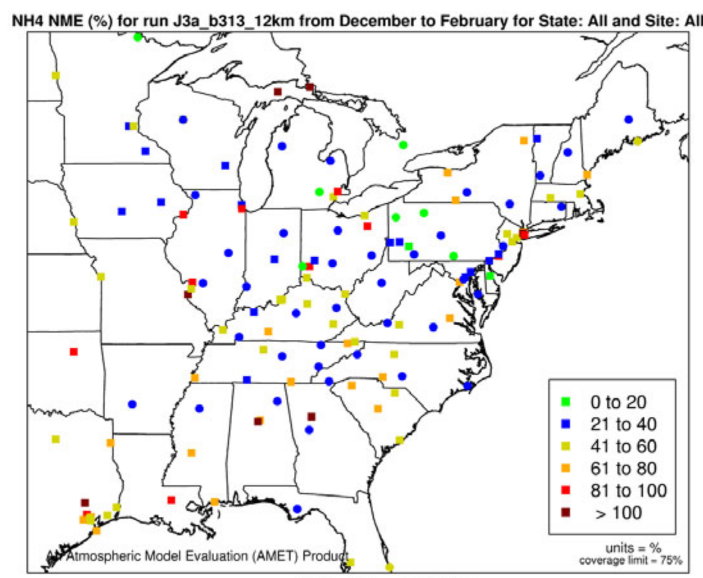


Normalized Mean Bias (%) – Winter



square=STN; circle=CASTNet;

Normalized Mean Error (%) - Winter

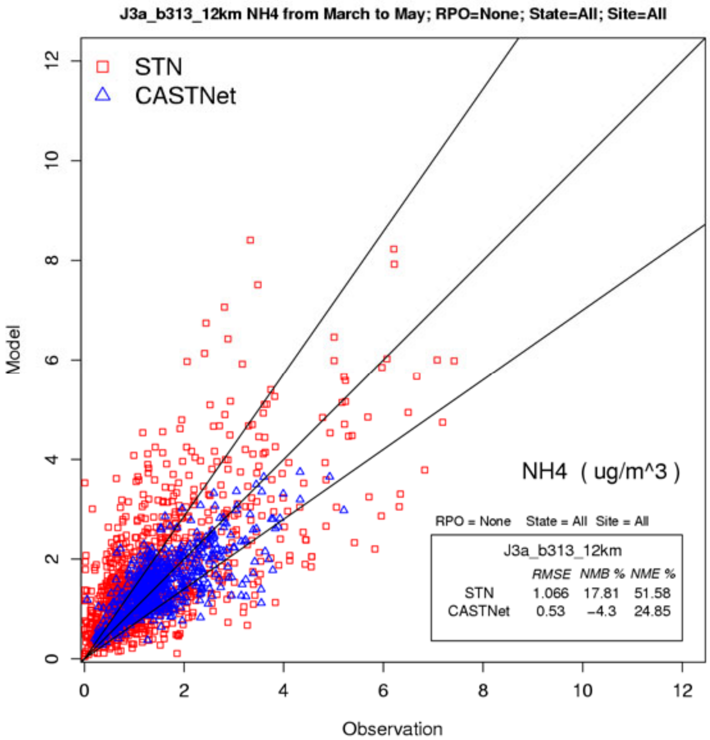


square=STN; circle=CASTNet;

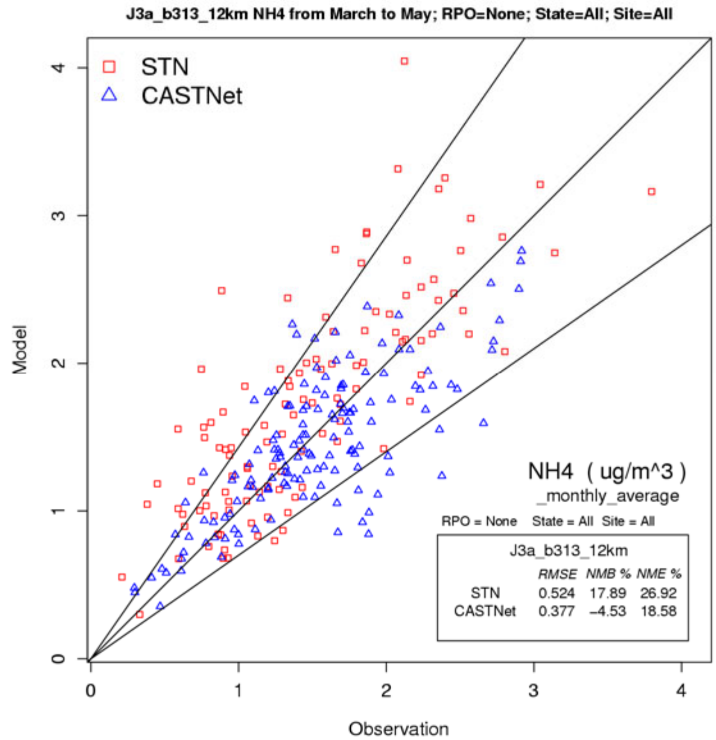
Network	# Obs	Mean Obs	Mean Model	SDEV Obs	SDEV Model	R	RMSE	NMB (%)	NME (%)
STN	1051	1.31	1.69	1.12	1.33	0.63	1.34	28.5	60.7
CASTNet	589	1.43	1.25	0.80	0.60	0.81	0.51	-12.1	26.5

NH_4 - Spring

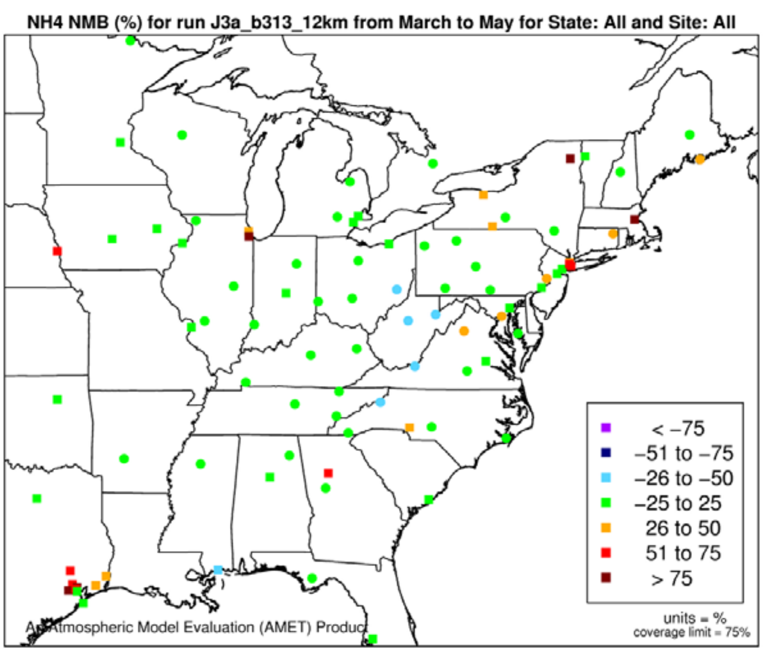
Scatter Plot – All Pairs



Scatter Plot – Monthly Average Pairs

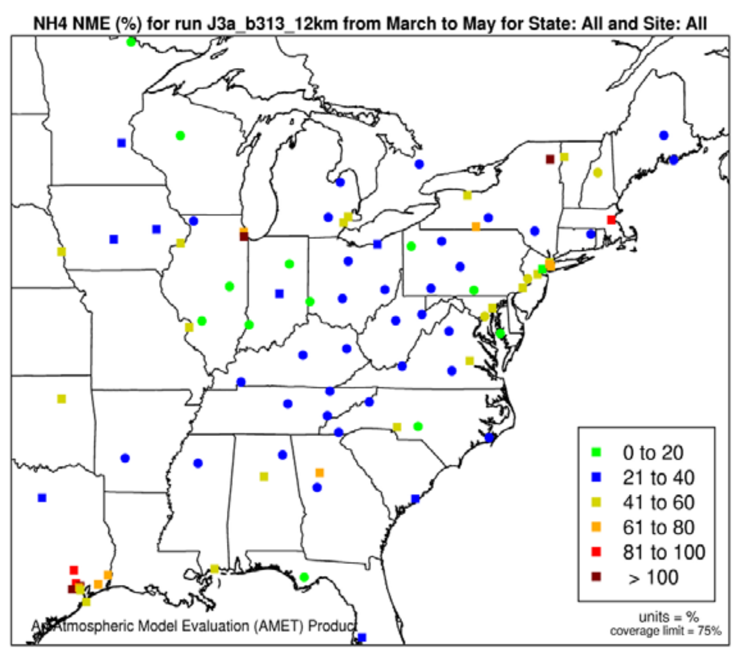


Normalized Mean Bias (%) –Spring



square=STN; circle=CASTNet;

Normalized Mean Error (%) - Spring

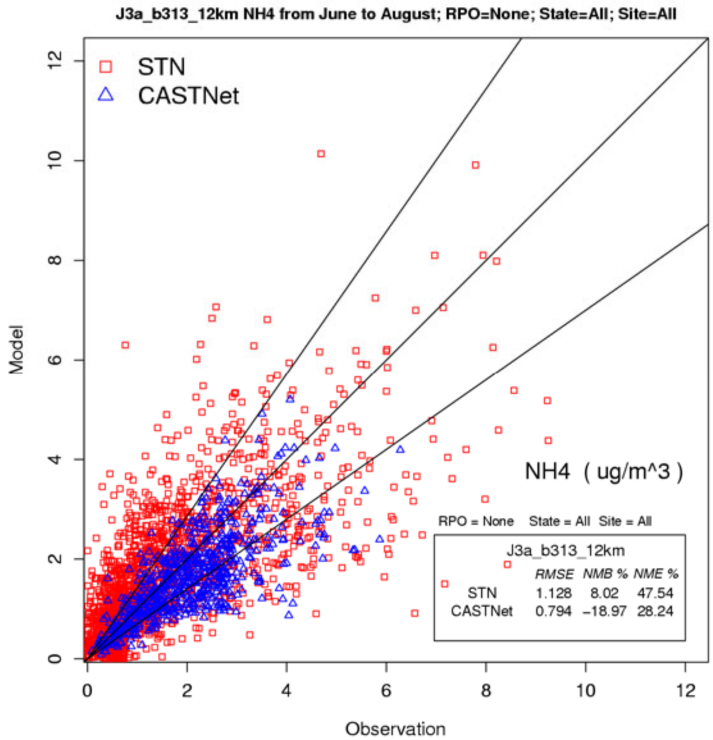


square=STN; circle=CASTNet;

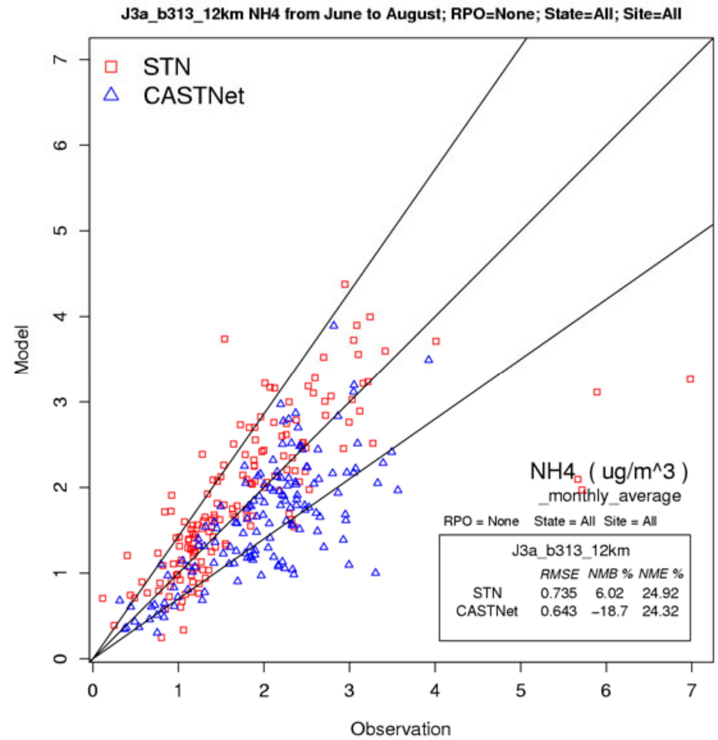
Network	# Obs	Mean Obs	Mean Model	SDEV Obs	SDEV Model	R	RMSE	NMB (%)	NME (%)
STN	984	1.46	1.72	1.28	1.26	0.67	1.07	17.8	51.6
CASTNet	623	1.52	1.45	0.79	0.61	0.74	0.53	-4.30	24.9

NH_4 - Summer

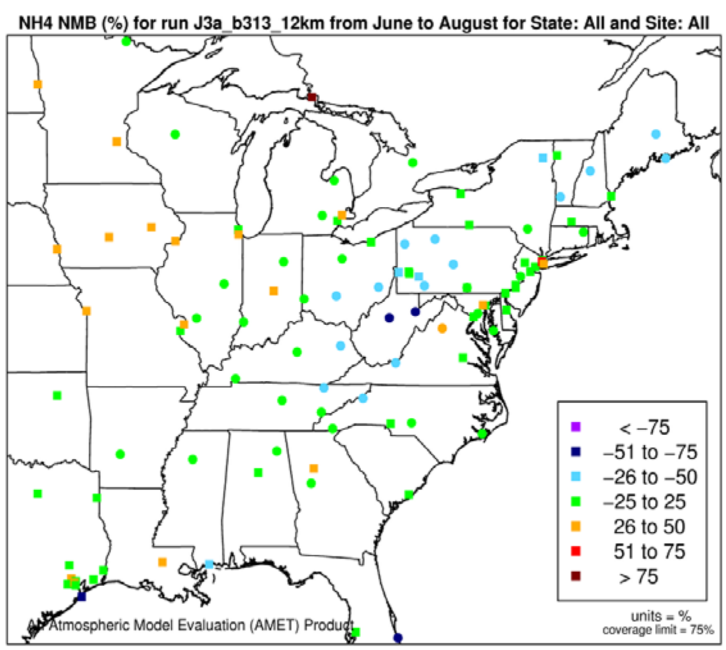
Scatter Plot – All Pairs



Scatter Plot – Monthly Average Pairs

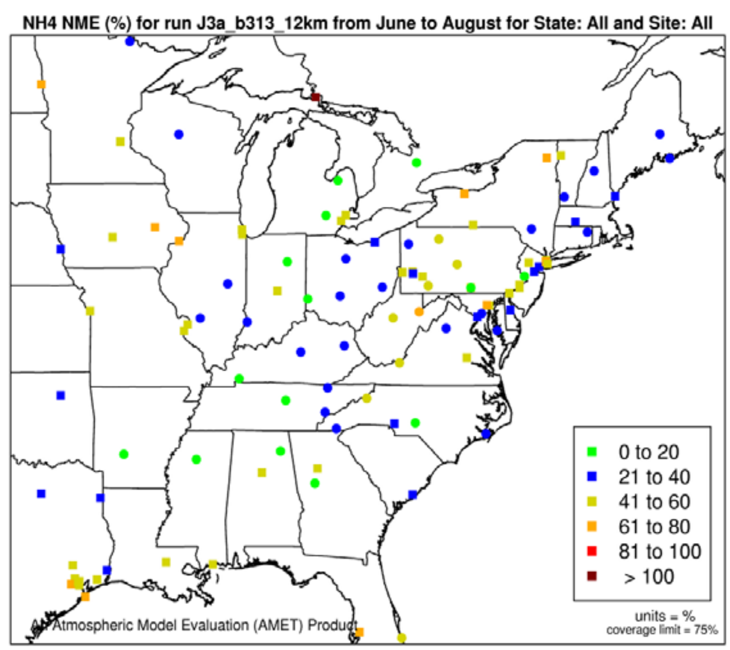


Normalized Mean Bias (%) –Summer



square=STN; circle=CASTNet;

Normalized Mean Error (%) - Summer

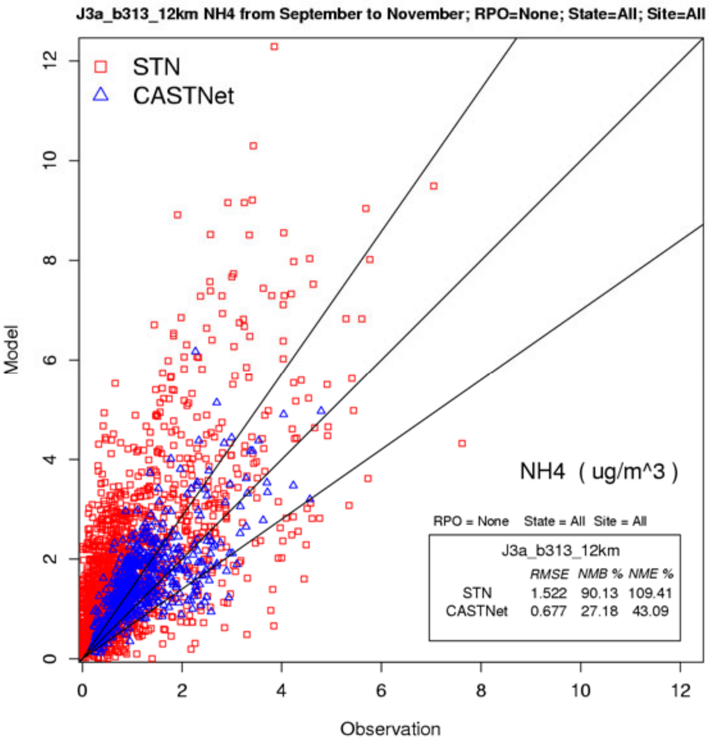


square=STN; circle=CASTNet;

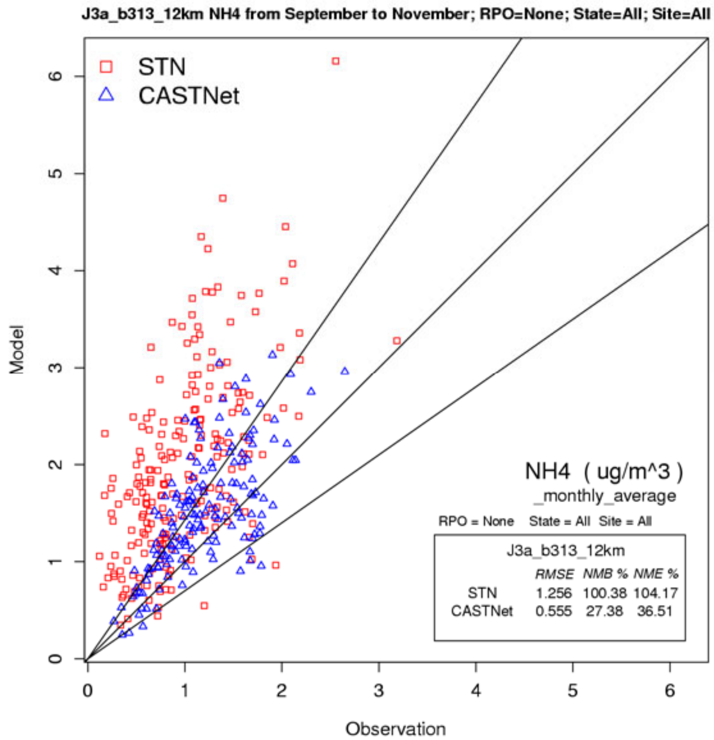
Network	# Obs	Mean Obs	Mean Model	SDEV Obs	SDEV Model	R	RMSE	NMB (%)	NME (%)
STN	1632	1.67	1.80	1.50	1.33	0.69	1.13	8.02	47.5
CASTNet	652	2.00	1.62	1.03	0.84	0.74	0.79	-19.0	28.2

NH_4 - Fall

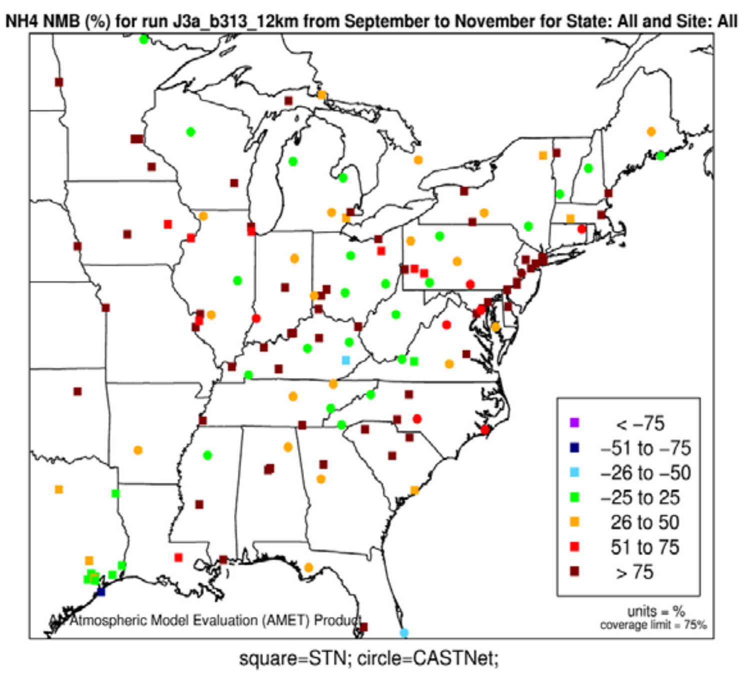
Scatter Plot – All Pairs



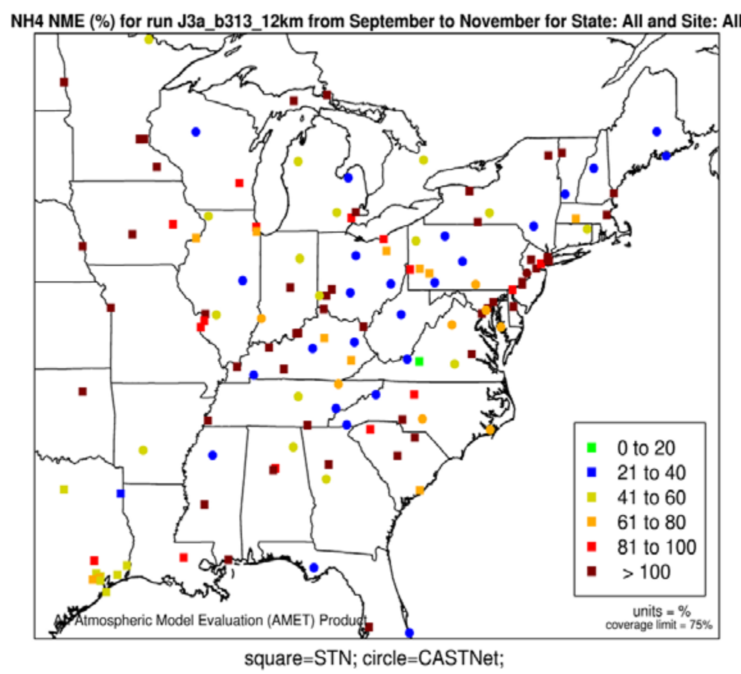
Scatter Plot – Monthly Average Pairs



Normalized Mean Bias (%) –Fall



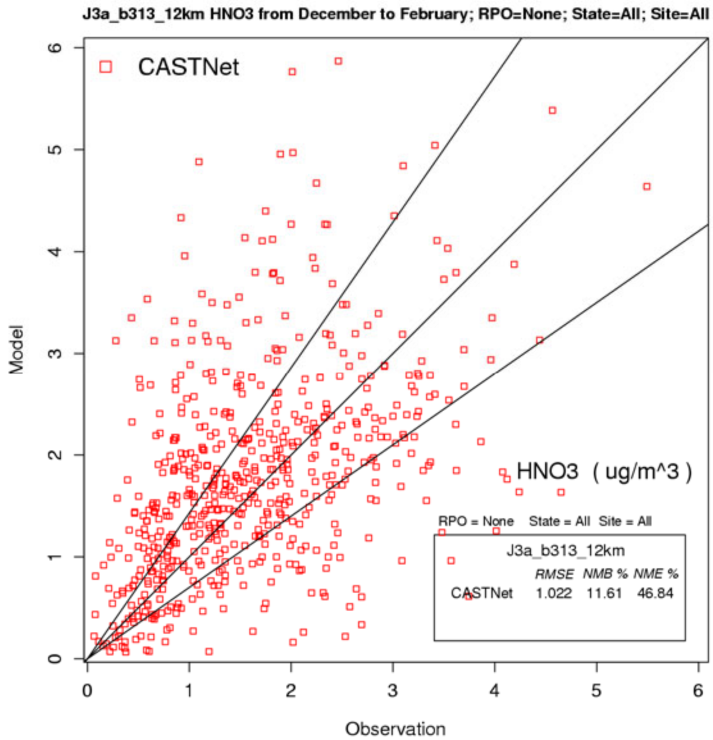
Normalized Mean Error (%) - Fall



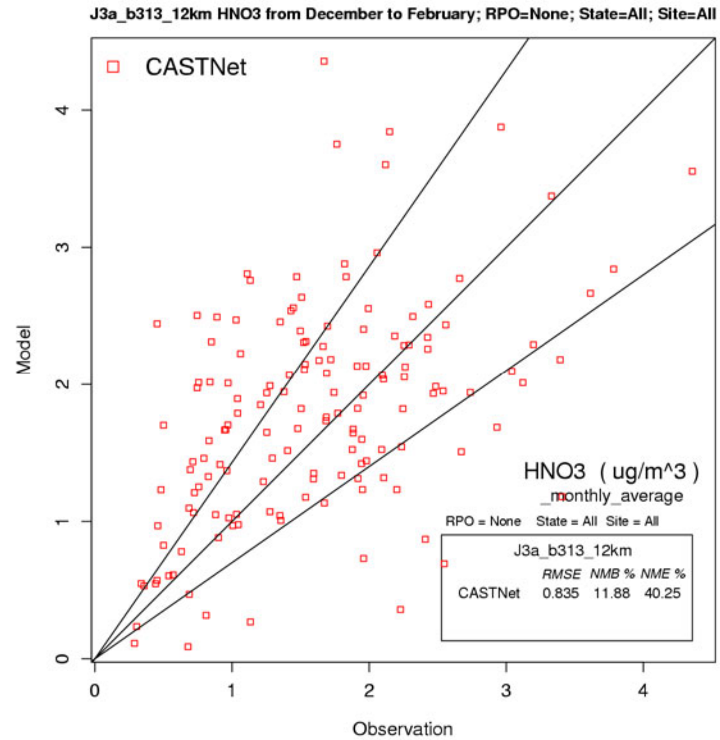
Network	# Obs	Mean Obs	Mean Model	SDEV Obs	SDEV Model	R	RMSE	NMB (%)	NME (%)
STN	1558	1.011	1.922	1.05	1.61	0.65	1.52	90.1	109
CASTNet	611	1.20	1.52	0.72	0.81	0.70	0.68	27.2	43.1

HNO_3 - Winter

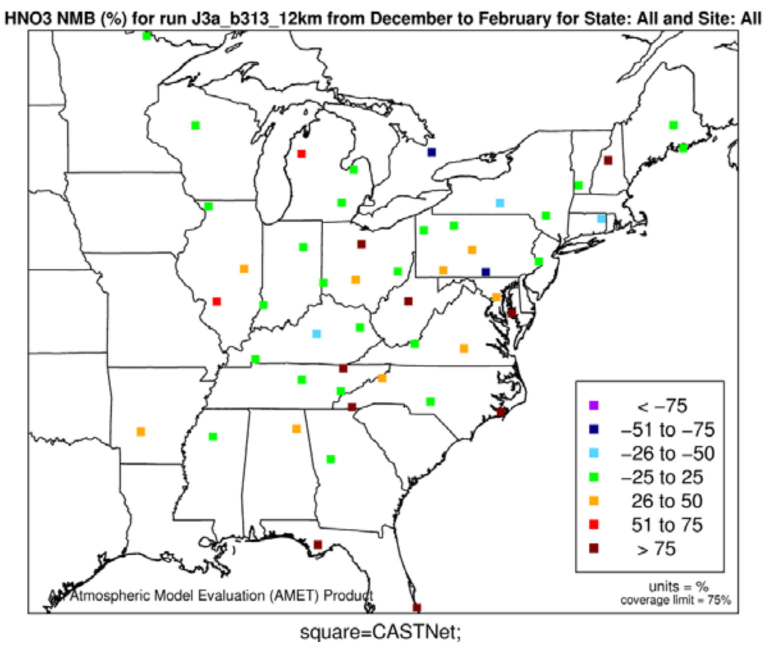
Scatter Plot – All Pairs



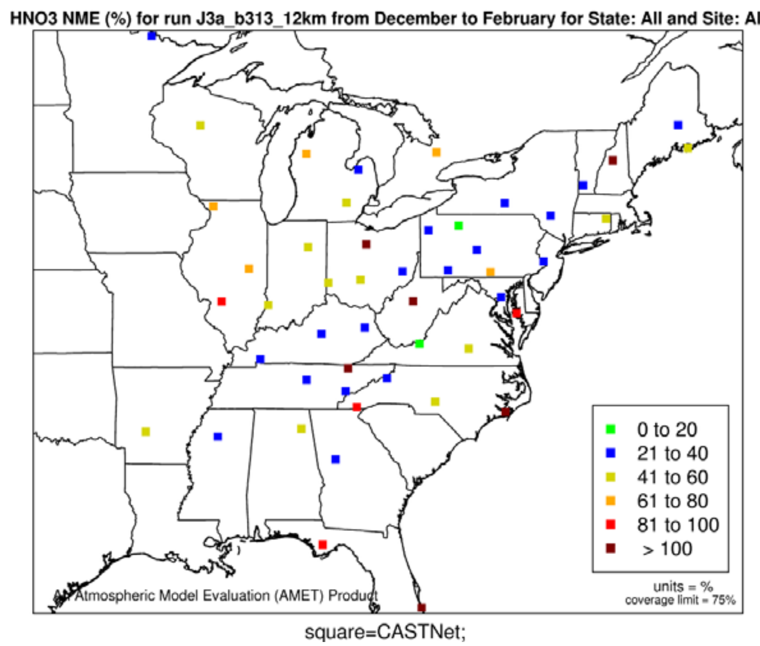
Scatter Plot – Monthly Average Pairs



Normalized Mean Bias (%) –Winter



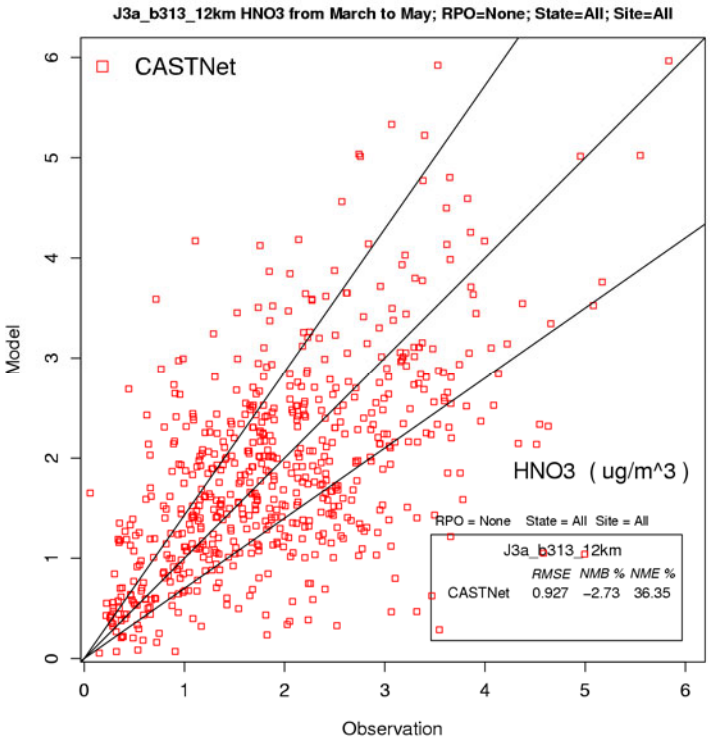
Normalized Mean Error (%) - Winter



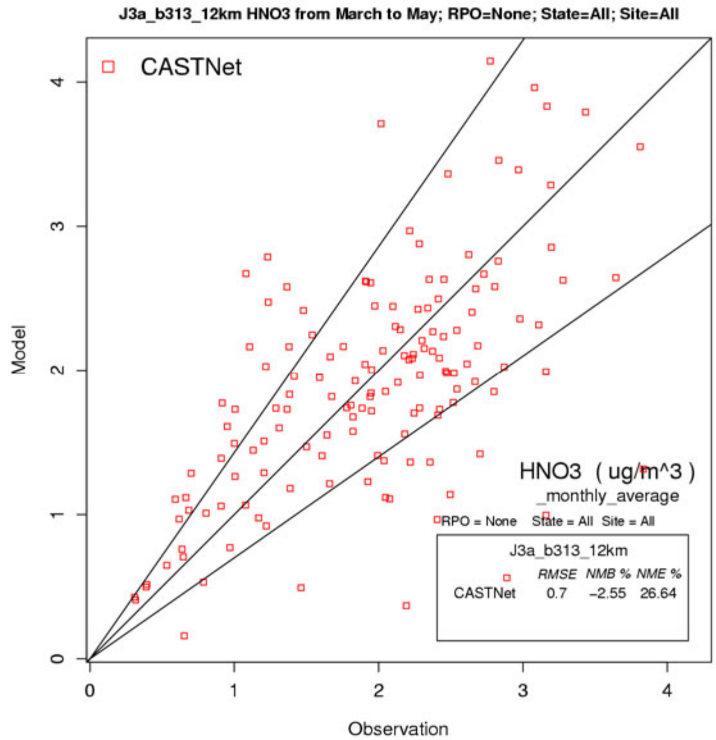
Network	# Obs	Mean Obs	Mean Model	SDEV Obs	SDEV Model	R	RMSE	NMB (%)	NME (%)
CASTNet	591	1.60	1.78	0.92	1.01	0.46	1.02	11.6	46.8

HNO_3 - Spring

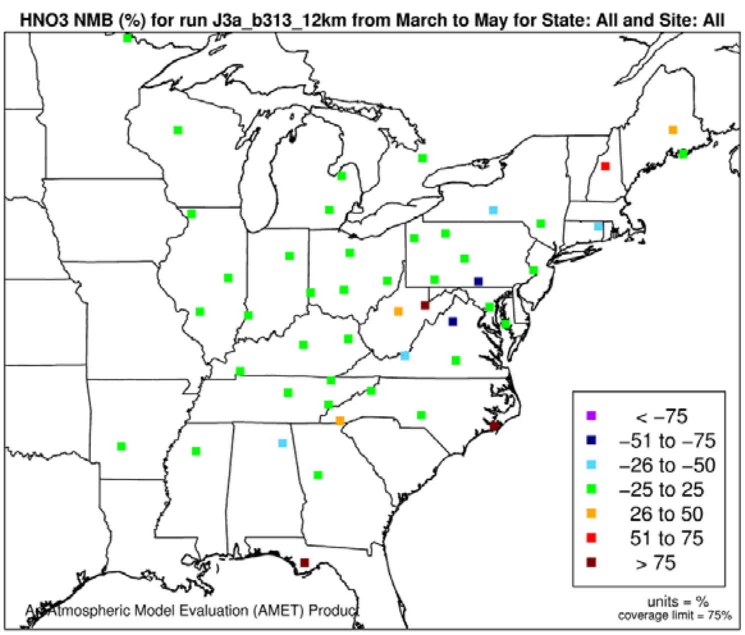
Scatter Plot – All Pairs



Scatter Plot – Monthly Average Pairs

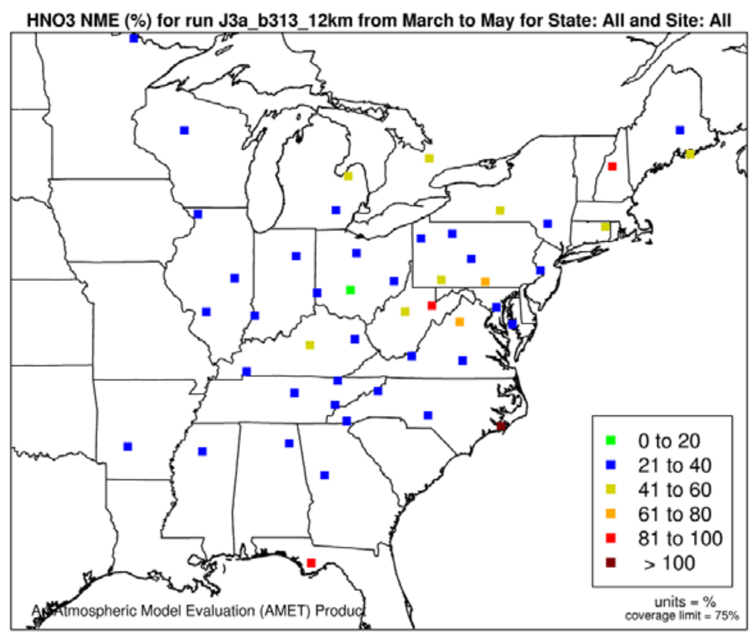


Normalized Mean Bias (%) –Spring



square=CASTNet;

Normalized Mean Error (%) - Spring

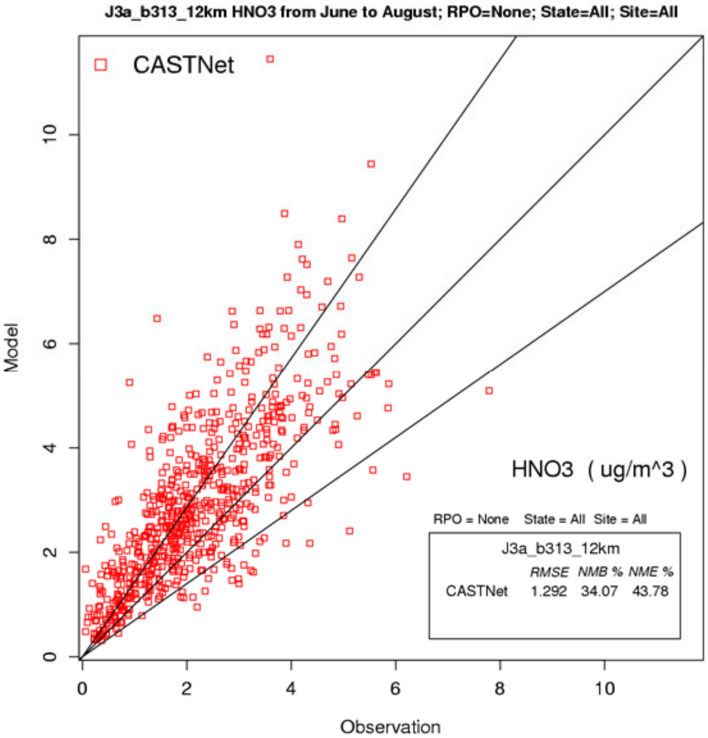


square=CASTNet;

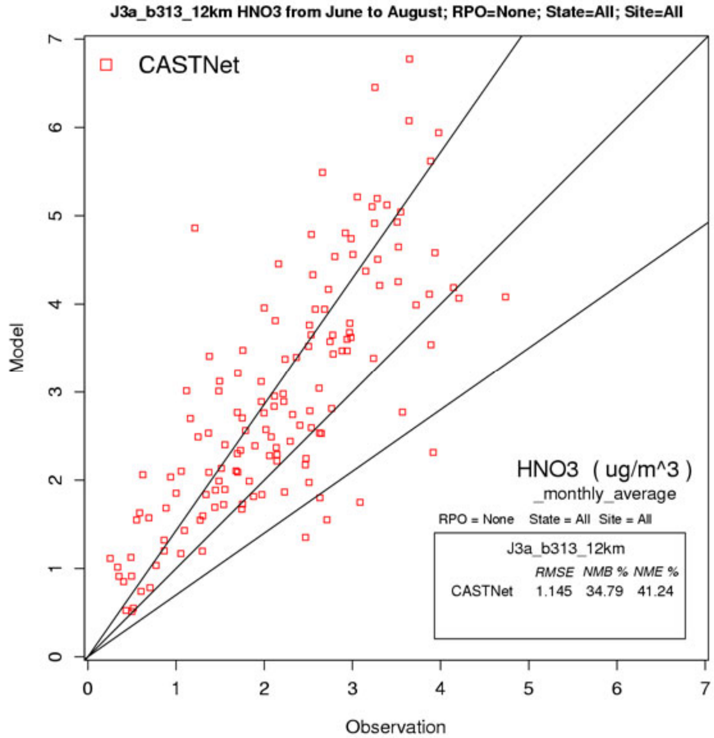
Network	# Obs	Mean Obs	Mean Model	SDEV Obs	SDEV Model	R	RMSE	NMB (%)	NME (%)
CASTNet	622	1.92	1.87	1.03	1.01	0.59	0.93	-2.73	36.4

HNO_3 - Summer

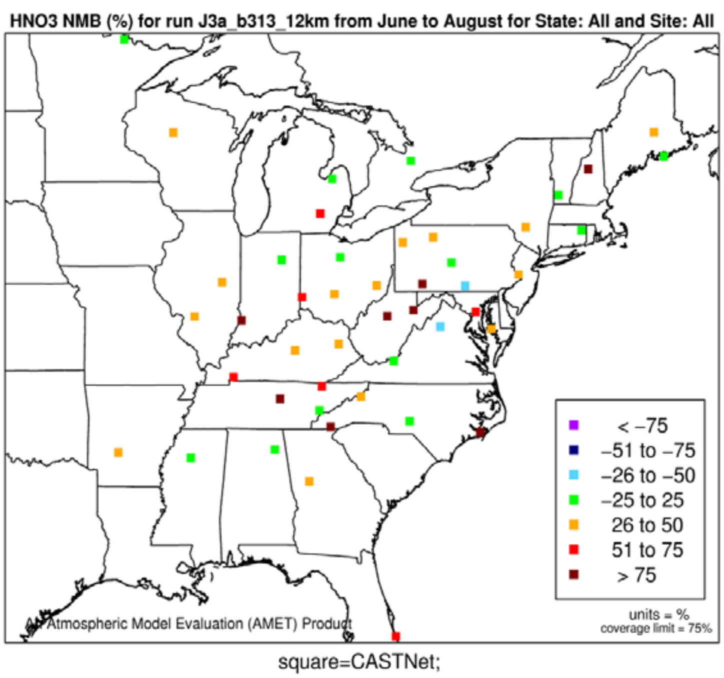
Scatter Plot – All Pairs



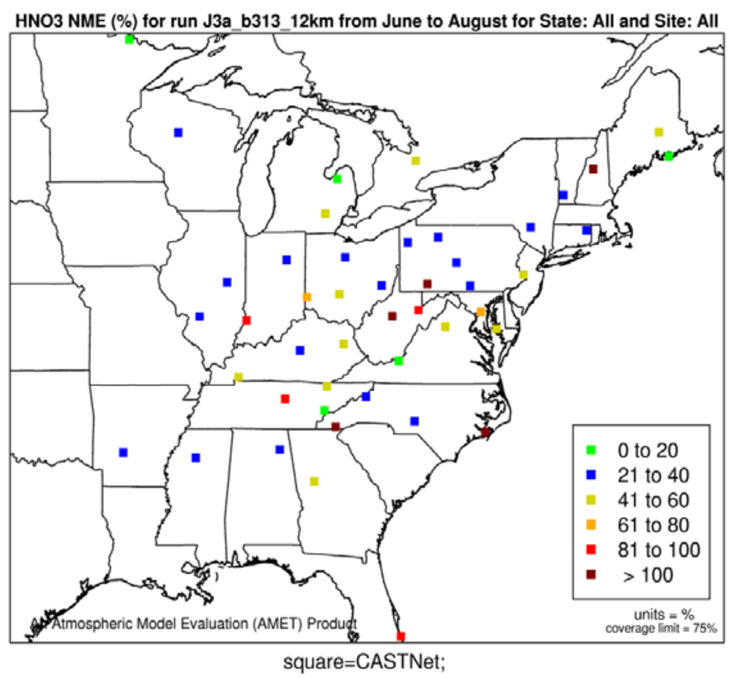
Scatter Plot – Monthly Average Pairs



Normalized Mean Bias (%) –Spring



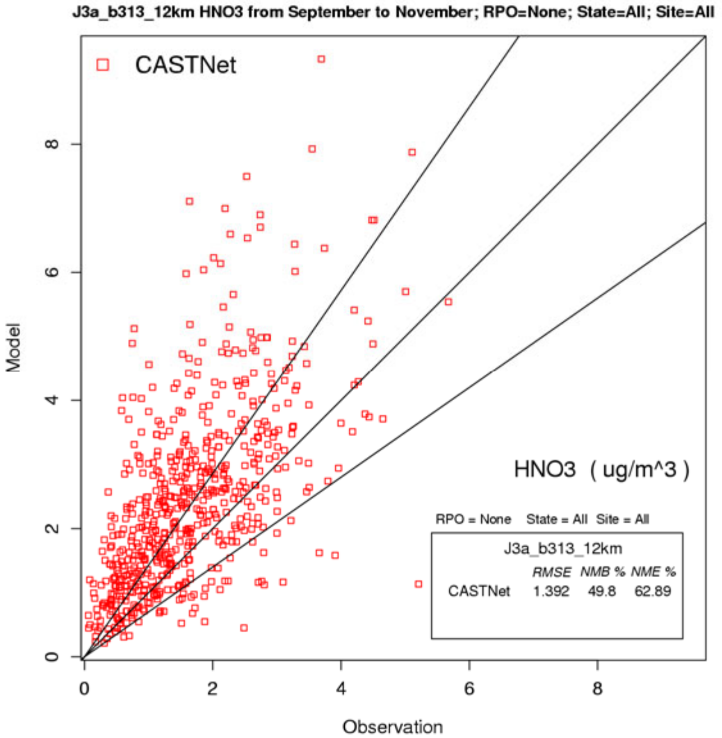
Normalized Mean Error (%) - Spring



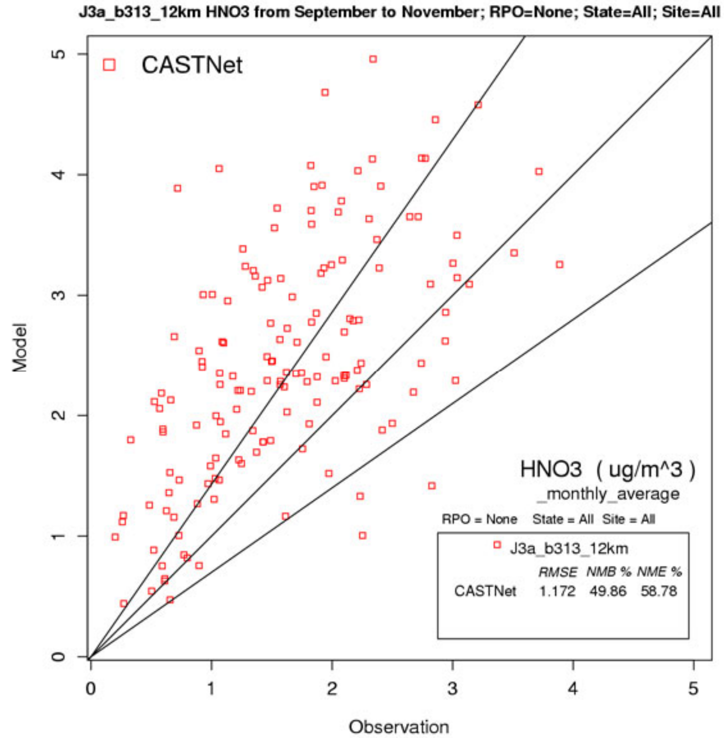
Network	# Obs	Mean Obs	Mean Model	SDEV Obs	SDEV Model	R	RMSE	NMB (%)	NME (%)
CASTNet	652	2.19	2.93	1.25	1.61	0.76	1.29	34.1	43.8

HNO_3 - Fall

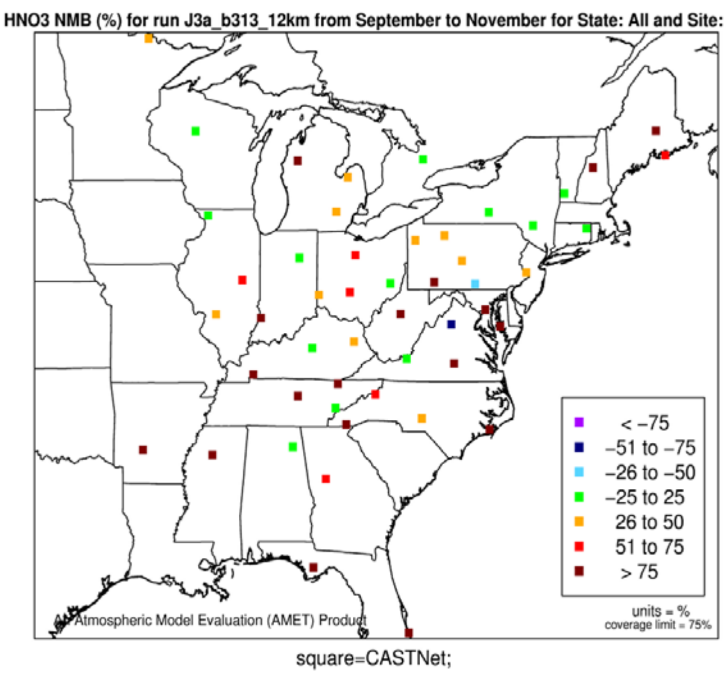
Scatter Plot – All Pairs



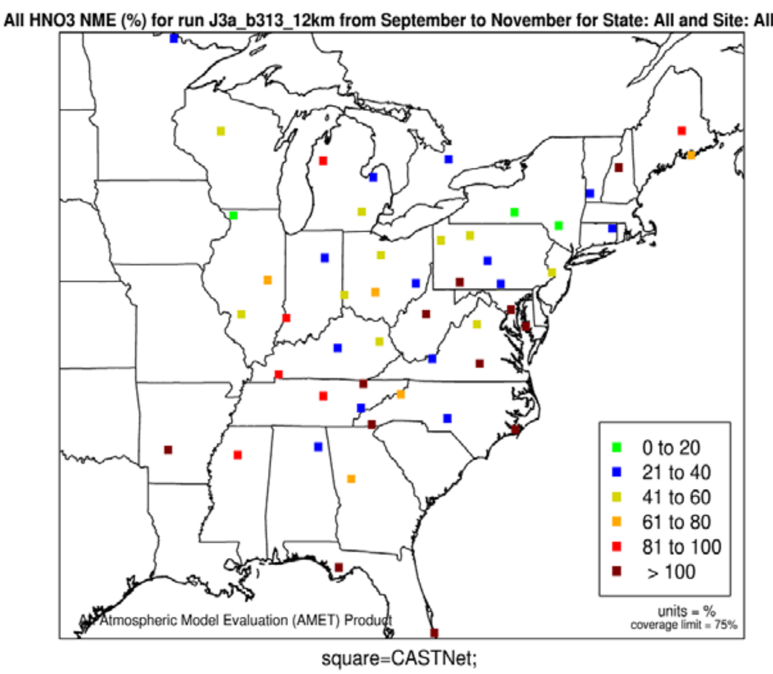
Scatter Plot – Monthly Average Pairs



Normalized Mean Bias (%) –Spring



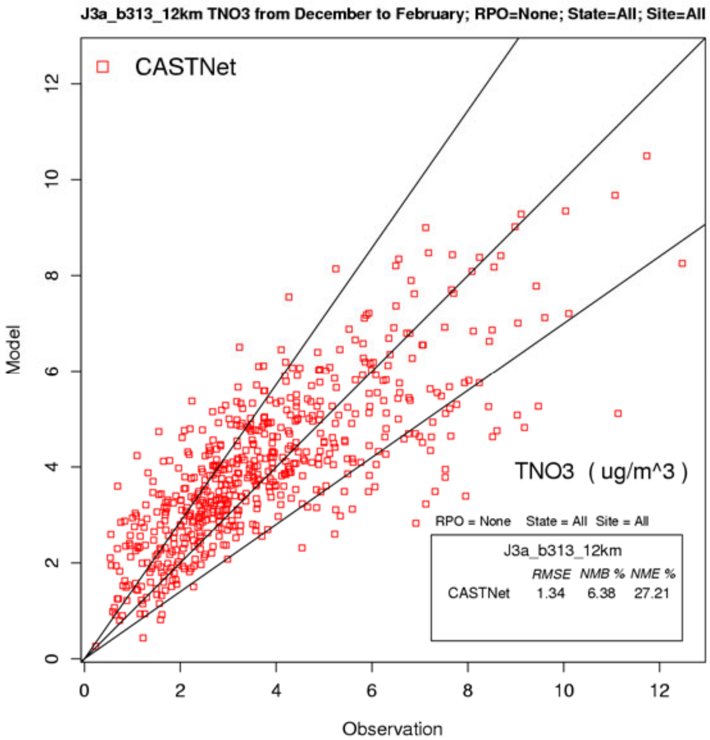
Normalized Mean Error (%) - Spring



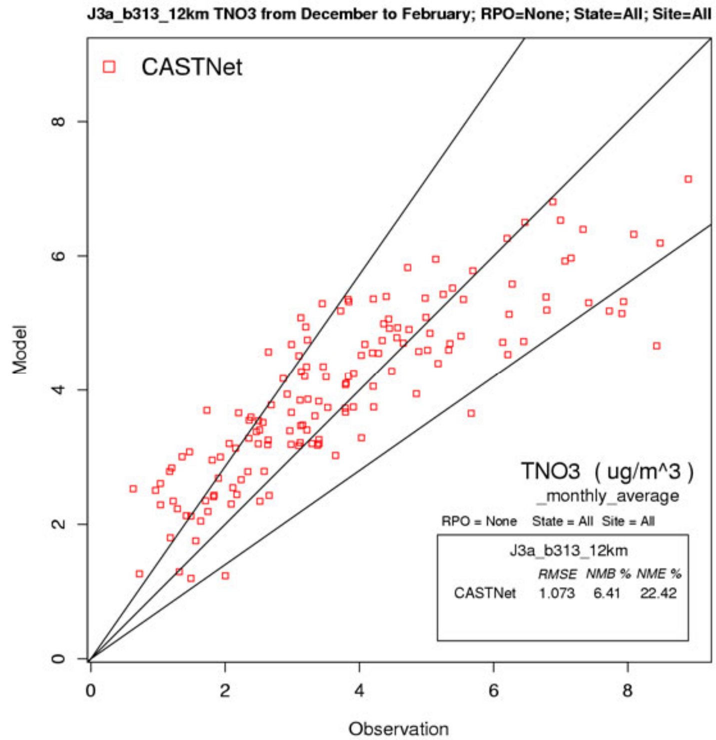
Network	# Obs	Mean Obs	Mean Model	SDEV Obs	SDEV Model	R	RMSE	NMB (%)	NME (%)
CASTNet	611	1.63	2.44	0.97	1.43	0.62	1.39	49.8	62.9

Total NO_3 - Winter

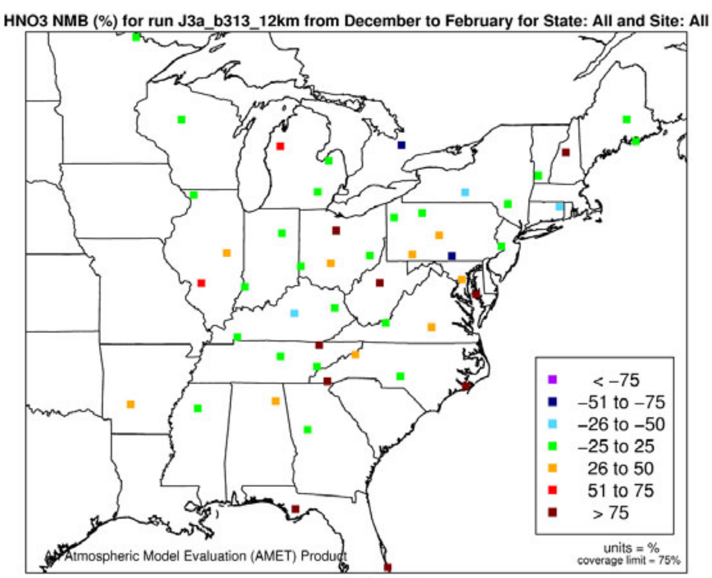
Scatter Plot – All Pairs



Scatter Plot – Monthly Average Pairs

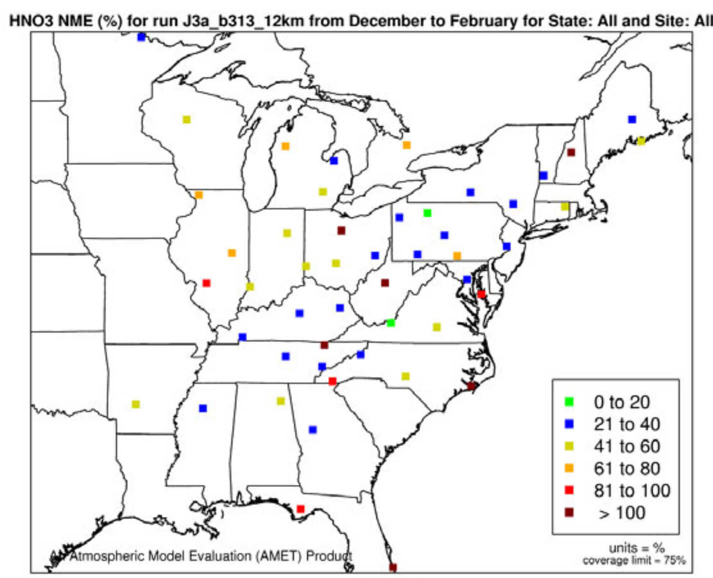


Normalized Mean Bias (%) –Winter



square=CASTNet;

Normalized Mean Error (%) - Winter

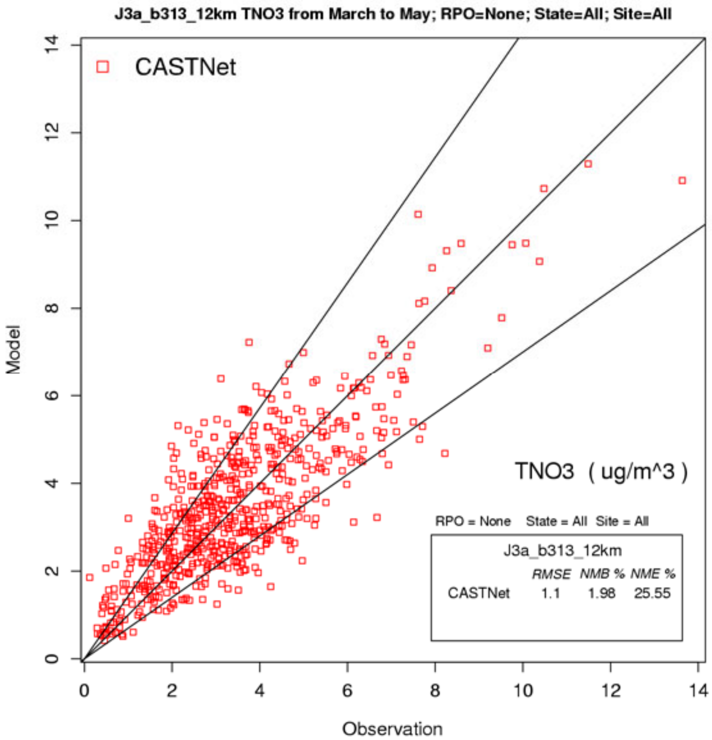


square=CASTNet;

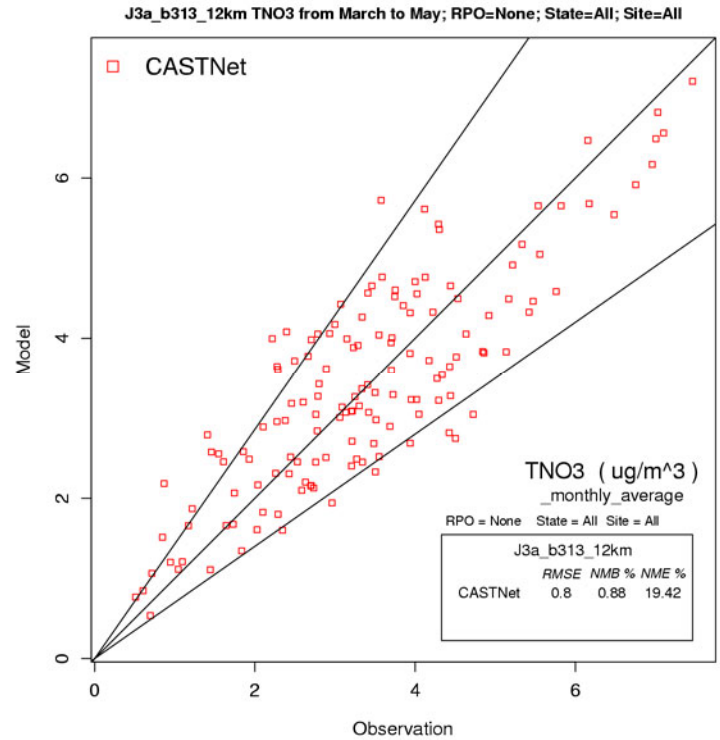
Network	# Obs	Mean Obs	Mean Model	SDEV Obs	SDEV Model	R	RMSE	NMB (%)	NME (%)
CASTNet	588	3.75	3.99	2.10	1.63	0.78	1.34	6.38	27.2

Total NO_3 - Spring

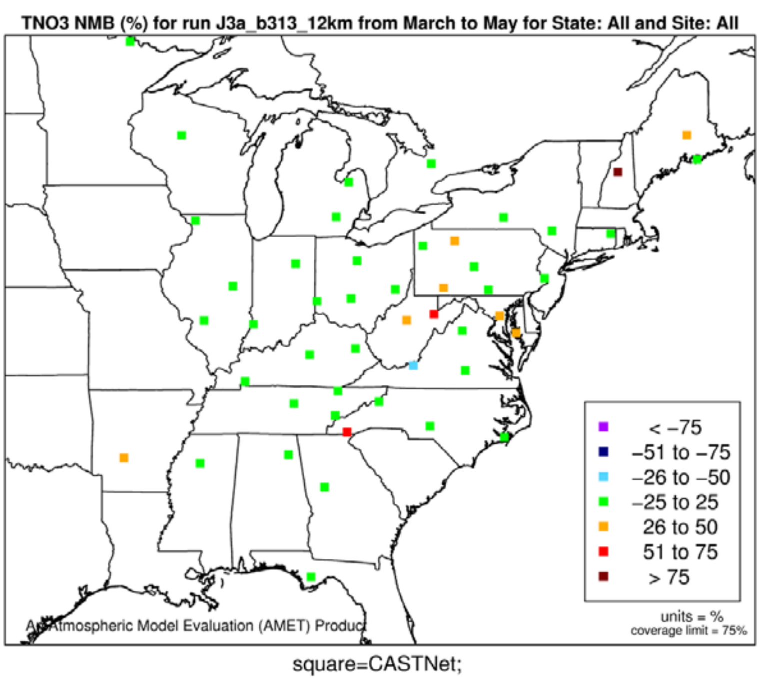
Scatter Plot – All Pairs



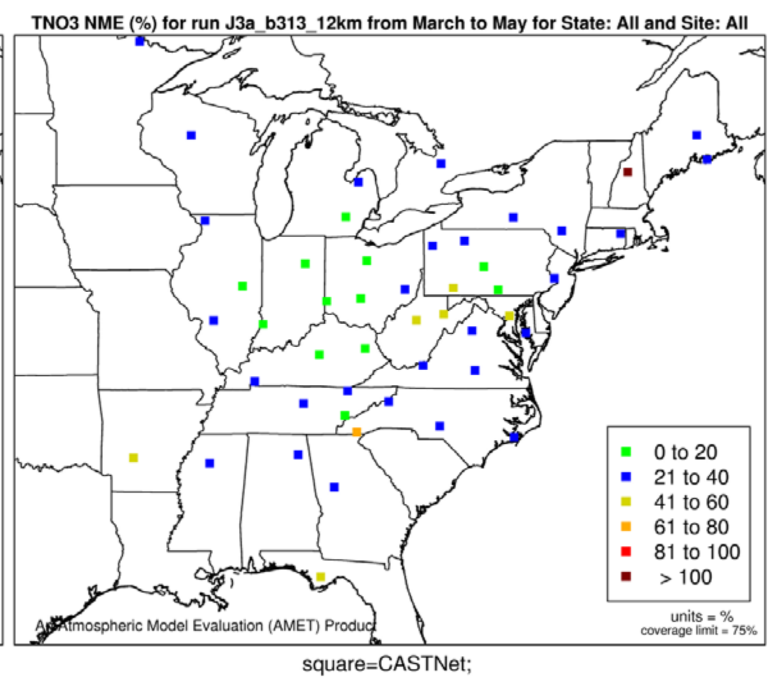
Scatter Plot – Monthly Average Pairs



Normalized Mean Bias (%) –Spring



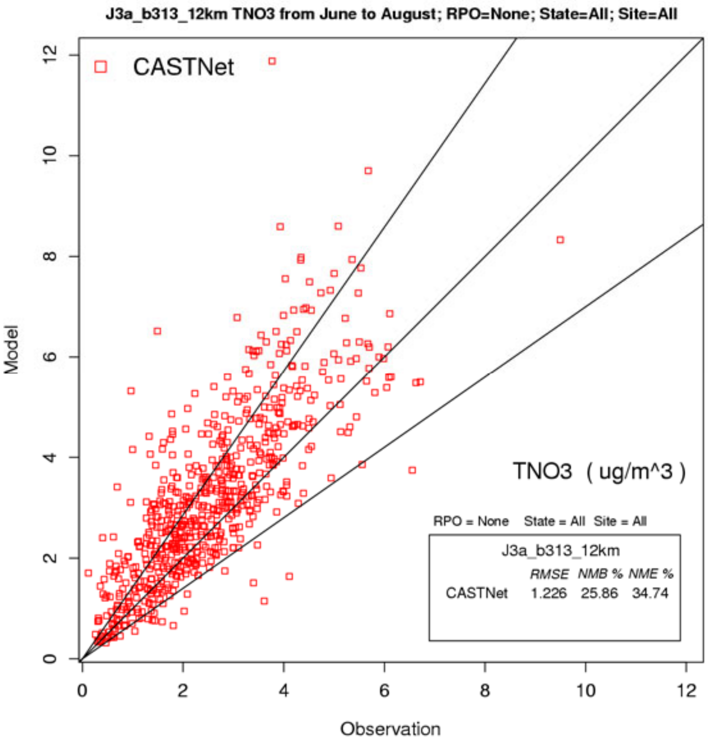
Normalized Mean Error (%) - Spring



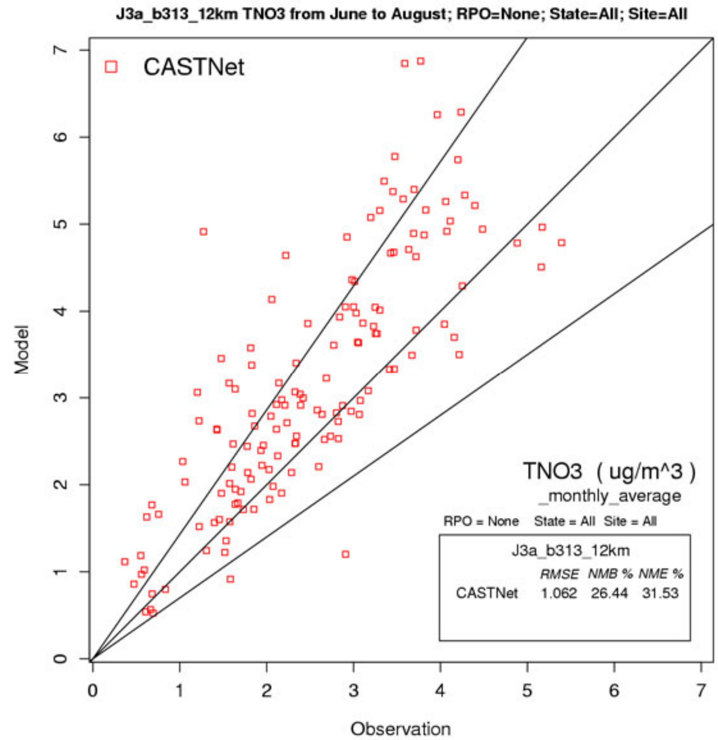
Network	# Obs	Mean Obs	Mean Model	SDEV Obs	SDEV Model	R	RMSE	NMB (%)	NME (%)
CASTNet	622	3.42	3.49	1.86	1.71	0.81	1.10	1.98	25.6

Total NO_3 - Summer

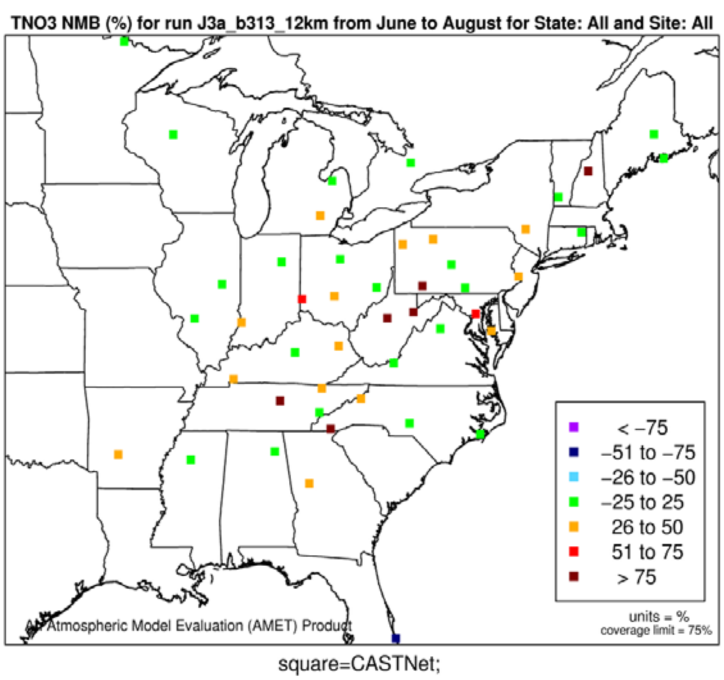
Scatter Plot – All Pairs



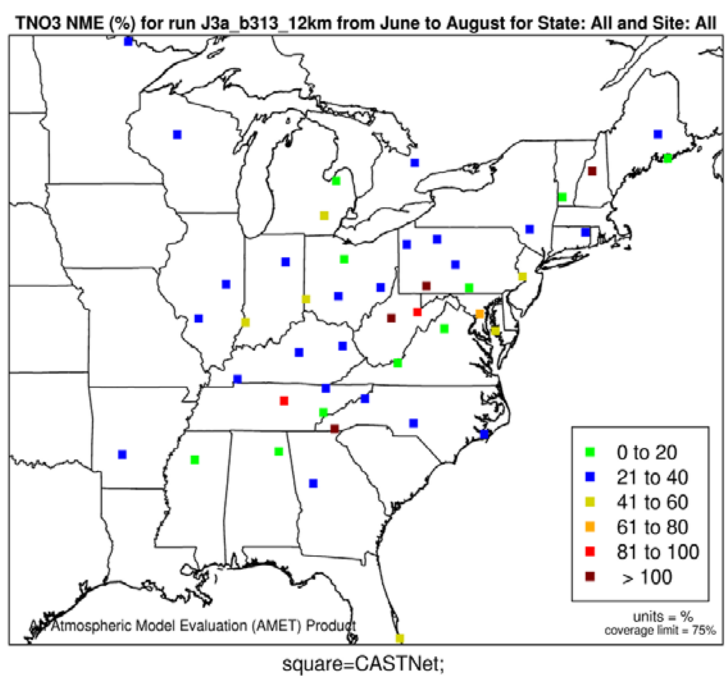
Scatter Plot – Monthly Average Pairs



Normalized Mean Bias (%) –Summer



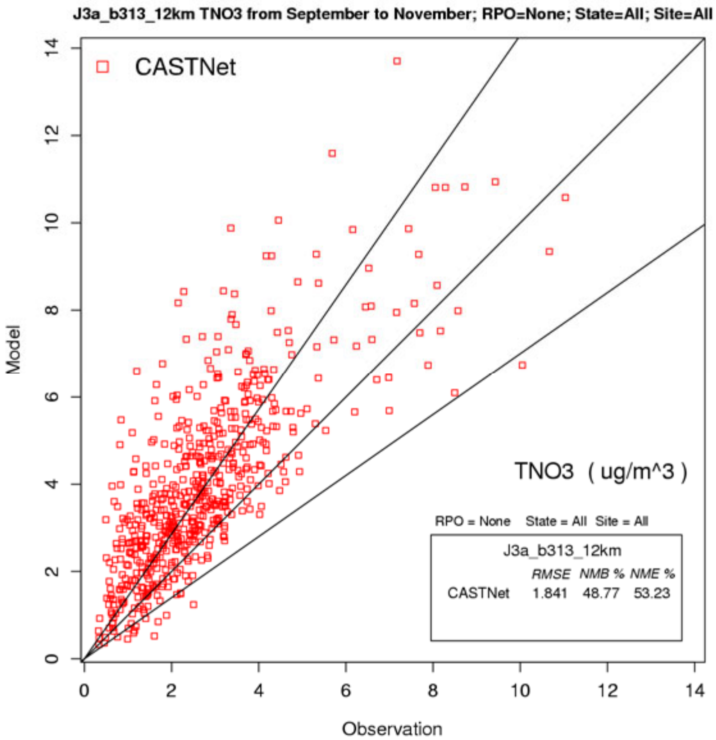
Normalized Mean Error (%) - Summer



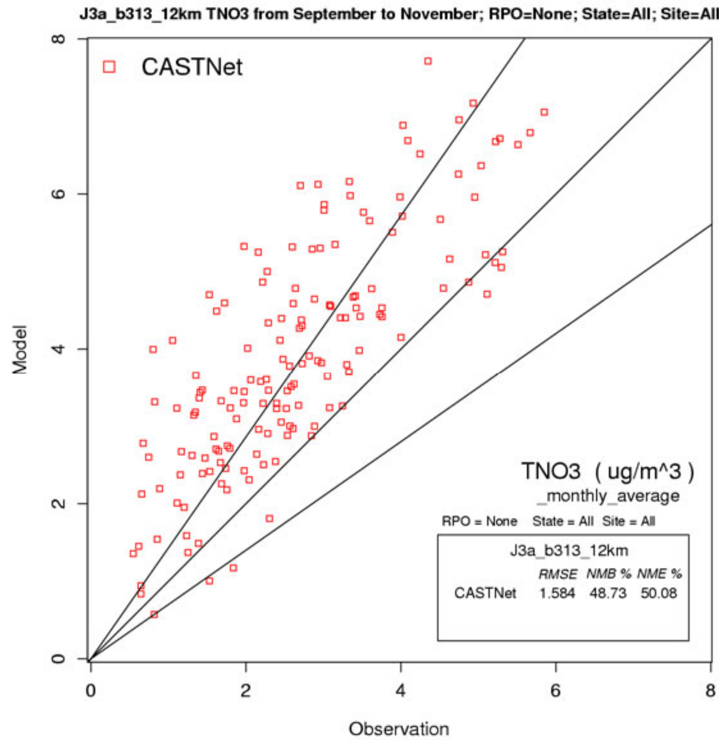
Network	# Obs	Mean Obs	Mean Model	SDEV Obs	SDEV Model	R	RMSE	NMB (%)	NME (%)
CASTNet	652	2.54	3.19	1.34	1.70	0.79	1.23	25.9	34.7

Total NO_3 - Fall

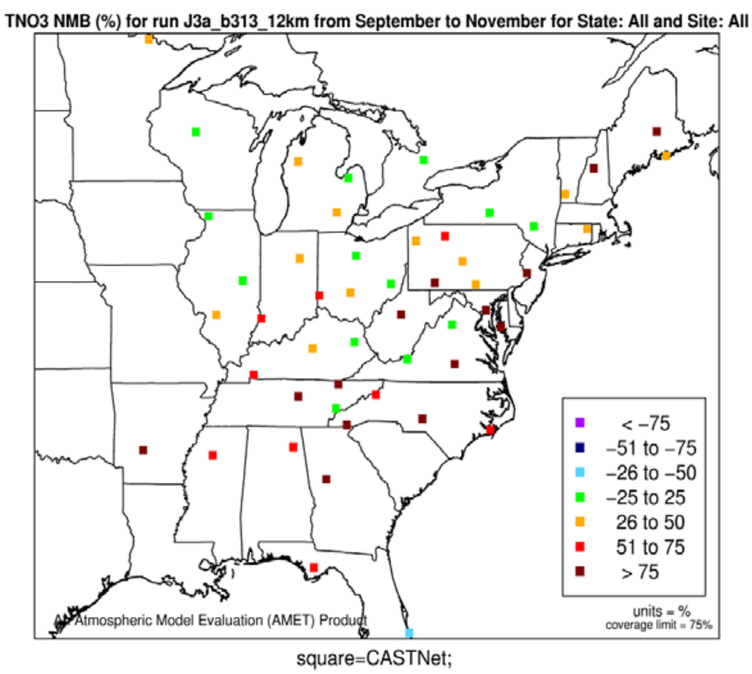
Scatter Plot – All Pairs



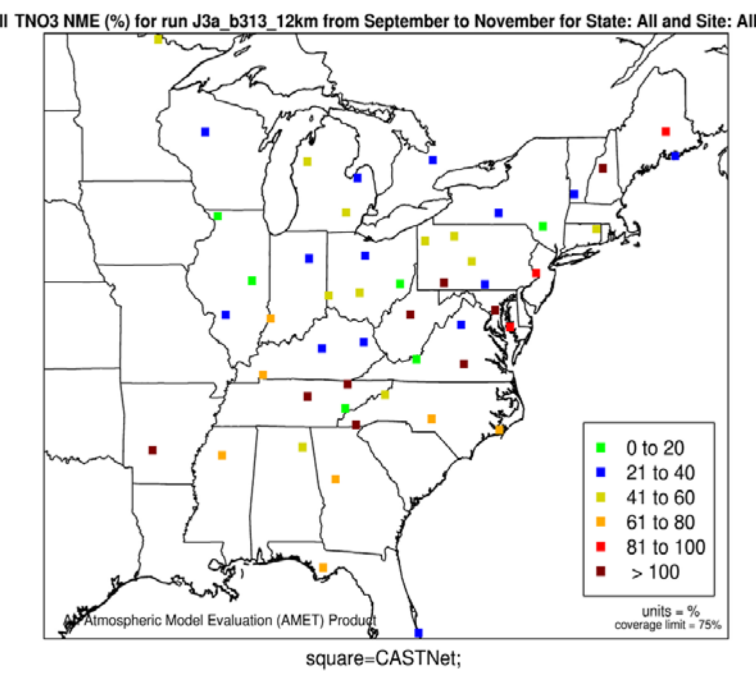
Scatter Plot – Monthly Average Pairs



Normalized Mean Bias (%) –Fall



Normalized Mean Error (%) - Fall



Network	# Obs	Mean Obs	Mean Model	SDEV Obs	SDEV Model	R	RMSE	NMB (%)	NME (%)
CASTNet	610	2.65	3.94	1.60	2.05	0.77	1.84	48.8	53.2

Evaluation of CMAQ version 4.5: 12km×12km Eastern United States Organic Aerosols: Elemental Carbon (EC) and Organic Carbon (OC)

Available Networks:

IMPROVE – Elemental Carbon, Organic Carbon
STN – Elemental Carbon, Organic Carbon

Organic Aerosol Performance: Introduction

The list below covers the plots and metrics available for the inorganic aerosol analysis for each of the four seasons (winter, spring, summer, fall):

- Seasonal model to observation scatter plot of various species using all pairs
- Seasonal model to observation scatter plot of various species using monthly averaged pairs
- Spatial Plot of NMB (%) and NME (%) of various species
- Table of select statistical metrics for various species

Where applicable, multiple networks are plotted on each scatter plot and spatial plot. Legends are provided on each plot to help identify each network.

Note that for comparison of organic carbon, the complete unit is μgC/m^3, although on plots the units are labeled as μg/m^3.

Organic Aerosol Performance: Summary

Since elemental carbon is a primary aerosol that is directly emitted into the atmosphere as elemental carbon, emission inputs to the CMAQ simulations have a strong influence on these predictions. Both primary organic aerosols as well as secondary organic aerosols contribute to the total organic carbon concentrations; therefore, both inputs and chemical transformations in the atmosphere have a substantial influence on these predictions. Major emission sources for carbonaceous aerosols include diesel and gasoline-fueled mobile sources, meat cooking, as well as wild fire sources that have a high level of uncertainty. Many research efforts are ongoing to improve fire emission estimates, as well as to improve modeling approaches for secondary organic aerosols.

Winter Season (December, January and February)

Elemental carbon for the winter season is slightly over-predicted for the IMPROVE network (NMB of 6.69% and NME of 51.0%), and also significantly over-predicted at STN sites (NMB of 117% and NME of 137%). Differences in model comparisons with IMPROVE and with STN could be attributed to both the rural versus urban representativeness of these networks as well as differences in the methodology between IMPROVE and STN (e.g., blank correction factors). Over-predictions are more evident at the Northeast, Midwest, and Texas sites. Organic carbon for the winter season was only slightly over-predicted at both IMPROVE and STN, with NMBs of 5.31% and 10.5% and NMEs of 48.6% and 58.0%. The mean concentration of observed organic carbon for the winter season for IMPROVE sites is about 3.8 times higher than elemental carbon concentrations, while at STN sites the mean concentration of observed organic carbon is about 4.8 times higher than that of elemental carbon.

Spring Season (March, April and May)

Elemental carbon for the spring season is under-predicted for the IMPROVE network (NMB of -19.6% and NME of 49.6%), while at STN sites elemental carbon is significantly over-predicted (NMB of 121% and NME of 144%). Organic carbon for under-predicted by roughly the same amount at IMPROVE (NMB = -24.9%, NME = 52.9%) and STN (NMB = -26.3% and NME = 51.4%). The mean concentration of observed organic for IMPROVE is about 4.4 times higher than that of elemental carbon, while for STN sites the mean concentration of observed organic carbon is 5.8 times higher than that of elemental carbon.

Summer Season (June, July and August)

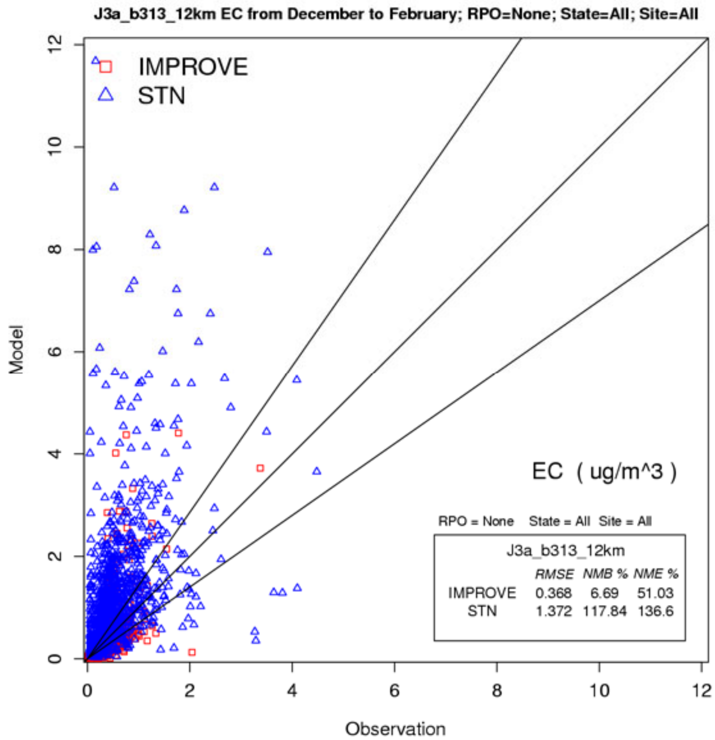
Elemental carbon for the summer season is again under predicted for the IMPROVE network (NMB of -30.3% and NME of 43.6%), while a significant over-prediction for STN sites is again noted (NMB of 82.6% and NME of 103%). Organic carbon is also again under-predicted for both IMPROVE and STN, and again by roughly the same amount, with a NMB of -44.1% and NME of 52.1% for IMPROVE and a NMB of -44.6% and NME of 52.7% for STN. IMPROVE observed organic carbon concentrations are about 4.8 times higher than that of elemental carbon for summer, while STN sites observed organic carbon concentrations are about 5.7 times than that of elemental carbon.

Fall Season (September, October and November)

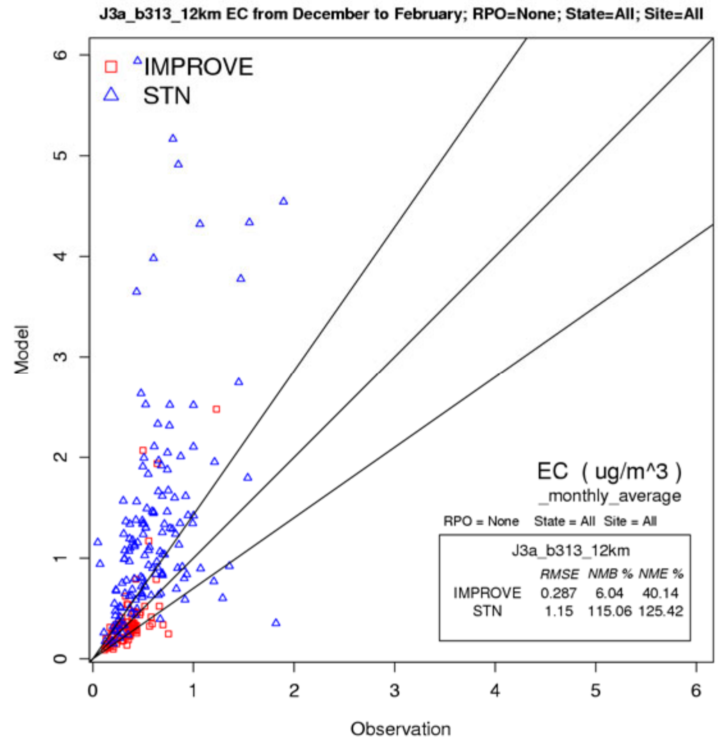
Elemental carbon for the fall season is slightly under-predicted for the IMPROVE network (NMB of -11.8% and NME of 45.2%), while for STN sites the over-prediction of elemental carbon continues, although the bias is lower than the winter, spring and summer seasons, with a NMB of 66.4% and NME of 95.5%. Organic carbon is moderately under-predicted at both IMPROVE and STN sites, with NMB values of -17.1% and -20.3% and NME values of 44.7% and 47.6% respectively. Observed concentrations of organic carbon for IMPROVE are 4.4 times higher than that of elemental carbon, while observed concentrations of organic carbon for STN sites are 4.6 times higher than that of elemental carbon.

Elemental Carbon - Winter

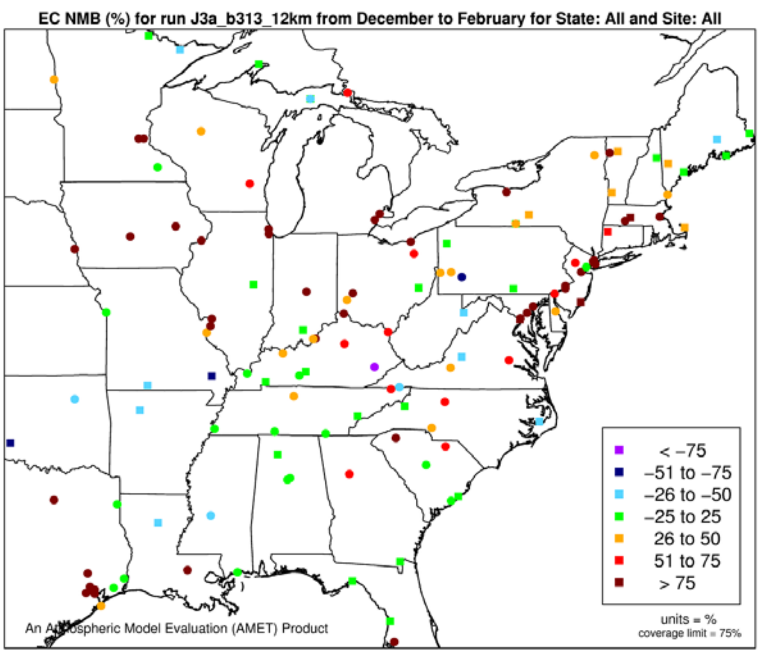
Scatter Plot – All Pairs



Scatter Plot – Monthly Average Pairs

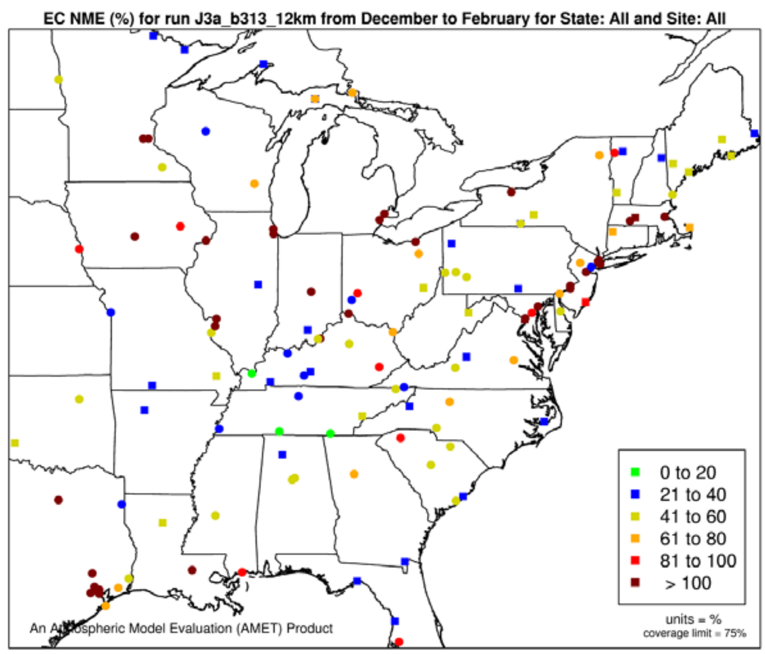


Normalized Mean Bias (%) –Winter



square=IMPROVE; circle=STN;

Normalized Mean Error (%) - Winter

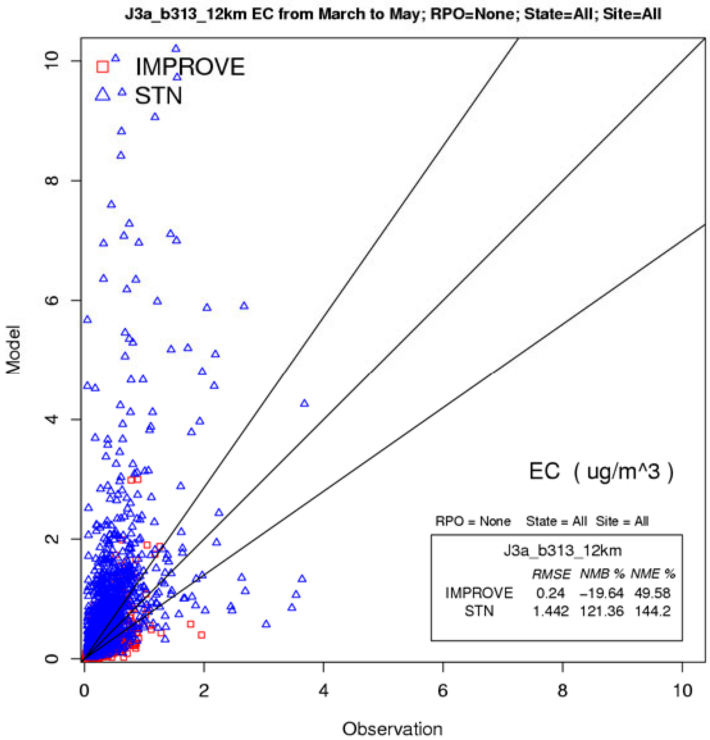


square=IMPROVE; circle=STN;

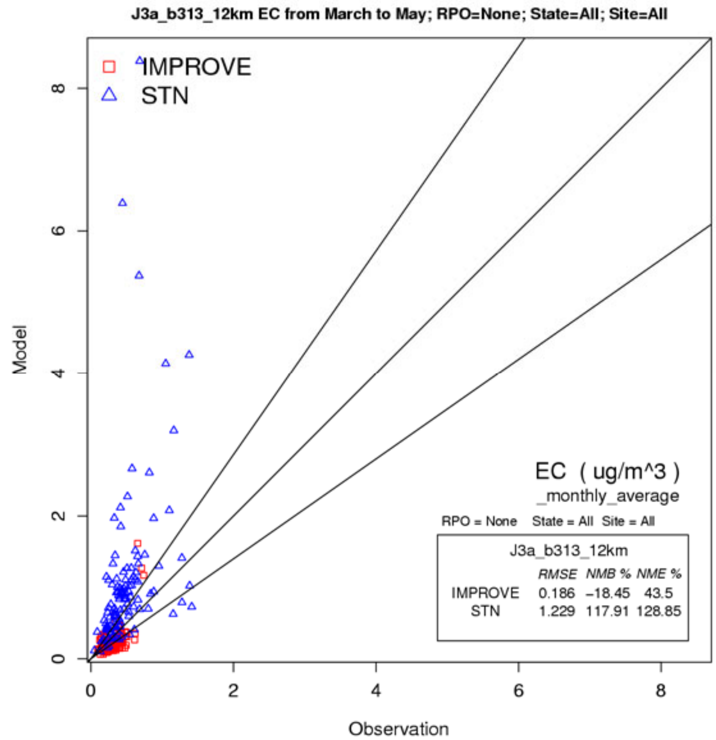
Network	# Obs	Mean Obs	Mean Model	SDEV Obs	SDEV Model	R	RMSE	NMB (%)	NME (%)
IMPROVE	929	0.35	0.37	0.25	0.46	0.60	0.37	6.69	51.0
STN	1050	0.59	1.28	0.53	1.32	0.44	1.37	118	137

Elemental Carbon - Spring

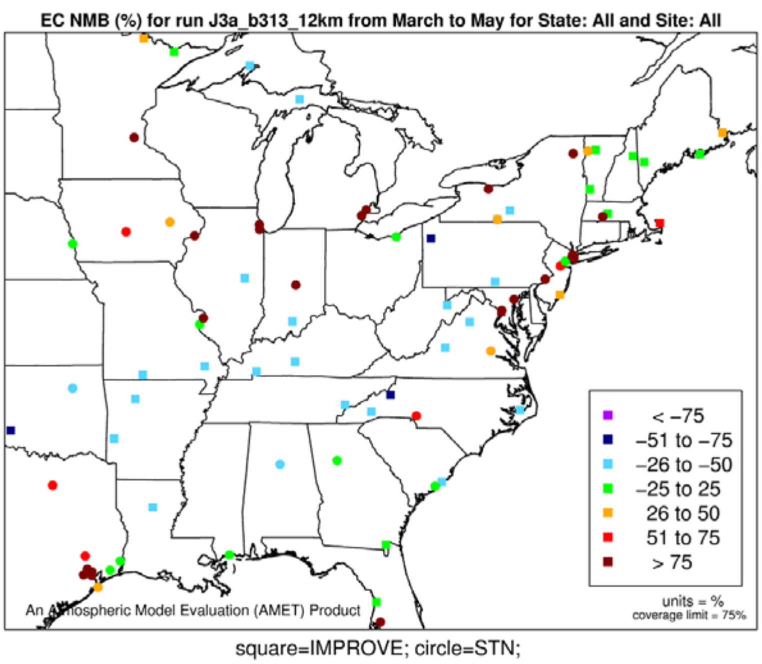
Scatter Plot – All Pairs



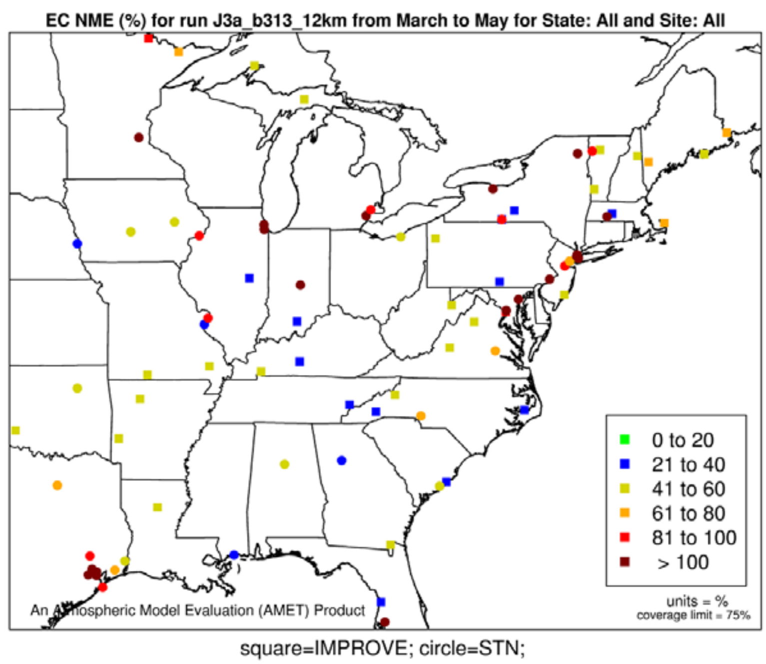
Scatter Plot – Monthly Average Pairs



Normalized Mean Bias (%) –Spring



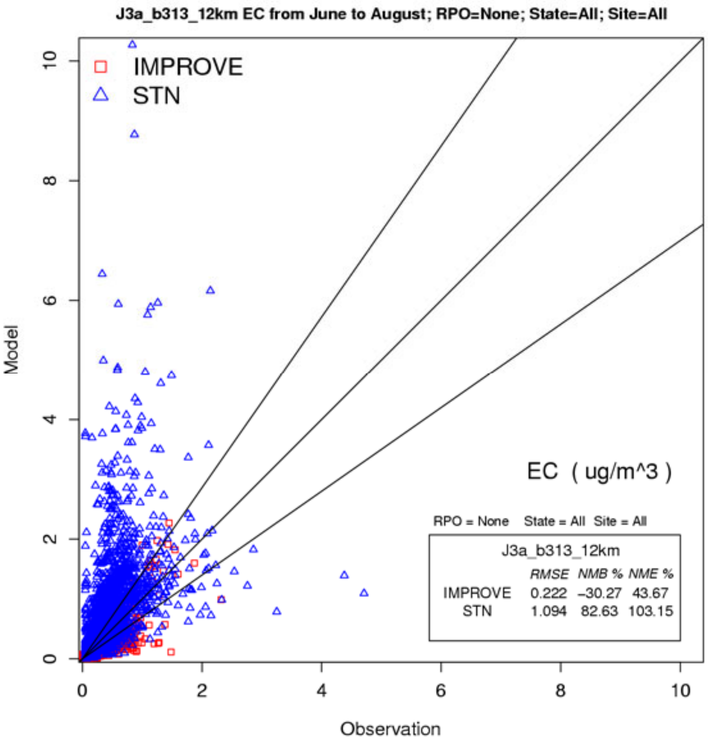
Normalized Mean Error (%) - Spring



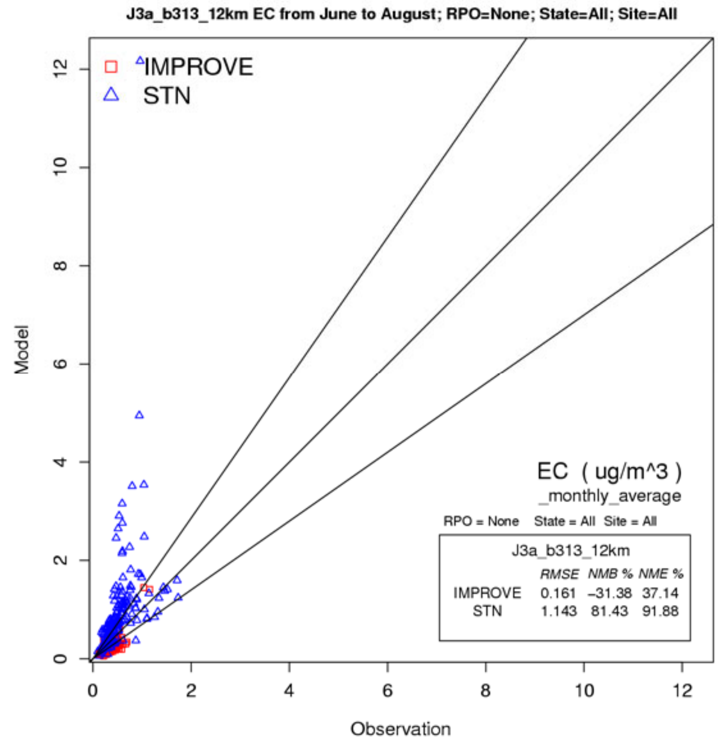
Network	# Obs	Mean Obs	Mean Model	SDEV Obs	SDEV Model	R	RMSE	NMB (%)	NME (%)
IMPROVE	1130	0.32	0.26	0.21	0.26	0.54	0.24	-19.6	49.6
STN	1014	0.49	1.09	0.43	1.39	0.33	1.44	121	144

Elemental Carbon - Summer

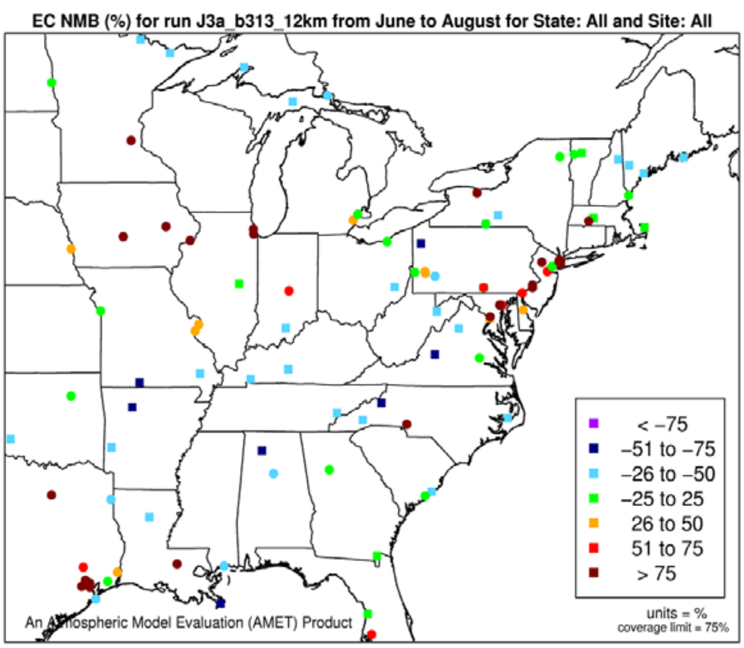
Scatter Plot – All Pairs



Scatter Plot – Monthly Average Pairs

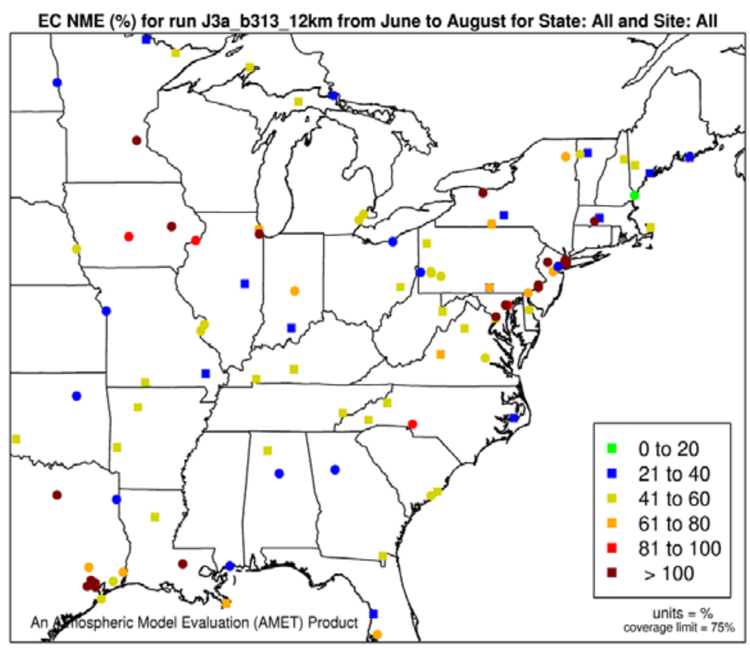


Normalized Mean Bias (%) –Summer



square=IMPROVE; circle=STN;

Normalized Mean Error (%) - Summer

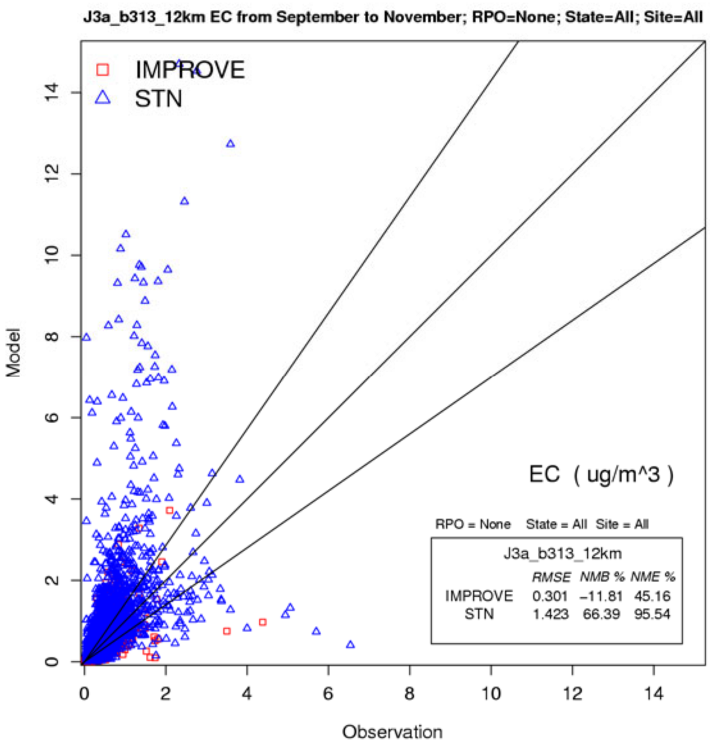


square=IMPROVE; circle=STN;

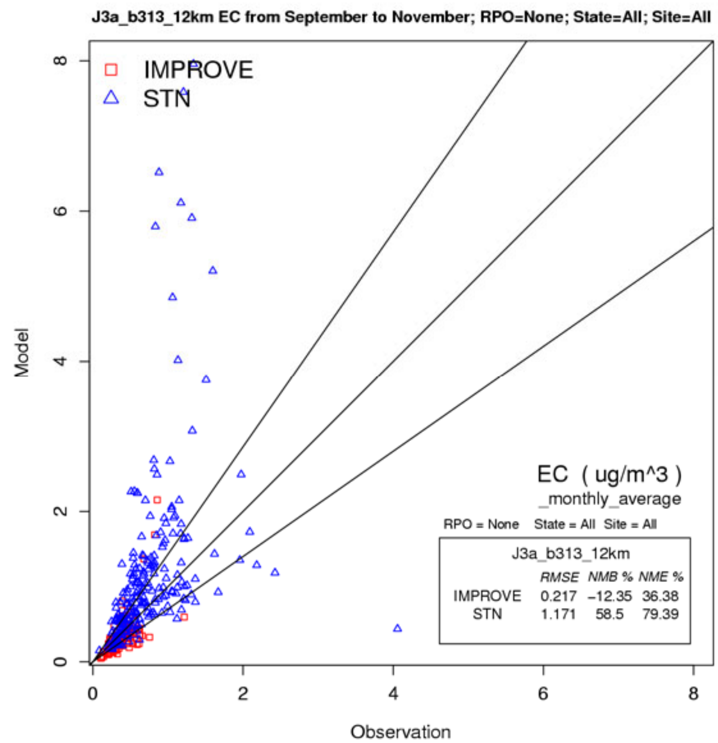
Network	# Obs	Mean Obs	Mean Model	SDEV Obs	SDEV Model	R	RMSE	NMB (%)	NME (%)
IMPROVE	1213	0.37	0.26	0.24	0.24	0.68	0.22	-30.3	43.6
STN	1659	0.52	0.95	0.40	1.08	0.35	1.09	82.6	103

Elemental Carbon - Fall

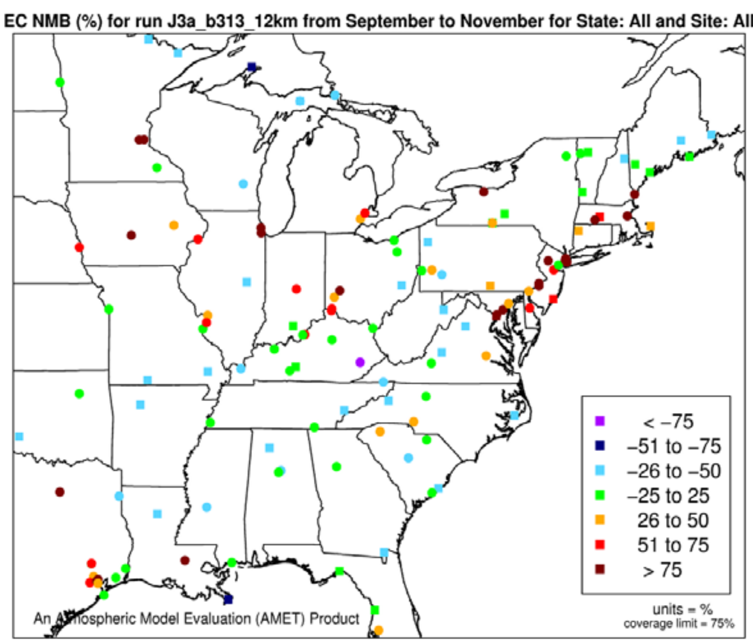
Scatter Plot – All Pairs



Scatter Plot – Monthly Average Pairs

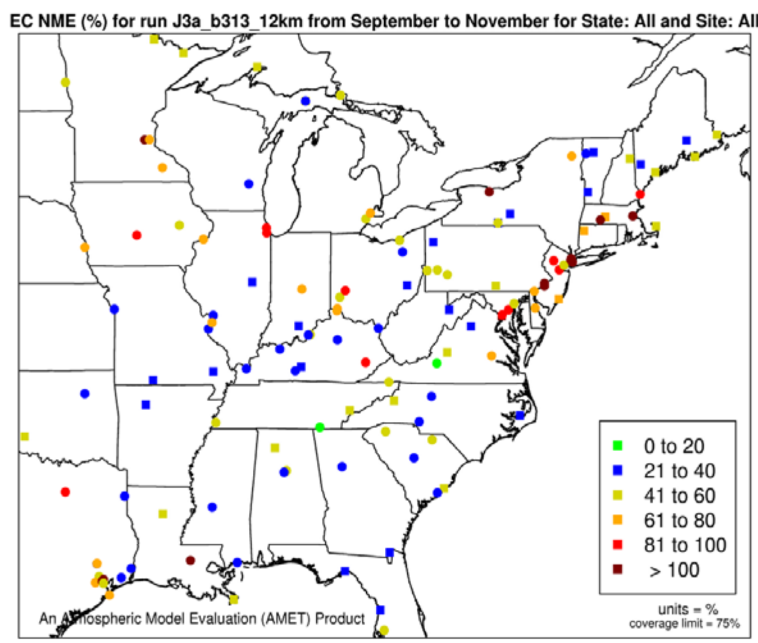


Normalized Mean Bias (%) –Fall



square=IMPROVE; circle=STN;

Normalized Mean Error (%) - Fall

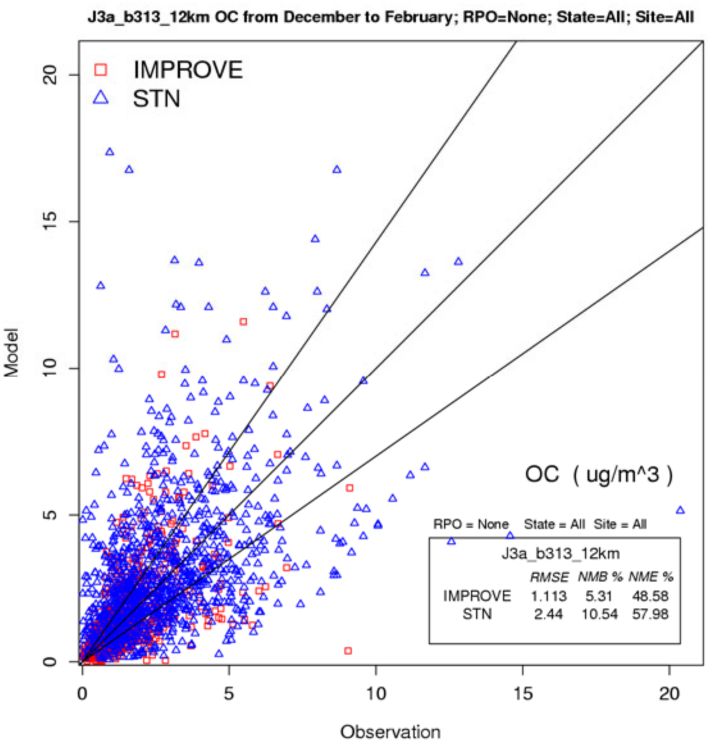


square=IMPROVE; circle=STN;

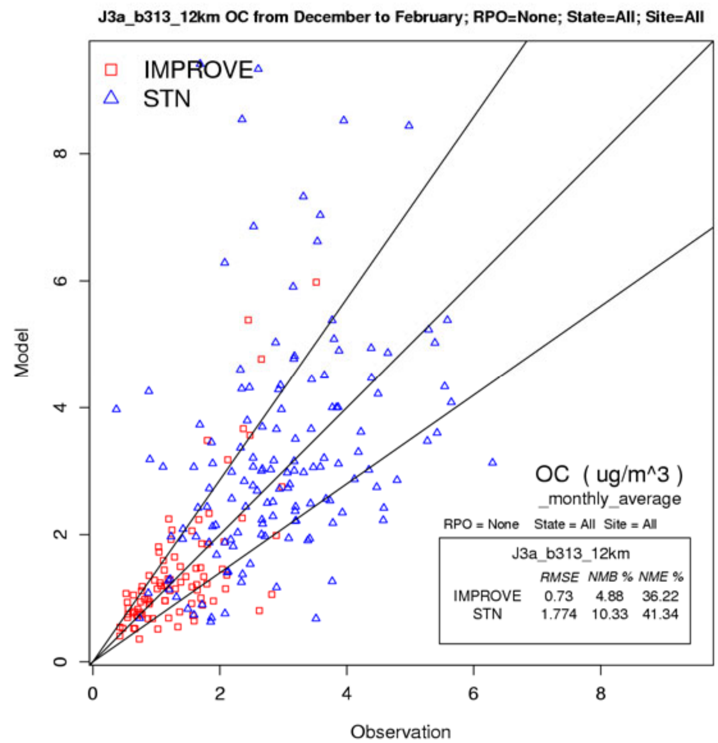
Network	# Obs	Mean Obs	Mean Model	SDEV Obs	SDEV Model	R	RMSE	NMB (%)	NME (%)
IMPROVE	1320	0.38	0.33	0.30	0.36	0.61	0.30	-11.8	45.2
STN	1580	0.72	1.20	0.61	1.49	0.43	1.42	66.4	95.5

Organic Carbon - Winter

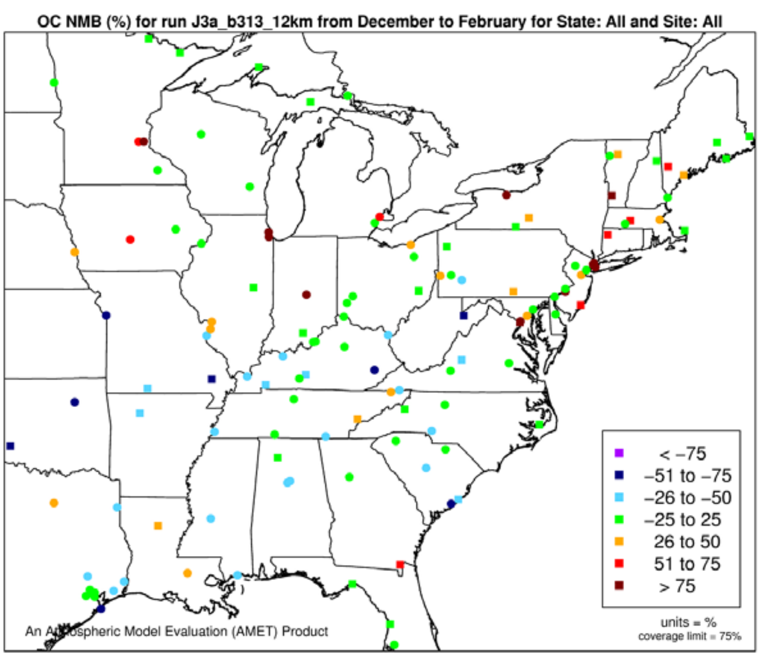
Scatter Plot – All Pairs



Scatter Plot – Monthly Average Pairs

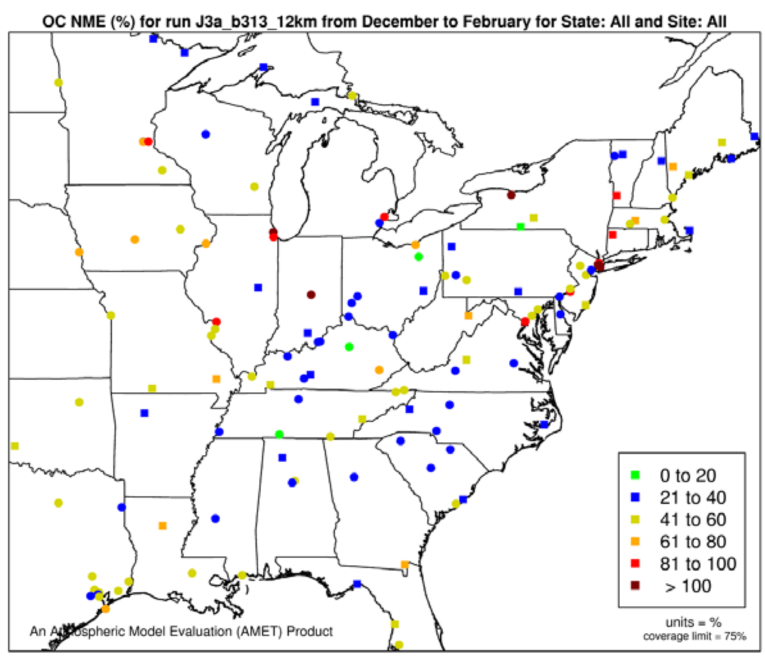


Normalized Mean Bias (%) –Winter



square=IMPROVE; circle=STN;

Normalized Mean Error (%) - Winter

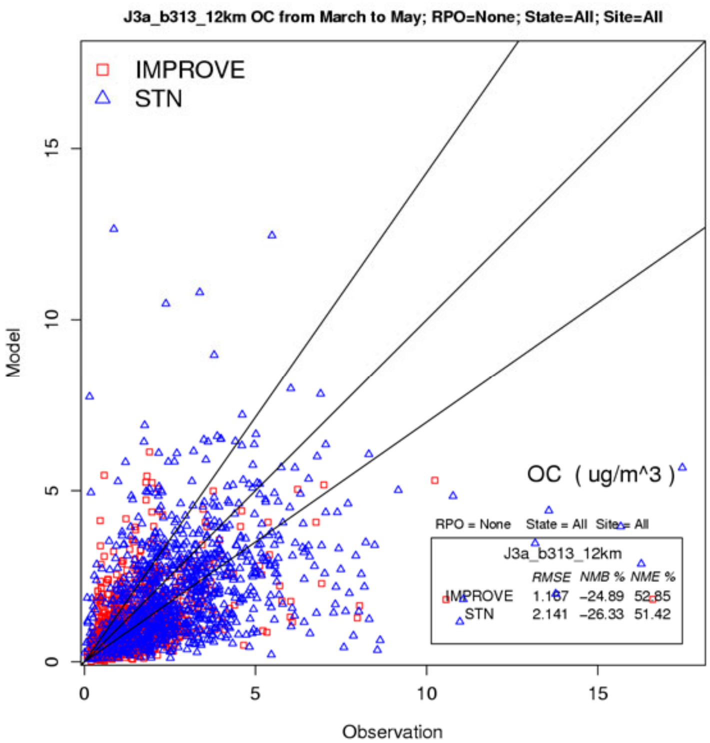


square=IMPROVE; circle=STN;

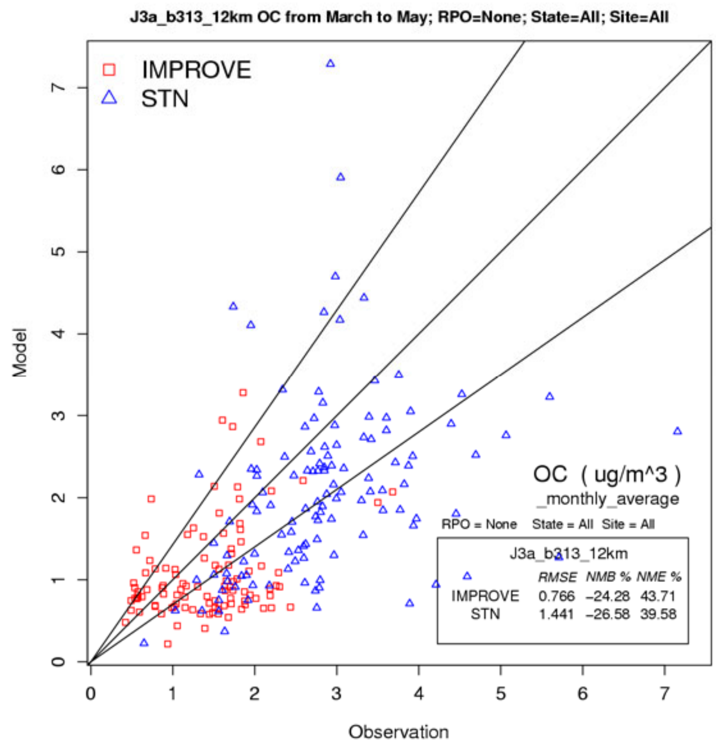
Network	# Obs	Mean Obs	Mean Model	SDEV Obs	SDEV Model	R	RMSE	NMB (%)	NME (%)
IMPROVE	929	1.34	1.41	1.09	1.37	0.61	1.11	5.31	48.6
STN	1012	2.84	3.14	2.10	2.42	0.43	2.44	10.5	58.0

Organic Carbon - Spring

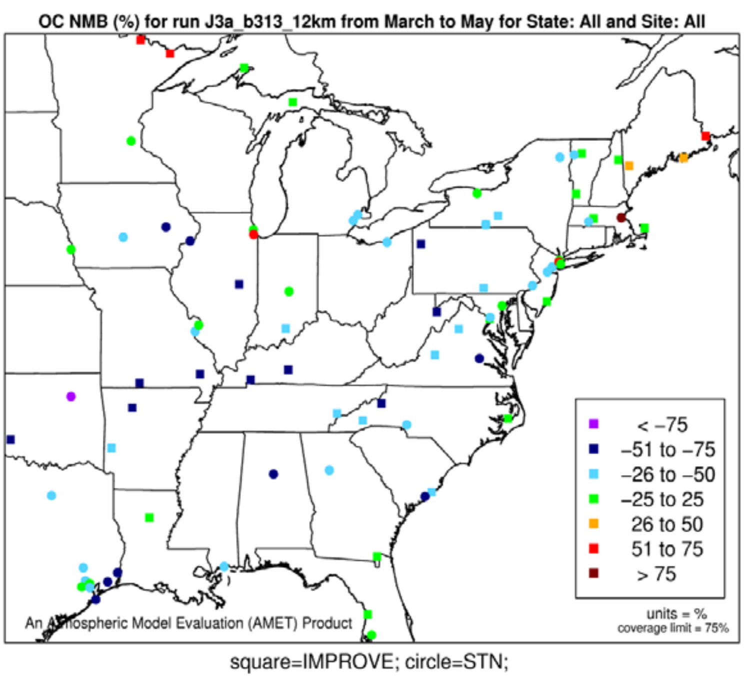
Scatter Plot – All Pairs



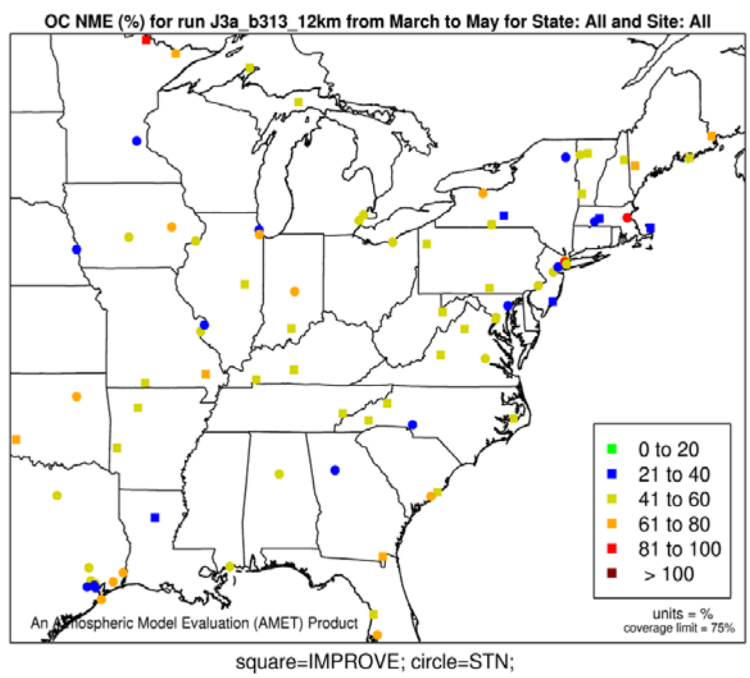
Scatter Plot – Monthly Average Pairs



Normalized Mean Bias (%) –Summer



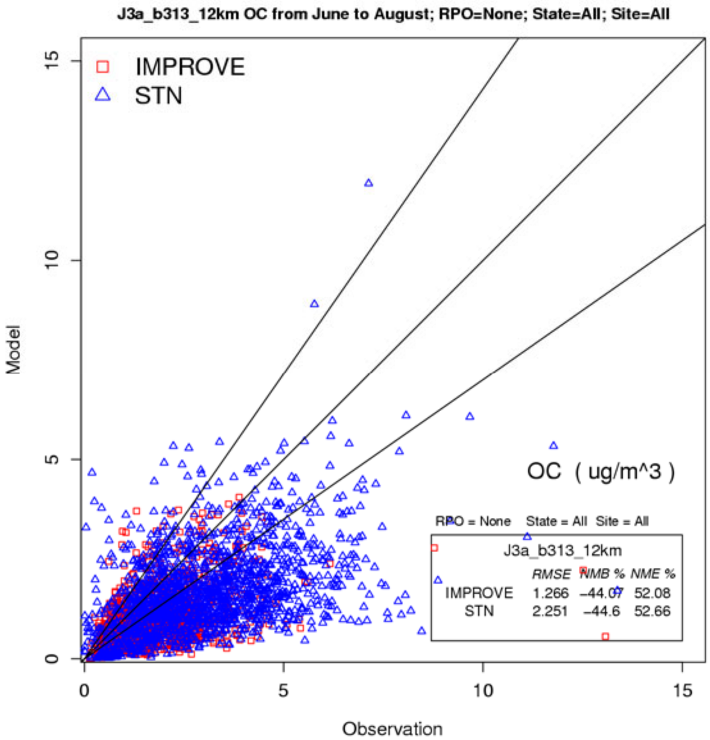
Normalized Mean Error (%) - Summer



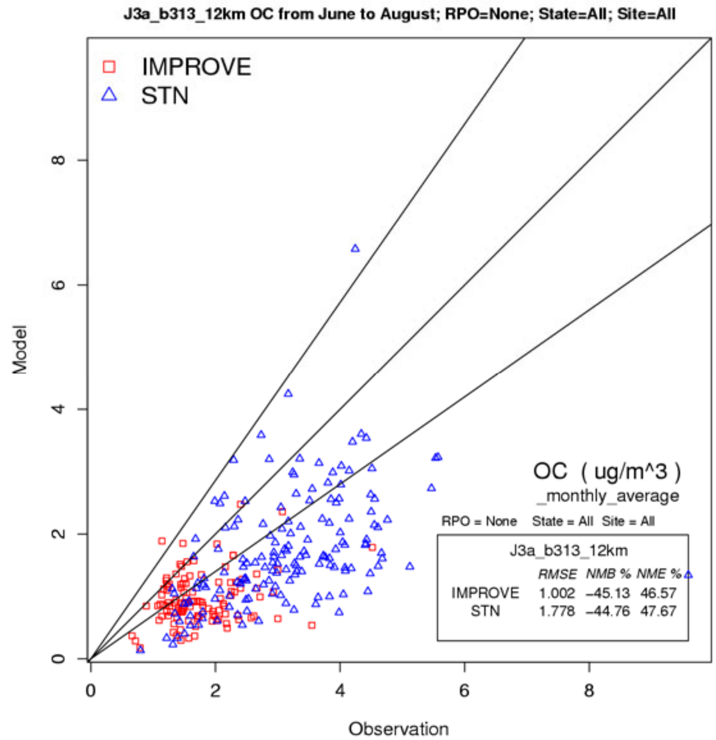
Network	# Obs	Mean Obs	Mean Model	SDEV Obs	SDEV Model	R	RMSE	NMB (%)	NME (%)
IMPROVE	1130	1.41	1.06	1.18	0.89	0.45	1.17	-24.9	52.9
STN	997	2.83	2.09	1.94	1.55	0.36	2.14	-26.3	51.4

Organic Carbon - Summer

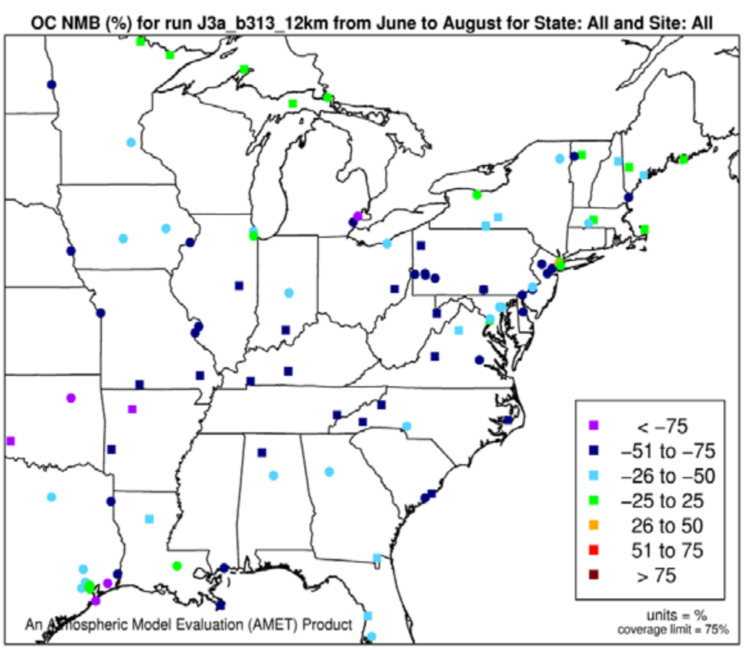
Scatter Plot – All Pairs



Scatter Plot – Monthly Average Pairs

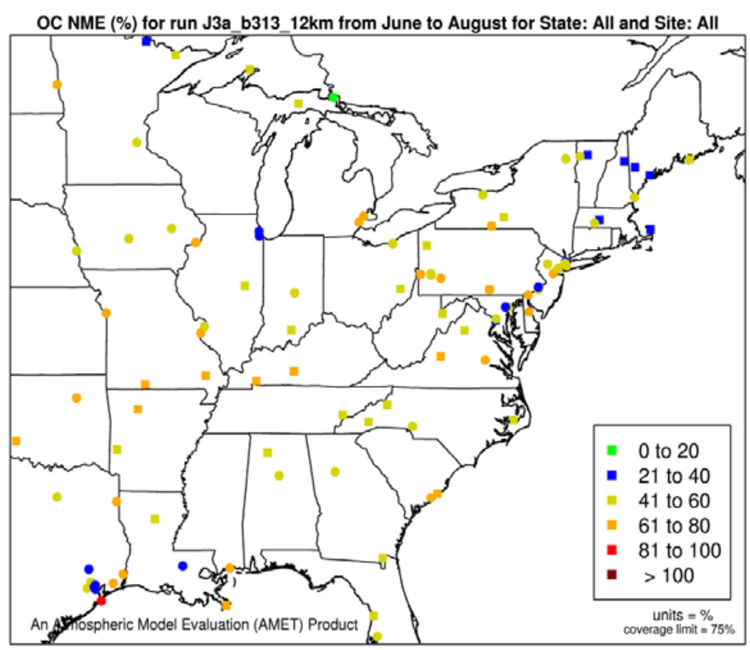


Normalized Mean Bias (%) –Summer



square=IMPROVE; circle=STN;

Normalized Mean Error (%) - Summer



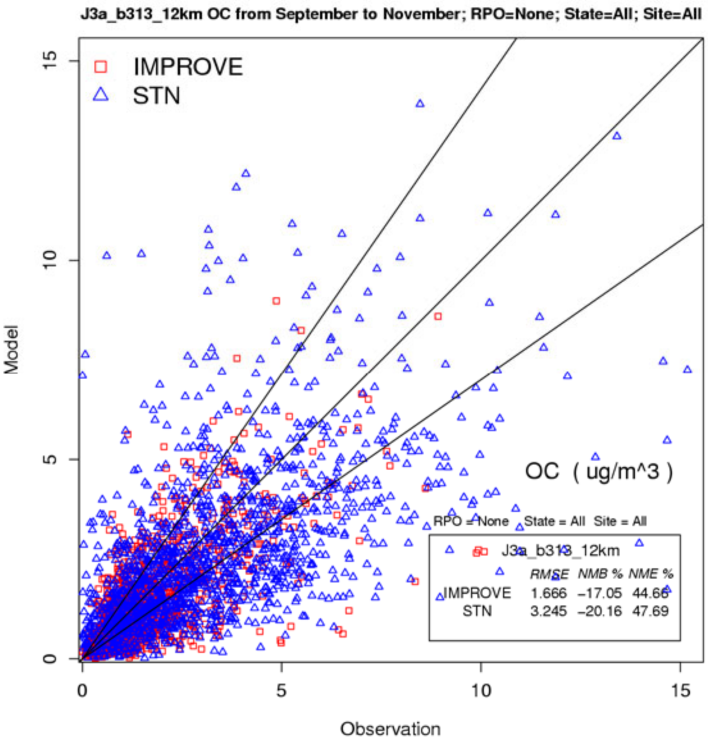
square=IMPROVE; circle=STN;

Network	# Obs	Mean Obs	Mean Model	SDEV Obs	SDEV Model	R	RMSE	NMB (%)	NME (%)
IMPROVE	1216	1.78	0.99	1.07	0.69	0.43	1.27	-44.1	52.1
STN	1629	2.98	1.65	1.95	1.07	0.39	2.25	-44.6	52.7

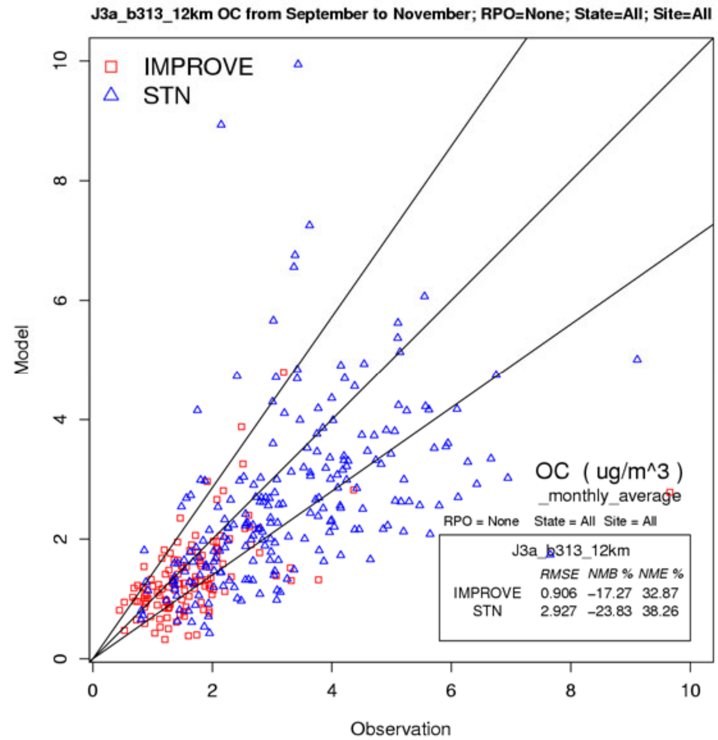
]

Organic Carbon - Fall

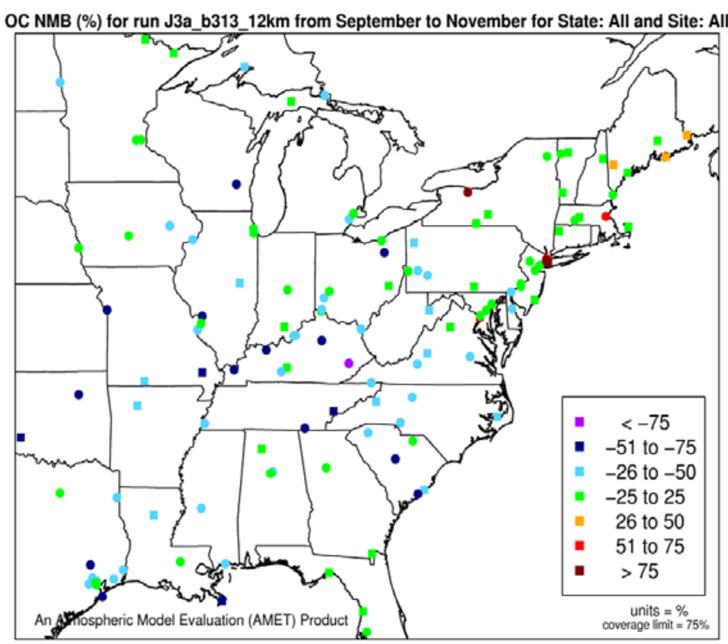
Scatter Plot – All Pairs



Scatter Plot – Monthly Average Pairs

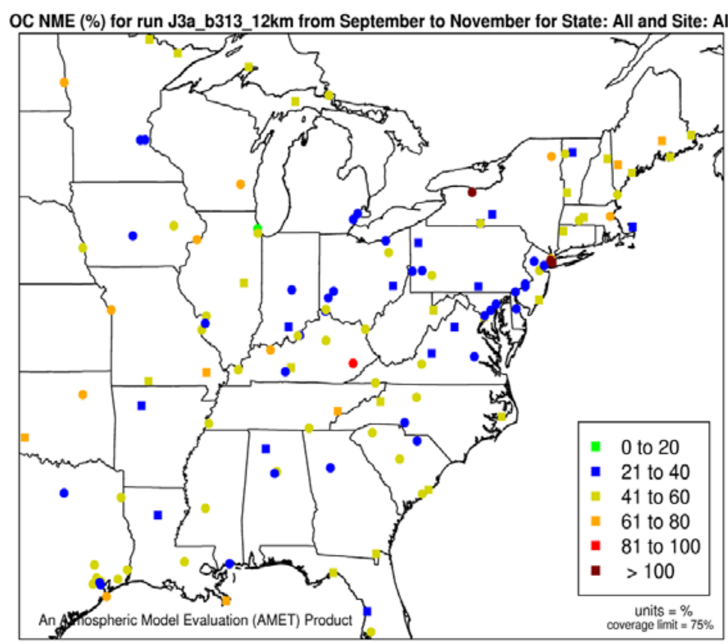


Normalized Mean Bias (%) –Summer



square=IMPROVE; circle=STN;

Normalized Mean Error (%) - Summer



square=IMPROVE; circle=STN;

Network	# Obs	Mean Obs	Mean Model	SDEV Obs	SDEV Model	R	RMSE	NMB (%)	NME (%)
IMPROVE	1319	1.68	1.39	1.95	1.23	0.55	1.67	-17.1	44.7
STN	1526	3.30	2.63	3.39	2.09	0.41	3.24	-20.3	47.6

Evaluation of CMAQ version 4.5: 12km×12km Eastern United States Total $PM_{2.5}$ Mass

Available Networks:

IMPROVE – Total PM2.5 Mass
STN – Total PM2.5 Mass

Total $PM_{2.5}$ Mass Performance: Introduction

The list below covers the plots and metrics available for the total $PM_{2.5}$ mass analysis for each of the four seasons (winter, spring, summer, fall). Monthly box plots (covering the entire year) are provided, which show the 25% and 75% quartiles (shading) and the median values (lines) for model and observation concentrations. Two scatter plots are provided, one showing all model-observation pairs (and corresponding statistics) and one showing monthly averaged model-observation pairs (with corresponding statistics). Spatial plots of NMB(%) and NME(%), along with a table of statistics are also provided. Where applicable, multiple networks are plotted on each scatter plot and spatial plot. Legends are provided on each plot to help identify each network.

- Monthly box plots (covering the entire year) showing 25% and 75% quartiles and median values
- Seasonal model to observation scatter plot of various species using all pairs
- Seasonal model to observation scatter plot of various species using monthly averaged pairs
- Spatial plots of NMB (%) and NME (%) of various species
- Table of select statistical metrics for various species

The monthly box plots are provided to show the variability in monthly performance for each specie and network. Sulfate is generally under-predicted for the first half of the year and over-predicted for the last half of the year. Nitrate is over-predicted in the cooler months and under-predicted in the warmer months (although concentrations are relatively low). Ammonium is over-predicted throughout the year at STN sites, while at CASTNet sites there is a slight over-prediction for the cooler months and an under-prediction in the warmer months. Elemental carbon throughout the year is consistently over-predicted at STN sites and under-predicted at IMPROVE sites. Organic carbon is generally under-predicted throughout the year at both IMPROVE and STN sites. $PM_{2.5}$ performance varies throughout the year, with over-predictions for several months, under-predictions for several months and nearly unbiased performance for several months.

Note that for comparison of organic carbon, the complete unit is μgC/m^3, although on plots the units are labeled as μg/m^3.

Total $PM_{2.5}$ Mass Performance: Summary

Winter Season (December, January and February)

Total $PM_{2.5}$ mass is over-predicted for the winter season, with a NMB of 30.0%, NME of 49.5% and a correlation of 0.67 for IMPROVE sites and a NMB of 46.3%, NME of 67.2% and a correlation of 0.57 for STN sites. Mean observed concentrations of $PM_{2.5}$ are roughly twice as high for STN sites as IMPROVE sites, implying the differences between the urban STN and rural IMPROVE network. $PM_{2.5}$ performance tends to be slightly worse in the Northeast as compared to the rest of the domain.

Spring Season (March, April and May)

Total $PM_{2.5}$ mass performance is mixed for the spring season, with an slight under-prediction for the IMPROVE network (NMB = -9.51, NME = 37.8%, R = 0.65) and a slight over-prediction for STN (NMB = 10.4%, NME = 49.2%, R = 0.50). The mean observed concentration of $PM_{2.5}$ mass for STN is about 40% higher than the mean observed PM2.5 for IMPROVE.

Summer Season (June, July and August)

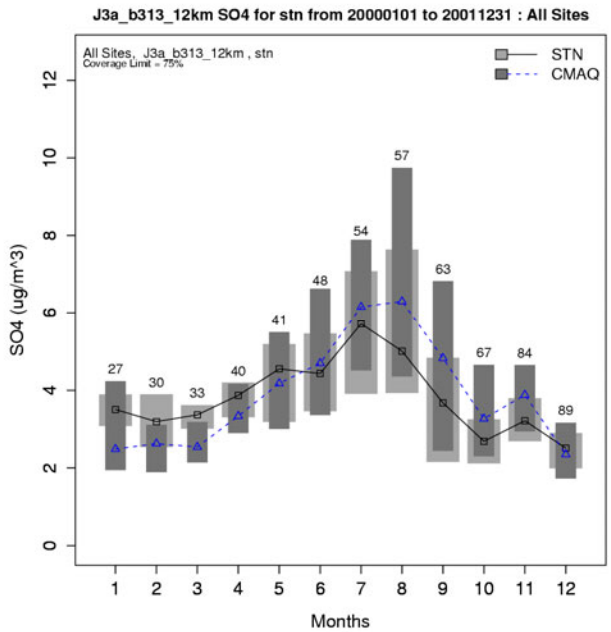
Total $PM_{2.5}$ mass is under-predicted for the summer season, with IMPROVE showing a moderate under-prediction (NMB = -24.1%, NME = 33.7%, R = 0.79) and STN showing a slight under-prediction (NMB = -4.14%, NME = 35.6%, R = 0.68). Mean observed concentrations of $PM_{2.5}$ mass for STN is about 18% higher than that of IMPROVE. Spatially, performance was consistent throughout the majority of the modeled domain.

Fall Season (September, October and November)

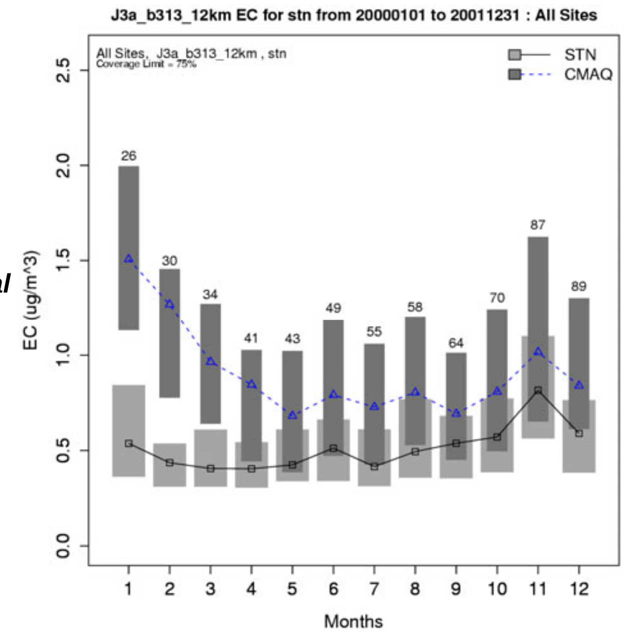
Total $PM_{2.5}$ mass is over-predicted for the winter season, with a NMB of 21.2%, NME of 42.7% and correlation of 0.79 for IMPROVE and a NMB of 38.9%, NME of 57.0% and correlation of 0.66 for STN. Mean observed concentrations of $PM_{2.5}$ mass for STN is about 53% higher than that of IMPROVE. Spatially, performance was slightly worse in the Northeast and Ohio Valley regions when compared to the rest of the modeled domain.

STN Network Monthly Box Plots

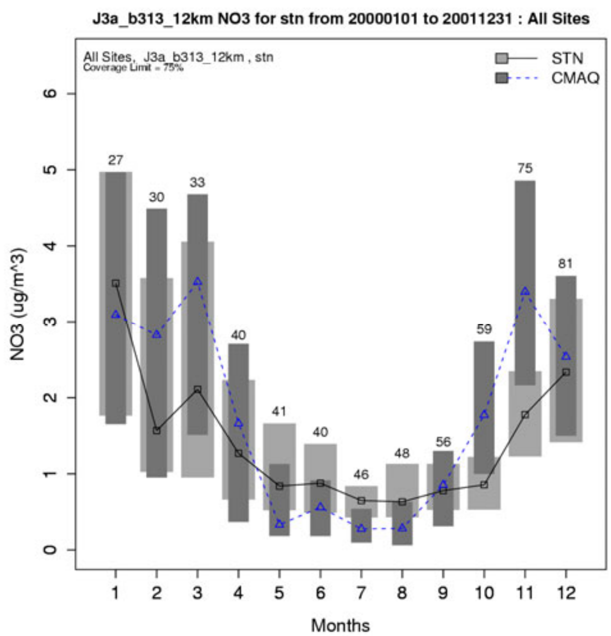
Sulfate



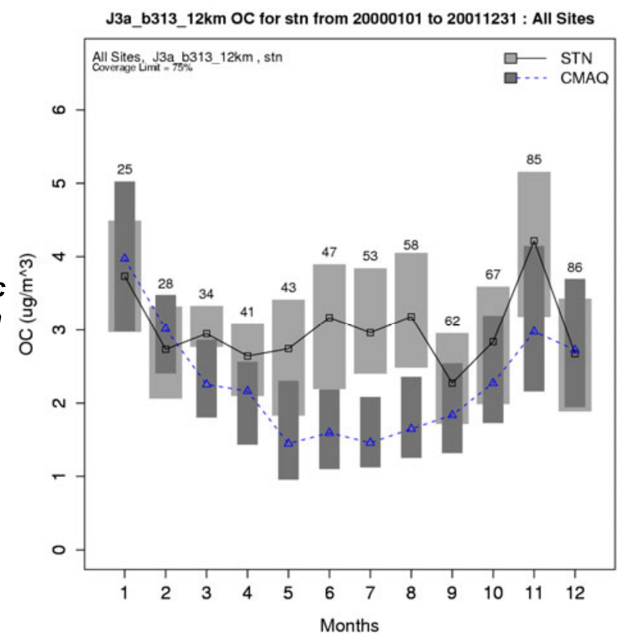
Elemental Carbon



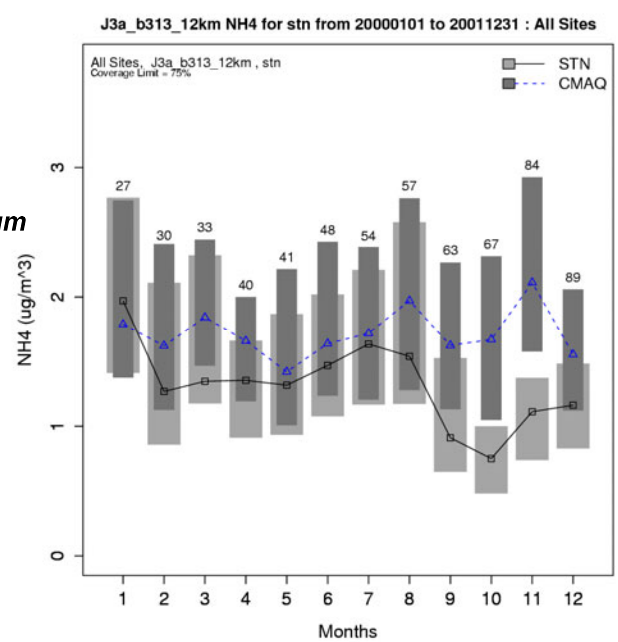
Nitrate



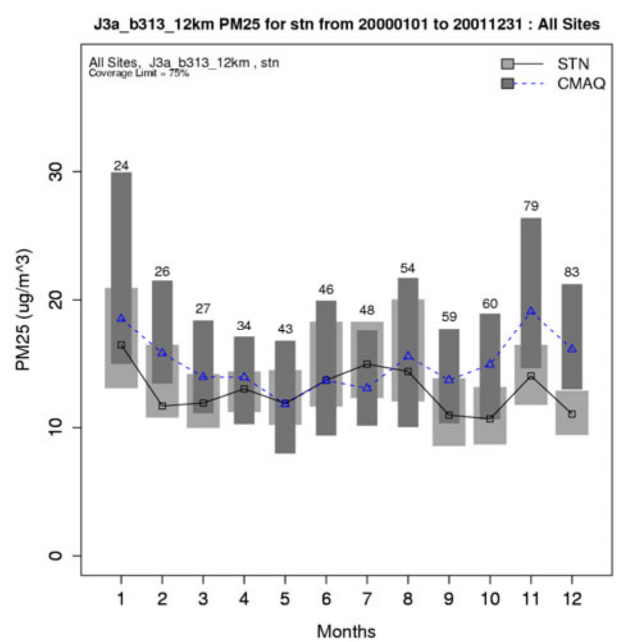
Organic Carbon



Ammonium

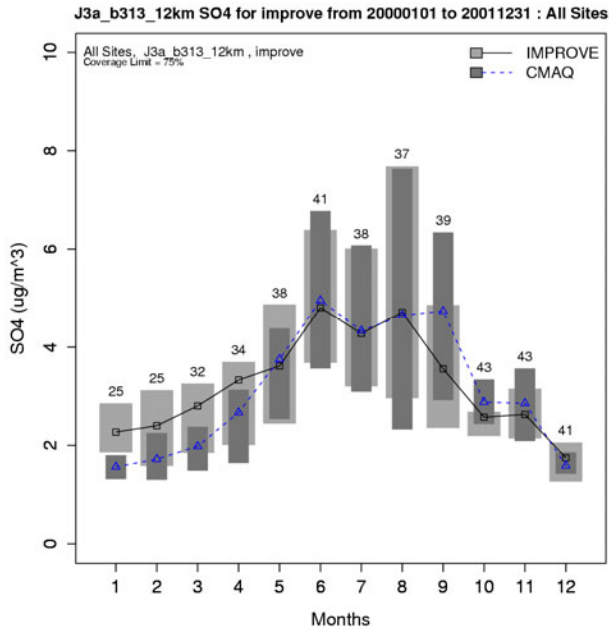


$PM_{2.5}$

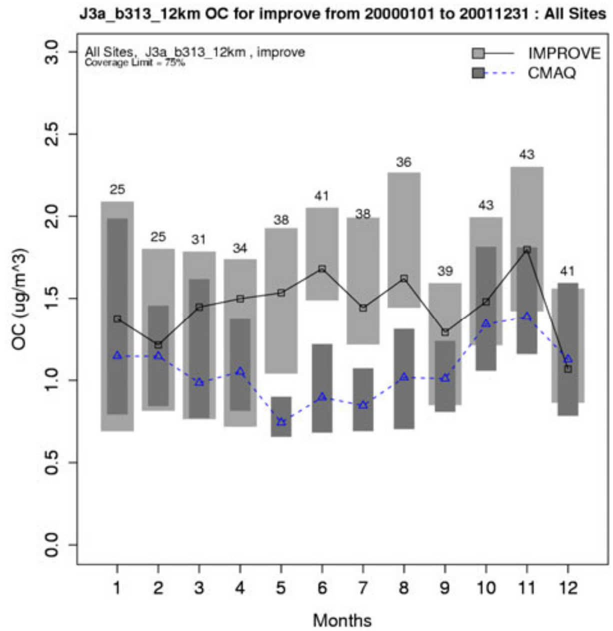


IMPROVE Network Monthly Box Plots

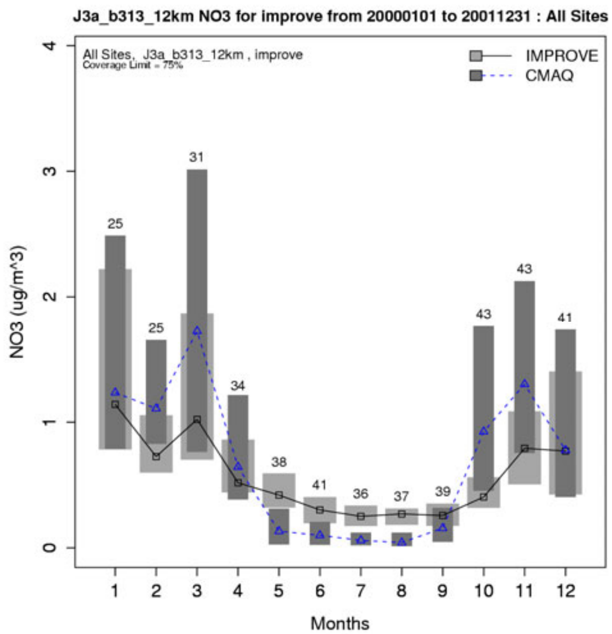
Sulfate



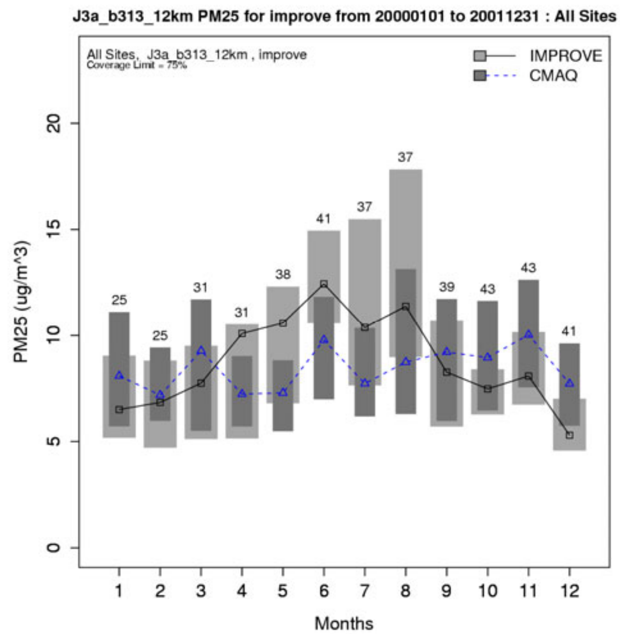
Organic Carbon



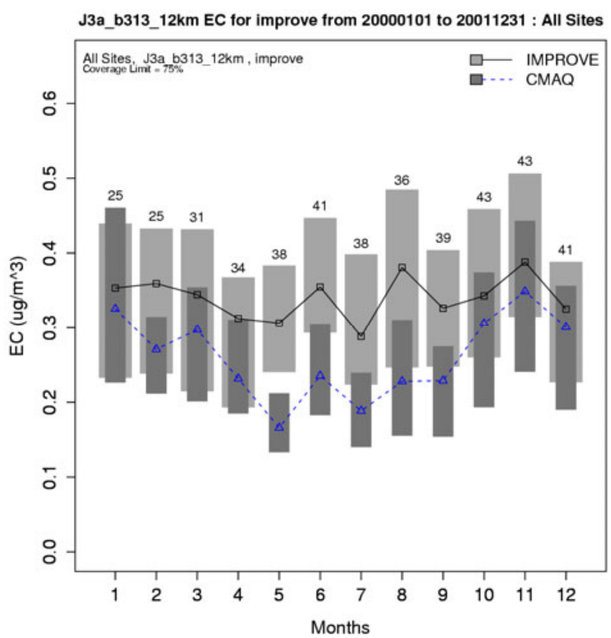
Nitrate



$PM_{2.5}$

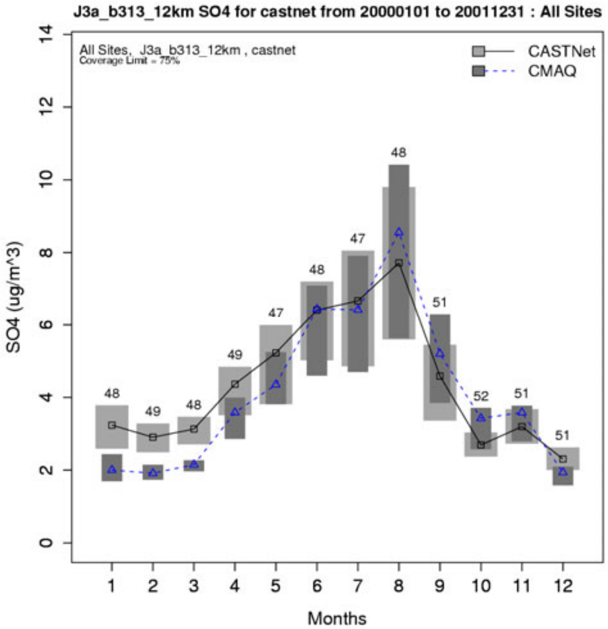


Elemental Carbon

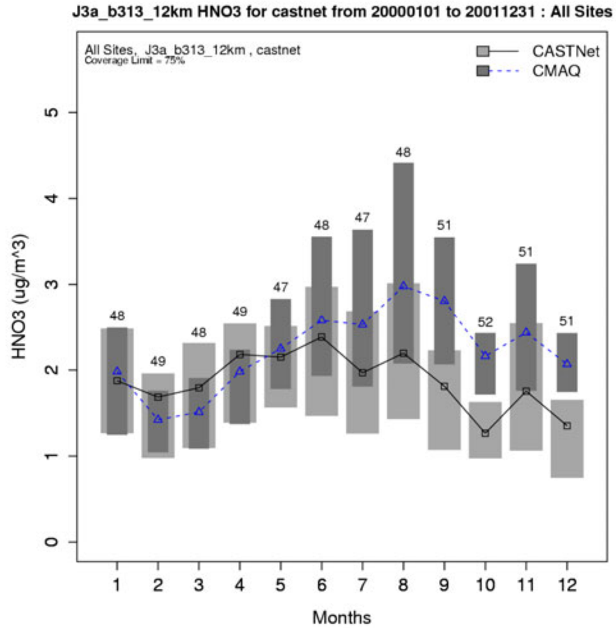


CASTNet Network Monthly Box Plots

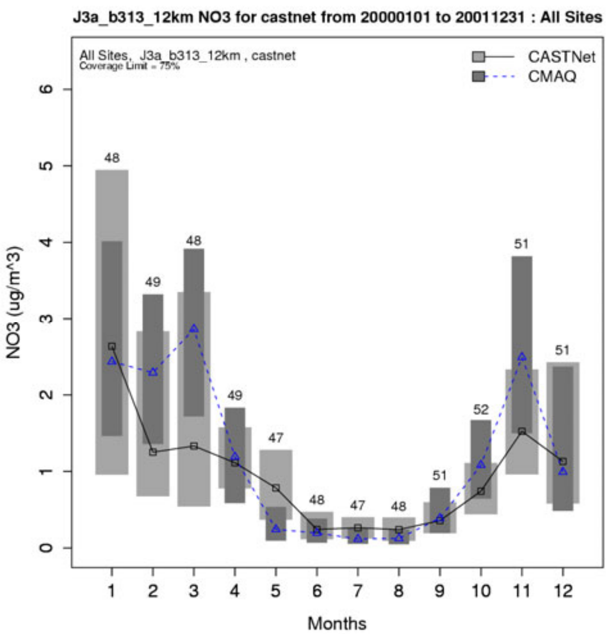
Sulfate



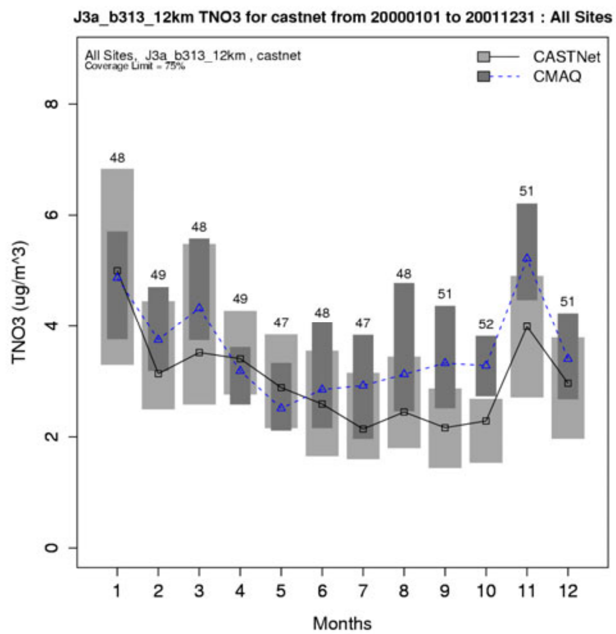
Nitric Acid



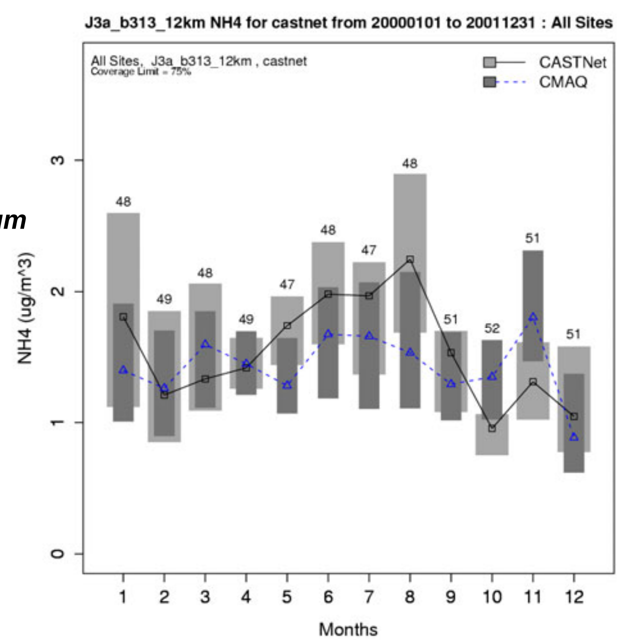
Nitrate



Total Nitrate

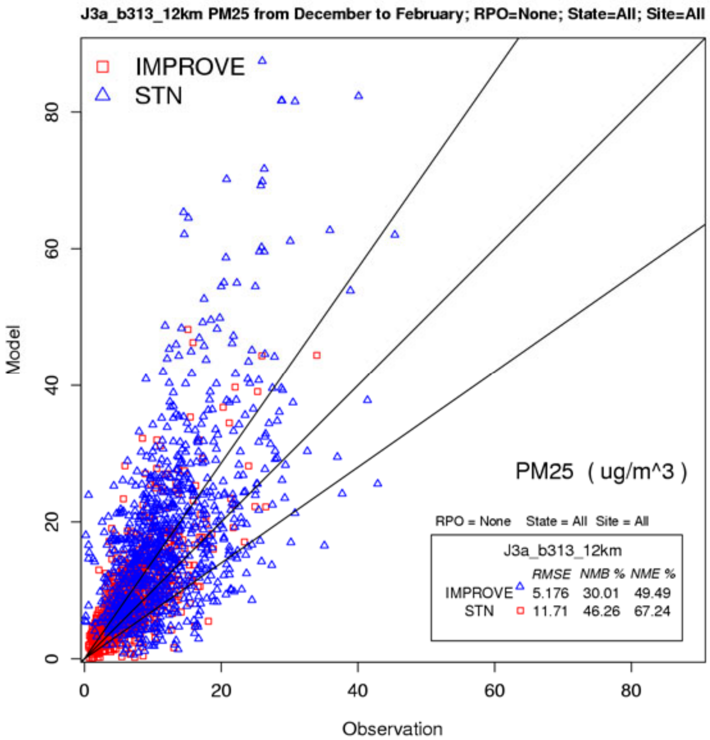


Ammonium

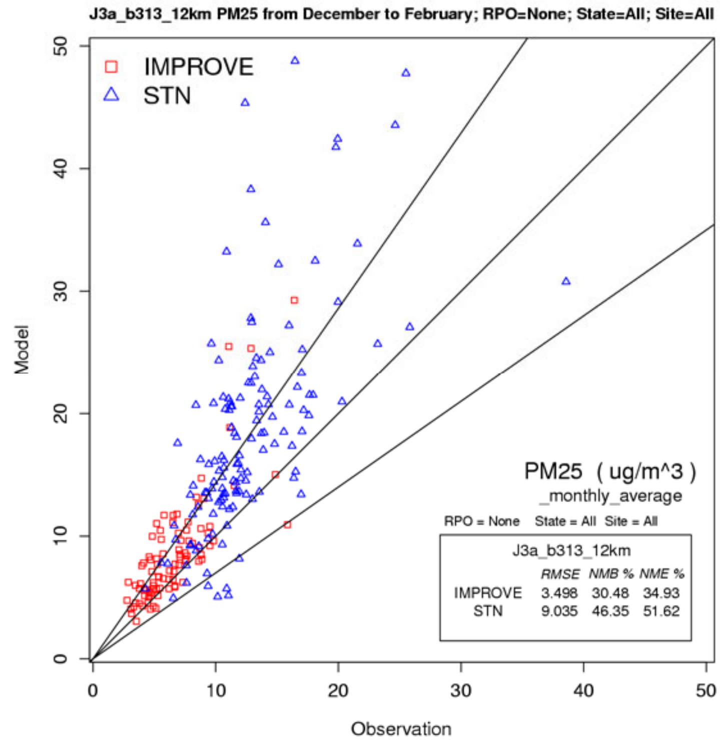


Total $PM_{2.5}$ - Winter

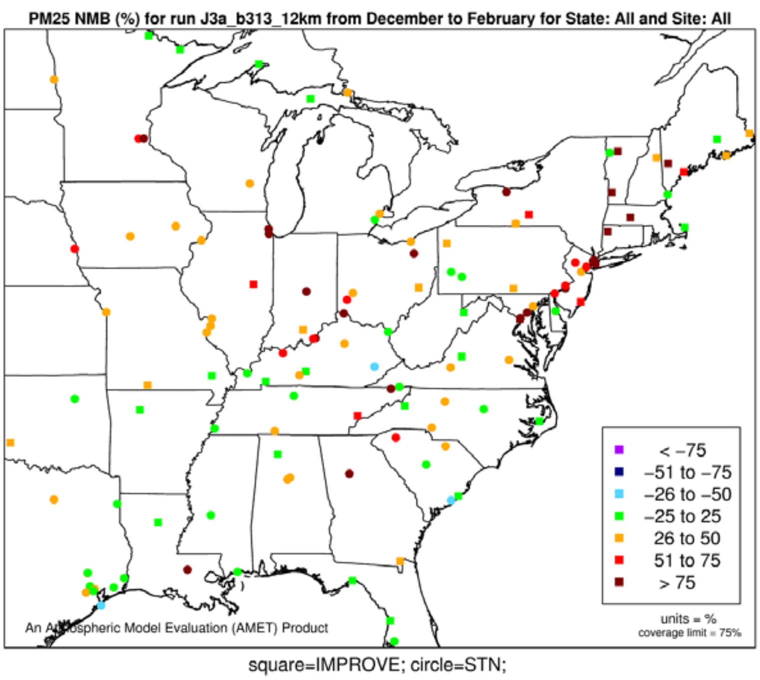
Scatter Plot – All Pairs



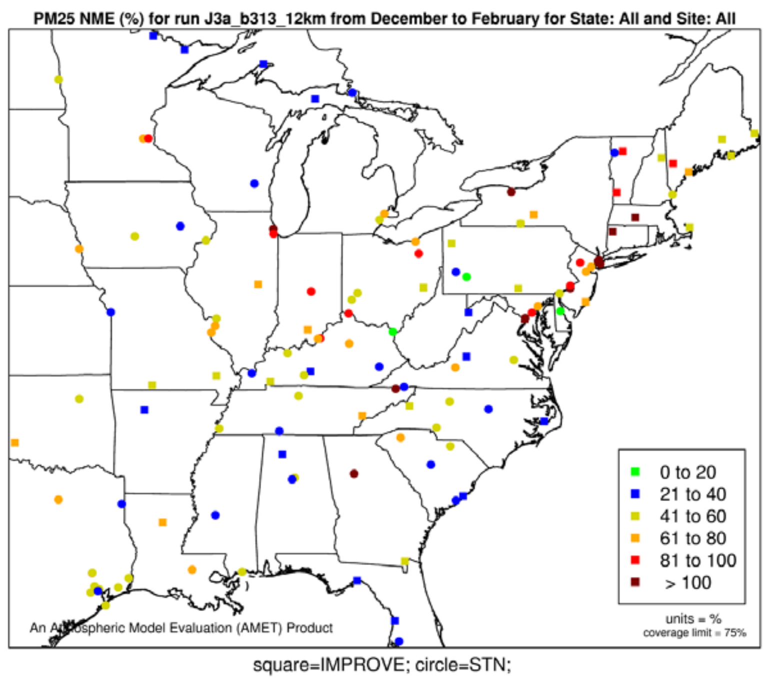
Scatter Plot – Monthly Average Pairs



Normalized Mean Bias (%) –Winter



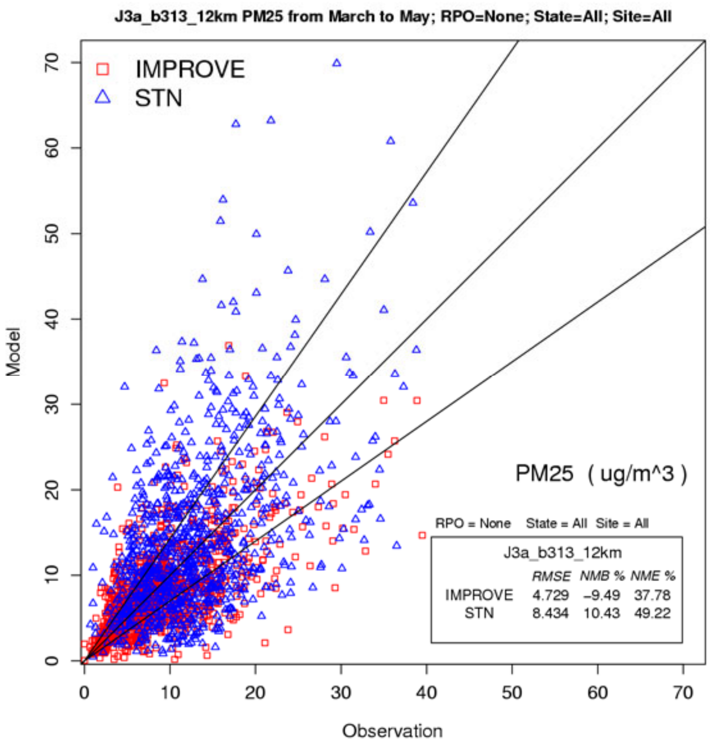
Normalized Mean Error (%) - Winter



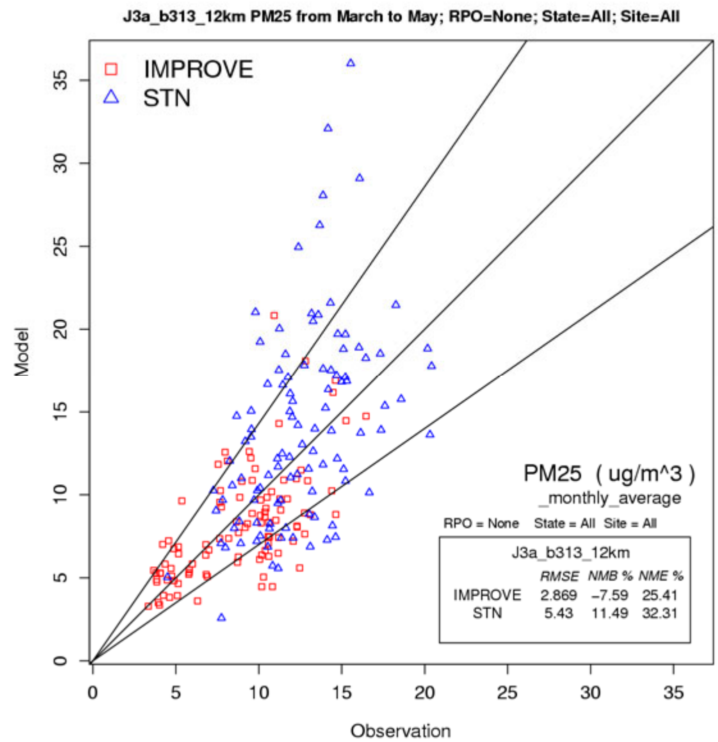
Network	# Obs	Mean Obs	Mean Model	SDEV Obs	SDEV Model	R	RMSE	NMB (%)	NME (%)
IMPROVE	927	6.55	8.52	4.60	6.42	0.67	5.18	30.0	49.5
STN	966	12.1	17.7	6.86	12.5	0.57	11.7	46.3	67.2

Total $PM_{2.5}$ - Spring

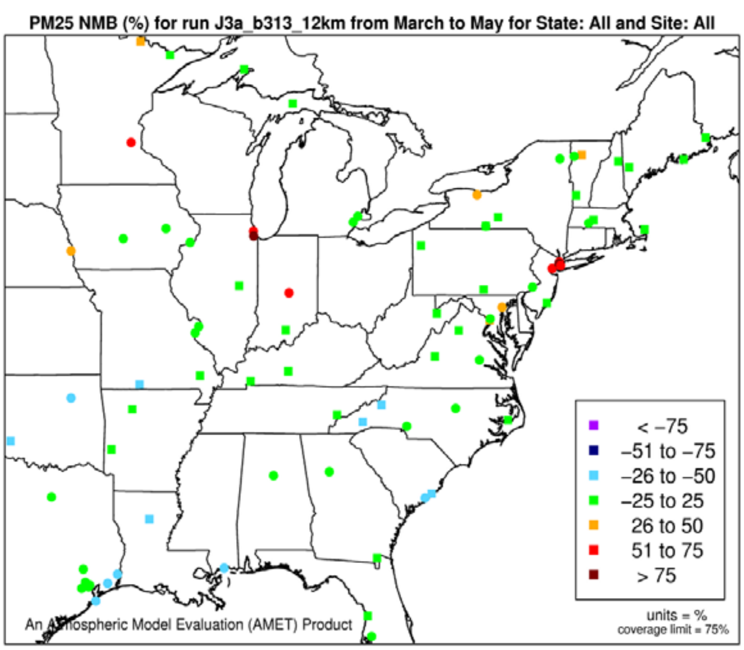
Scatter Plot – All Pairs



Scatter Plot – Monthly Average Pairs

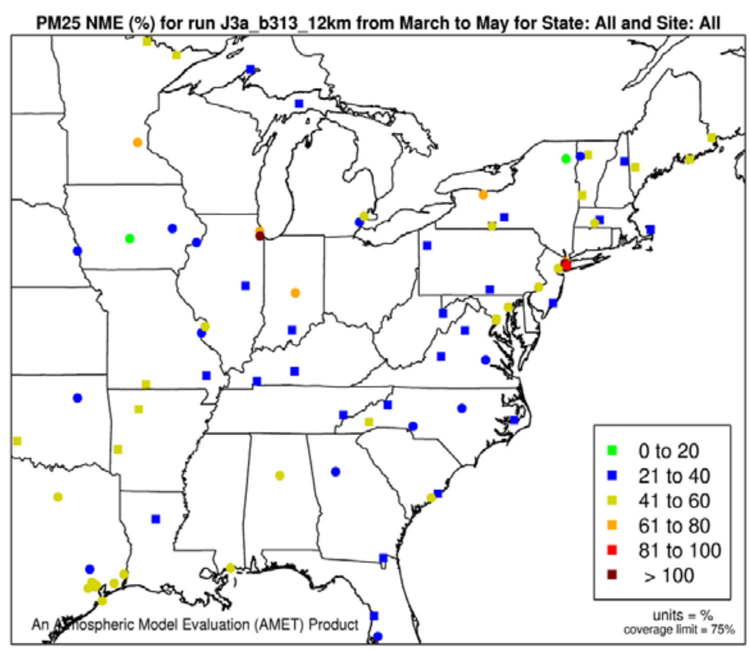


Normalized Mean Bias (%) –Spring



square=IMPROVE; circle=STN;

Normalized Mean Error (%) - Spring

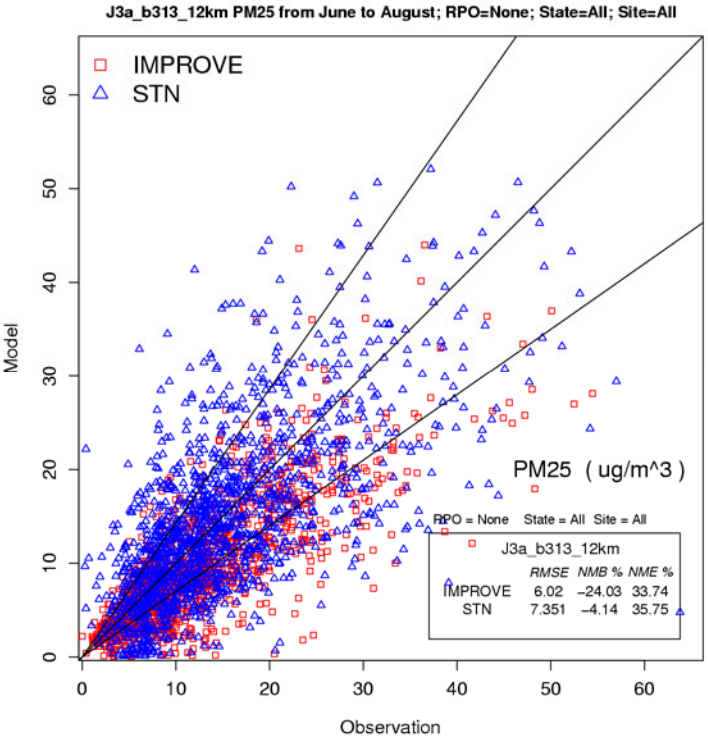


square=IMPROVE; circle=STN;

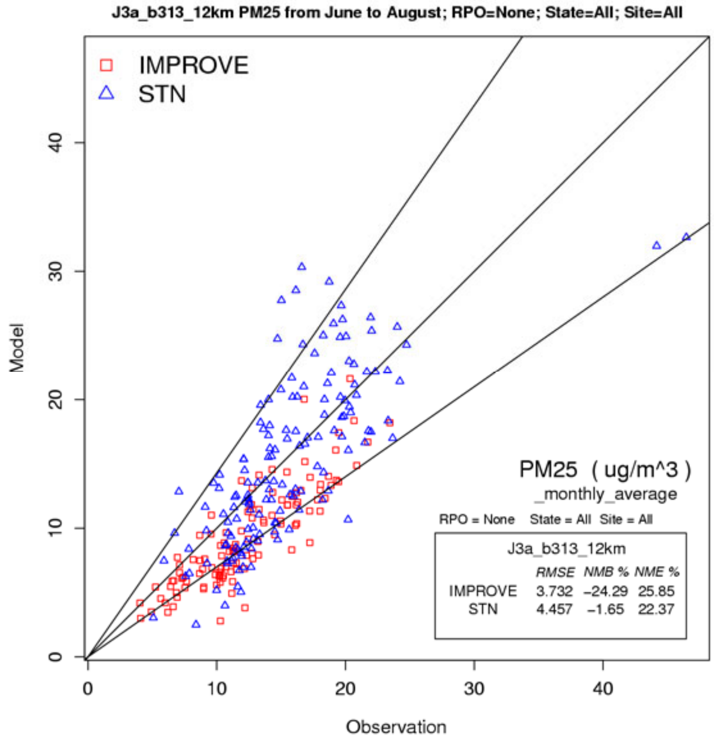
Network	# Obs	Mean Obs	Mean Model	SDEV Obs	SDEV Model	R	RMSE	NMB (%)	NME (%)
IMPROVE	1112	8.77	7.94	5.85	5.26	0.65	4.73	-9.51	37.8
STN	922	12.5	13.8	6.48	9.40	0.50	8.43	10.4	49.2

Total $PM_{2.5}$ - Summer

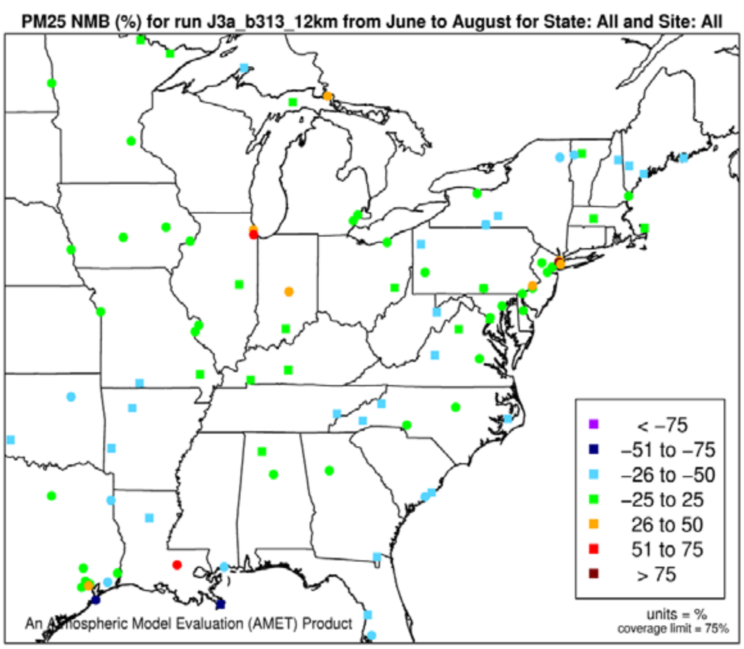
Scatter Plot – All Pairs



Scatter Plot – Monthly Average Pairs

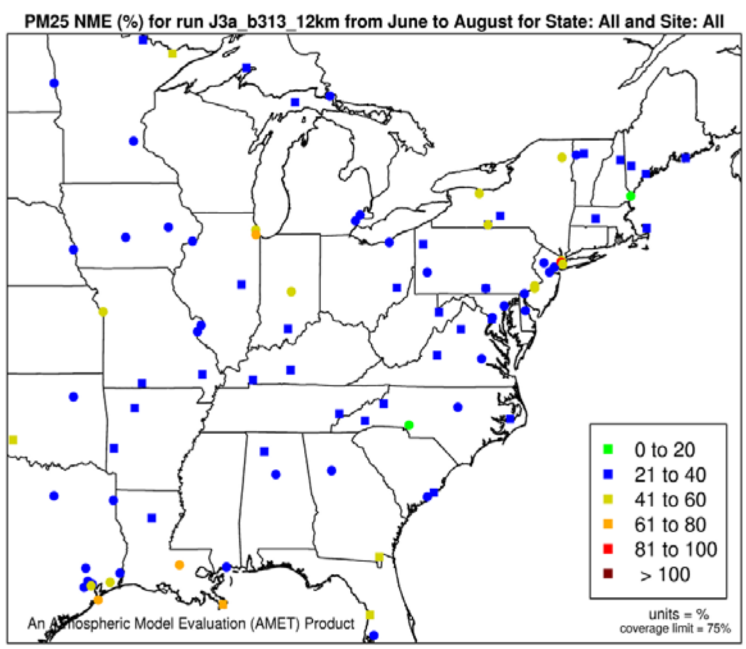


Normalized Mean Bias (%) –Summer



square=IMPROVE; circle=STN;

Normalized Mean Error (%) - Summer

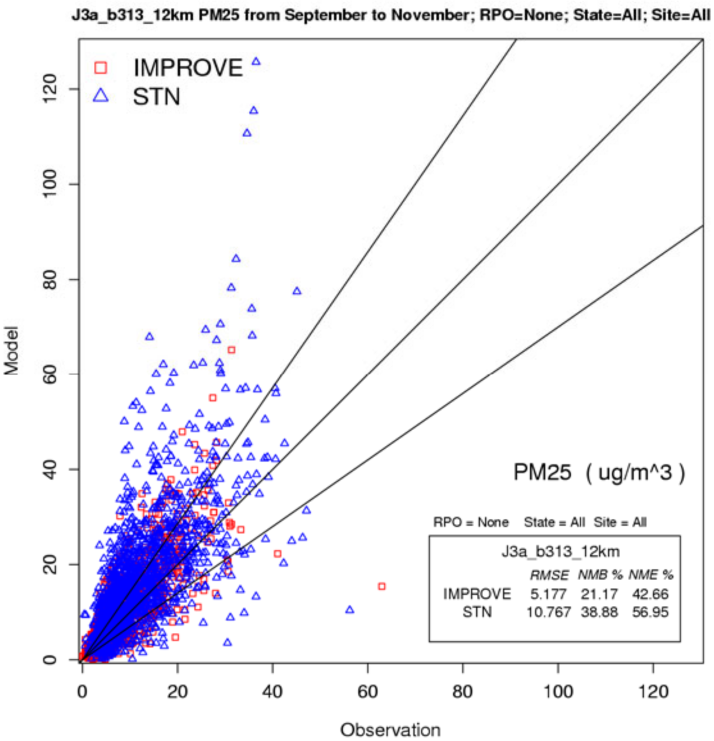


square=IMPROVE; circle=STN;

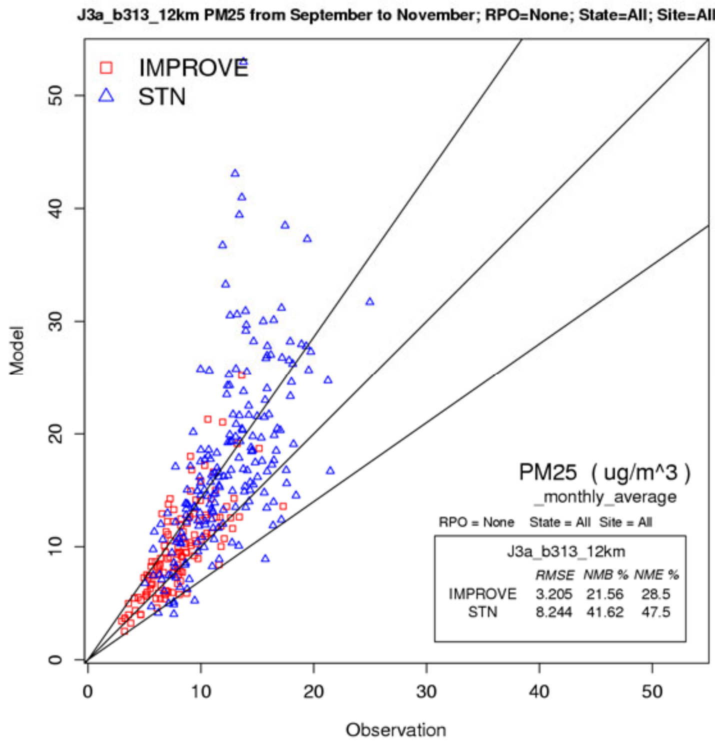
Network	# Obs	Mean Obs	Mean Model	SDEV Obs	SDEV Model	R	RMSE	NMB (%)	NME (%)
IMPROVE	1205	12.6	9.60	8.49	6.72	0.79	6.02	-24.1	33.7
STN	1485	14.9	14.3	9.01	9.12	0.68	7.35	-4.14	35.6

Total $PM_{2.5}$ - Fall

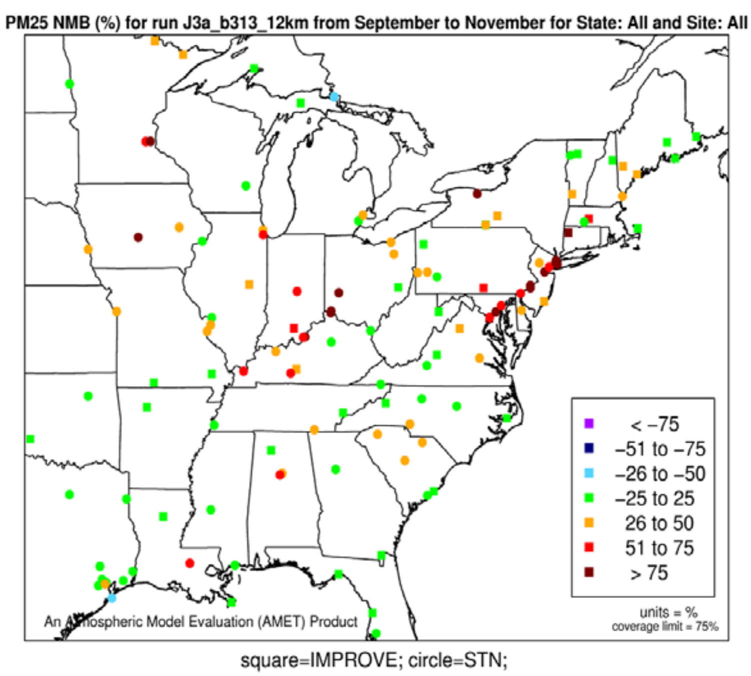
Scatter Plot – All Pairs



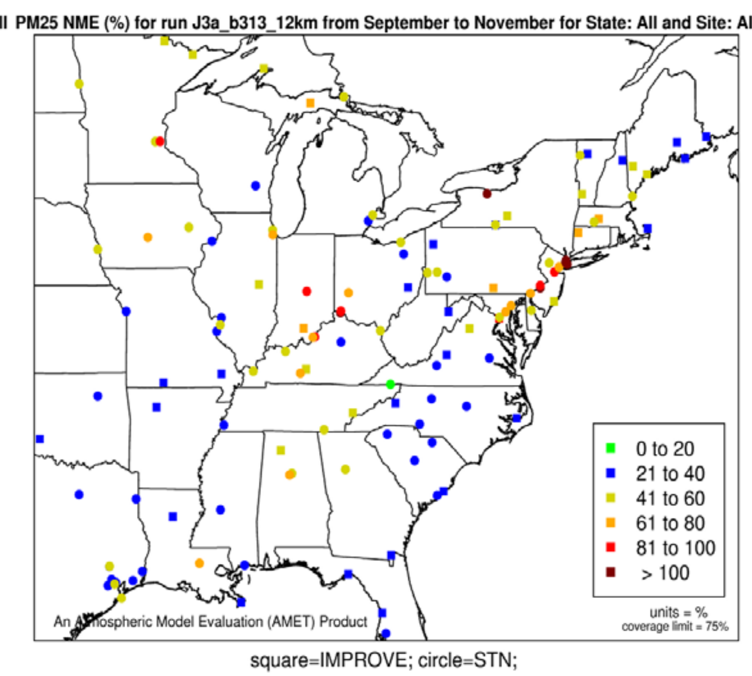
Scatter Plot – Monthly Average Pairs



Normalized Mean Bias (%) –Fall



Normalized Mean Error (%) - Fall



Network	# Obs	Mean Obs	Mean Model	SDEV Obs	SDEV Model	R	RMSE	NMB (%)	NME (%)
IMPROVE	1308	8.03	9.73	6.14	7.92	0.79	5.18	21.2	42.7
STN	1444	12.3	17.1	7.95	12.9	0.66	10.7	38.9	57.0

Evaluation of CMAQ version 4.5: 12km×12km Eastern United States Wet Deposition Sulfate (SO_4^{2-}), Nitrate (NO_3^-), Ammonium (NH_4^+)

Available Networks:

NADP – SO_4^{2-}, $NO3^-$, $NH4^+$ and precipitation

Precipitation Chemistry Performance: Introduction

Box plots of sulfate, nitrate, ammonium and precipitation are provided. These box plots show the monthly 25% to 75% quartiles (shading) and median values (points and lines) for NADP network observed and model predicted values for each species. The list below covers the plots and metrics available for the precipitation chemistry analysis for each of the four seasons (winter, spring, summer, fall). Two scatter plots are provided, one showing all model-observation pairs (and corresponding statistics) and one showing monthly averaged model-observation pairs (with corresponding statistics). Spatial plots of NMB(%) and NME(%), along with a table of statistics are also provided.

- Monthly box plots (covering the entire year) showing 25% and 75% quartiles and median values
- Seasonal model to observation scatter plot of various species using all pairs
- Seasonal model to observation scatter plot of various species using monthly averaged pairs
- Spatial plots of NMB (%) and NME (%) of various species
- Table of select statistical metrics for various species

Precipitation Chemistry Performance: Summary

Winter Season (December, January and February)

Wet deposition sulfate is slightly over-predicted for the winter, with a NMB of 3.74%, NME of 65.5% and correlation of 0.72. Wet deposition nitrate is moderately over-predicted, with a NMB of 15.6%, NME of 63.8% and correlation of 0.60. Spatially, wet deposition nitrate performance was slightly better in the Northeast when compared to the rest of the domain. Wet deposition ammonium is under-predicted, with a NMB of -23.8%, NME of 63.7% and correlation of 0.43. Precipitation performance at the NADP sites for the winter season is fairly good, with a slight under-prediction (NMB of -6.65%), NME of 42.1% and correlation of 0.83.

Spring Season (March, April and May)

Wet deposition sulfate is slightly under-predicted for the spring, with a NMB of -6.43%, NME of 54.1% and correlation of 0.67. Wet deposition nitrate is under-predicted, with a NMB of -29.5%, NME of 52.7% and correlation of 0.59. Wet deposition ammonium is also under-predicted, with a NMB of -33.0%, NME of 56.0% and correlation of 0.60. Precipitation is slightly under-predicted for the spring season (NMB = -5.26%) and NME of 54.7% (correlation = 0.67).

Summer Season (June, July and August)

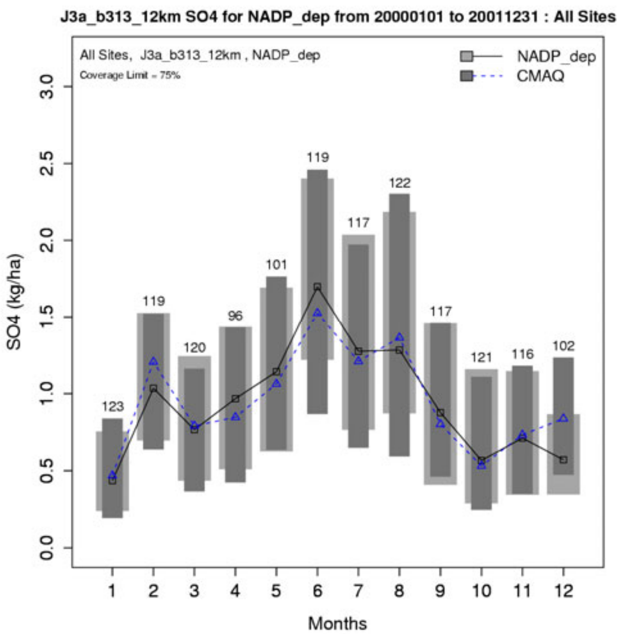
Wet deposition sulfate is again slightly under-predicted for the summer, with a NMB of -5.50% and NME of 70.2%. Wet deposition nitrate is under-predicted, with a NMB of -45.9%, NME of 62.6% and correlation of 0.41. Wet deposition ammonium is also under-predicted, with a NMB of -21.1%, NME of 68.8% and a relatively low correlation of 0.32. Precipitation for the summer season is slightly under-predicted (NMB = -5.06%), with a NME of 71.5% and correlation of 0.46.

Fall Season (September, October and November)

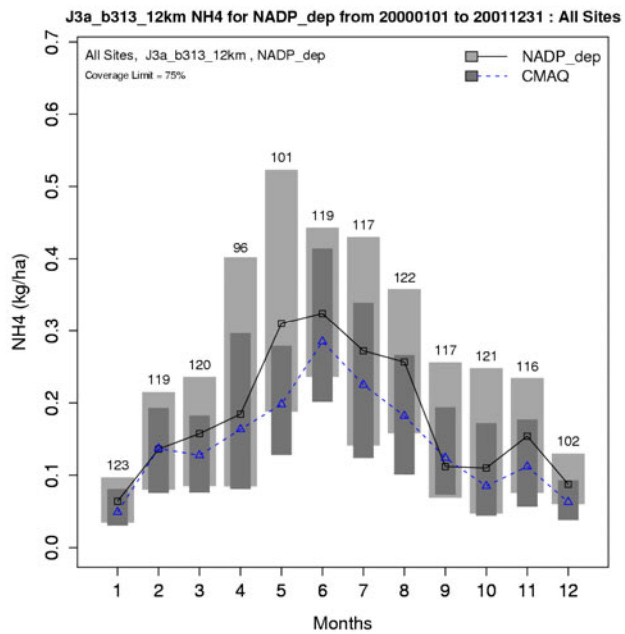
Wet deposition sulfate for the fall season is slightly over-predicted (although the error is rather large), with a NMB of 3.74 and NME of 65.5%. Wet deposition nitrate is slightly under-predicted (NMB = -9.53%), with a rather large NME of 61.5% and a correlation of 0.55. Wet deposition ammonium is moderately under-predicted, with a NMB of -23.3%, NME of 61.7% and correlation of 0.56. Precipitation for the fall season is significantly more under-predicted than the other three seasons, with a NMB of -23.8%. However, the NME of 53.3% is similar to that of the other seasons, and the correlation of 0.73 is the highest of all the seasons.

NADP Deposition (kg/ha)

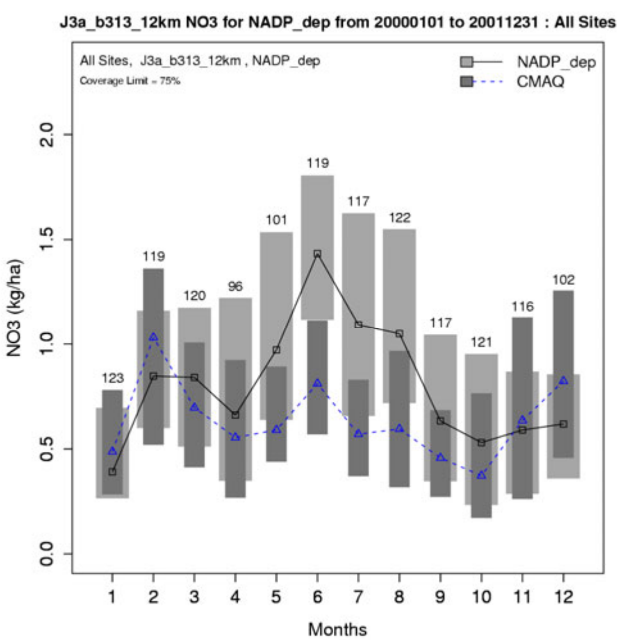
Sulfate



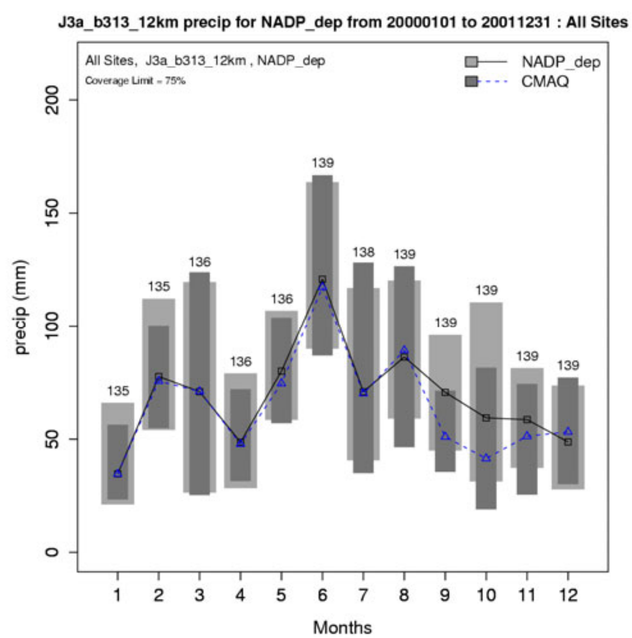
Ammonium



Nitrate

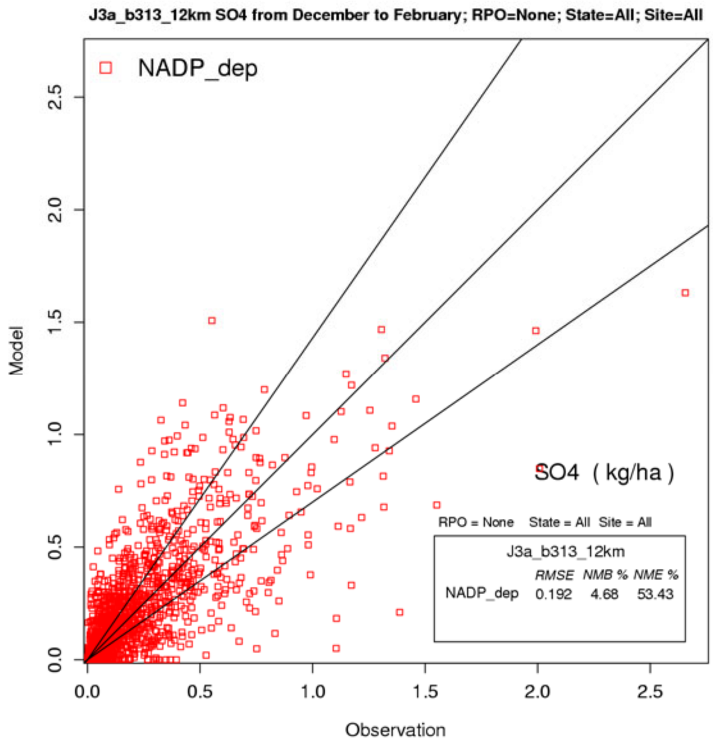


Precipitation

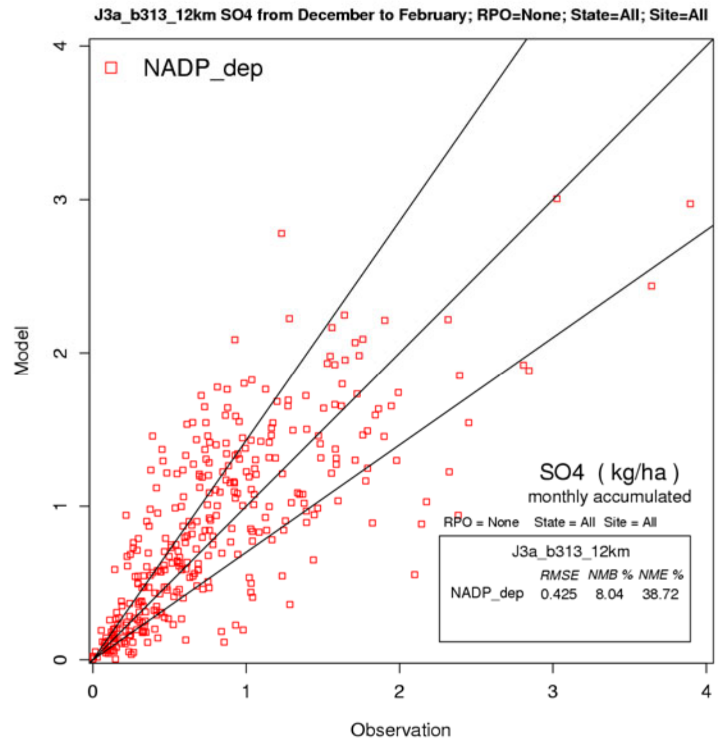


NADP Deposition SO_4^{2-} - Winter

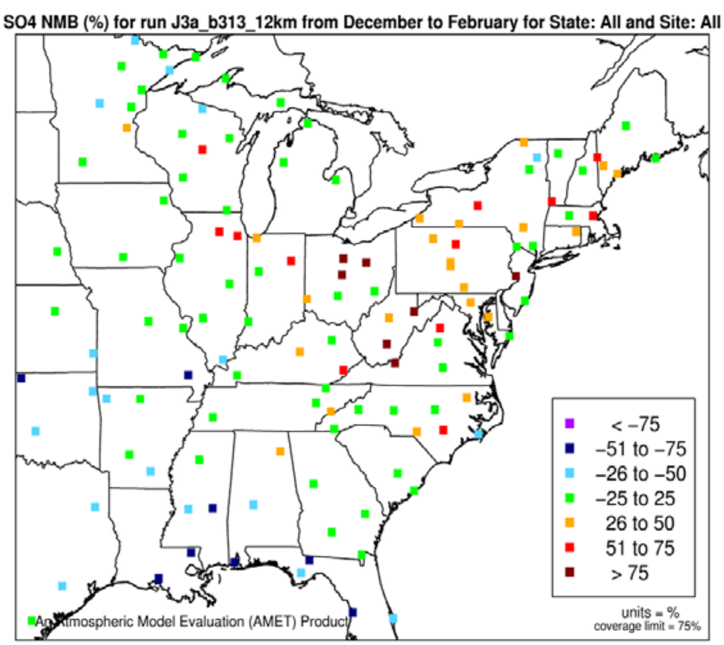
Scatter Plot – All Pairs



Scatter Plot – Monthly Accumulated Pairs

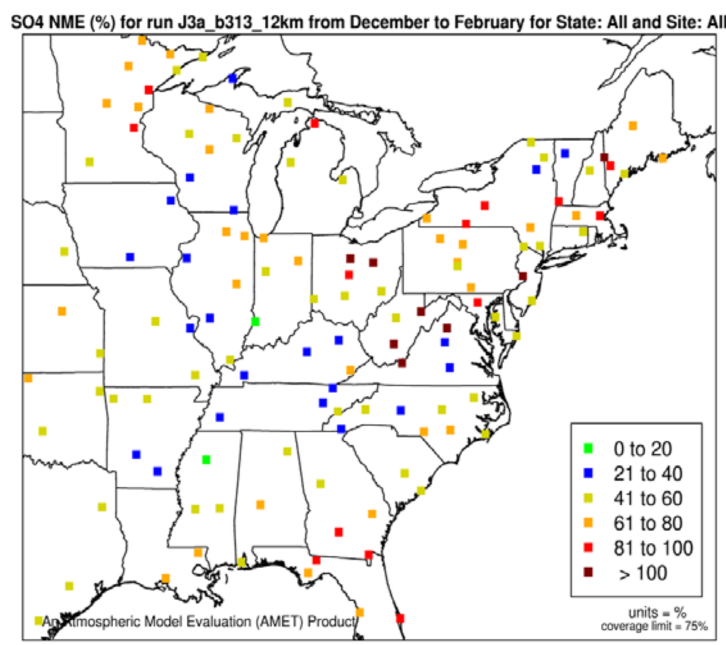


Normalized Mean Bias (%) - Winter



square=NADP_dep;

Normalized Mean Error (%) - Winter

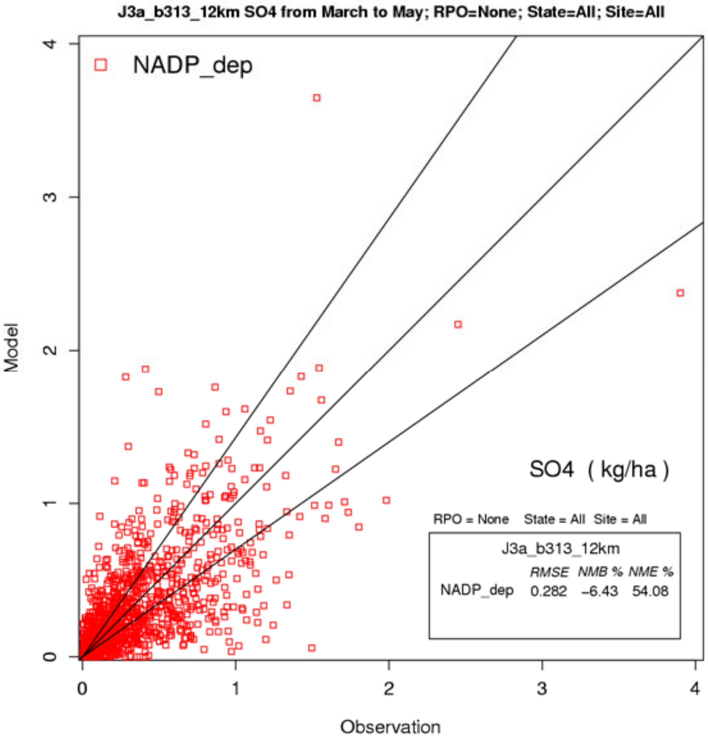


square=NADP_dep;

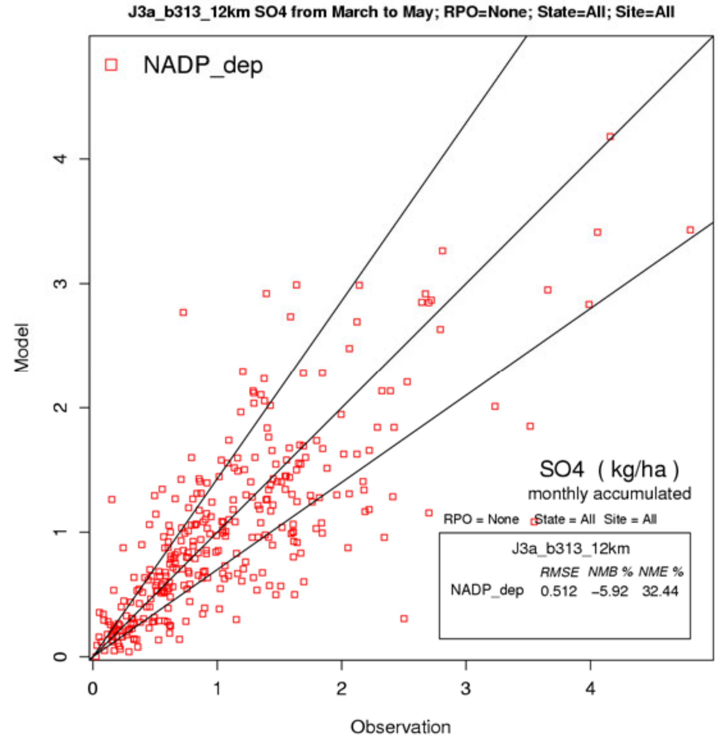
Network	# Obs	Mean Obs (kg/ha)	Mean Model (kg/ha)	SDEV Obs (kg/ha)	SDEV Model (kg/ha)	R	RMSE (kg/ha)	NMB (%)	NME (%)
NADP Dep	1270	0.236	0.247	0.261	0.252	0.72	0.192	4.68	53.4

NADP Deposition SO_4^{2-} - Spring

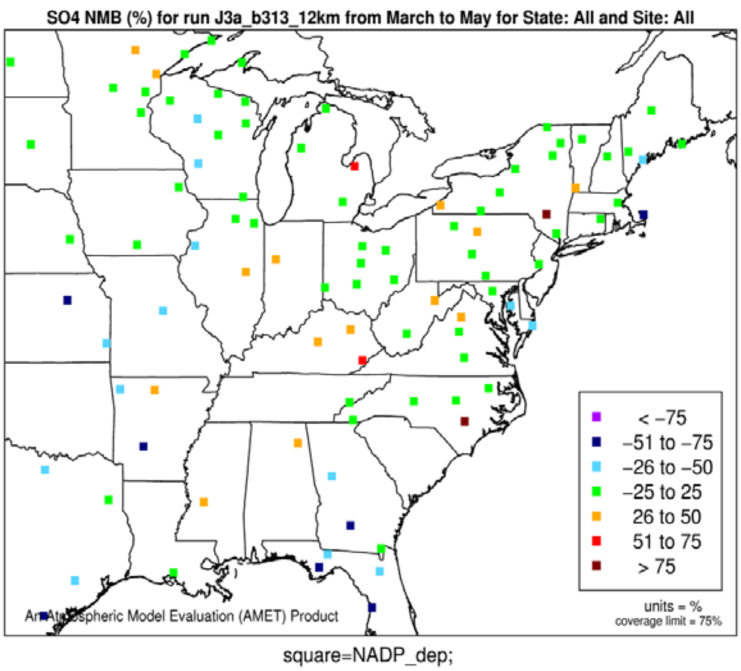
Scatter Plot – All Pairs



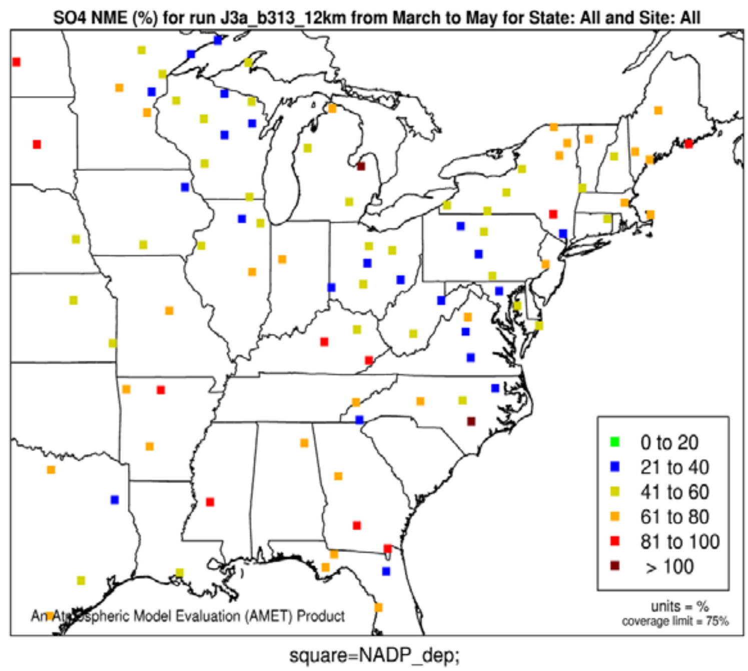
Scatter Plot – Monthly Accumulated Pairs



Normalized Mean Bias (%) - Spring



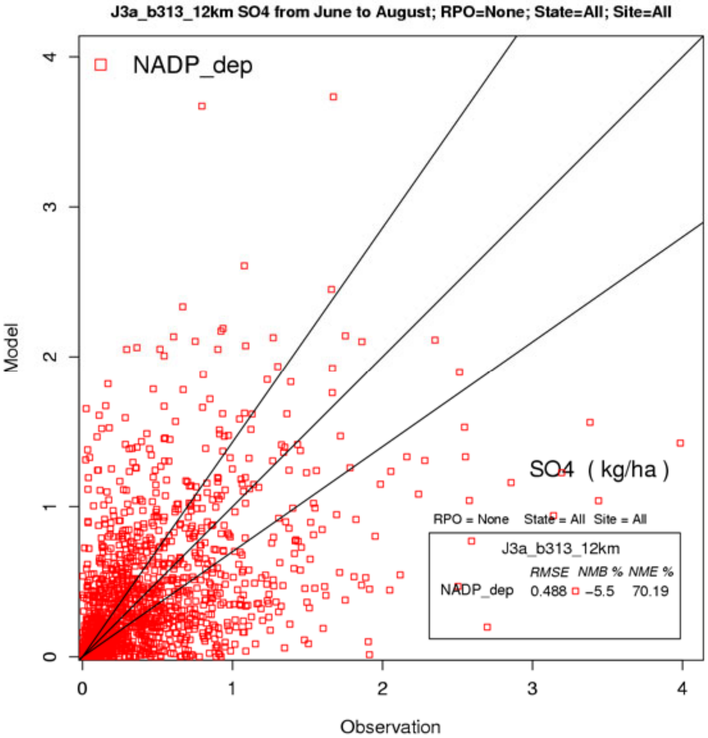
Normalized Mean Error (%) - Spring



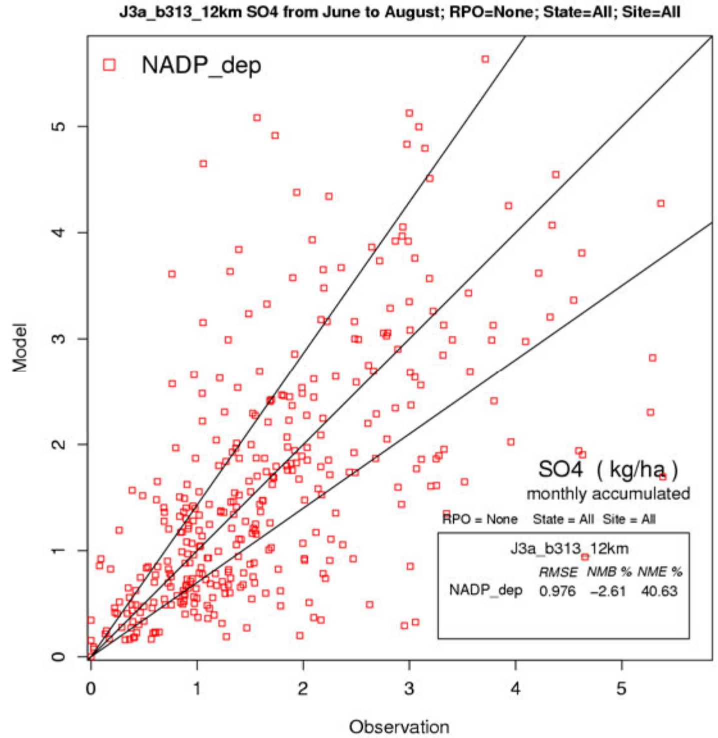
Network	# Obs	Mean Obs (kg/ha)	Mean Model (kg/ha)	SDEV Obs (kg/ha)	SDEV Model (kg/ha)	R	RMSE (kg/ha)	NMB (%)	NME (%)
NADP Dep	1148	0.346	0.324	0.348	0.345	0.67	0.282	-6.43	54.1

NADP Deposition SO_4^{2-} - Summer

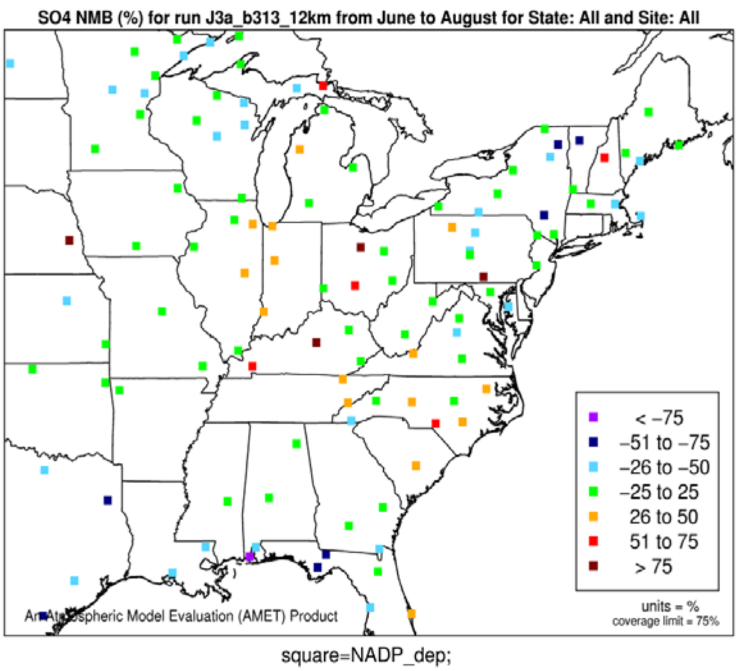
Scatter Plot – All Pairs



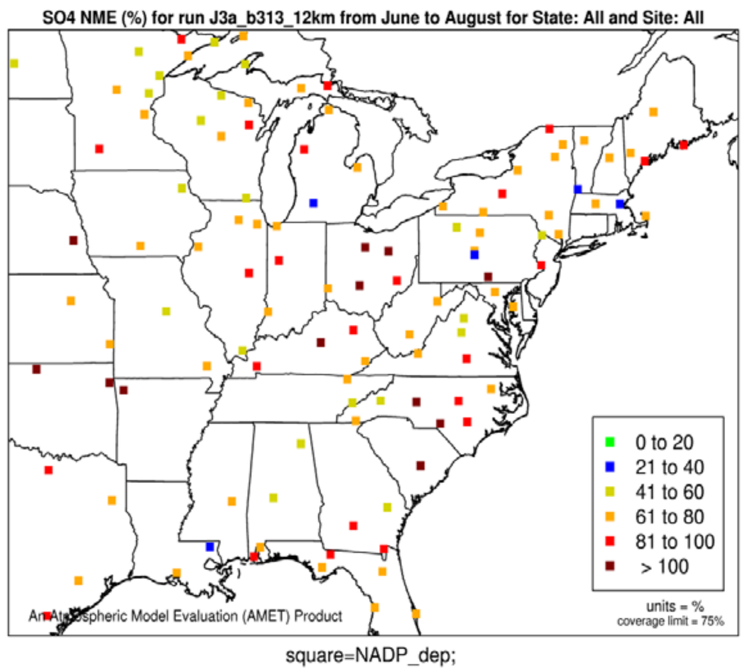
Scatter Plot – Monthly Accumulated Pairs



Normalized Mean Bias (%) - Summer



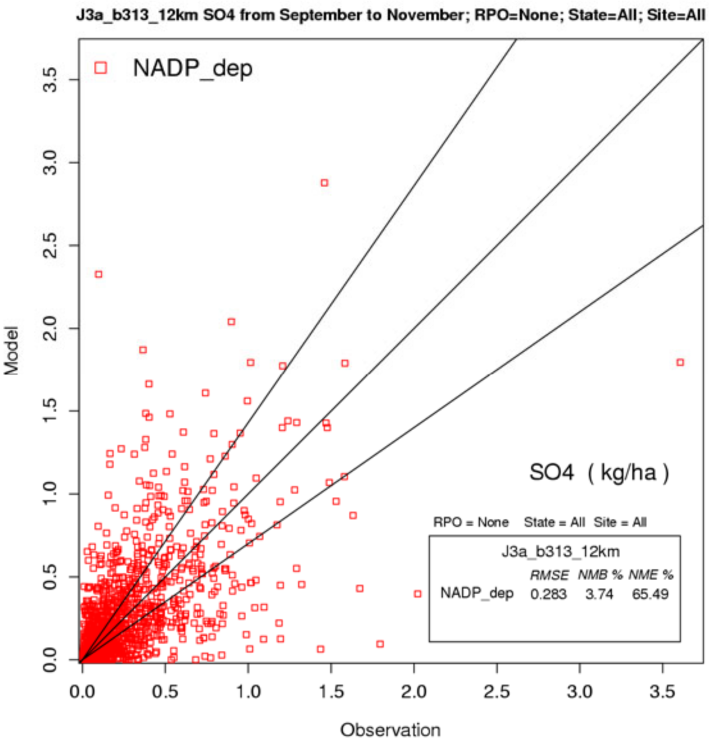
Normalized Mean Error (%) - Summer



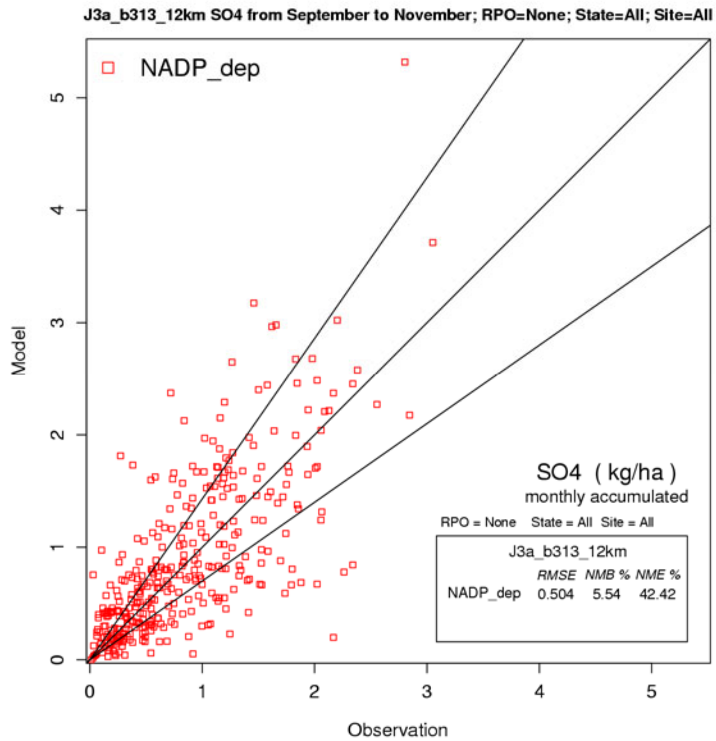
Network	# Obs	Mean Obs (kg/ha)	Mean Model (kg/ha)	SDEV Obs (kg/ha)	SDEV Model (kg/ha)	R	RMSE (kg/ha)	NMB (%)	NME (%)
NADP Dep	1431	0.457	0.432	0.476	0.448	0.44	0.488	-5.50	70.2

NADP Deposition SO_4^{2-} - Fall

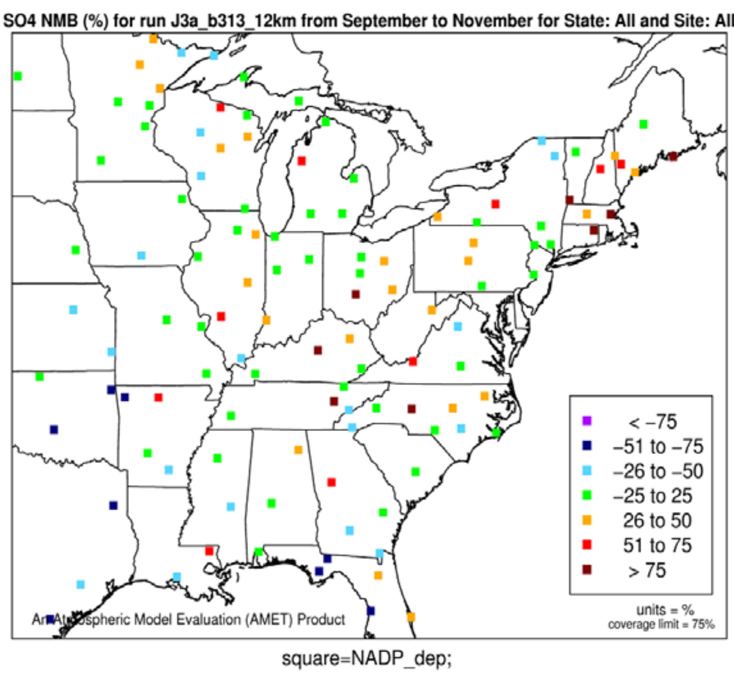
Scatter Plot – All Pairs



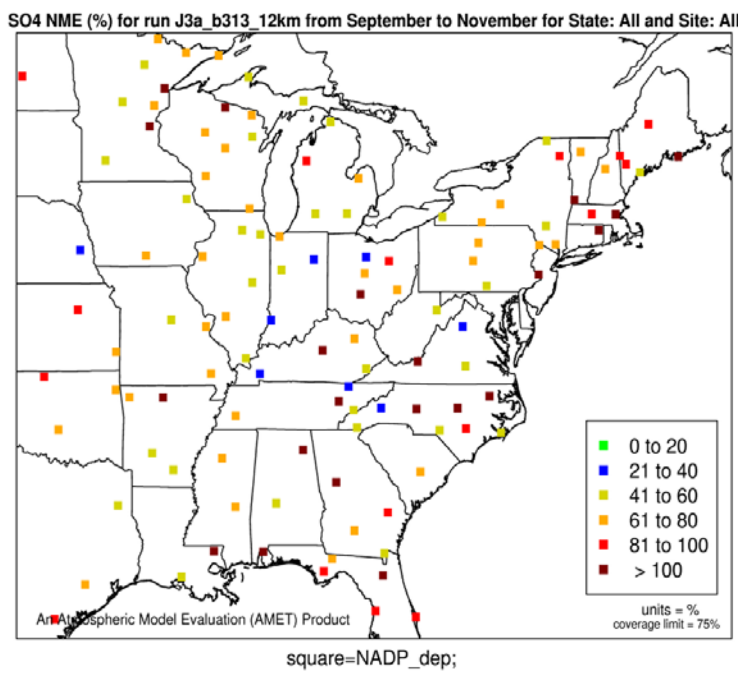
Scatter Plot – Monthly Accumulated Pairs



Normalized Mean Bias (%) - Fall



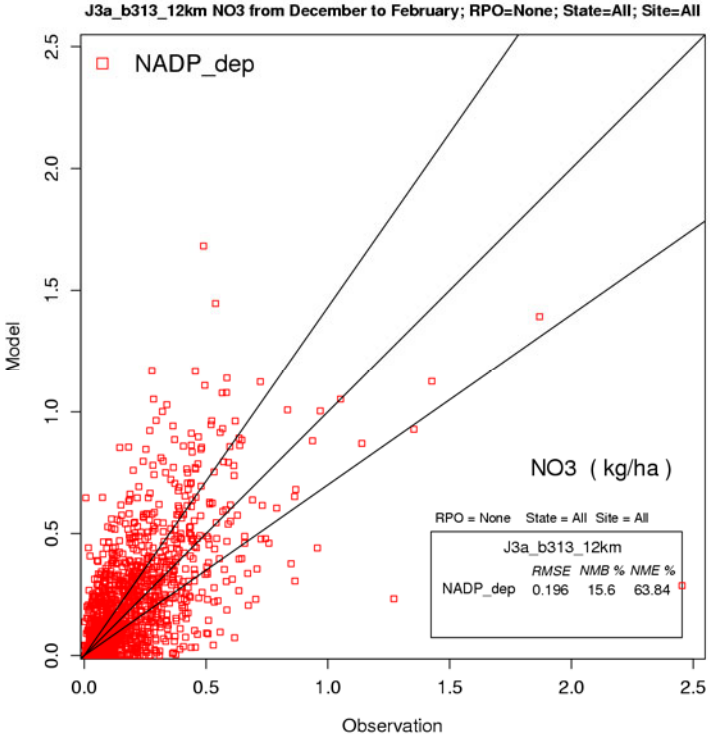
Normalized Mean Error (%) - Fall



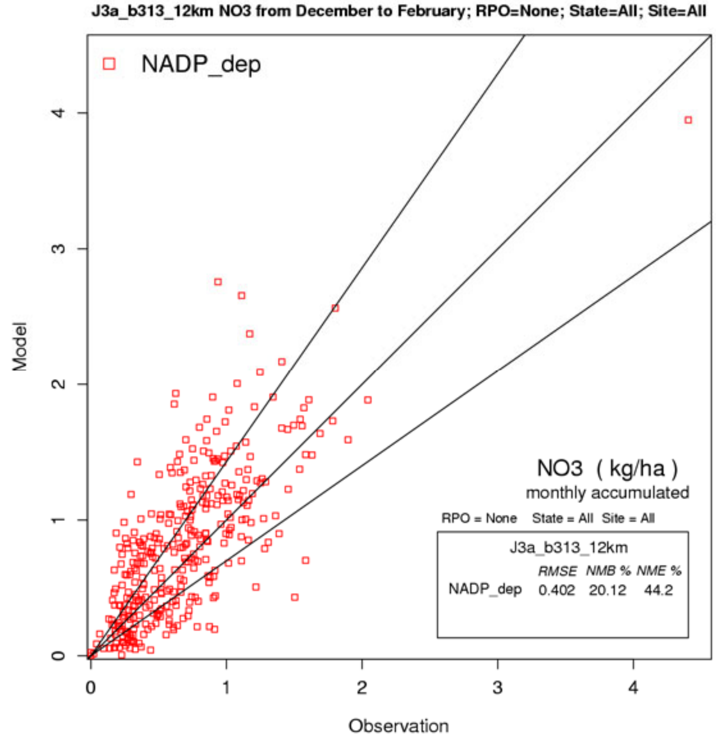
Network	# Obs	Mean Obs (kg/ha)	Mean Model (kg/ha)	SDEV Obs (kg/ha)	SDEV Model (kg/ha)	R	RMSE (kg/ha)	NMB (%)	NME (%)
NADP Dep	1216	0.267	0.277	0.299	0.324	0.59	0.283	3.74	65.5

NADP Deposition NO_3 - Winter

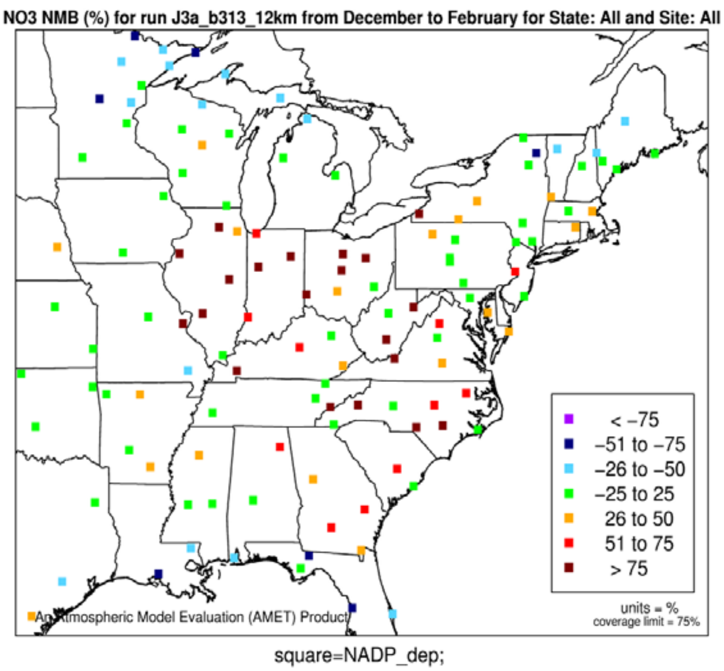
Scatter Plot – All Pairs



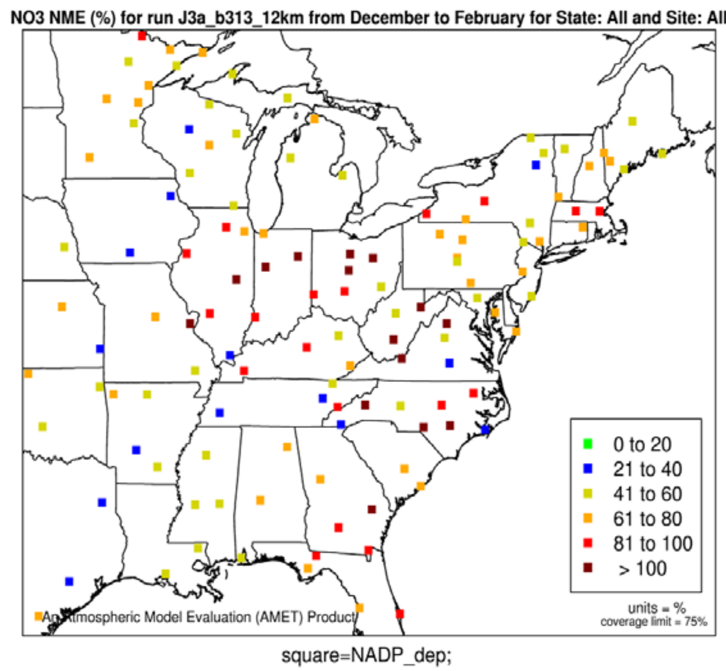
Scatter Plot – Monthly Accumulated Pairs



Normalized Mean Bias (%) - Winter



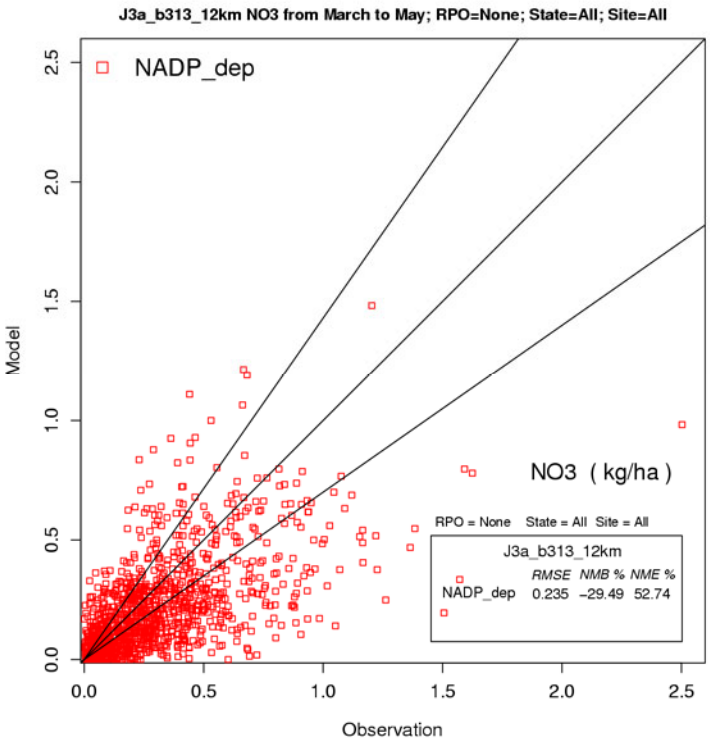
Normalized Mean Error (%) - Winter



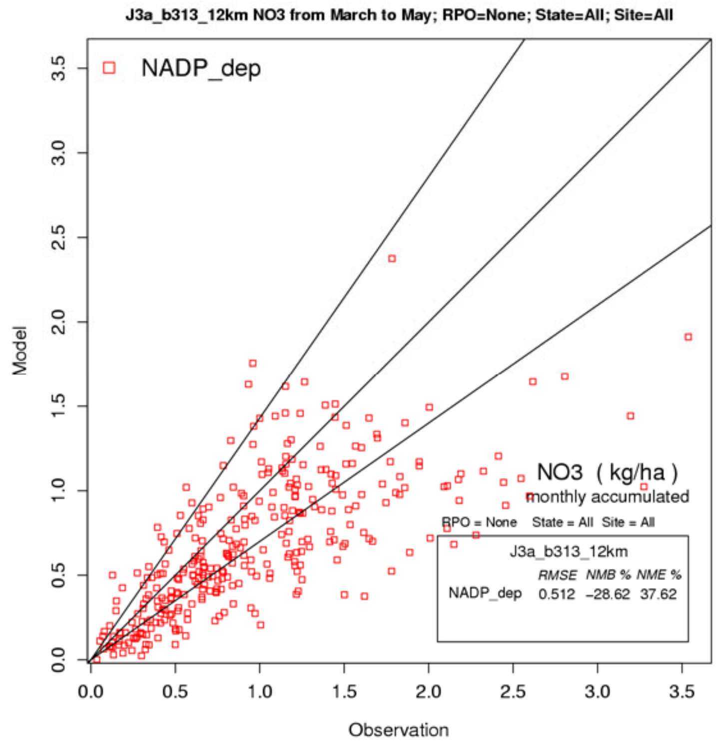
Network	# Obs	Mean Obs (kg/ha)	Mean Model (kg/ha)	SDEV Obs (kg/ha)	SDEV Model (kg/ha)	R	RMSE (kg/ha)	NMB (%)	NME (%)
NADP Dep	1270	0.204	0.235	0.192	0.231	0.60	0.196	15.6	63.8

NADP Deposition NO_3 - Spring

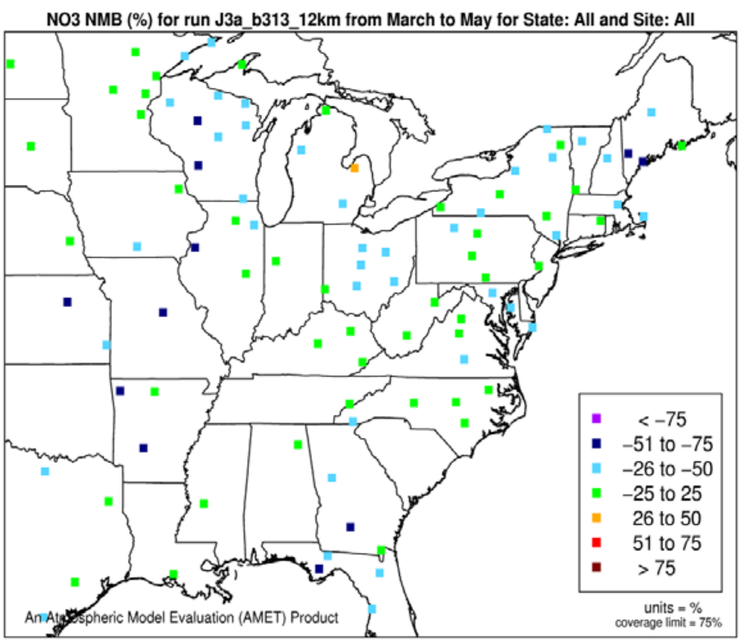
Scatter Plot – All Pairs



Scatter Plot – Monthly Accumulated Pairs

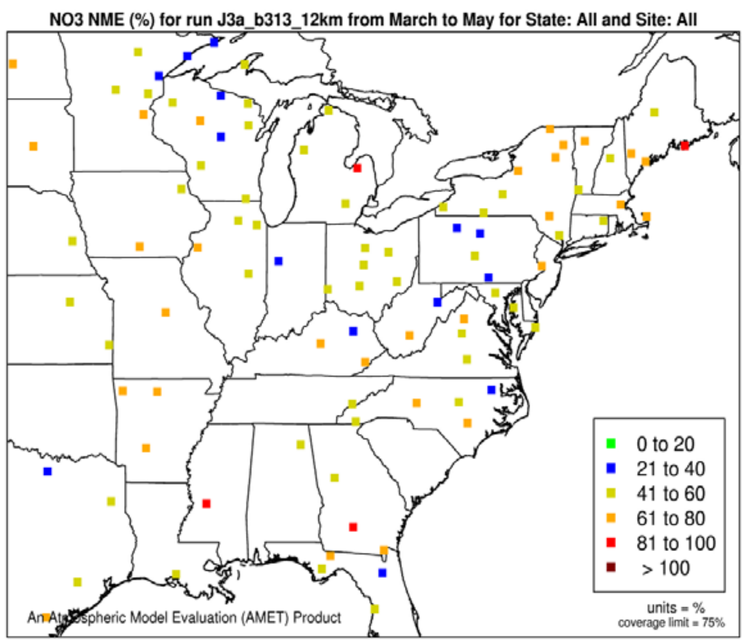


Normalized Mean Bias (%) - Spring



square=NADP_dep;

Normalized Mean Error (%) - Spring

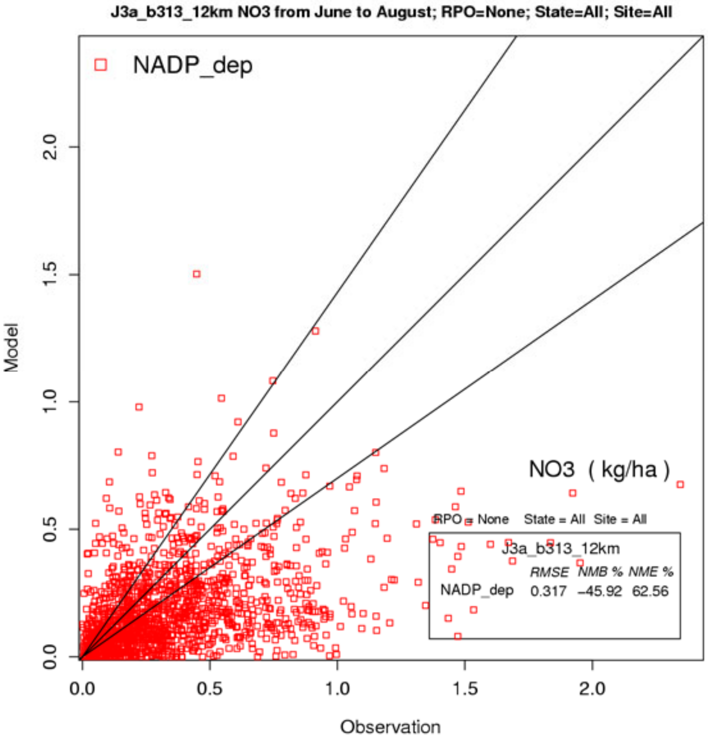


square=NADP_dep;

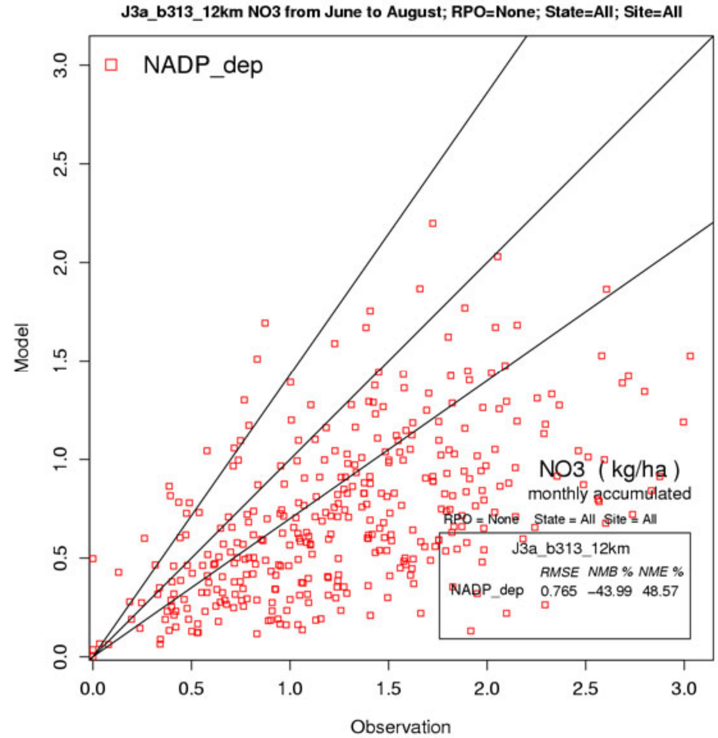
Network	# Obs	Mean Obs (kg/ha)	Mean Model (kg/ha)	SDEV Obs (kg/ha)	SDEV Model (kg/ha)	R	RMSE (kg/ha)	NMB (%)	NME (%)
NADP Dep	1148	0.303	0.214	0.266	0.197	0.59	0.235	-29.5	52.7

NADP Deposition NO_3 - Summer

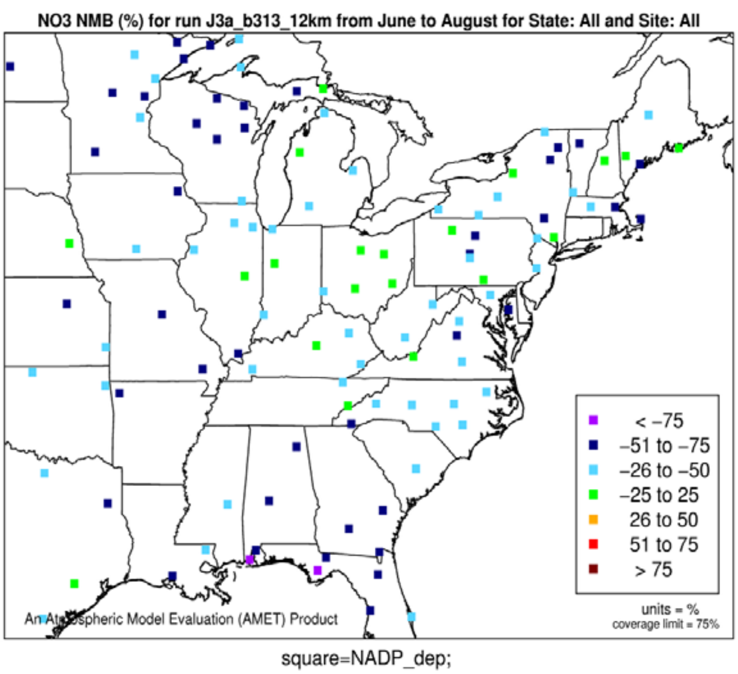
Scatter Plot – All Pairs



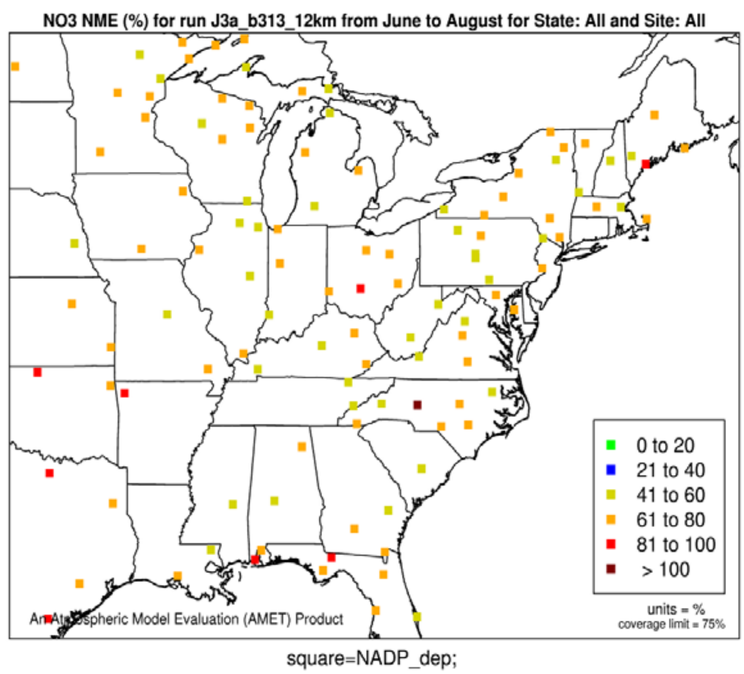
Scatter Plot – Monthly Accumulated Pairs



Normalized Mean Bias (%) - Summer



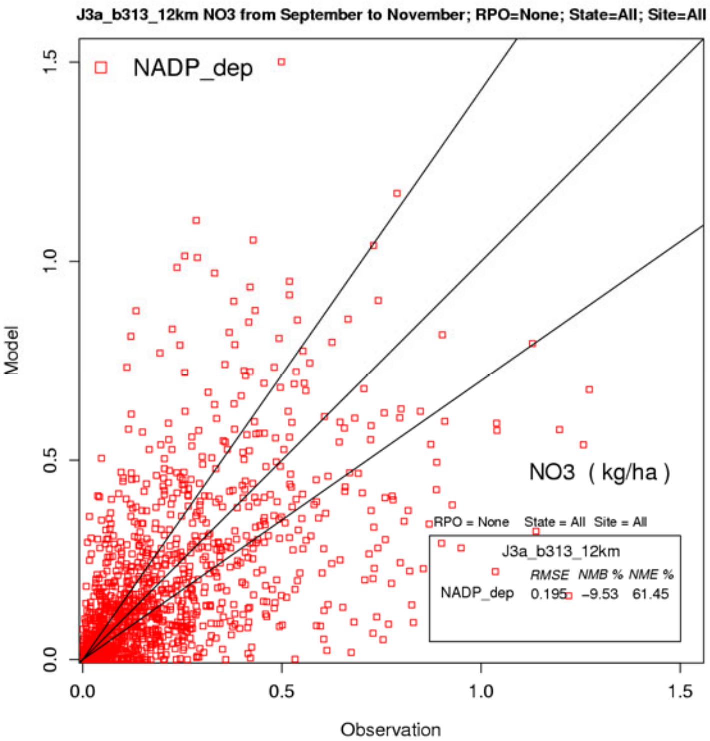
Normalized Mean Error (%) - Summer



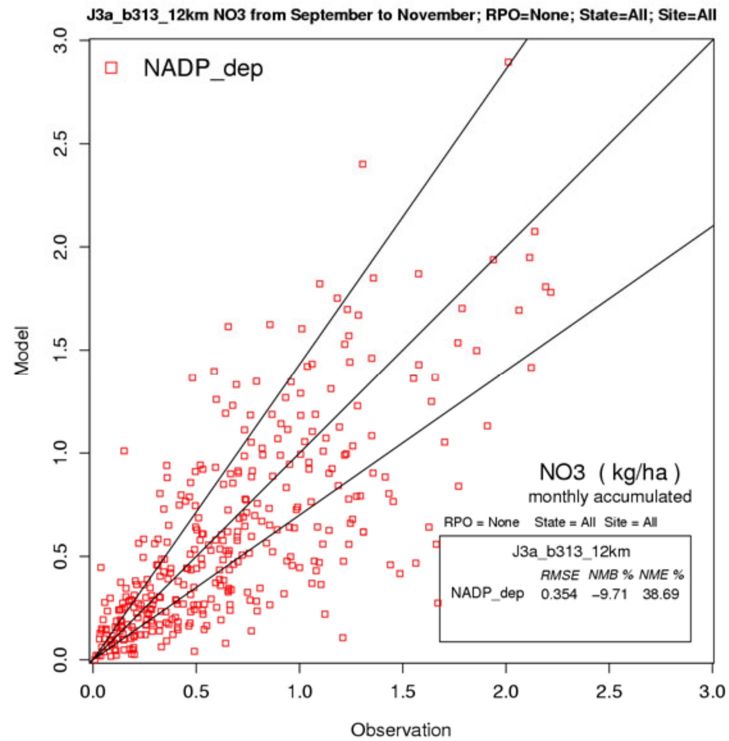
Network	# Obs	Mean Obs (kg/ha)	Mean Model (kg/ha)	SDEV Obs (kg/ha)	SDEV Model (kg/ha)	R	RMSE (kg/ha)	NMB (%)	NME (%)
NADP Dep	1431	0.348	0.188	0.295	0.171	0.41	0.317	-45.9	62.6

NADP Deposition NO_3 - Fall

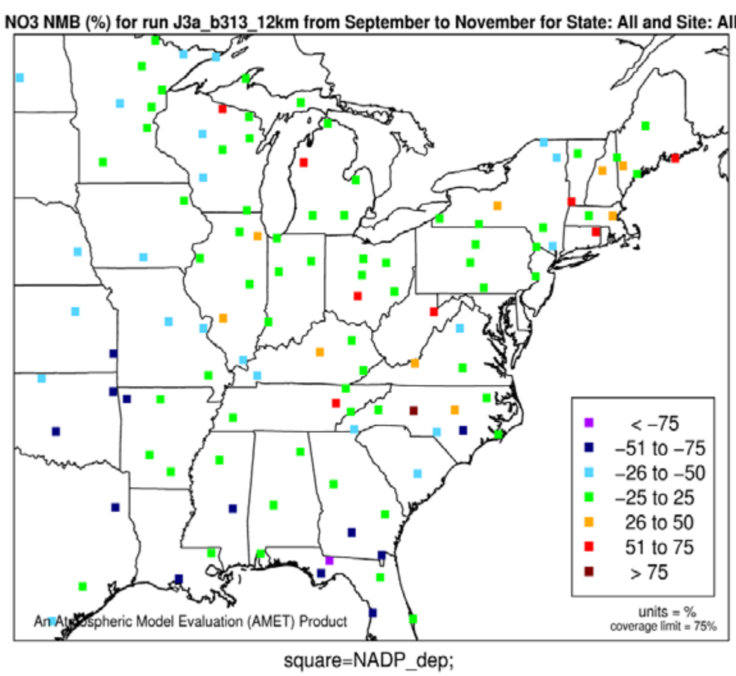
Scatter Plot – All Pairs



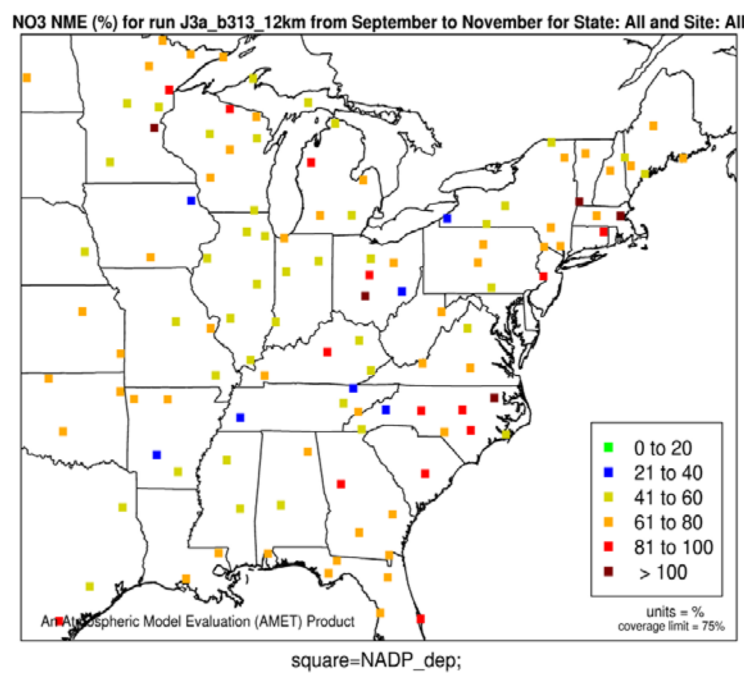
Scatter Plot – Monthly Accumulated Pairs



Normalized Mean Bias (%) - Fall



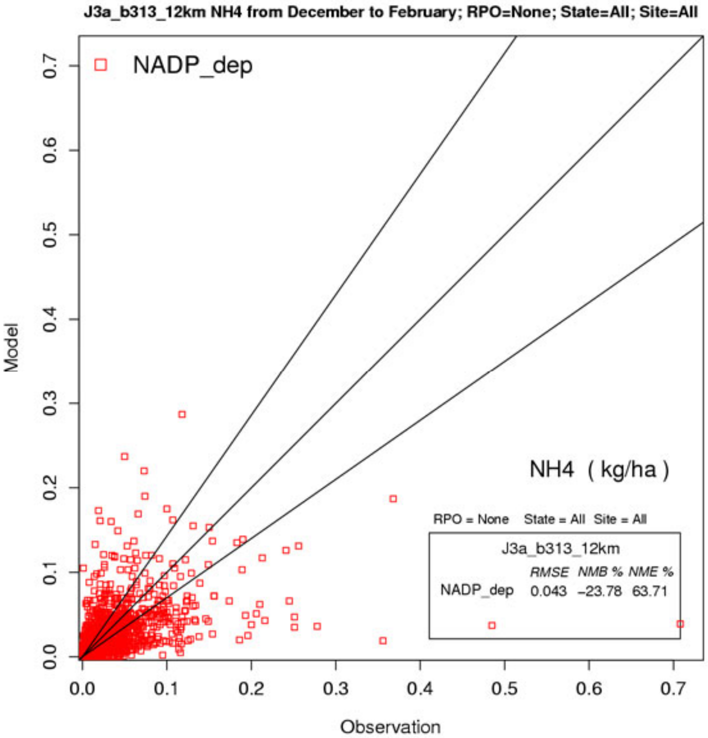
Normalized Mean Error (%) - Fall



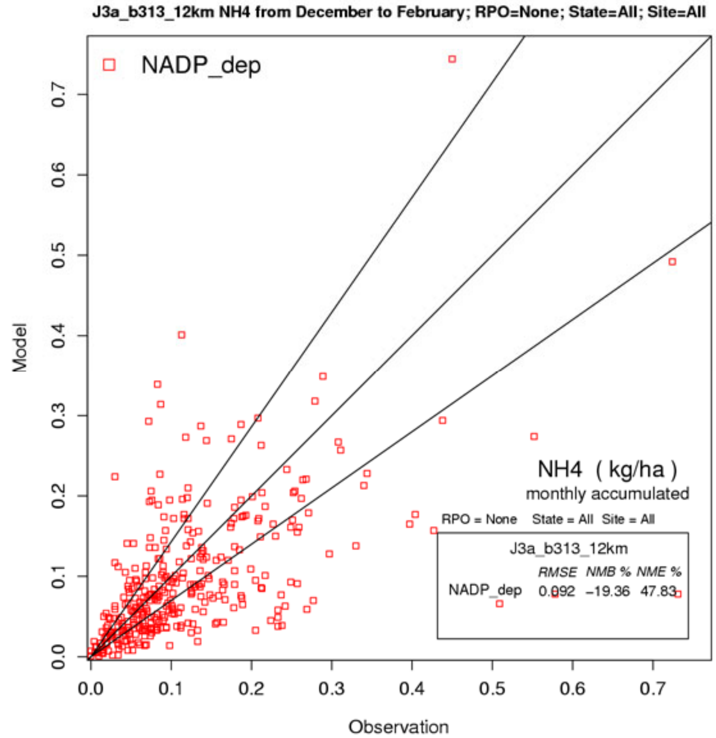
Network	# Obs	Mean Obs (kg/ha)	Mean Model (kg/ha)	SDEV Obs (kg/ha)	SDEV Model (kg/ha)	R	RMSE (kg/ha)	NMB (%)	NME (%)
NADP Dep	1216	0.209	0.189	0.207	0.202	0.55	0.195	-9.53	61.5

NADP Deposition NH_4 - Winter

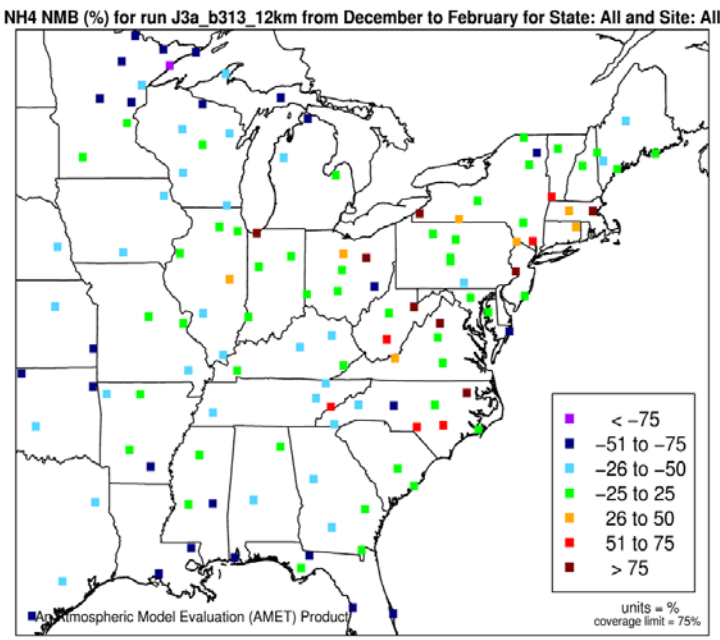
Scatter Plot – All Pairs



Scatter Plot – Monthly Accumulated Pairs

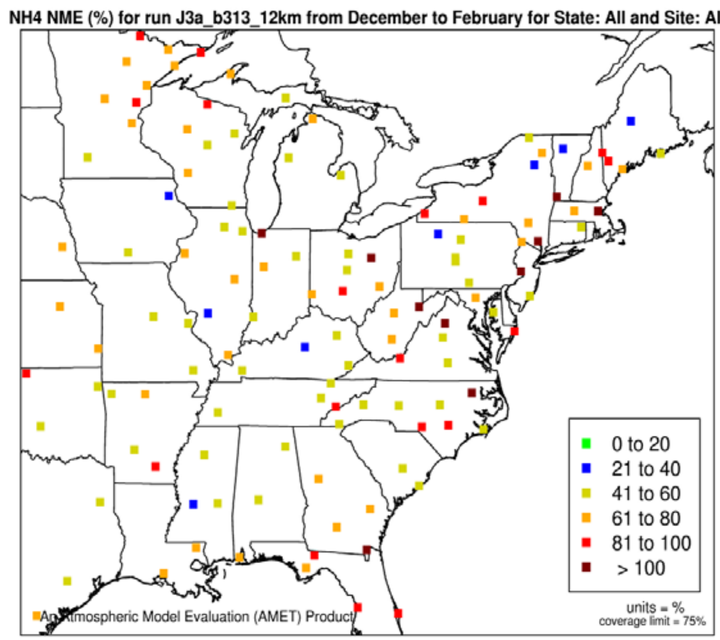


Normalized Mean Bias (%) - Winter



square=NADP_dep;

Normalized Mean Error (%) - Winter

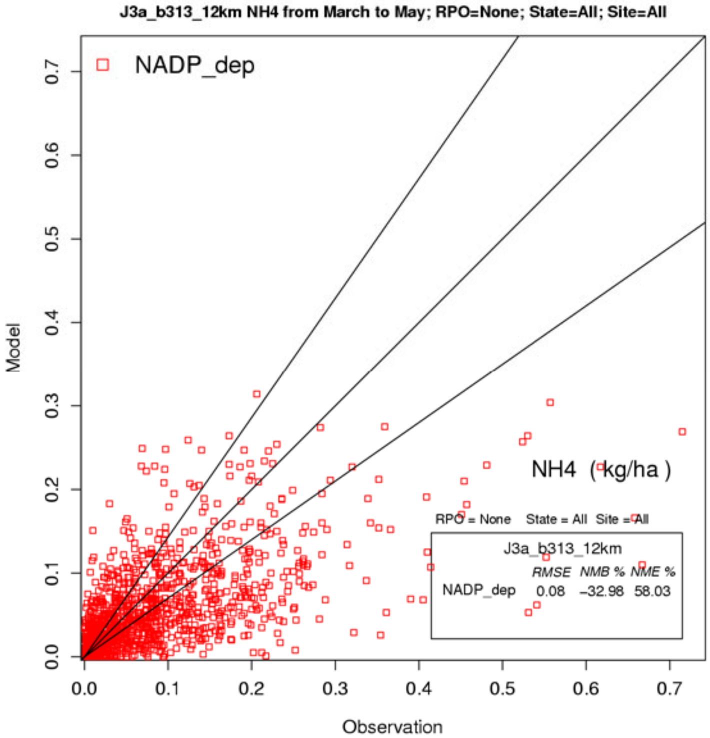


square=NADP_dep;

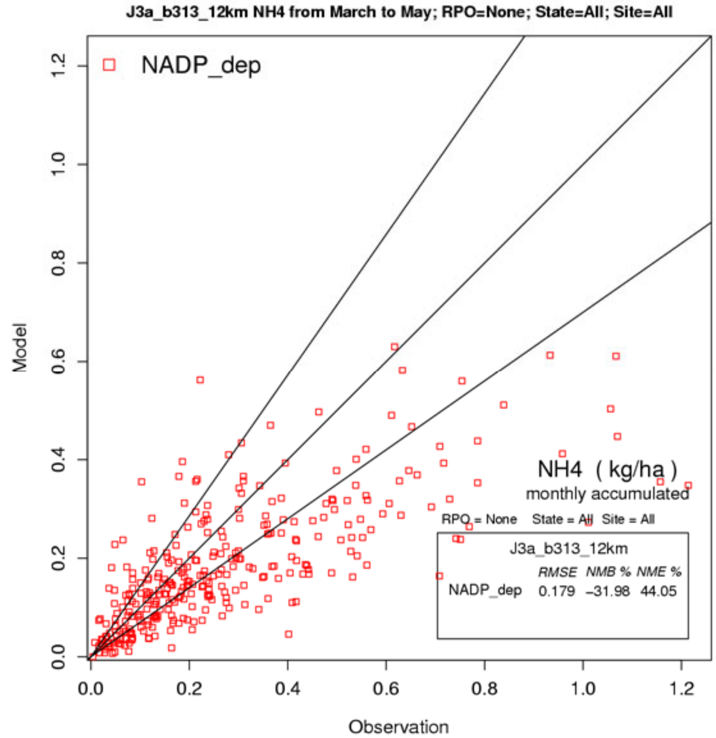
Network	# Obs	Mean Obs (kg/ha)	Mean Model (kg/ha)	SDEV Obs (kg/ha)	SDEV Model (kg/ha)	R	RMSE (kg/ha)	NMB (%)	NME (%)
NADP Dep	1262	0.036	0.027	0.046	0.030	0.43	0.043	-23.8	63.6

NADP Deposition NH_4 - Spring

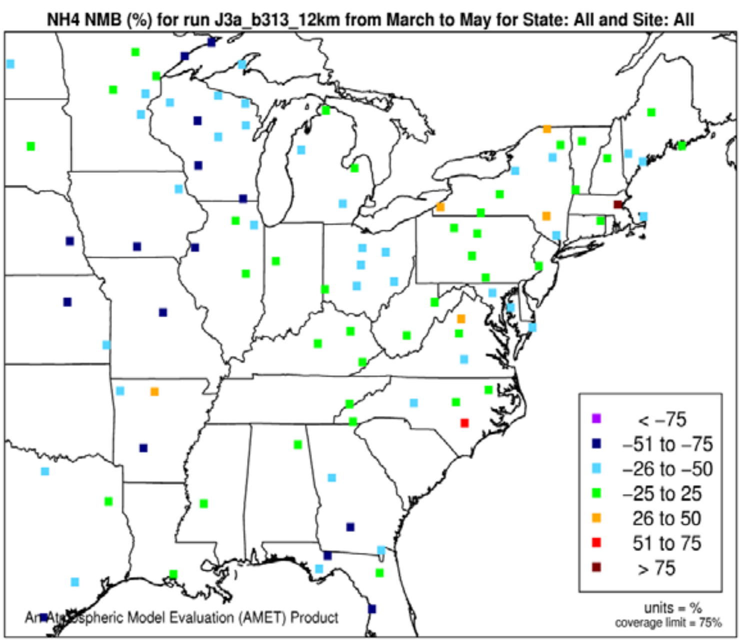
Scatter Plot – All Pairs



Scatter Plot – Monthly Accumulated Pairs

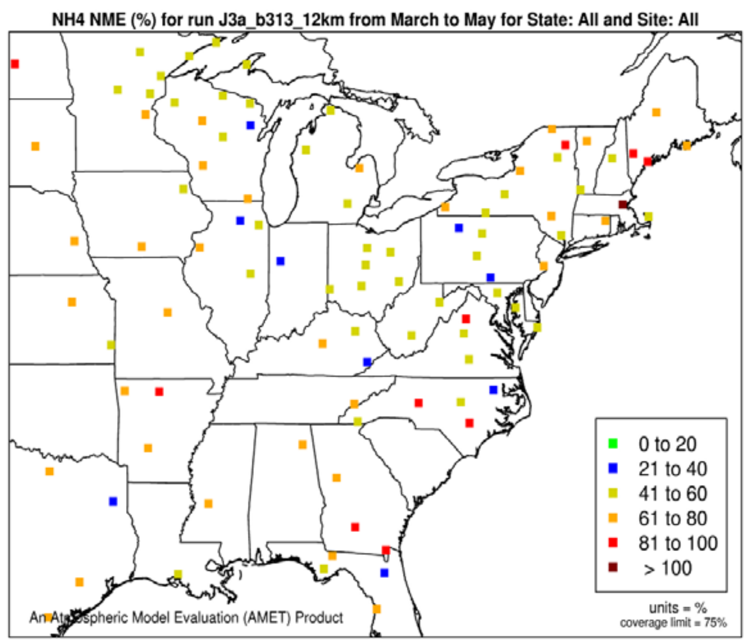


Normalized Mean Bias (%) - Spring



square=NADP_dep;

Normalized Mean Error (%) - Spring

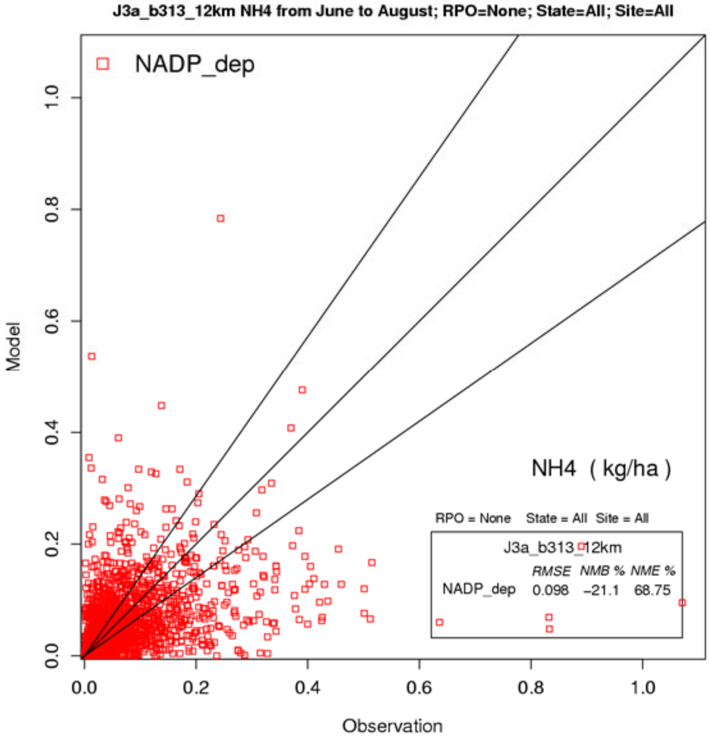


square=NADP_dep;

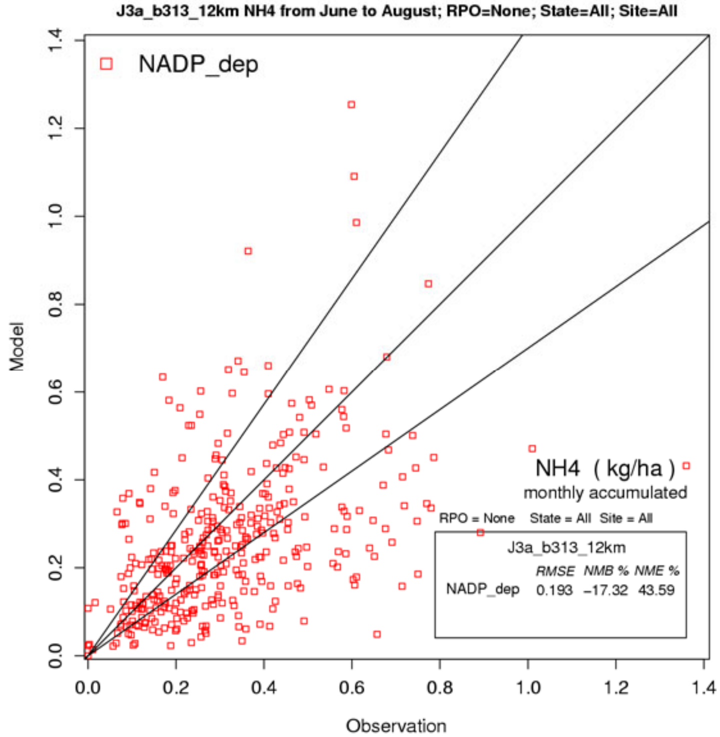
Network	# Obs	Mean Obs (kg/ha)	Mean Model (kg/ha)	SDEV Obs (kg/ha)	SDEV Model (kg/ha)	R	RMSE (kg/ha)	NMB (%)	NME (%)
NADP Dep	1147	0.085	0.057	0.093	0.054	0.60	0.080	-33.0	58.0

NADP Deposition NH_4 - Summer

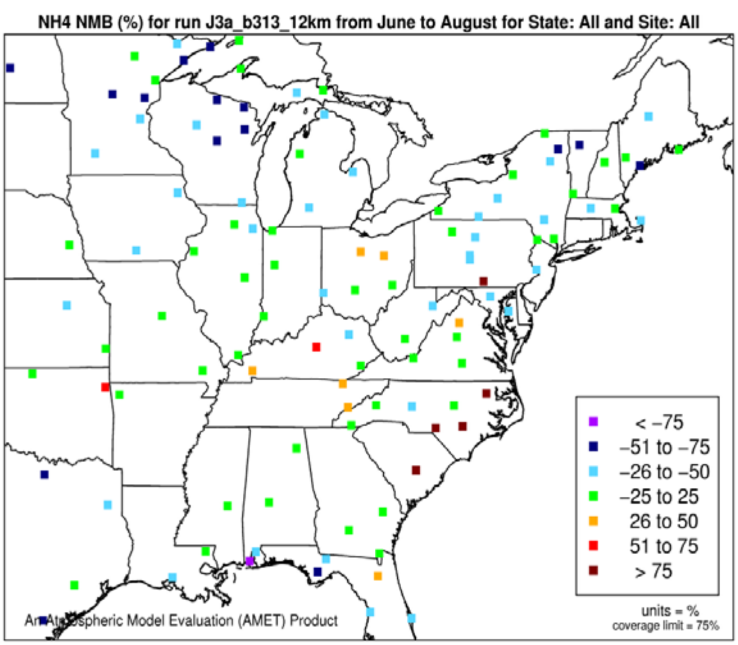
Scatter Plot – All Pairs



Scatter Plot – Monthly Accumulated Pairs

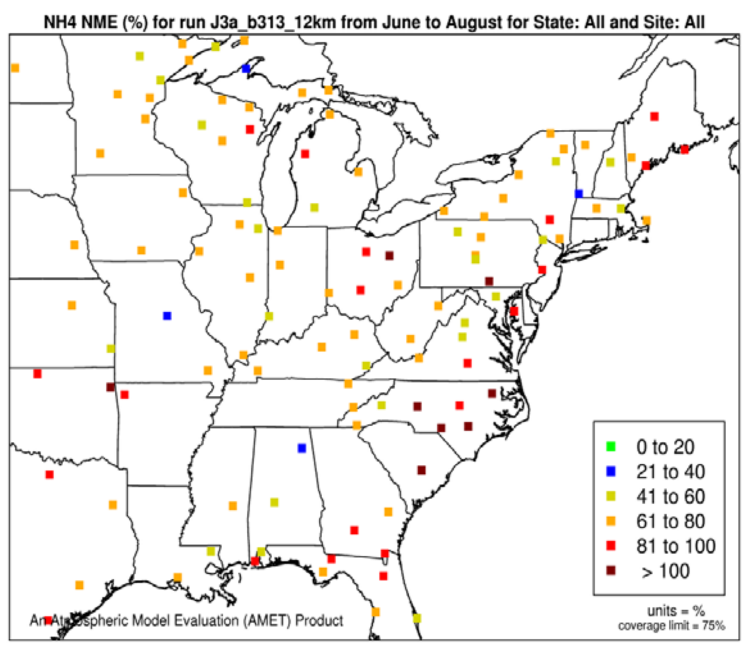


Normalized Mean Bias (%) - Summer



square=NADP_dep;

Normalized Mean Error (%) - Summer

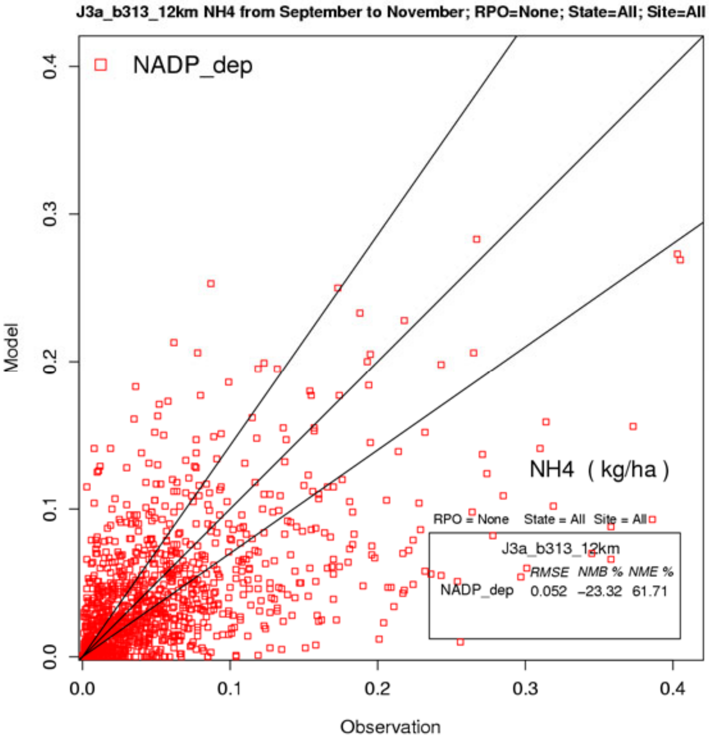


square=NADP_dep;

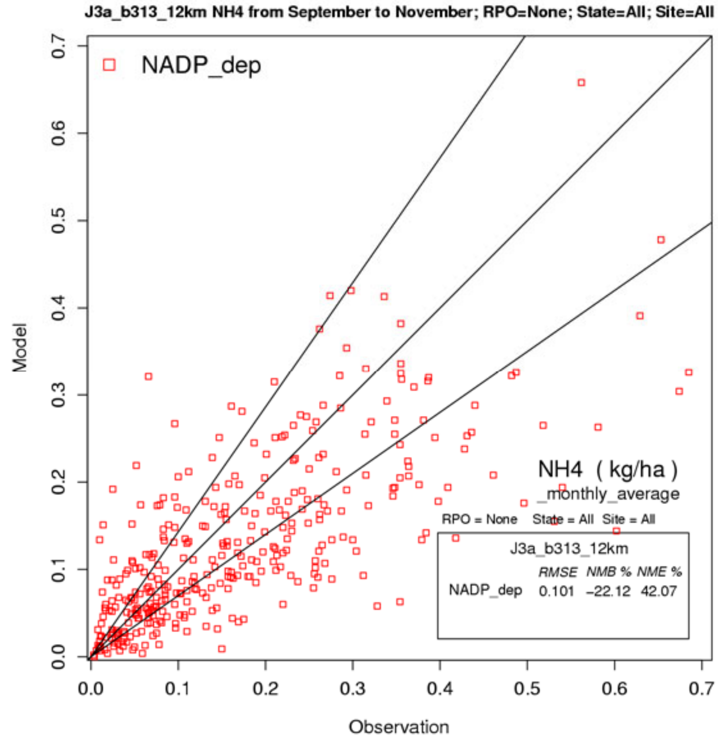
Network	# Obs	Mean Obs (kg/ha)	Mean Model (kg/ha)	SDEV Obs (kg/ha)	SDEV Model (kg/ha)	R	RMSE (kg/ha)	NMB (%)	NME (%)
NADP Dep	1429	0.087	0.069	0.094	0.067	0.32	0.098	-21.1	68.7

NADP Deposition NH_4 - Fall

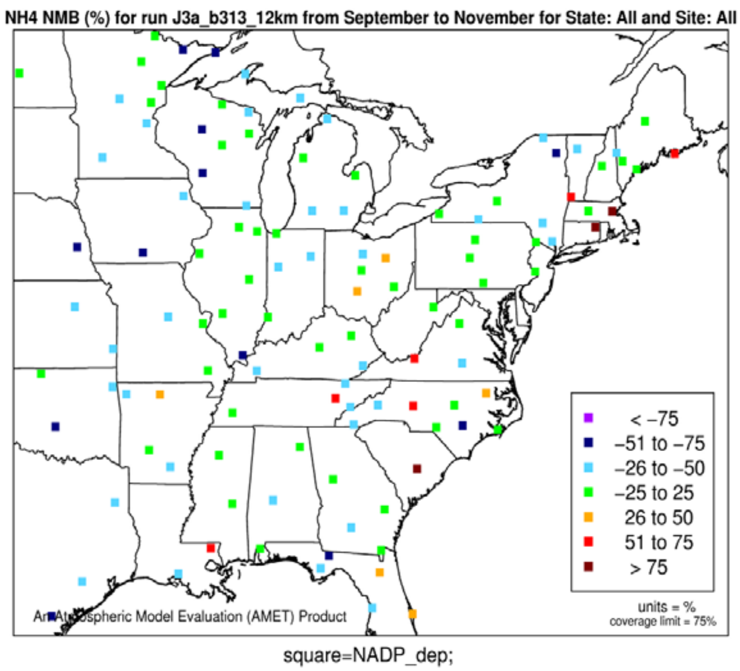
Scatter Plot – All Pairs



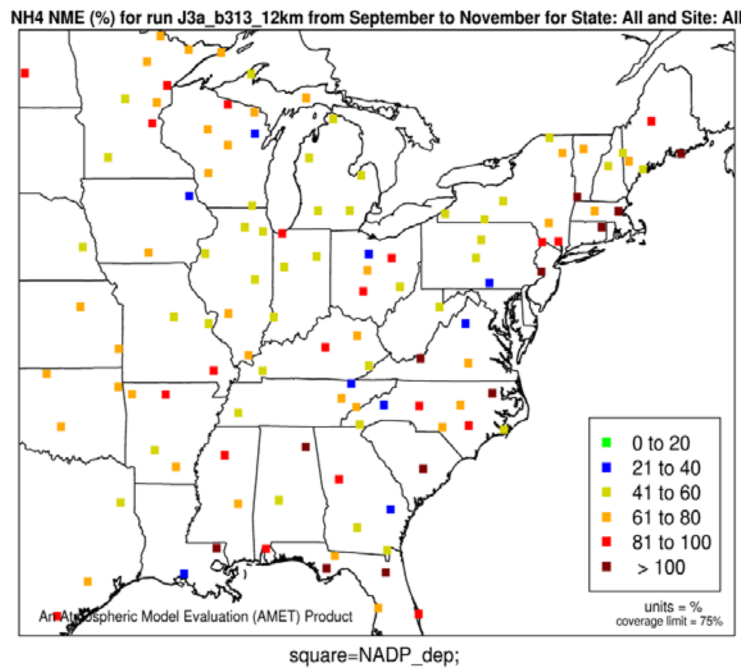
Scatter Plot – Monthly Accumulated Pairs



Normalized Mean Bias (%) - Fall



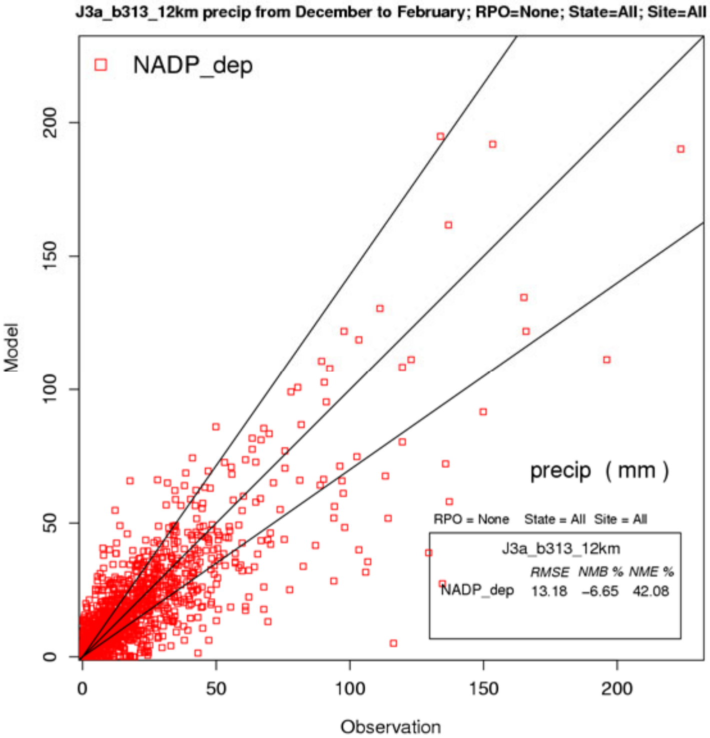
Normalized Mean Error (%) - Fall



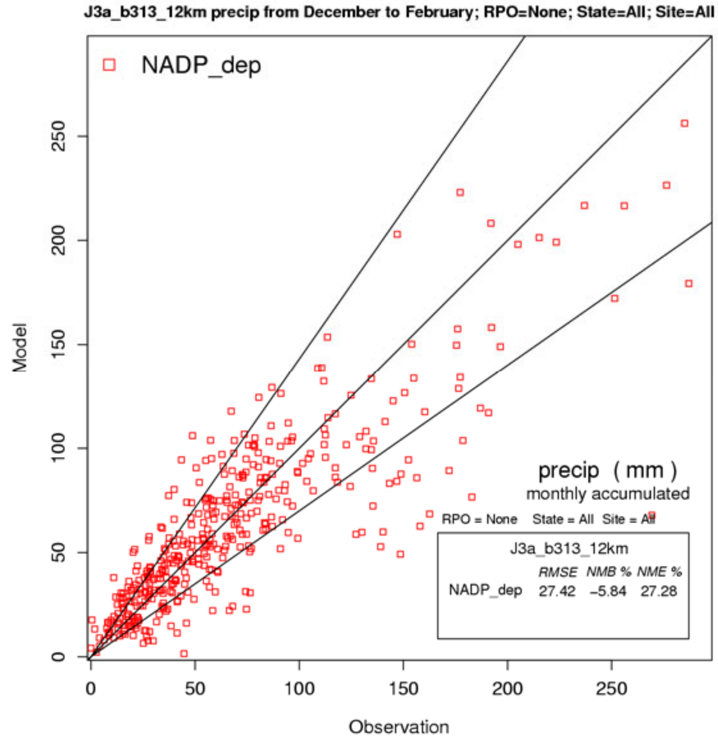
Network	# Obs	Mean Obs (kg/ha)	Mean Model (kg/ha)	SDEV Obs (kg/ha)	SDEV Model (kg/ha)	R	RMSE (kg/ha)	NMB (%)	NME (%)
NADP Dep	1214	0.053	0.040	0.059	0.043	0.56	0.052	-23.3	61.7

NADP Precipitation (mm) - Winter

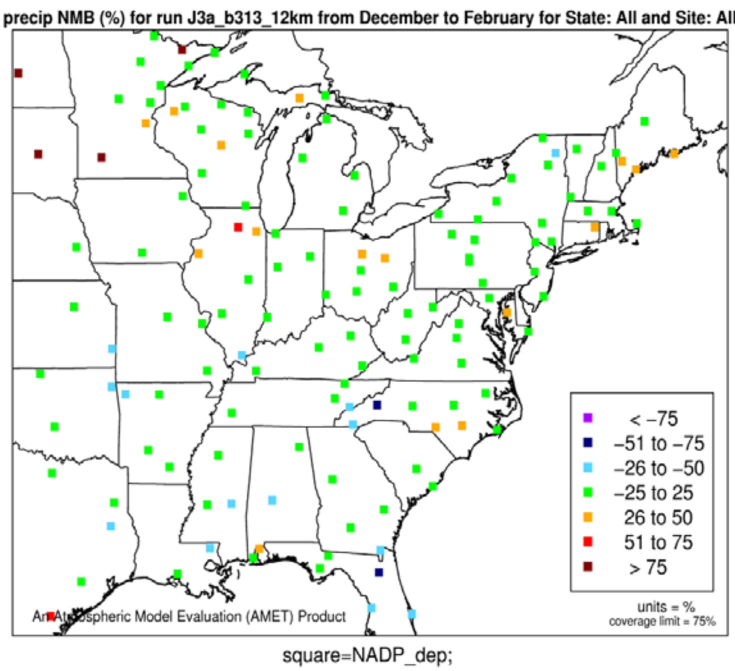
Scatter Plot – All Pairs



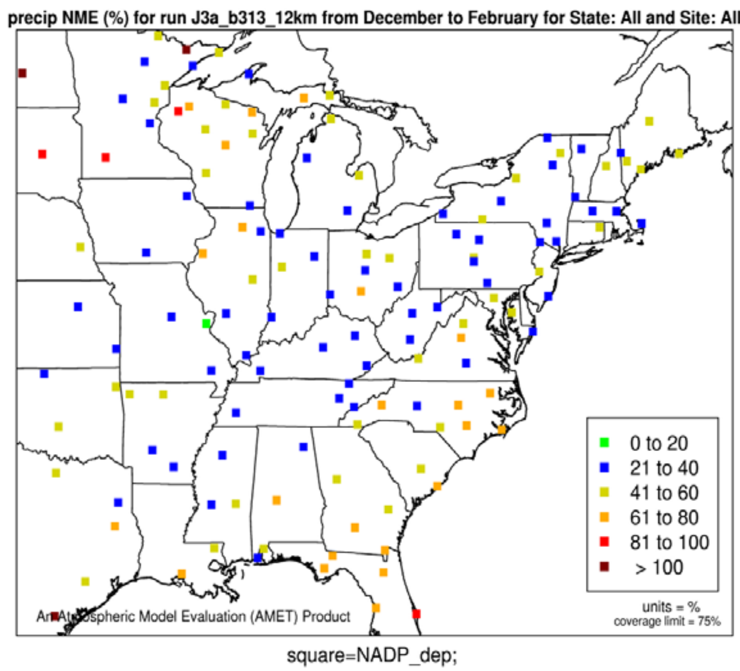
Scatter Plot – Monthly Accumulated Pairs



Normalized Mean Bias (%) - Winter



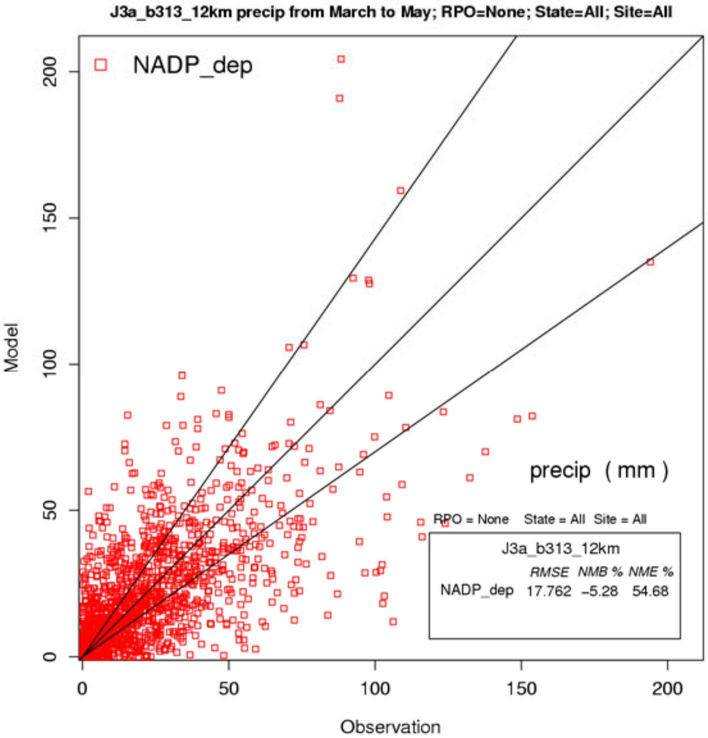
Normalized Mean Error (%) - Winter



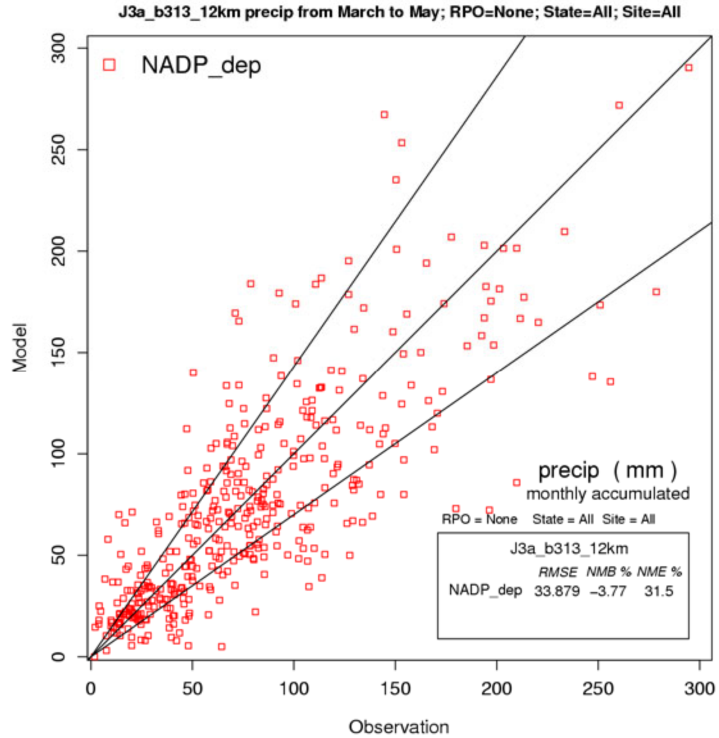
Network	# Obs	Mean Obs (mm)	Mean Model (mm)	SDEV Obs (mm)	SDEV Model (mm)	R	RMSE (mm)	NMB (%)	NME (%)
NADP Dep	1466	18.4	17.2	23.2	20.3	0.83	13.2	-6.65	42.1

NADP Precipitation - Spring

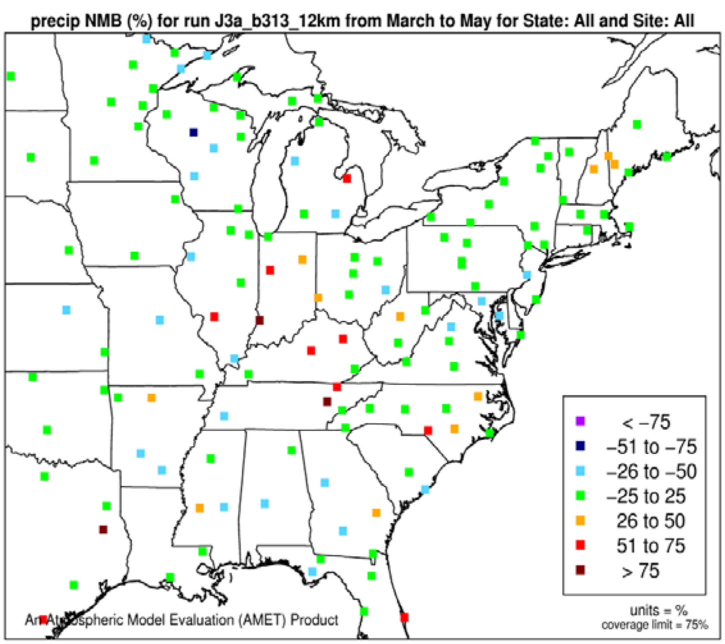
Scatter Plot – All Pairs



Scatter Plot – Monthly Accumulated Pairs

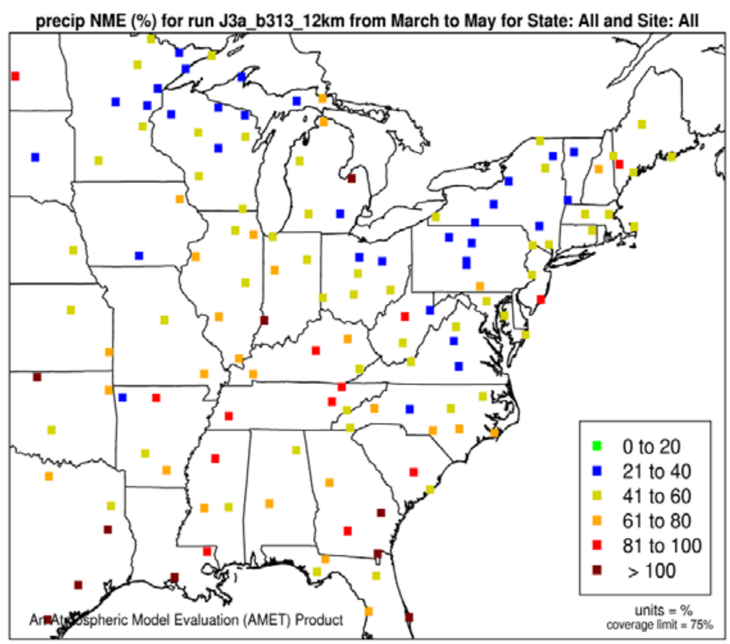


Normalized Mean Bias (%) - Winter



square=NADP_dep;

Normalized Mean Error (%) - Winter

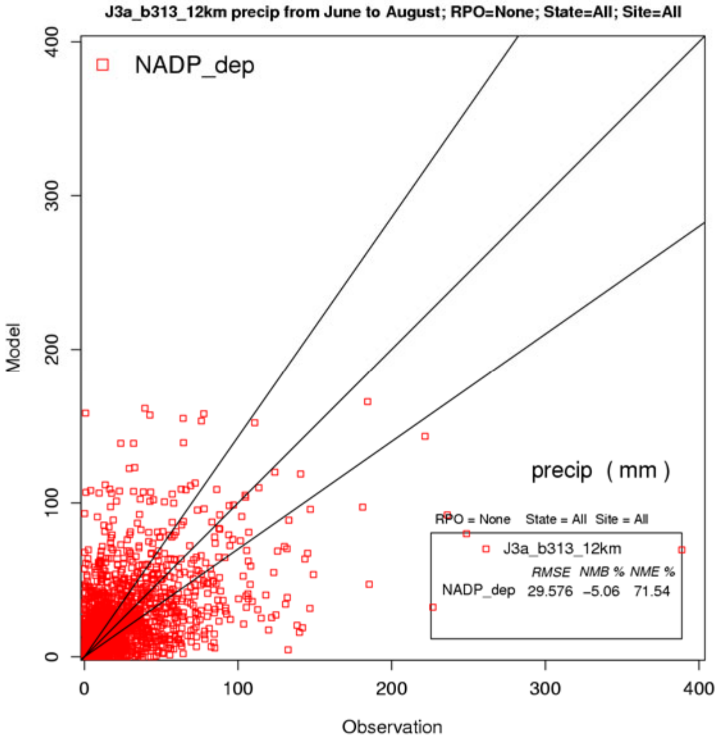


square=NADP_dep;

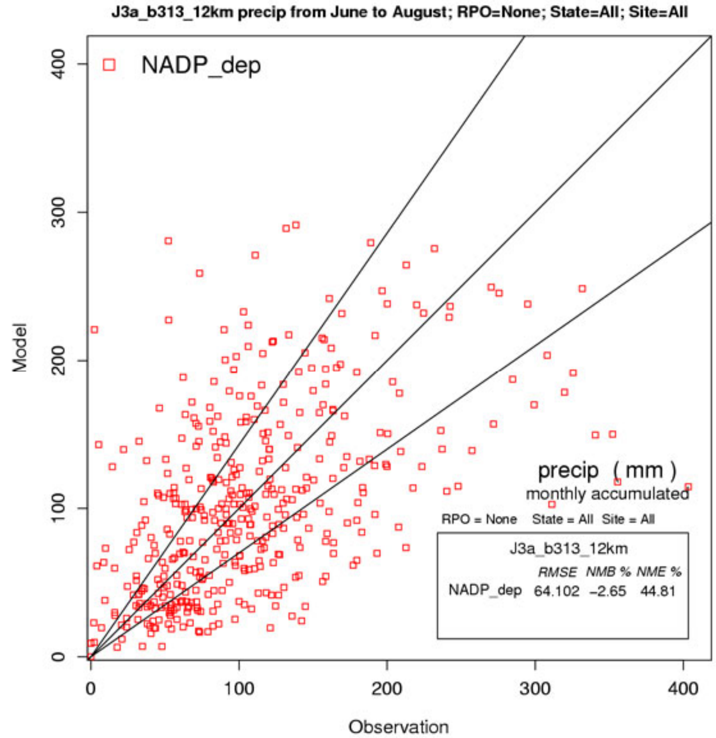
Network	# Obs	Mean Obs (mm)	Mean Model (mm)	SDEV Obs (mm)	SDEV Model (mm)	R	RMSE (mm)	NMB (%)	NME (%)
NADP Dep	1523	20.7	19.6	22.7	20.6	0.67	17.8	-5.28	54.7

NADP Precipitation - Summer

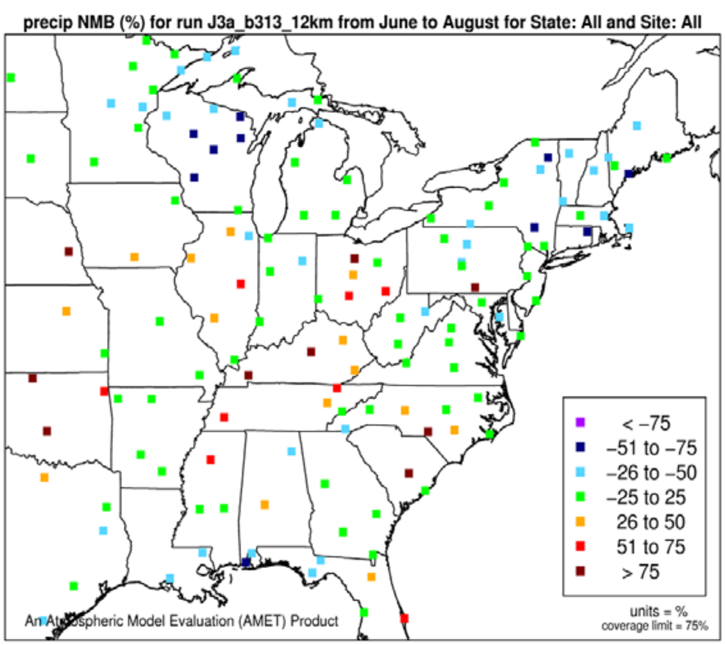
Scatter Plot – All Pairs



Scatter Plot – Monthly Accumulated Pairs

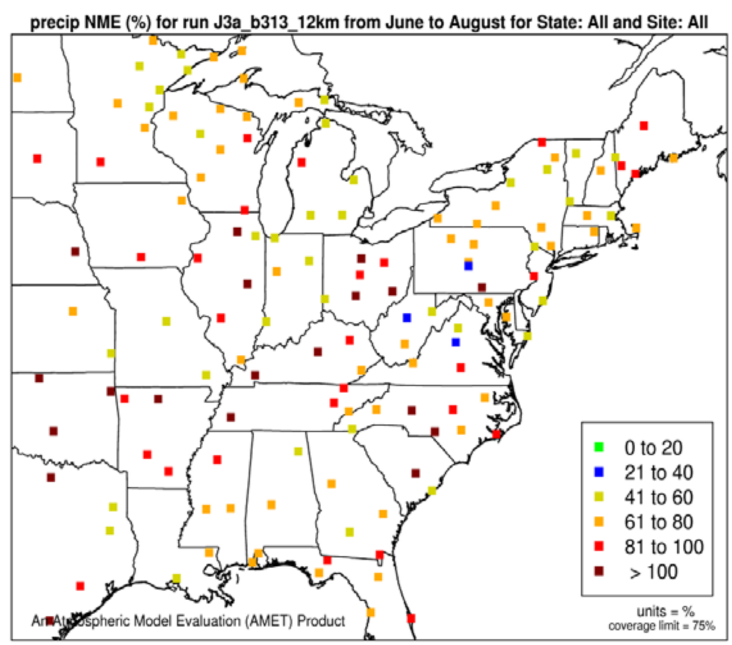


Normalized Mean Bias (%) - Summer



square=NADP_dep;

Normalized Mean Error (%) - Summer

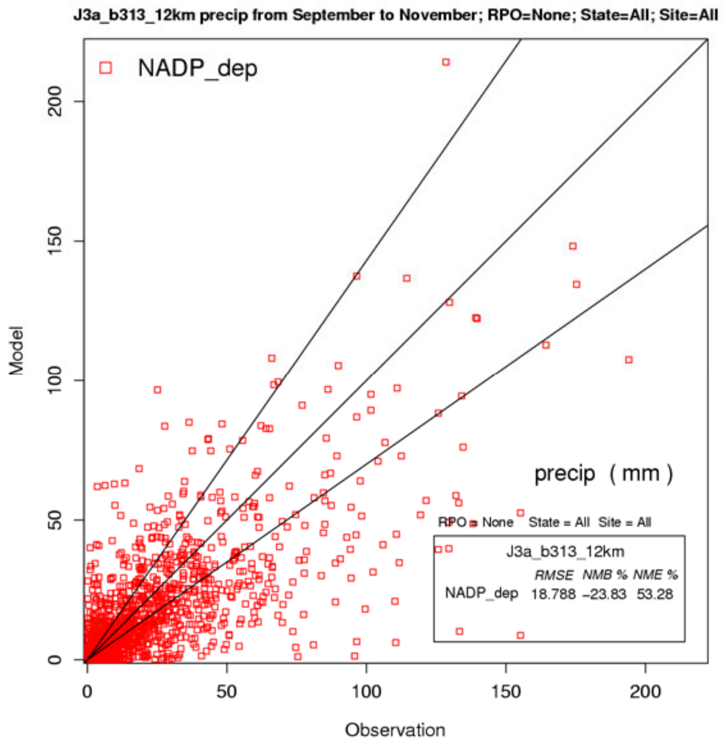


square=NADP_dep;

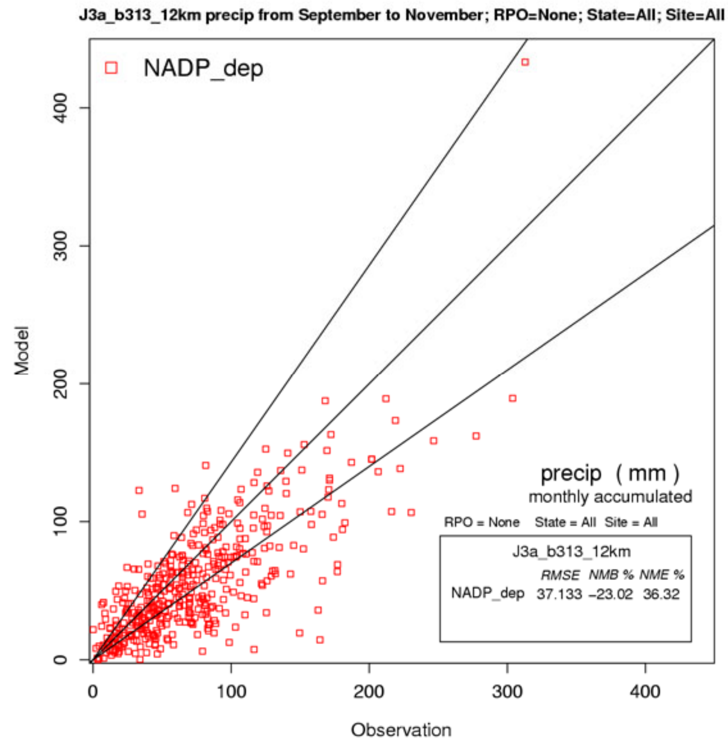
Network	# Obs	Mean Obs (mm)	Mean Model (mm)	SDEV Obs (mm)	SDEV Model (mm)	R	RMSE (mm)	NMB (%)	NME (%)
NADP Dep	1693	26.2	24.9	30.5	25.4	0.46	29.6	-5.06	71.5

NADP Precipitation - Fall

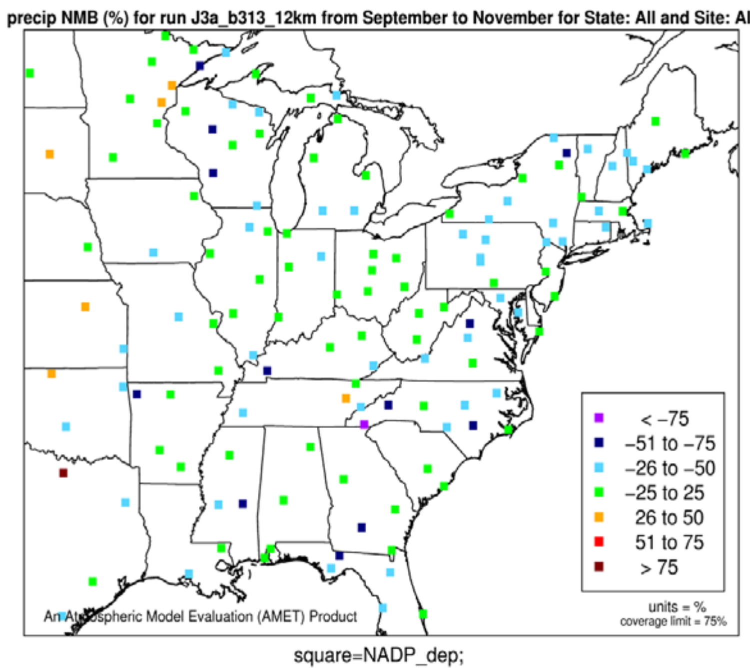
Scatter Plot – All Pairs



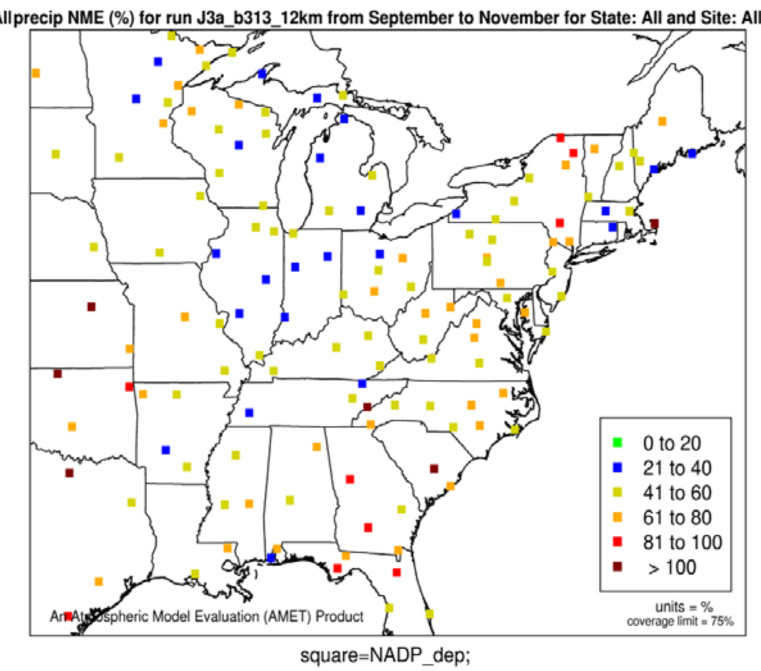
Scatter Plot – Monthly Accumulated Pairs



Normalized Mean Bias (%) - Fall



Normalized Mean Error (%) - Fall



Network	# Obs	Mean Obs (mm)	Mean Model (mm)	SDEV Obs (mm)	SDEV Model (mm)	R	RMSE (mm)	NMB (%)	NME (%)
NADP Dep	1486	20.5	15.6	26.3	20.6	0.73	18.8	-23.8	53.3

Comparison of CMAQ v4.4 vs. v4.5: 12km×12km Grid Cell Sizes

Networks and Species Used:

AQS - Ozone
IMPROVE – Sulfate, Nitrate
STN – Sulfate, Nitrate, Ammonium
CASTNet – Sulfate, Nitrate, Ammonium, Nitric Acid, Total Nitrate
NADP – wet deposition SO_4^{2-}, wet deposition NO_3^-, wet deposition NH_4^+

CMAQ v4.5 versus v4.4 Performance Comparison: Introduction

The following section deals with a comparison of the relative performance of the 2005 release version of CMAQ (v.4.5) and the 2004 release version of CMAQ (v4.4) at the 12-km horizontal resolution. In addition to the different versions of the model, there are also several other differences between the simulations, which are discussed in section 3 at the beginning of this report. Only the winter (December, January and February 2001) and summer (June, July and August 2001) seasons will be used in the comparison, which are sufficient for highlighting the changes between the two model versions.

- Ozone 8-hr max scatter plots, diurnal average plots and spatial NMB and NME plots
- Winter and summer model to observation scatter plots of organic and inorganic aerosols
- Winter and summer model to observation scatter plots of total $PM_{2.5}$ mass
- Winter and summer model to observation scatter plots of precipitation chemistry

Note that there is a small difference in the total number of observations included in the AQS statistics (one extra day for each site). The difference is indirectly due to the unavailability of the month of September when running site compare for CMAQ v4.4, which results in several more observations being included in the v4.5 analysis. The difference in the number of observations does not significantly impact the statistics.

Note that for comparison of organic carbon, the complete unit is µgC/m³, although on plots the units are labeled as µg/m³.

CMAQ v4.5 versus v4.4 Performance Comparison: Summary

The performance for ozone (8hr-max) is relatively unchanged between versions 4.4 and 4.5 of CMAQ. The diurnal profile at urban sites has improved slightly in v4.5 due to the modification in the minimum K_z values. There is virtually no change in the diurnal profile between the two versions at the selected rural sites.

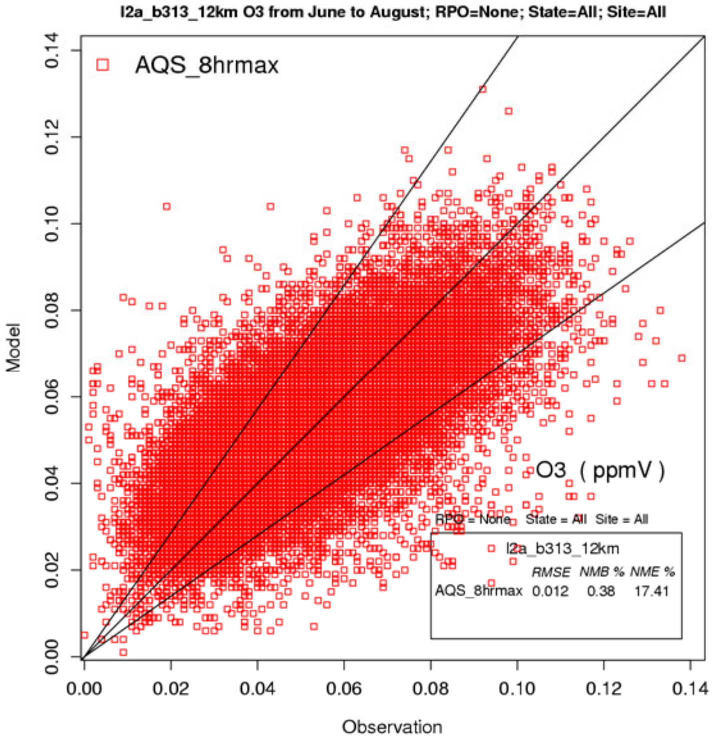
Inorganic sulfate performance for both the winter and summer seasons generally improved from v4.4 to v4.5, with marked improvements in bias and in some cases error as well. For winter, NMB and NME improved for STN and CASTNet, while the IMPROVE network performance remained fairly unchanged. For summer, NMB and NME values improved with the new version, with generally a 17-24% improvement in NMB and a roughly 8-10% decrease in NME. Inorganic nitrate showed a moderate to significant improvement in bias and error in the winter with v4.5, however bias and error values generally increased slightly in the summer. Ammonium performance for the winter was slightly worse with v4.5, as the bias and error values increased slightly. Ammonium performance for the summer was mixed, with an improvement at STN and poorer performance at CASTNet. Nitric acid performance at CASTNet sites was slightly worse for the winter, with a slight negative bias in v4.4 becoming a slight positive bias in v4.5 (NME values are virtually unchanged). Performance of nitric acid improved in the summer, with significant decreases in both NMB and NME in v4.5. There was a slight improvement in total nitrate performance in the winter and a larger improvement in the summer in v4.5.

Elemental carbon performance varies between the two versions of the model, with a small improvement at both IMPROVE and STN in the winter, while in the summer, performance improves slightly at STN and becomes slightly worse at IMPROVE. Significant over-predictions in EC at STN were observed in both model versions. The performance changes in organic carbon were similar to that of EC between the v4.4 and v4.5, with a slight improvement in the winter and a slight to moderate decrease in performance in the summer. OC is over-predicted in the winter and under-predicted in the summer in both versions of the model. Total PM2.5 mass performance improved slightly in the winter, with improvements in NMB and NME at both IMPROVE and STN. For the summer, under-predictions at IMPROVE became larger in v4.5, increasing NMB by roughly 16% (NME increased about 4%), while at STN a small positive NMB in v4.4 became a small negative NMB in v4.5 and NME remained roughly unchanged.

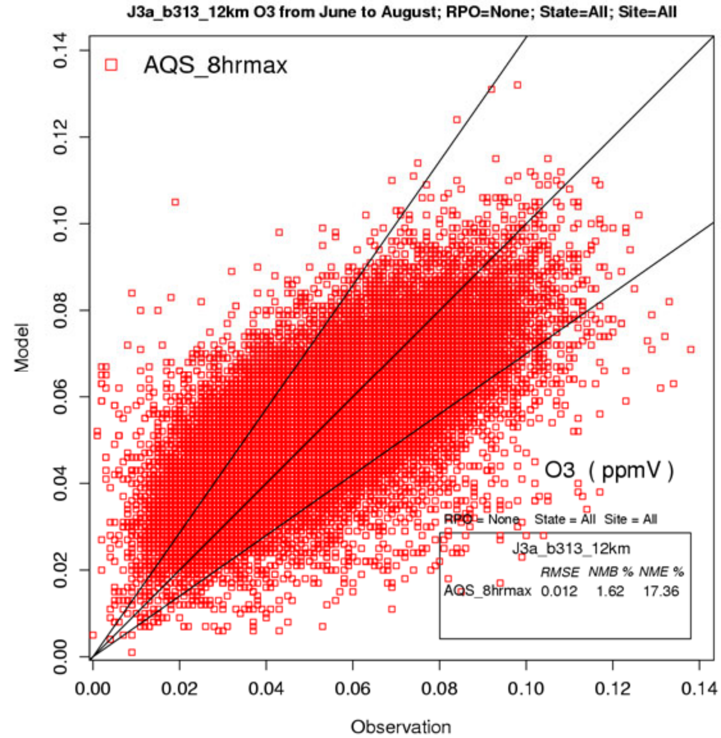
For precipitation chemistry, the NMB for wet deposition sulfate improved in both the winter and summer in v4.5, but NME increased for both seasons. Wet deposition nitrate was essentially unchanged in the winter between the two versions, while in the summer a slight improvement in both NMB and NME is observed in v4.5. Wet deposition ammonium saw a slight increase in NMB in the winter (NME was essentially unchanged) and a moderate improvement in NMB in the summer (NME was unchanged) with v4.5.

AQS 8-hr Max Ozone (ppm) - Summer

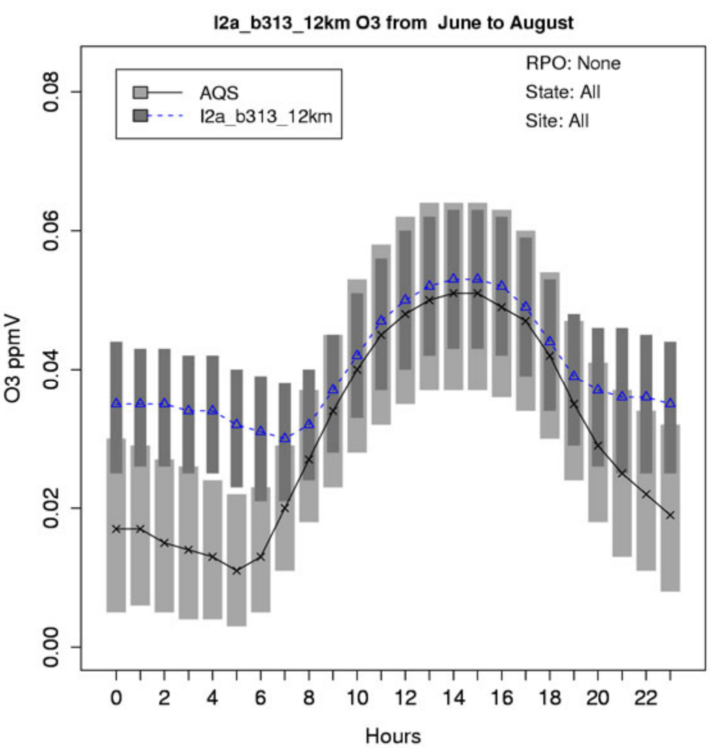
Scatter Plot – CMAQ v4.4 12 km



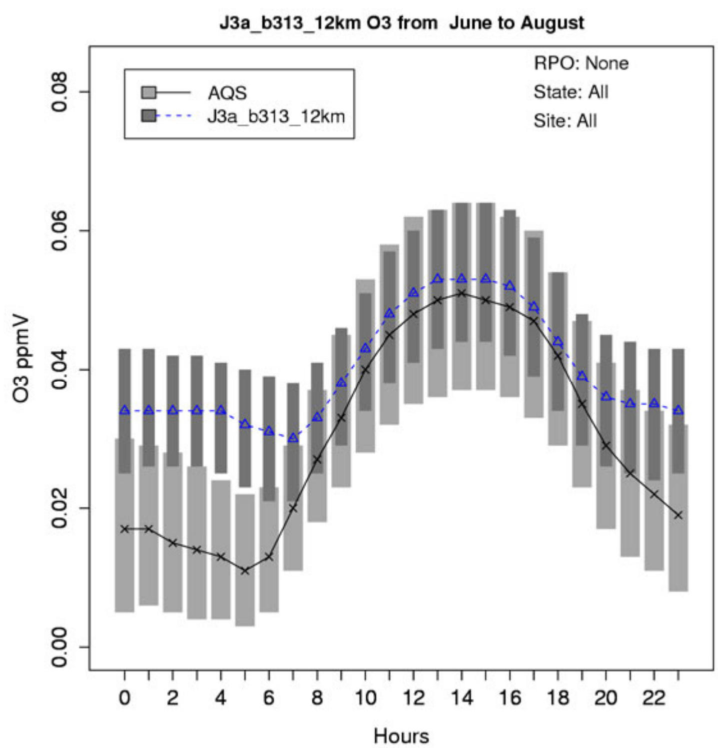
Scatter Plot – CMAQ v4.5 12 km



Diurnal Box Plot – CMAQ v4.4 12 km



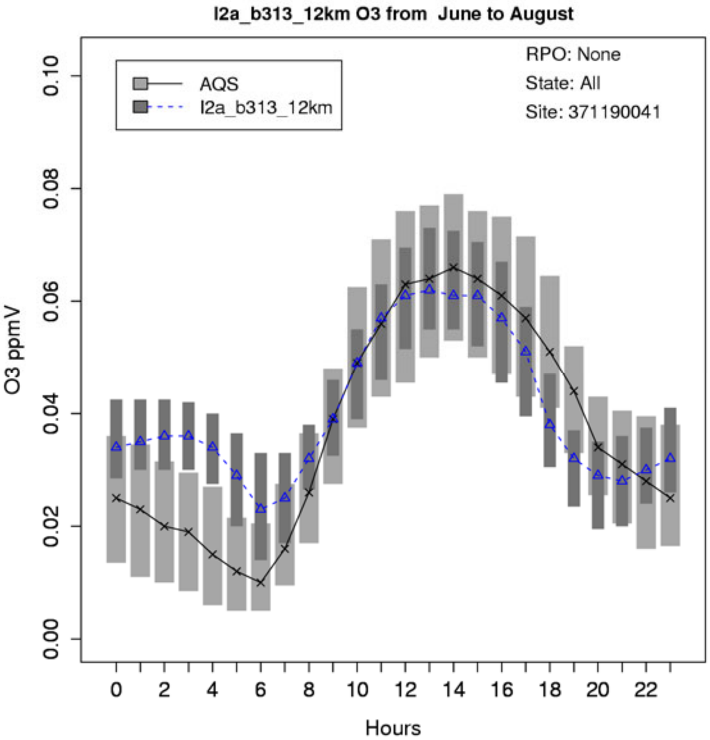
Diurnal Box Plot – CMAQ v4.5 12 km



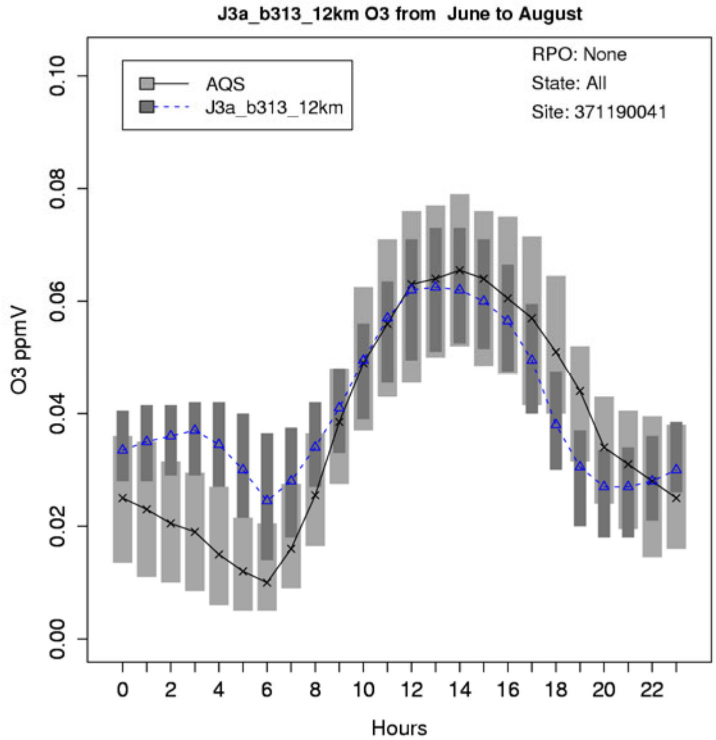
Network	# Obs	Mean Obs	Mean Model	SDEV Obs	SDEV Model	R	RMSE	NMB (%)	NME (%)
AQS (v4.4)	70499	0.053	0.053	0.017	0.013	0.73	0.012	0.38	17.4
AQS (v4.5)	71284	0.052	0.053	0.018	0.013	0.74	0.012	1.62	17.4

AQS Diurnal Box Plots (Urban) – Summer

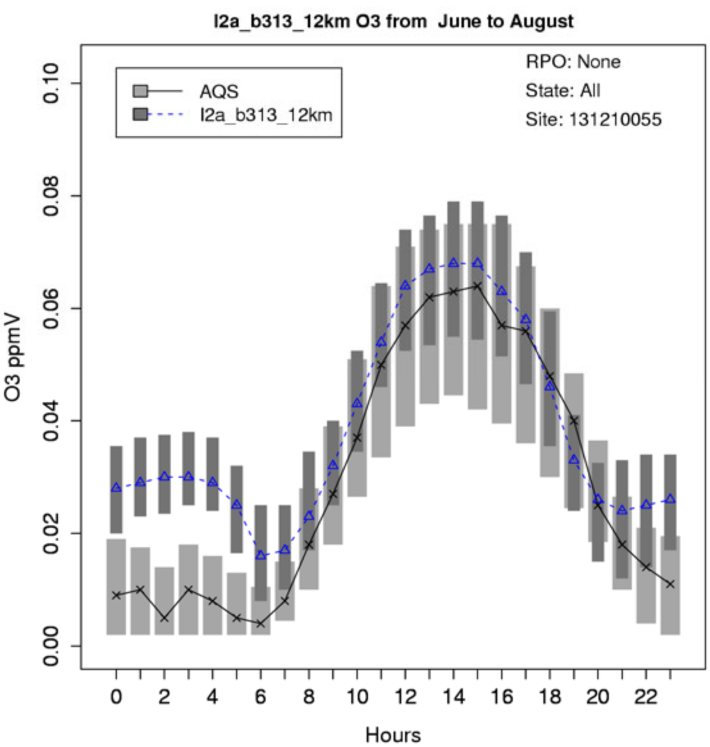
Diurnal Plot – CMAQ v4.4 12 km (Urban)



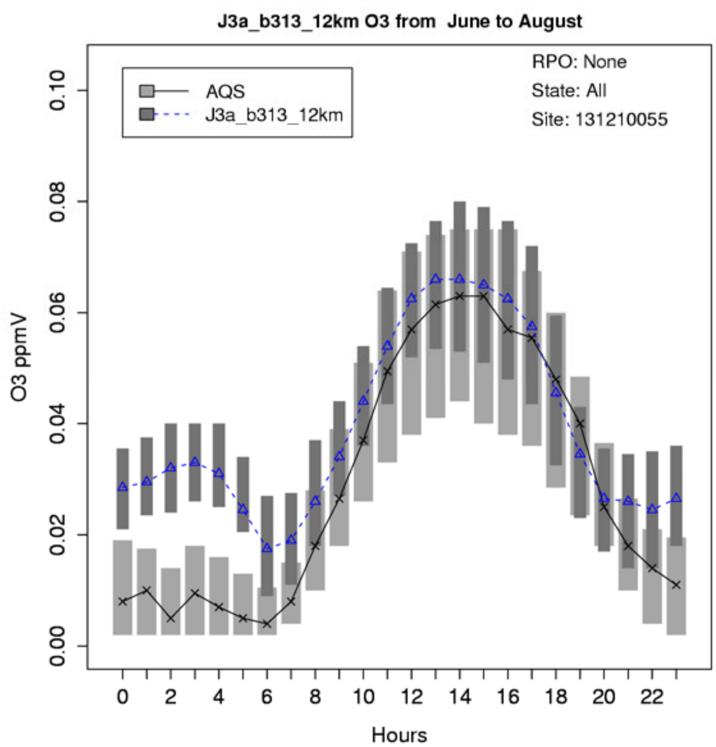
Diurnal Plot – CMAQ v4.5 12 km (Urban)



Diurnal Plot – CMAQ v4.4 12 km (Urban)

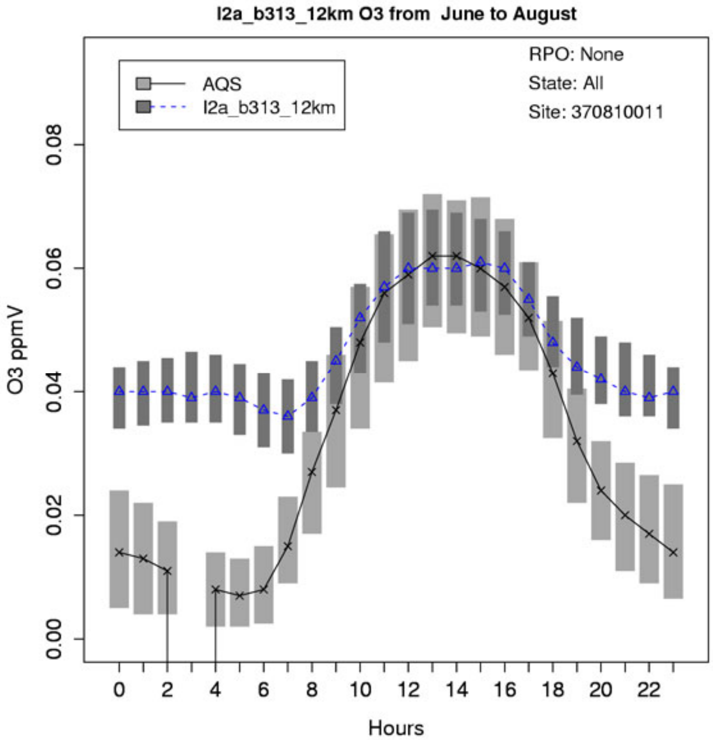


Diurnal Plot – CMAQ v4.5 12 km (Urban)

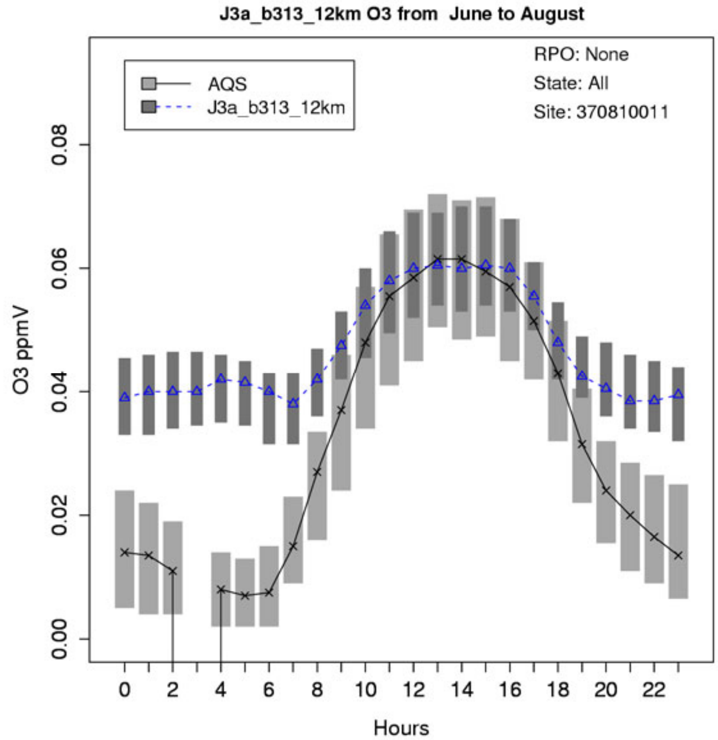


AQS Diurnal Box Plots (Rural) – Summer

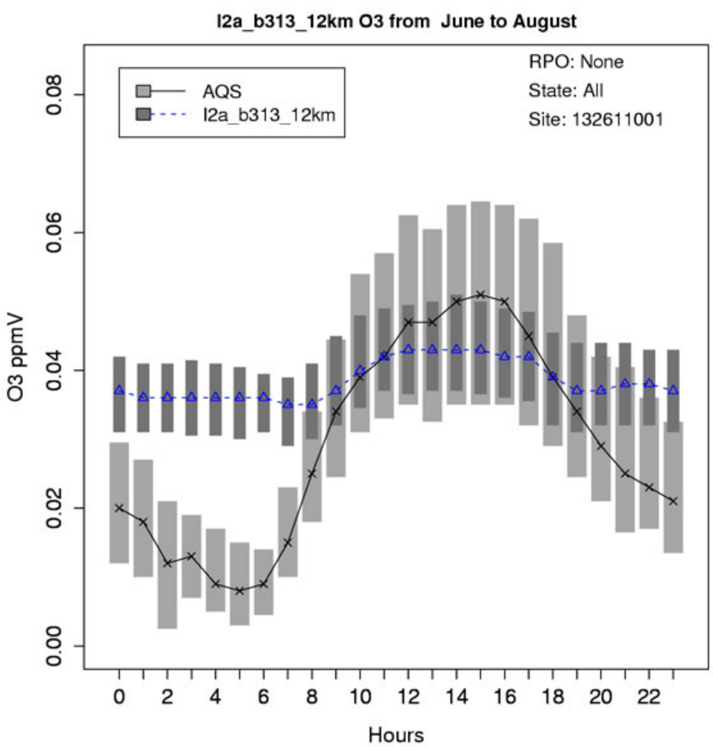
Diurnal Plot – CMAQ v4.4 12 km (Rural)



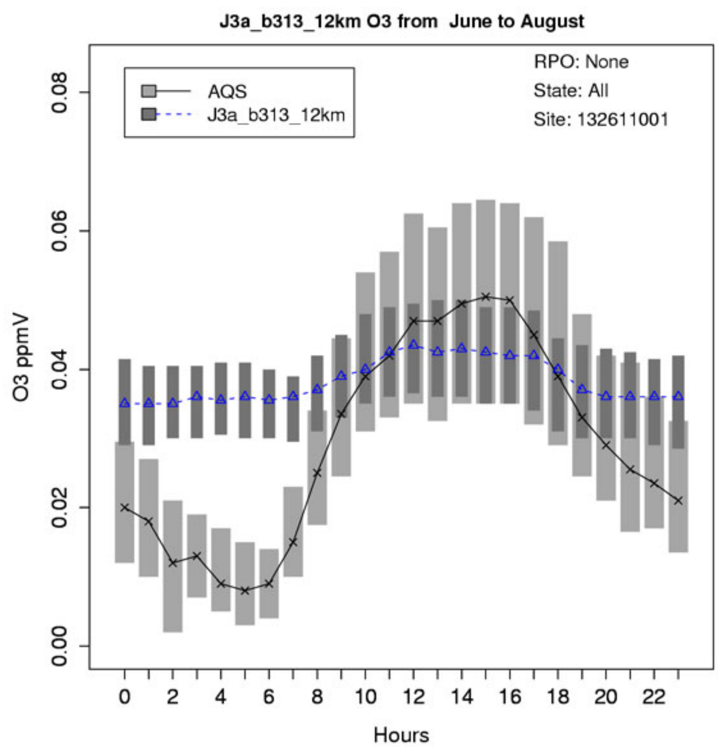
Diurnal Plot – CMAQ v4.5 12 km (Rural)



Diurnal Plot – CMAQ v4.4 12 km (Rural)

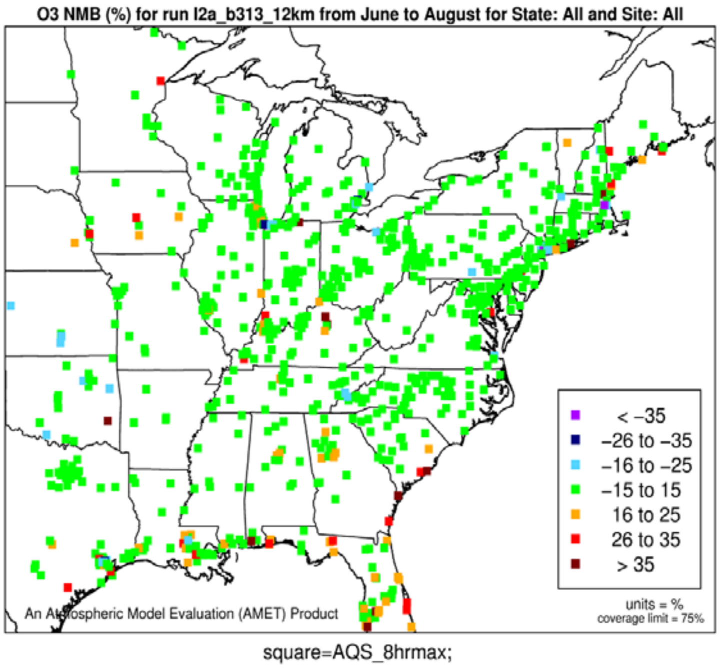


Diurnal Plot – CMAQ v4.5 12 km (Rural)

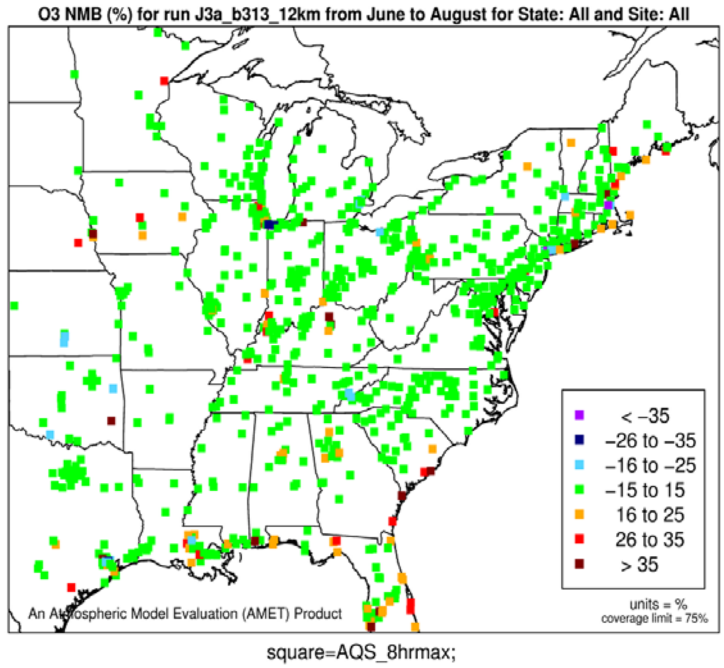


AQS 8-hr Max Ozone - Summer

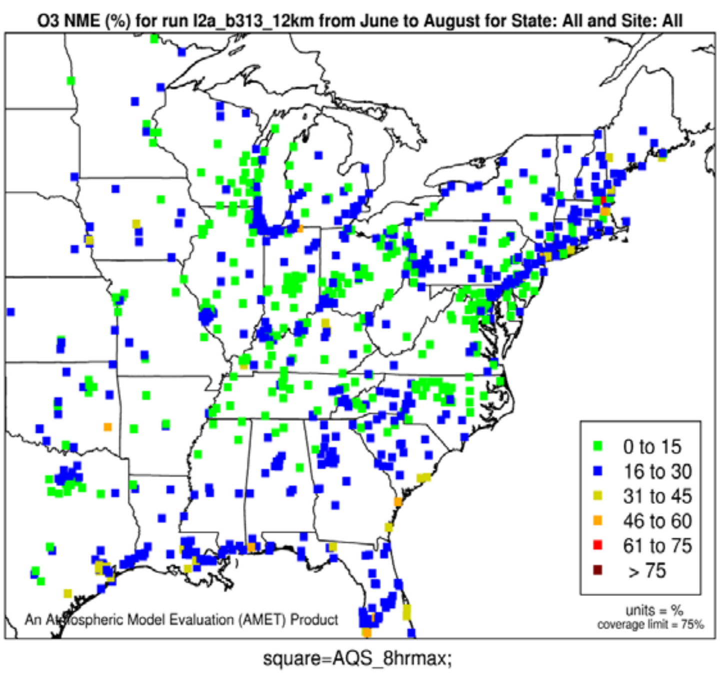
NMB (%) – CMAQ v4.4 12 km



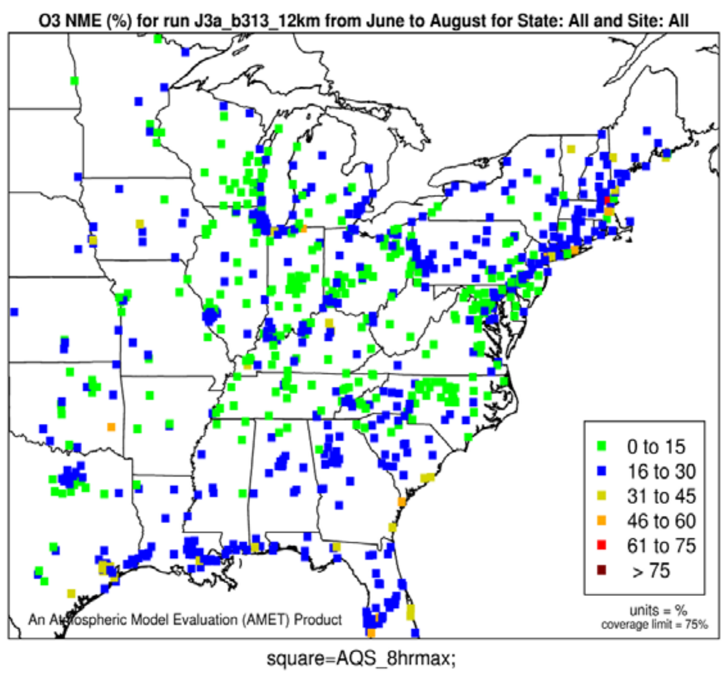
NMB (%) – CMAQ v4.5 12 km



NME (%) – CMAQ v4.4 12 km

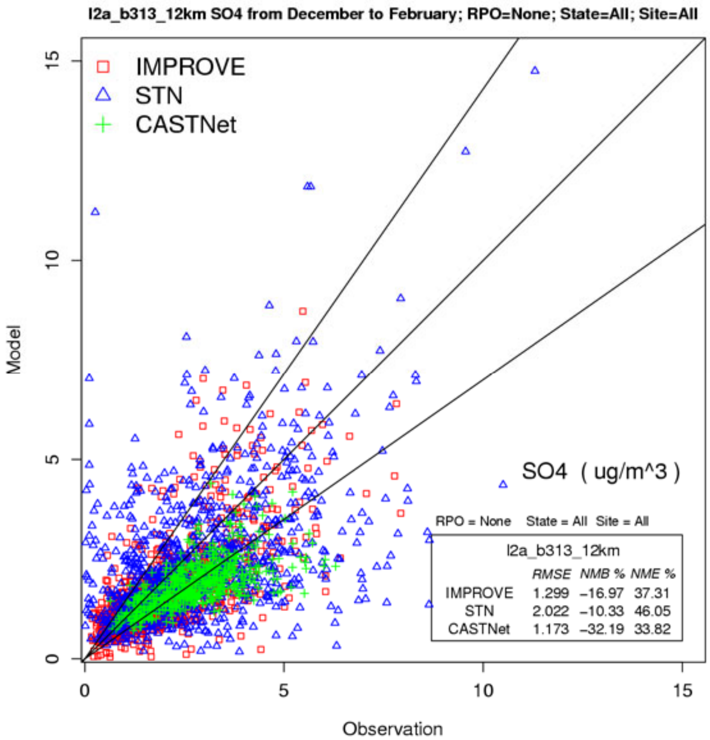


NME (%) – CMAQ v4.5 12 km

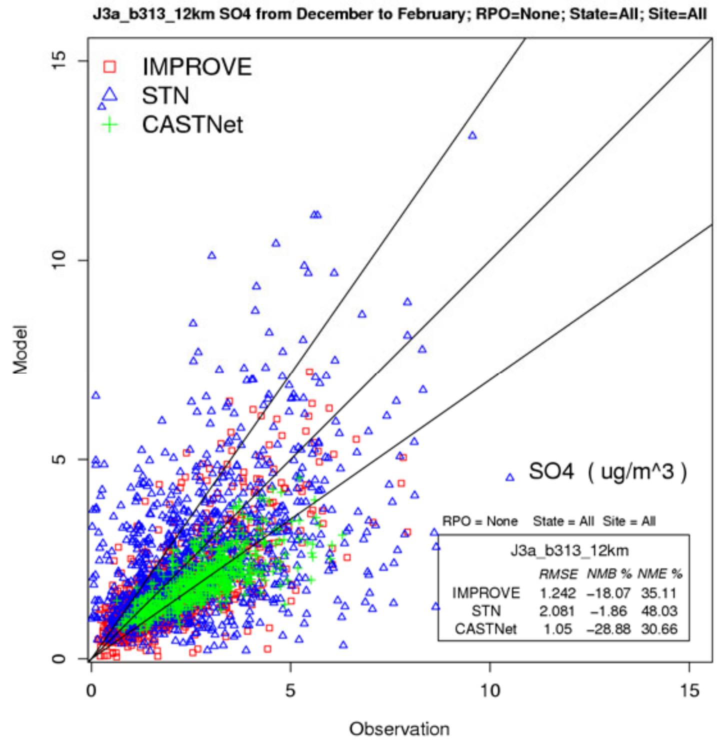


Sulfate (µg/m^3) – Winter

Scatter Plot – CMAQ v4.4 12 km

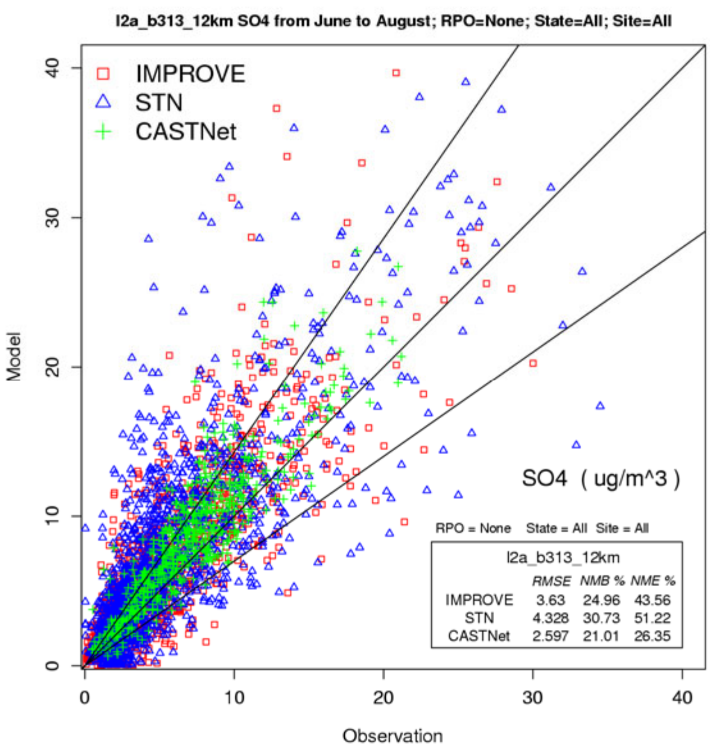


Scatter Plot – CMAQ v4.5 12 km

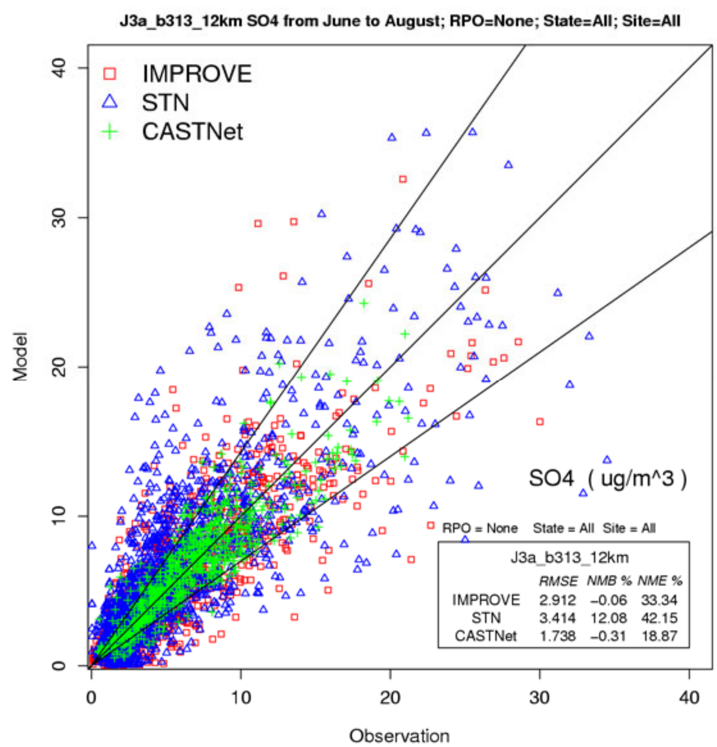


Sulfate (µg/m^3) - Summer

Scatter Plot – CMAQ v4.4 12 km

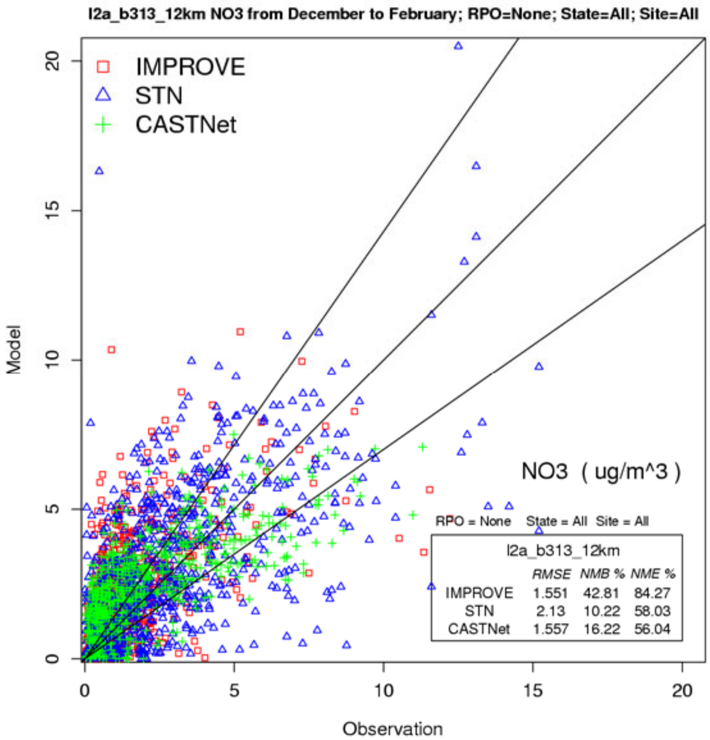


Scatter Plot – CMAQ v4.5 12 km

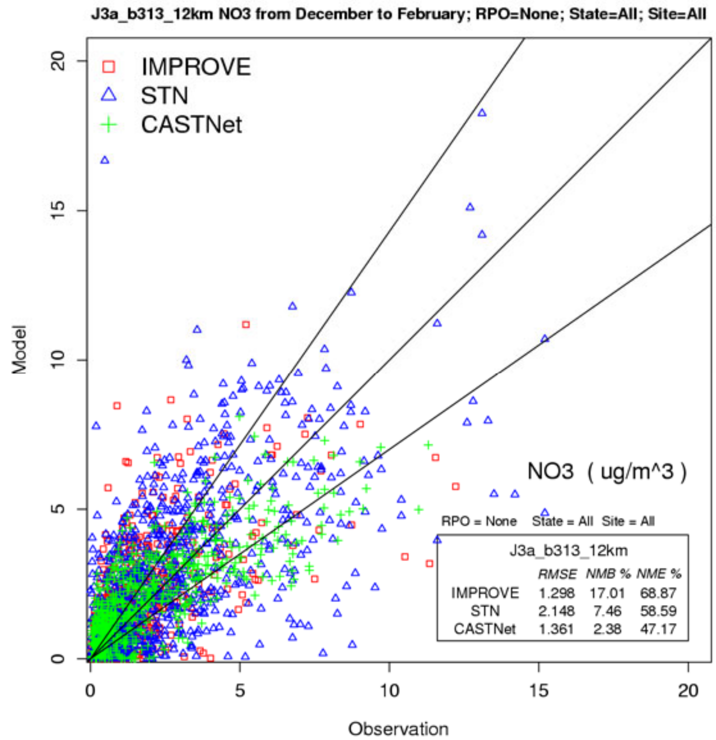


Nitrate (µg/m^3) – Winter

Scatter Plot – CMAQ v4.4 12 km

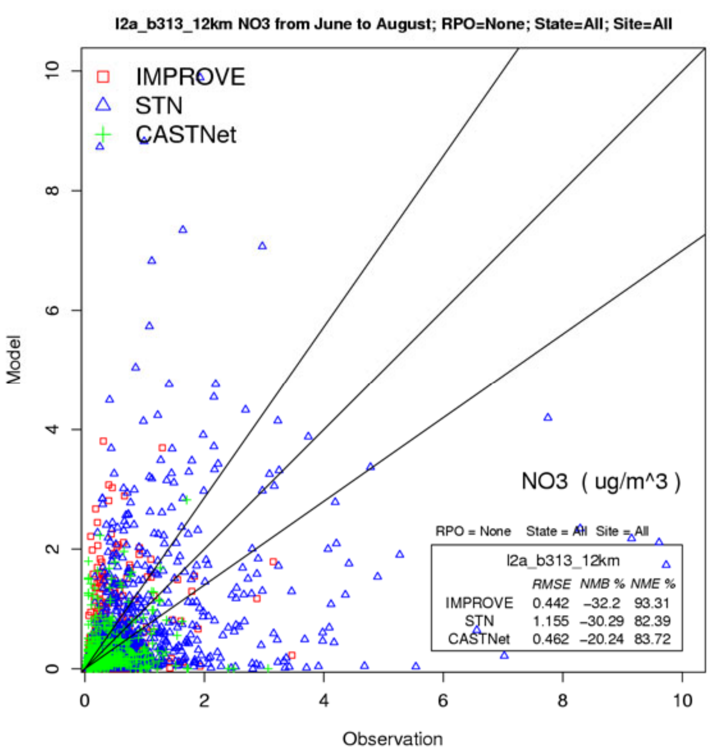


Scatter Plot – CMAQ v4.5 12 km

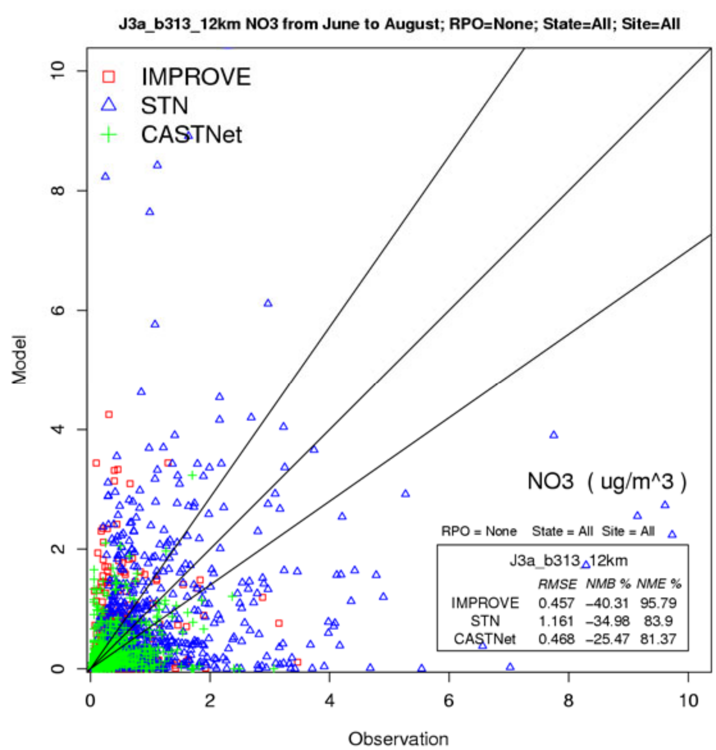


Nitrate (µg/m^3) - Summer

Scatter Plot – CMAQ v4.4 12 km

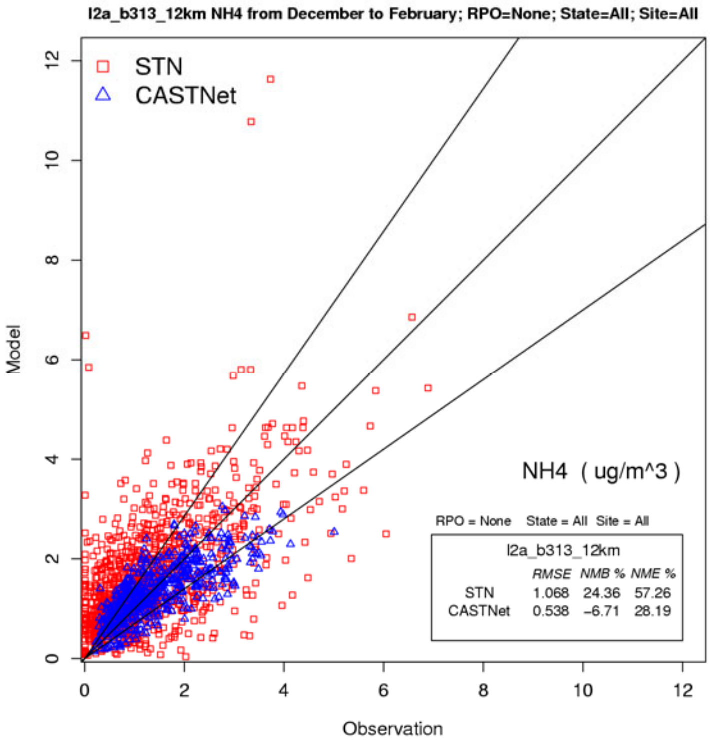


Scatter Plot – CMAQ v4.5 12 km

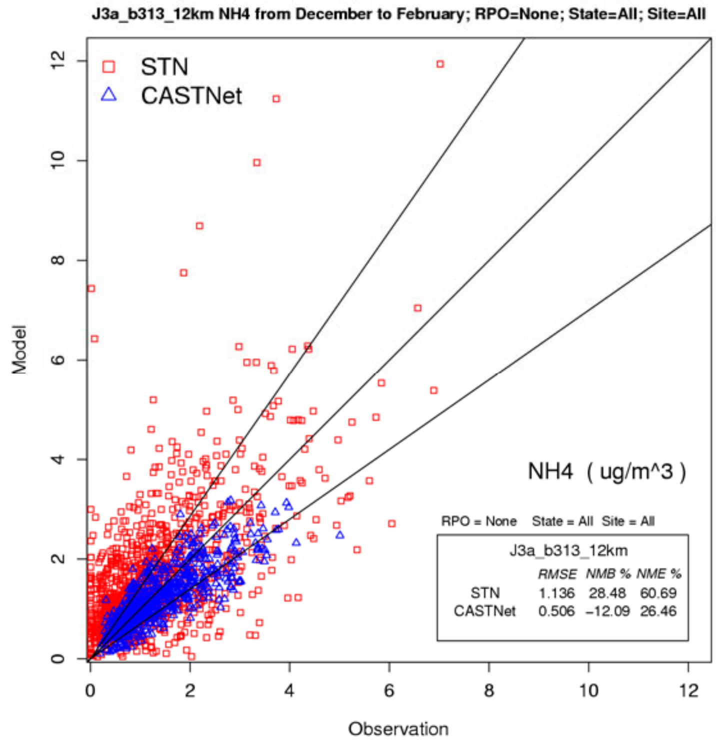


Ammonium (µg/m³) – Winter

Scatter Plot – CMAQ v4.4 12 km

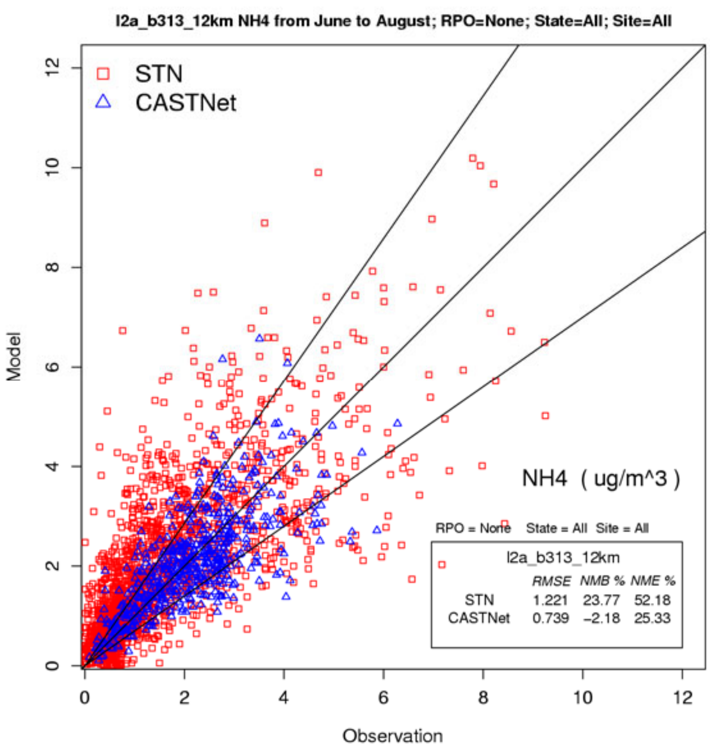


Scatter Plot – CMAQ v4.5 12 km

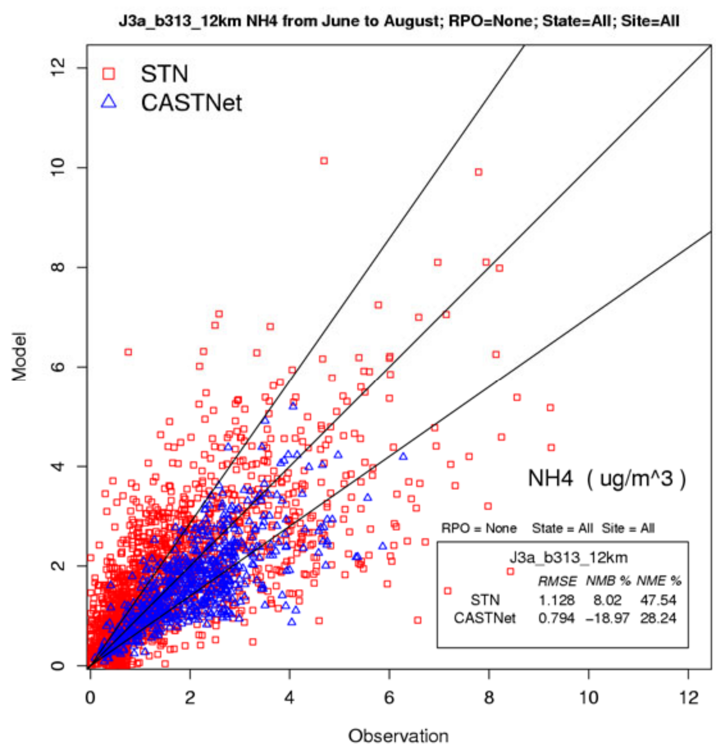


Ammonium (µg/m³) – Summer

Scatter Plot – CMAQ v4.4 12 km

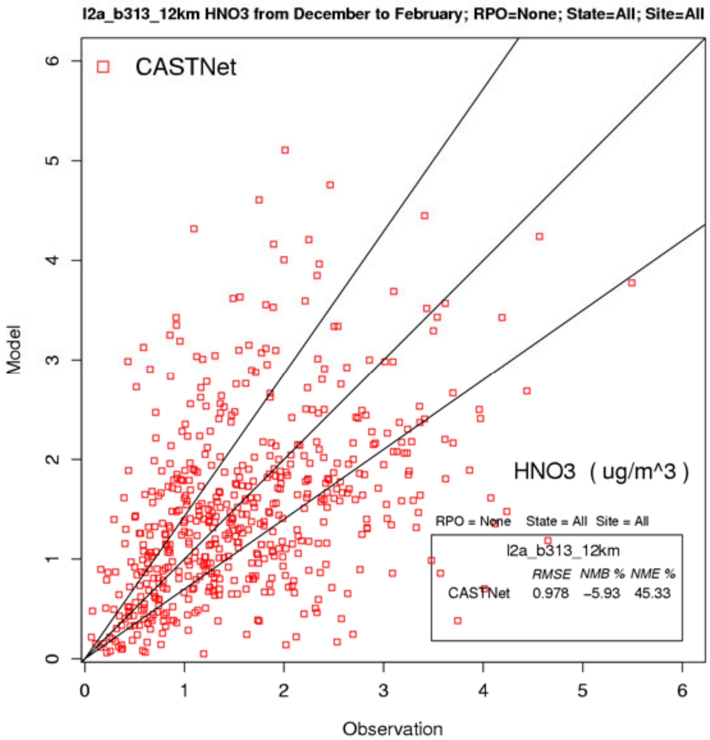


Scatter Plot – CMAQ v4.5 12 km

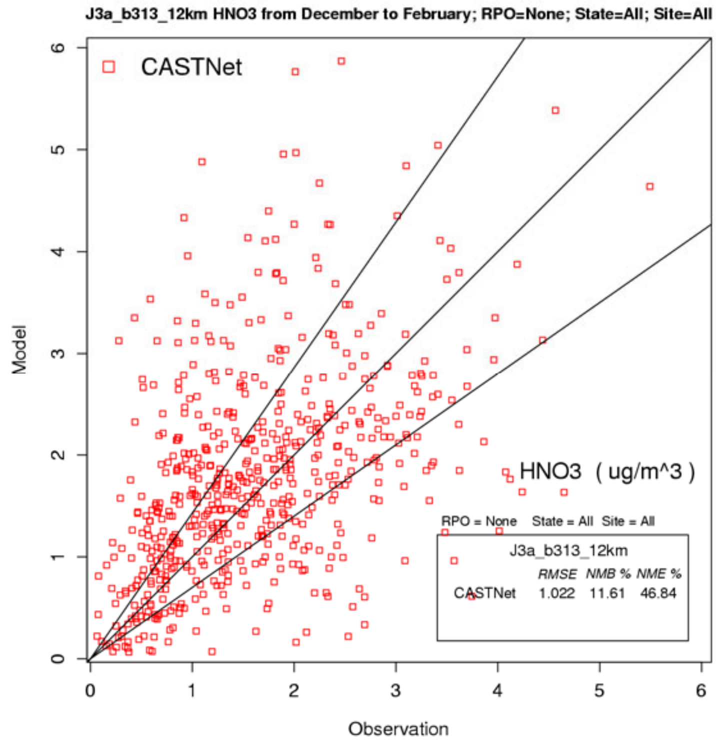


Nitric Acid (µg/m^3) – Winter

Scatter Plot – CMAQ v4.4 12 km

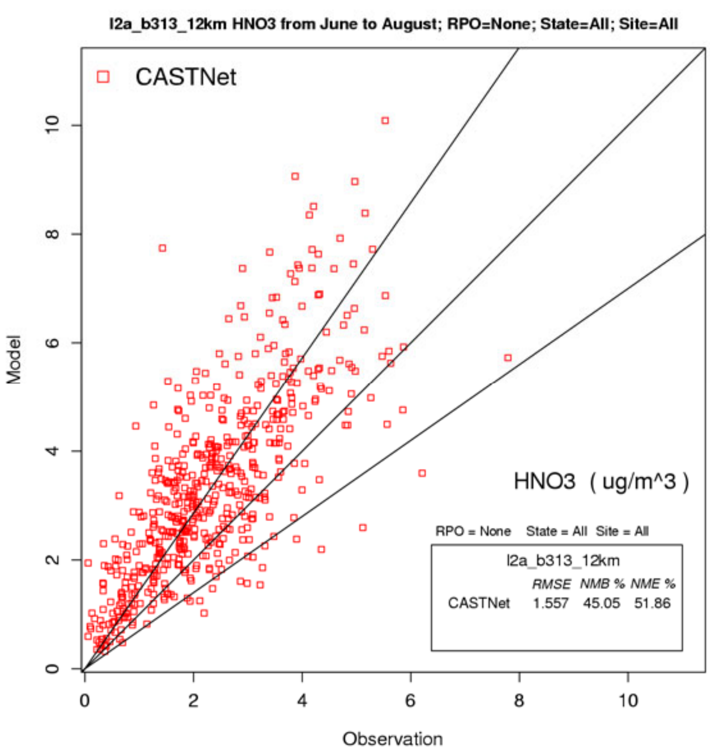


Scatter Plot – CMAQ v4.5 12 km

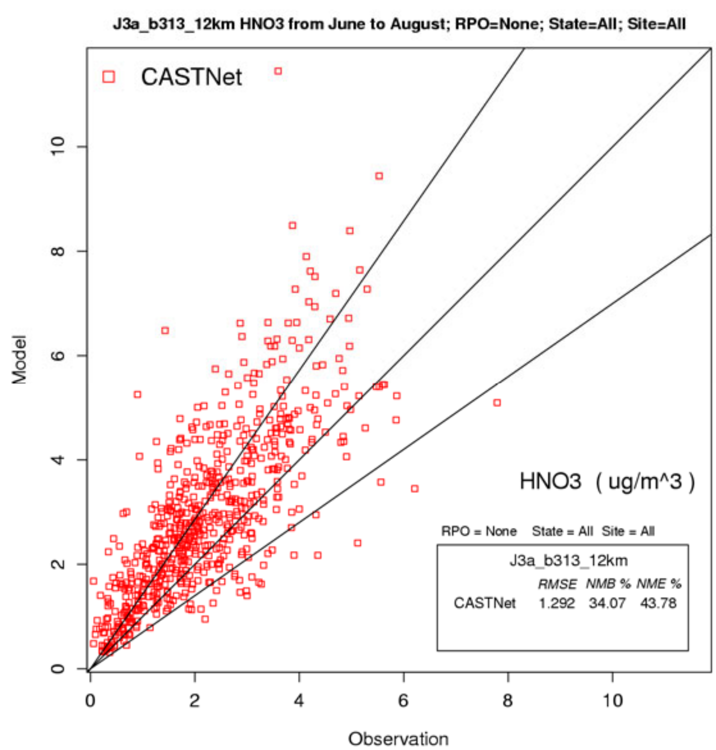


Nitric Acid (µg/m^3) – Summer

Scatter Plot – CMAQ v4.4 12 km

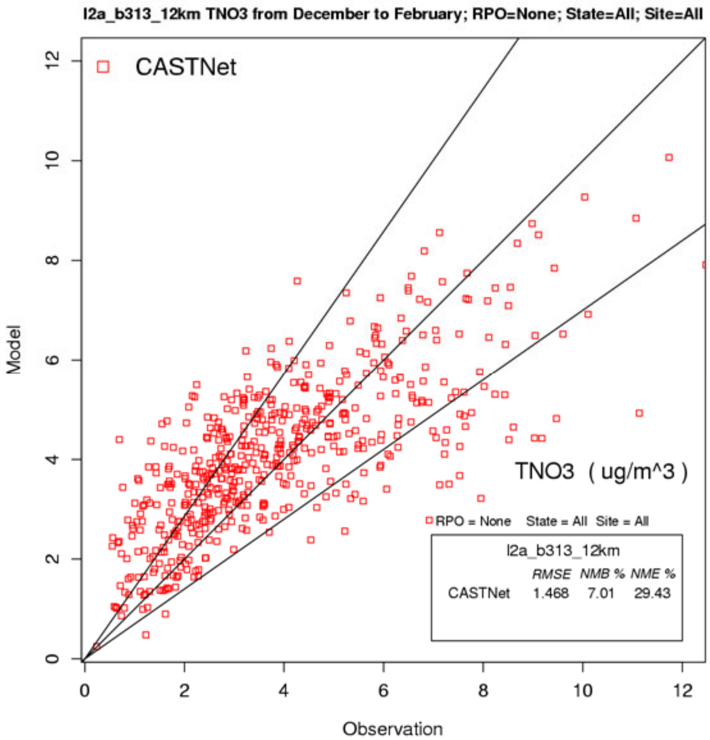


Scatter Plot – CMAQ v4.5 12 km

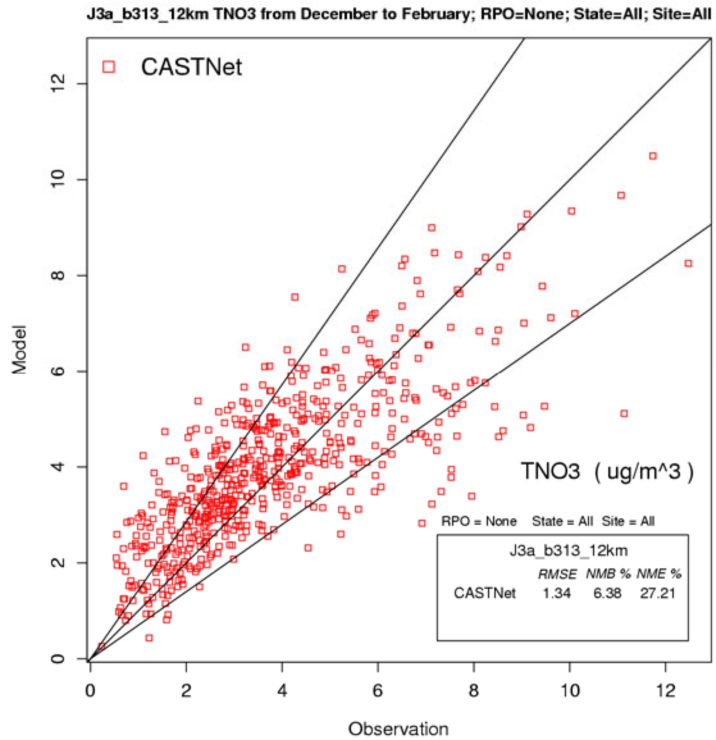


Total Nitrate (µg/m³) – Winter

Scatter Plot – CMAQ v4.4 12 km

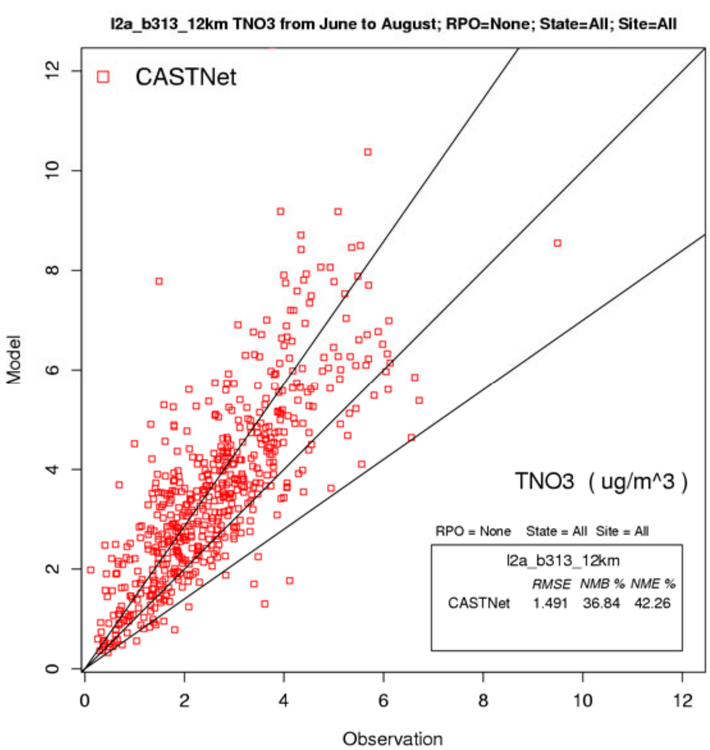


Scatter Plot – CMAQ v4.5 12 km

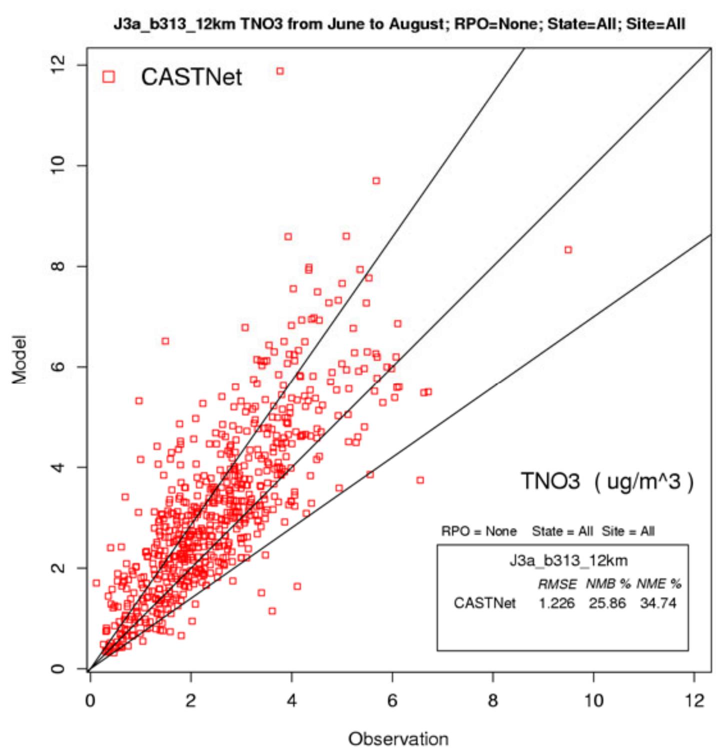


Total Nitrate (µg/m³) – Summer

Scatter Plot – CMAQ v4.4 12 km

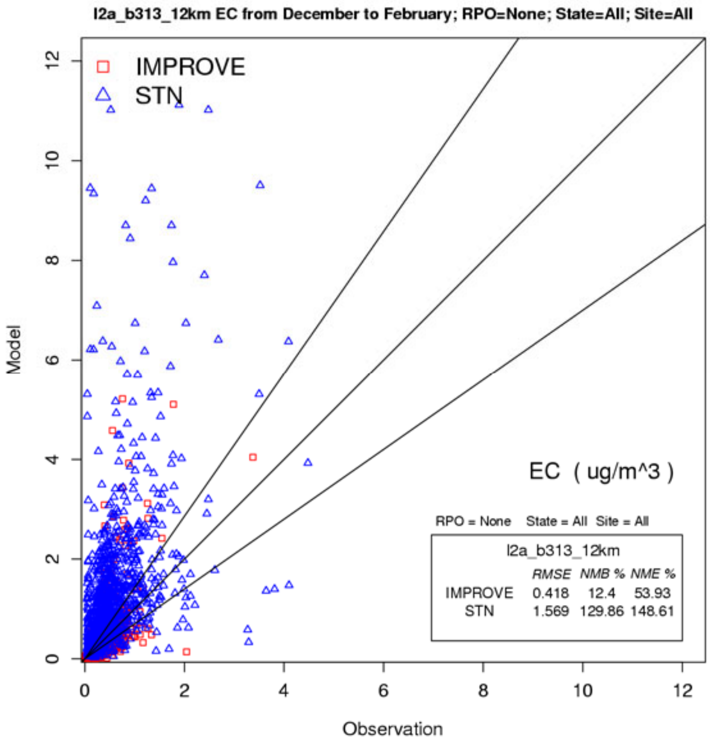


Scatter Plot – CMAQ v4.5 12 km

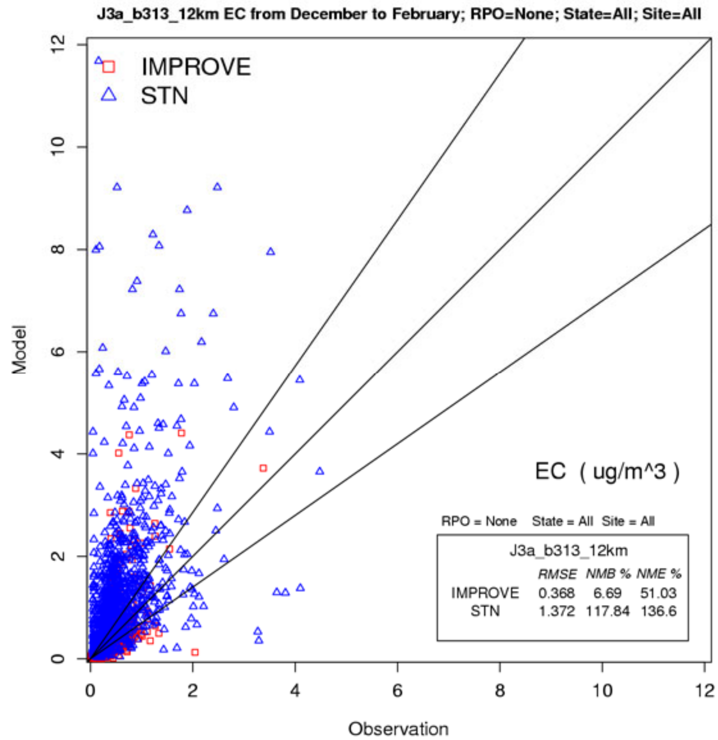


Elemental Carbon ($\mu g/m^3$) – Winter

Scatter Plot – CMAQ v4.4 12 km

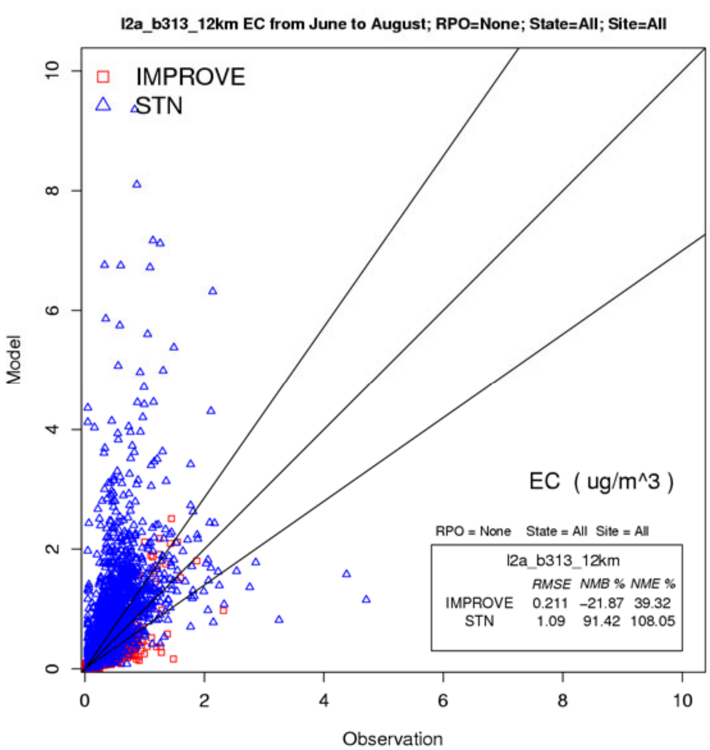


Scatter Plot – CMAQ v4.5 12 km

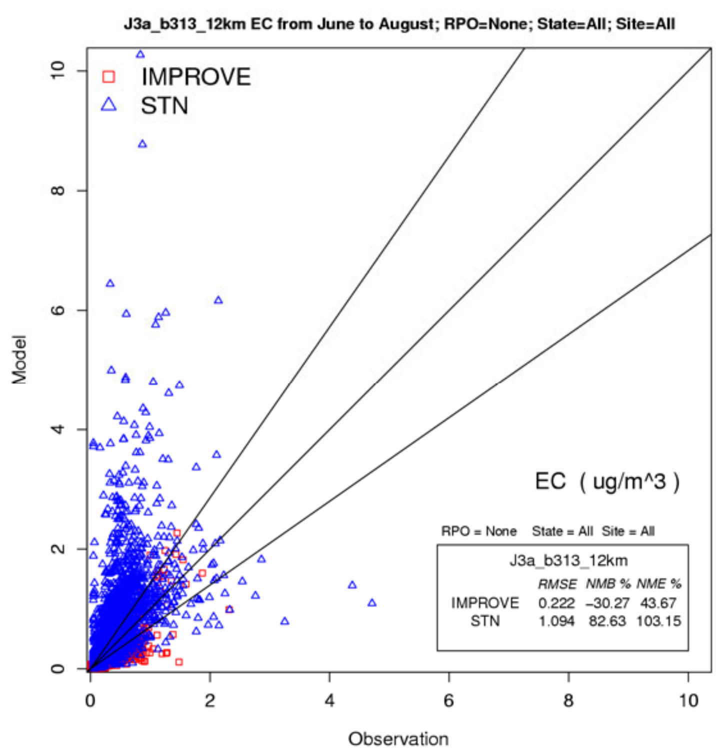


Elemental Carbon ($\mu g/m^3$) – Summer

Scatter Plot – CMAQ v4.4 12 km

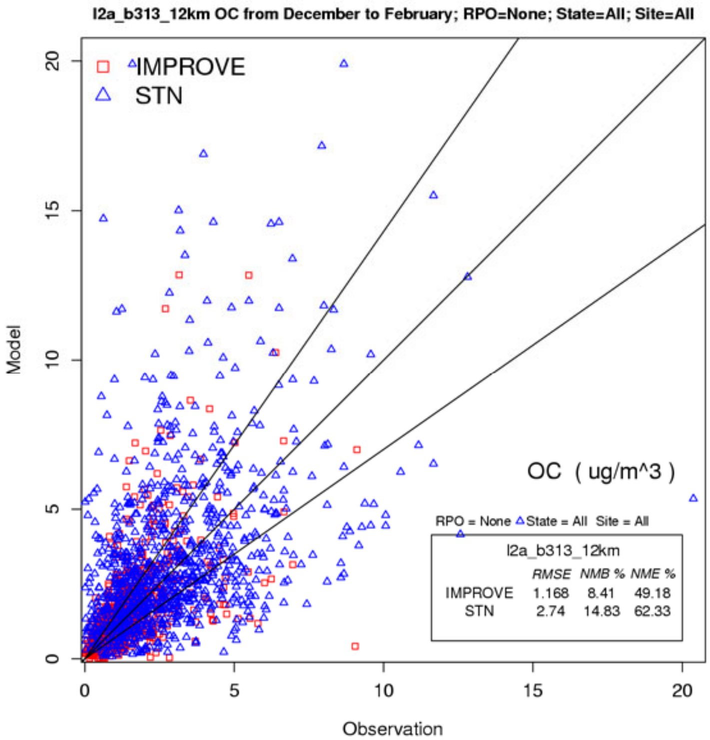


Scatter Plot – CMAQ v4.5 12 km

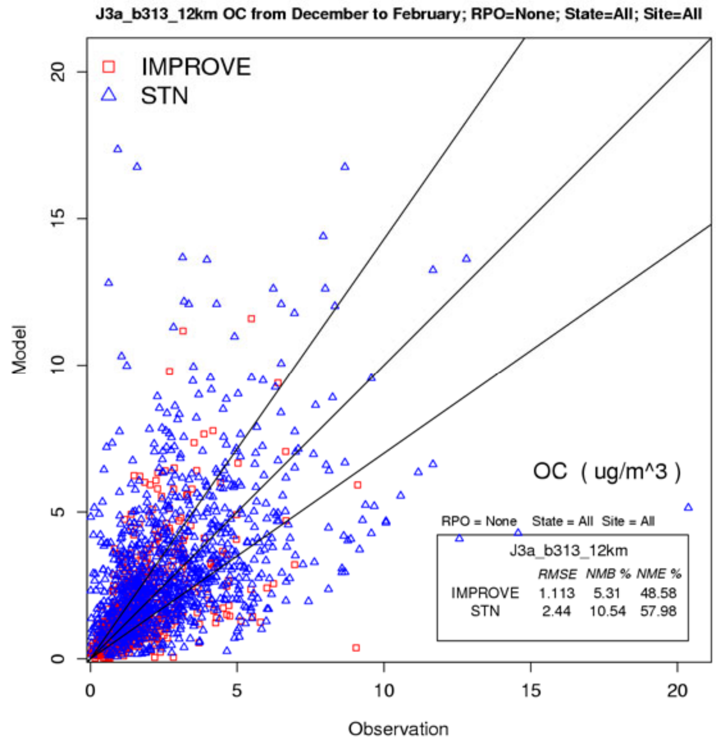


Organic Carbon (μg/m³) – Winter

Scatter Plot – CMAQ v4.4 12 km

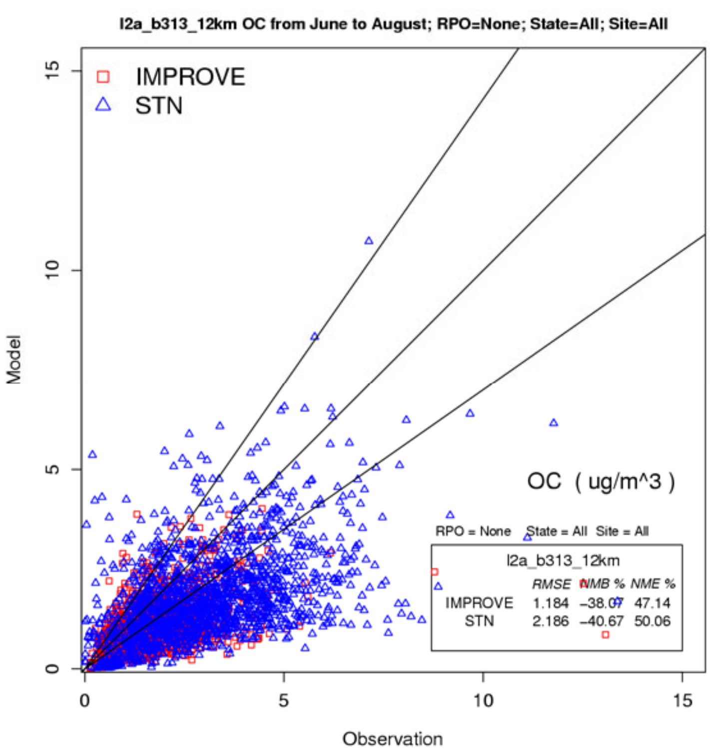


Scatter Plot – CMAQ v4.5 12 km

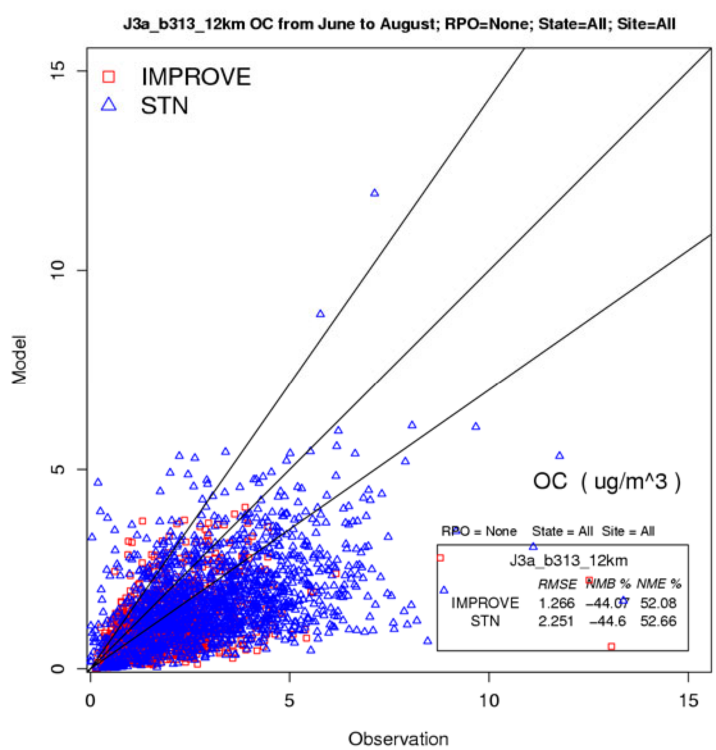


Organic Carbon (μg/m³) – Summer

Scatter Plot – CMAQ v4.4 12 km

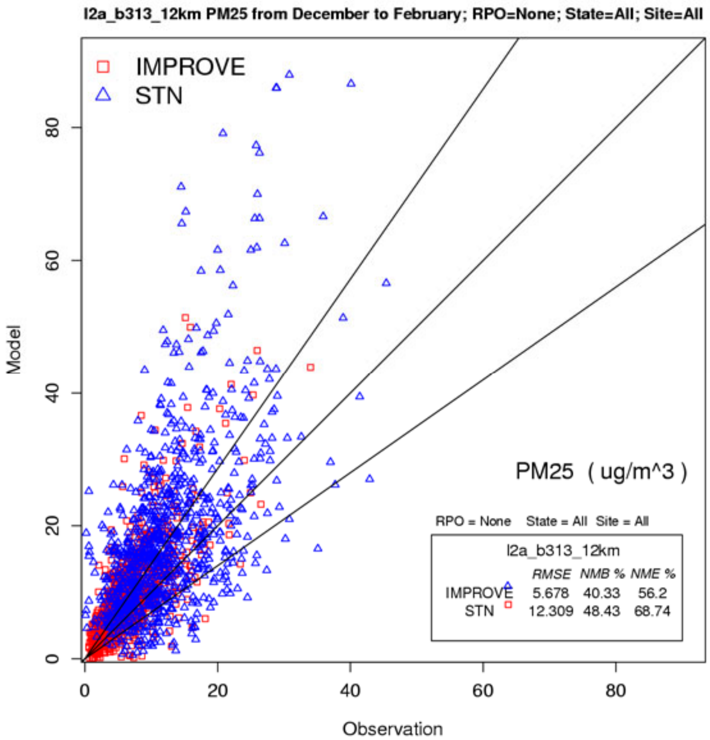


Scatter Plot – CMAQ v4.5 12 km

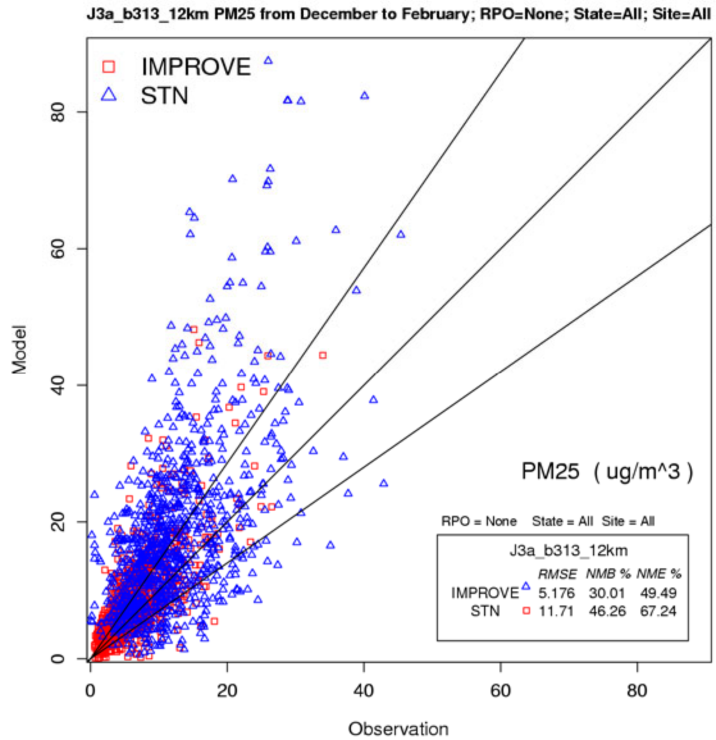


$PM_{2.5}$ ($\mu g/m^3$) – Winter

Scatter Plot – CMAQ v4.4 12 km

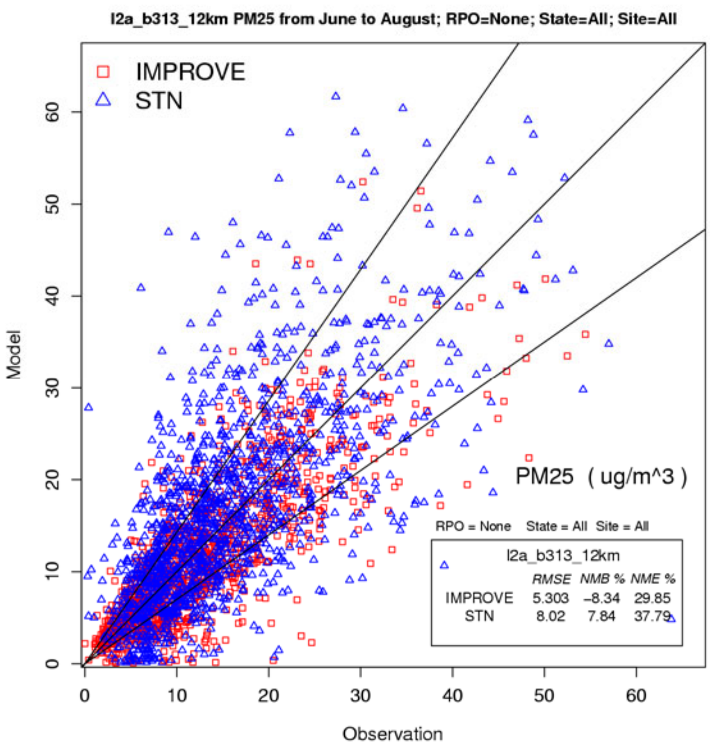


Scatter Plot – CMAQ v4.5 12 km

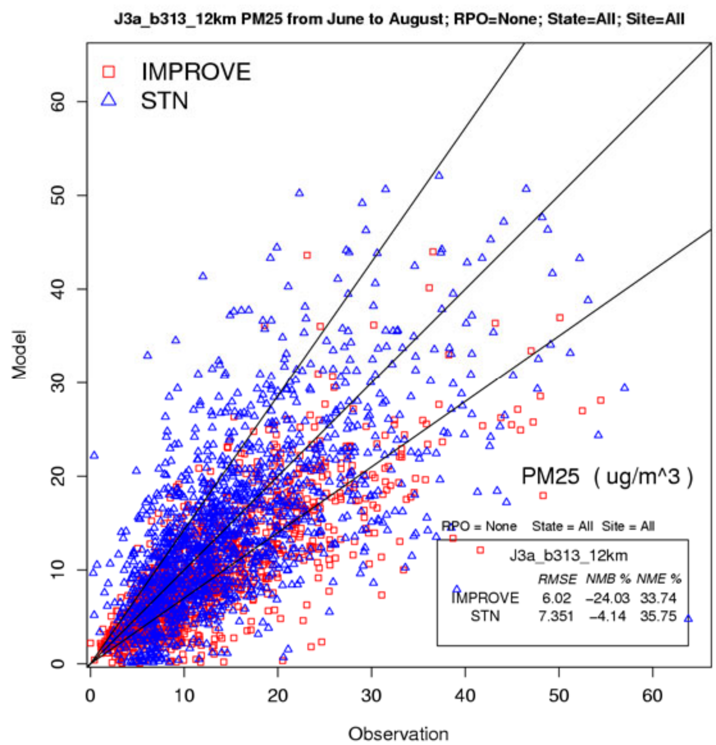


$PM_{2.5}$ ($\mu g/m^3$) – Summer

Scatter Plot – CMAQ v4.4 12 km

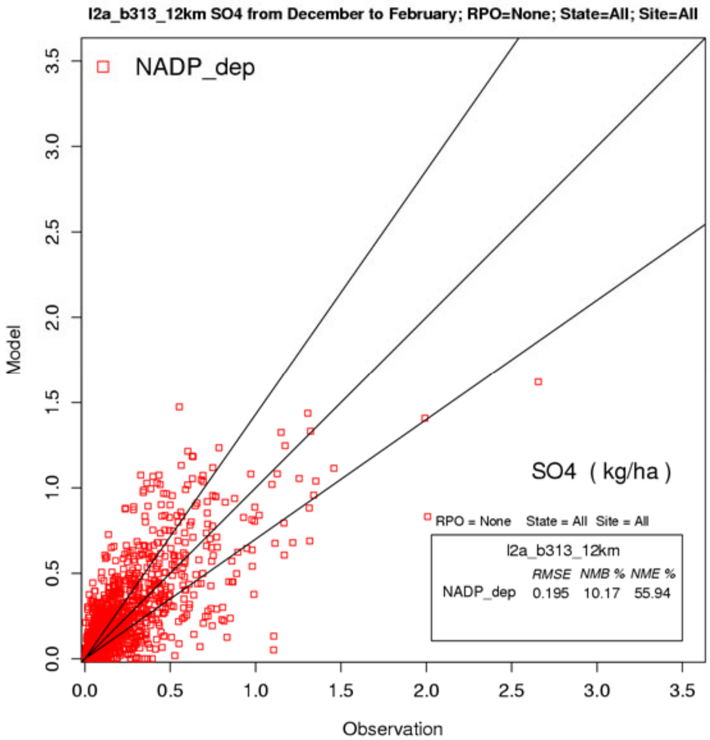


Scatter Plot – CMAQ v4.5 12 km

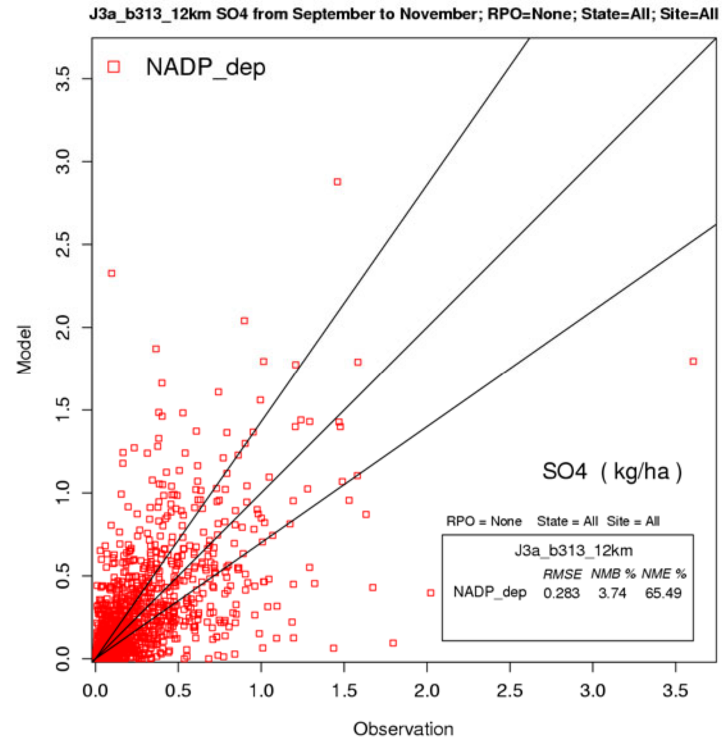


Wet Deposition Sulfate (kg/ha) - Winter

Scatter Plot – CMAQ v4.4 12 km

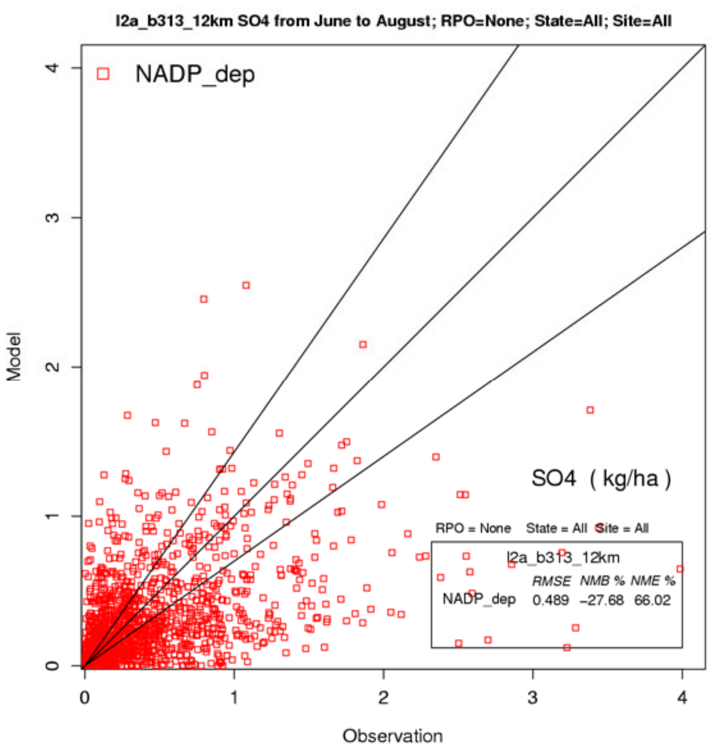


Scatter Plot – CMAQ v4.5 12 km

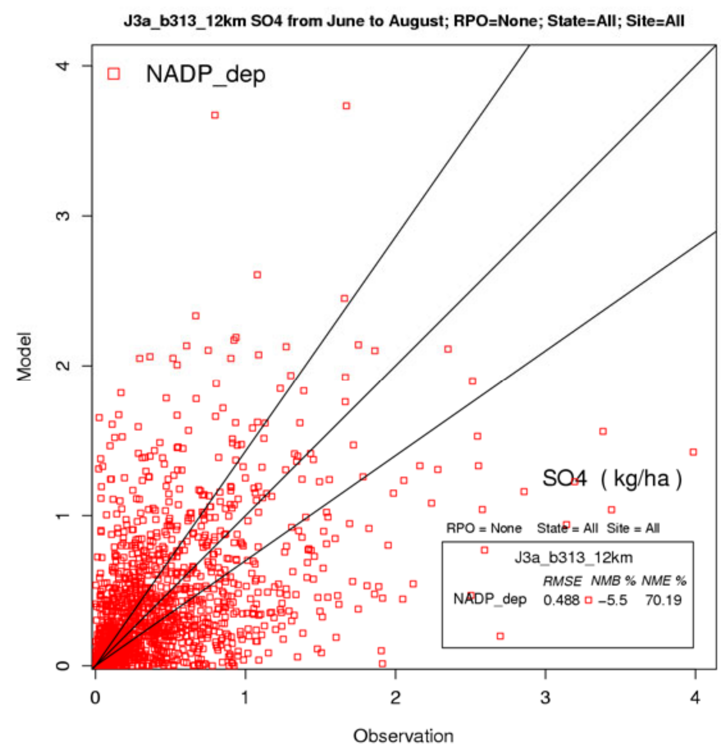


Wet Deposition Sulfate (kg/ha) - Summer

Scatter Plot – CMAQ v4.4 12 km

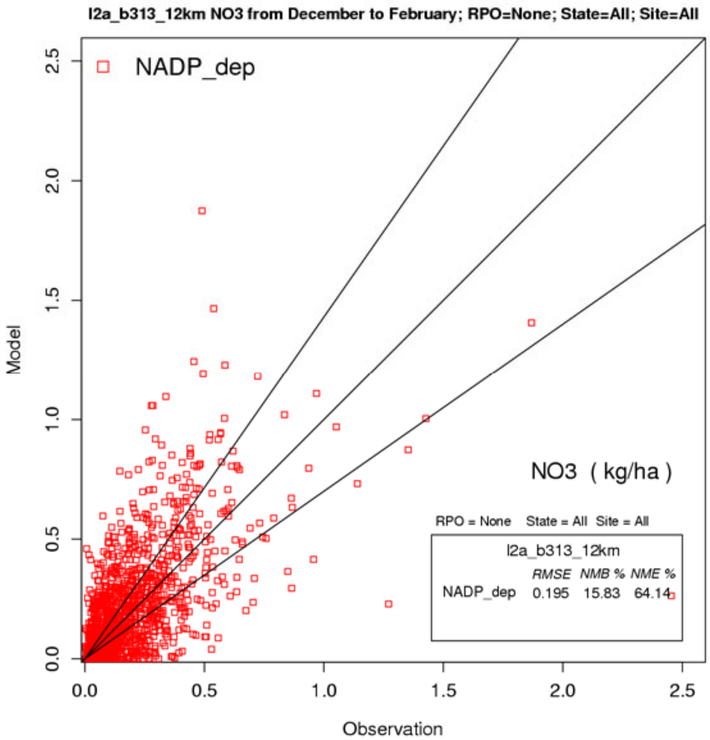


Scatter Plot – CMAQ v4.5 12 km

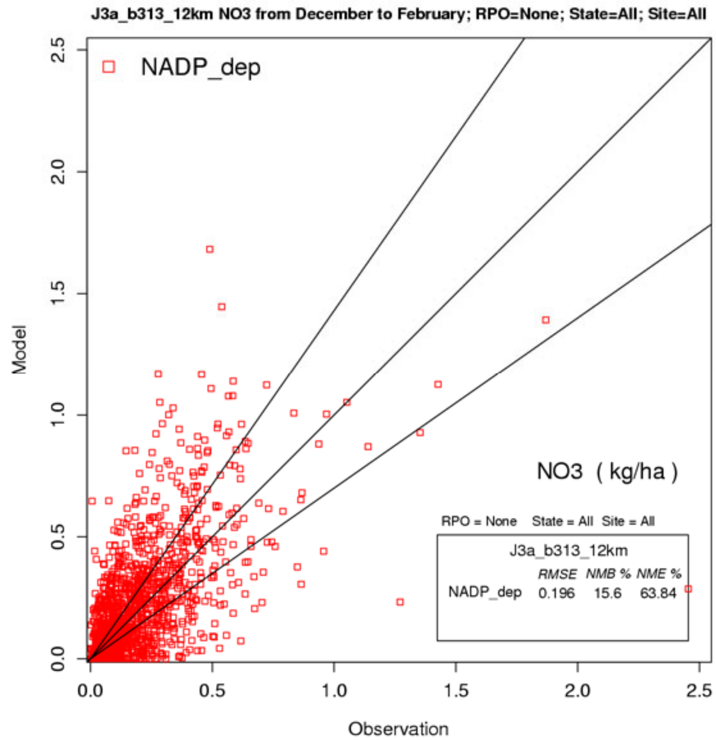


Wet Deposition Nitrate (kg/ha) - Winter

Scatter Plot – CMAQ v4.4 12 km

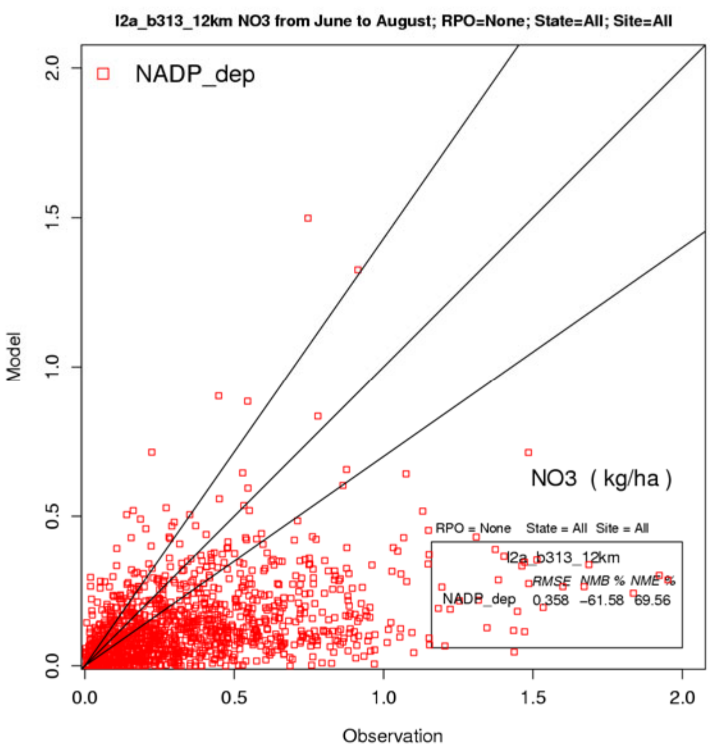


Scatter Plot – CMAQ v4.5 12 km

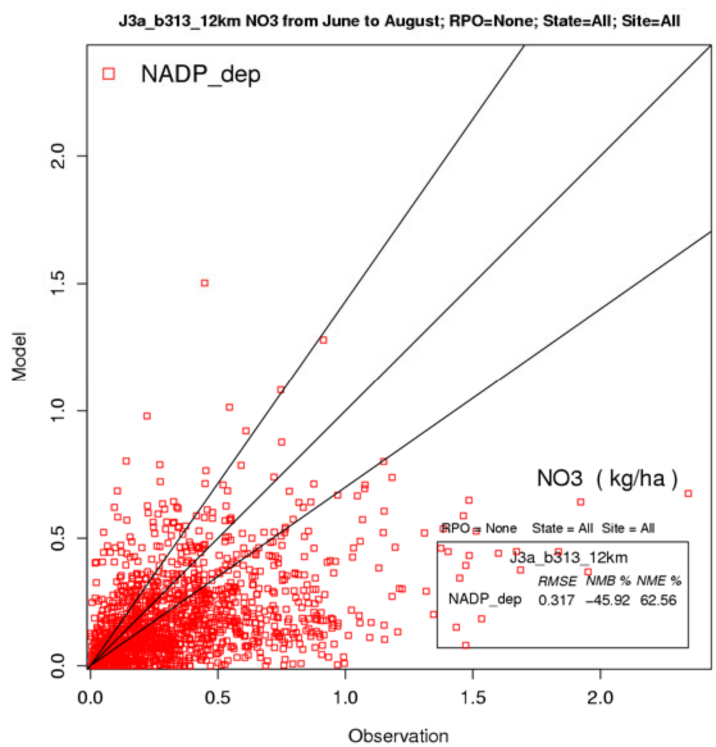


Wet Deposition Nitrate (kg/ha) - Summer

Scatter Plot – CMAQ v4.4 12 km

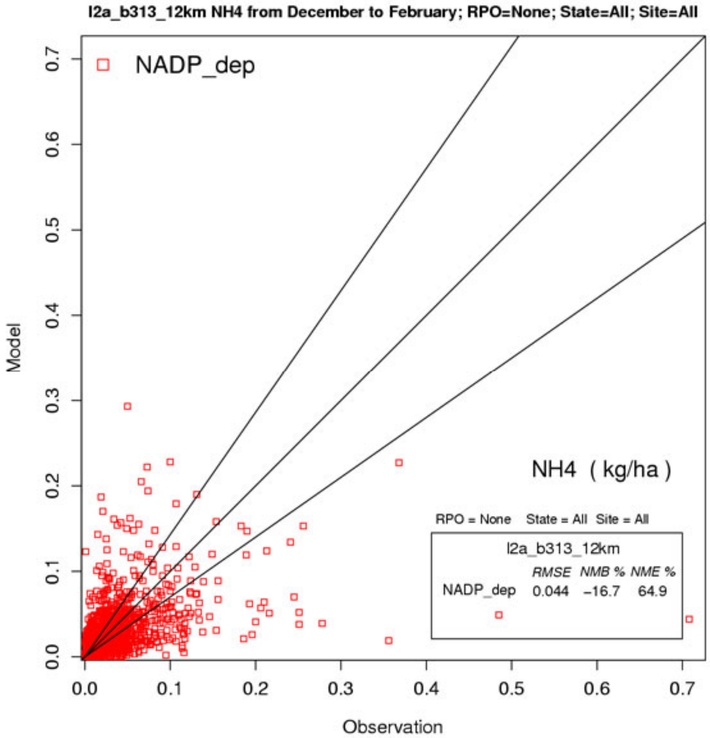


Scatter Plot – CMAQ v4.5 12 km

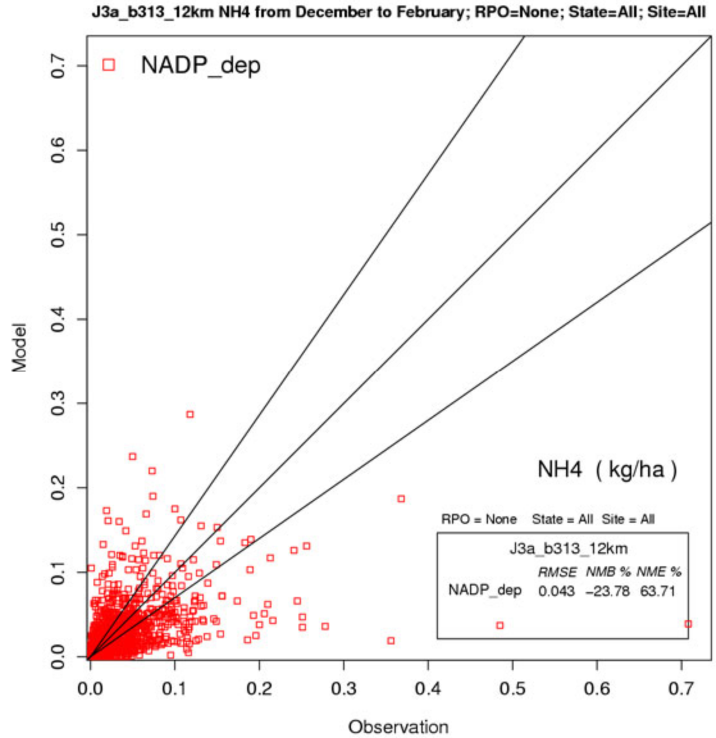


Wet Deposition Ammonium (kg/ha) - Winter

Scatter Plot – CMAQ v4.4 12 km

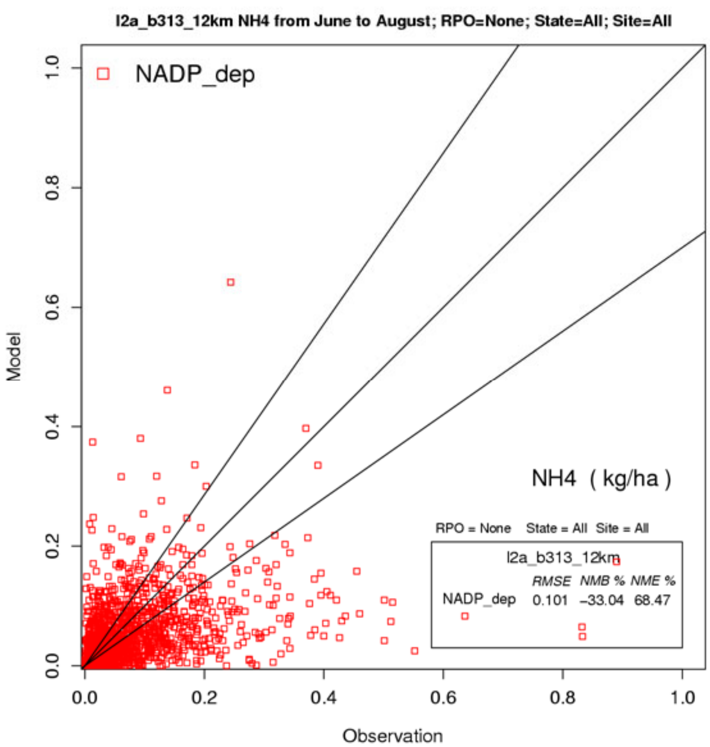


Scatter Plot – CMAQ v4.5 12 km

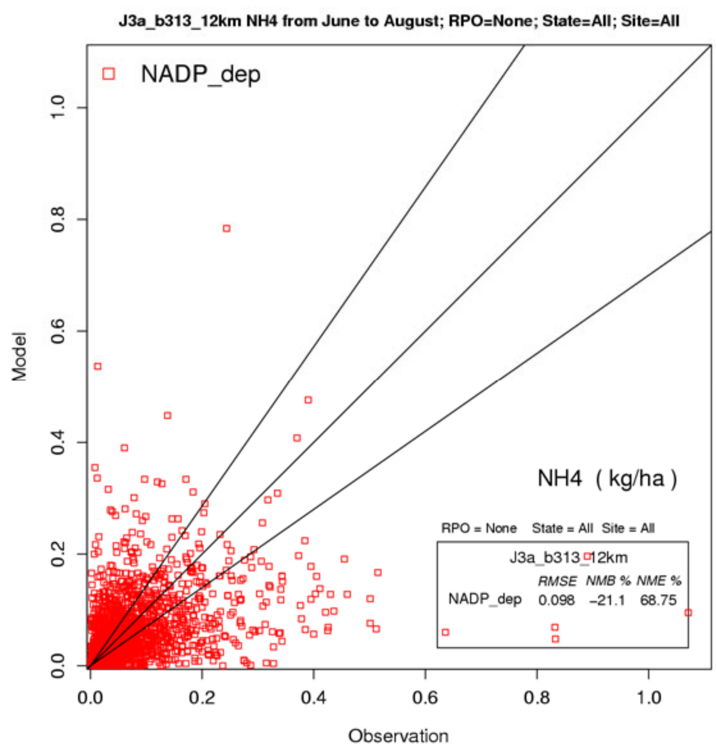


Wet Deposition Ammonium (kg/ha) - Summer

Scatter Plot – CMAQ v4.4 12 km



Scatter Plot – CMAQ v4.5 12 km



Comparison of CMAQ v4.5 36-km with 12-km Horizontal Grid Cell Sizes

Networks and Species Used:

AQS - Ozone
IMPROVE – Sulfate, Nitrate
STN – Sulfate, Nitrate, Ammonium
CASTNet – Sulfate, Nitrate, Ammonium, Nitric Acid, Total Nitrate
NADP – wet deposition SO_4^{2-}, wet deposition NO_3^-, wet deposition NH_4^+ and precipitation

CMAQ v4.5 36-km vs. 12-km Performance Comparison: Introduction

The following section will compare the performance of the 2005 release version of CMAQ (v.4.5) at the 36 km horizontal resolution and the 12 km horizontal resolution. Since the 36 km domain covers the entire continental United States, while the 12 km domain only covers the eastern portion of the United States, it was necessary to "window" the 36 km domain to as closely match that of the 12 km domain. The "windowing" was accomplished using a post-processing technique (no IOAPI tool was used) and as a result, for some observation networks, there is a small discrepancy (one or two sites usually) between the windowed 36 km domain and the whole 12 km domain. However, these differences do not significantly impact the evaluation results or the comparison of the two horizontal grid resolutions to each other. Below is a list of the plots and statistics included in this section.

- Ozone 8-hr max scatter plots, diurnal average plots and spatial NMB and NME plots
- Winter and summer model to observation scatter plots of organic and inorganic aerosols
- Winter and summer model to observation scatter plots of total $PM_{2.5}$ mass
- Winter and summer model to observation scatter plots of precipitation chemistry

Note that for comparison of organic carbon, the complete unit is μgC/m³, although on plots the units are labeled as μg/m³.

CMAQ v4.5 36-km vs. 12-km Performance Comparison: Summary

Ozone (8hr-max) performance improved when going from 36 km to 12 km, with a decrease in NMB from 8.94% at 36 km to 1.62% at 12 km while NME decreases by about 1.5%. The diurnal box plots show a much better agreement between model and observation concentrations at 12-km horizontal grids versus the 36-km grids, especially during the peak daylight hours. Spatially, there is improved performance at 12 km in areas where NMB and NME are relatively large at 36 km (e.g. coastal regions).

Inorganic sulfate performance is slightly worse at 12 km in the winter, while in the summer, performance is generally improved, especially for CASTNet, where the NMB improves while NME decreases by about 8%. Overall, sulfate in the summer goes from moderately under-predicted at 36 km to unbiased or slightly over-predicted at 12 km. Concentrations of inorganic nitrate increase slightly in the winter at 12 km when compared to 36 km, although changes are relatively small. In the summer, nitrate predictions decrease significantly at 12 km as compared to 36 km, with moderate negative NMB values (NME actually improve slightly versus 36 km). Ammonium predictions generally increase at 12 km, although in the winter CASTNet shows a slight decrease in NMB (NME improves however) in the winter. In the summer, ammonium NMB values increase approximately 10% at 12 km compared to 36 km, while NME values remain relatively unchanged. Nitric acid performance is very similar in the winter between the two resolutions, while in the summer, over-predictions at 36 km increase at 12 km, with increases in both NMB and NME values. Total nitrate performance is again very similar between the two resolutions in both the winter and summer seasons.

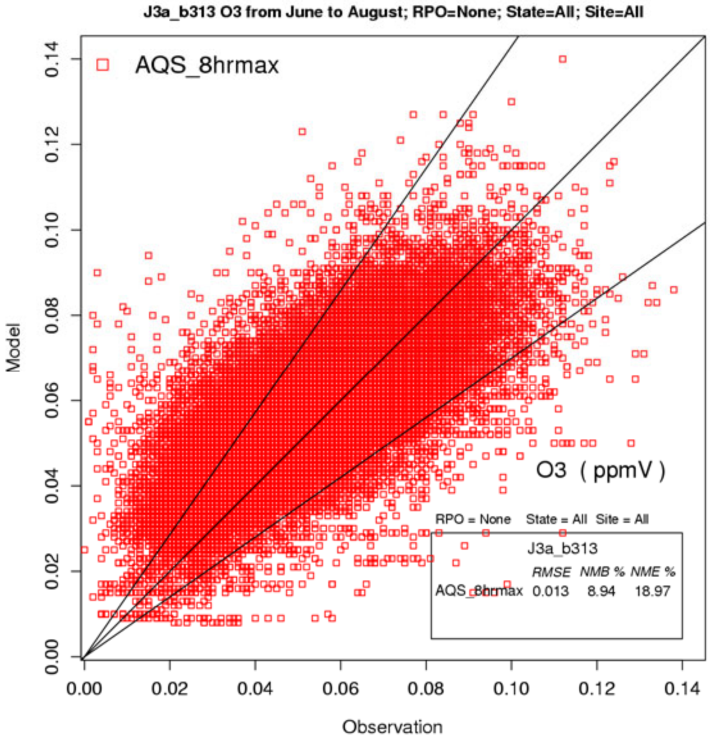
Performance of EC changes significantly between the two resolutions, especially at the urban STN sites. EC performance is relatively unchanged for IMPROVE between the two resolutions. However, STN shows a dramatic increase in NMB and NME (on top of an already significant over-prediction at 36 km) at

12 km when compared to 36 km. The large differences between the 36 km and 12 km grids are most likely a result of the higher resolution of the urban areas at 12 km, where there are usually significantly more emissions than in rural areas. The change is consistent in both the summer and winter seasons. OC performance is essentially the same at both resolutions, with only slight changes in both NMB and NME in both the summer and winter and at both IMPROVE and STN. Total PM2.5 mass follows the pattern of EC performance, with NMB and NME relatively unchanged at IMPROVE and relatively large changes at STN. For the winter, over-predictions in PM2.5 at 36 km increase at 12 km, although the increases are not as dramatic as those with EC. The under-predictions of PM2.5 mass in the summer at 36 km (NMB = -15.8%) improve at 12 km (NMB = -4.14%). The RMSE and NME values show only small changes between the two resolutions.

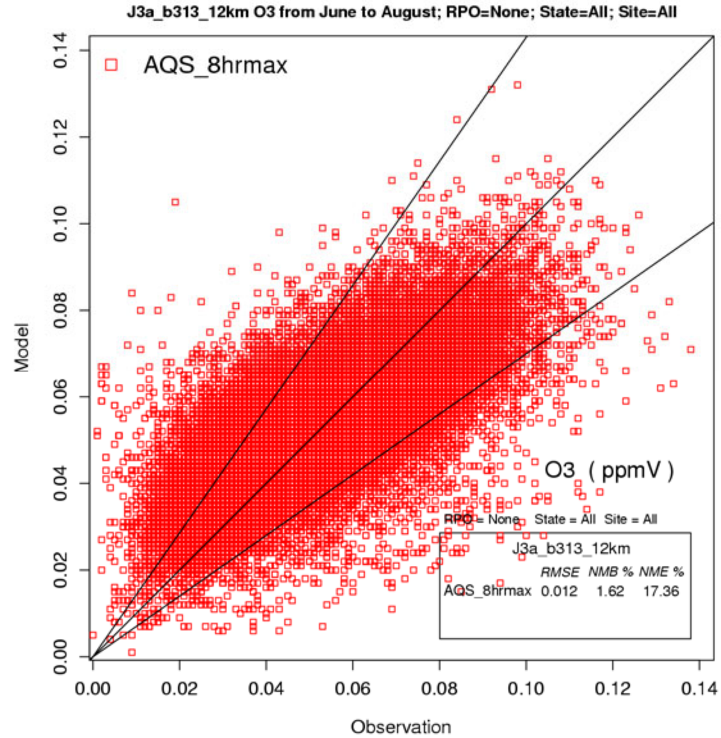
There is generally a decrease in the concentrations of wet deposition species in both the summer and winter. This is most likely due to the higher resolution of precipitating clouds at 12 km (note that precipitation performance is better at 12km than at 36km), which results in less deposition (and hence smaller concentrations of wet deposition species) within a single grid cell (precipitating cloud is covering a smaller percentage of the grid cell). Wet deposition sulfate shows a small improvement in NMB in the winter, although NME increases by about 12%. For the summer, the slight over-prediction at 36 km becomes a slight under-prediction at 12 km, while NME improves by approximately 3%. Wet deposition nitrate performance improves slightly in the winter at 12 km, while in the summer the under-prediction at 36 km becomes larger at 12 km (NME increases slightly). Wet deposition ammonium performance changes only slightly between the two resolutions, with moderate under-predictions observed in both the winter and summer seasons. Precipitation performance in the winter is very similar between the two resolutions, while in the summer, precipitation performance at 12 km is notably improved to that at 36 km. The NMB, which is 14.5% in the summer at 36 km, becomes -5.06% at 12 km, while the NME improves by roughly 10%.

AQS 8-hr Max Ozone (ppm) - Summer

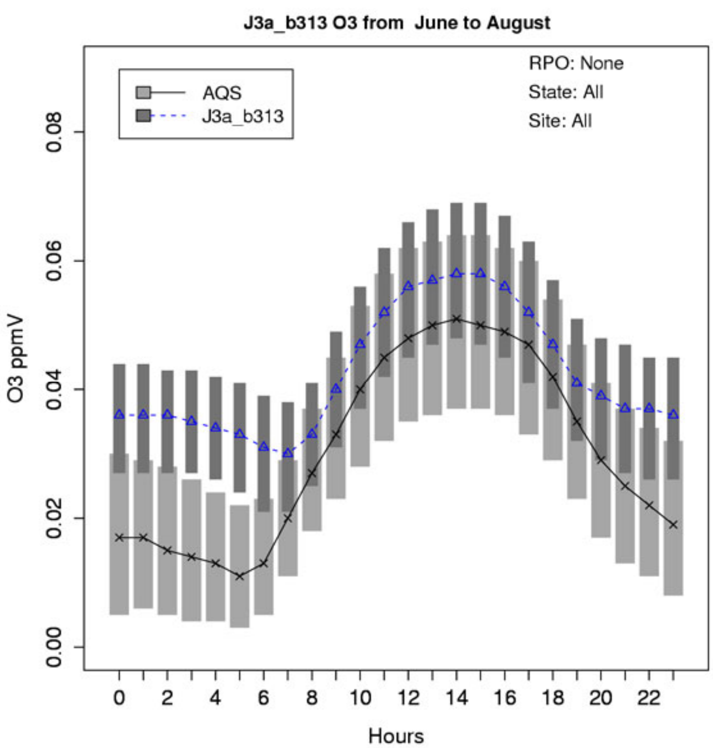
Scatter Plot – CMAQ v4.5 36 km



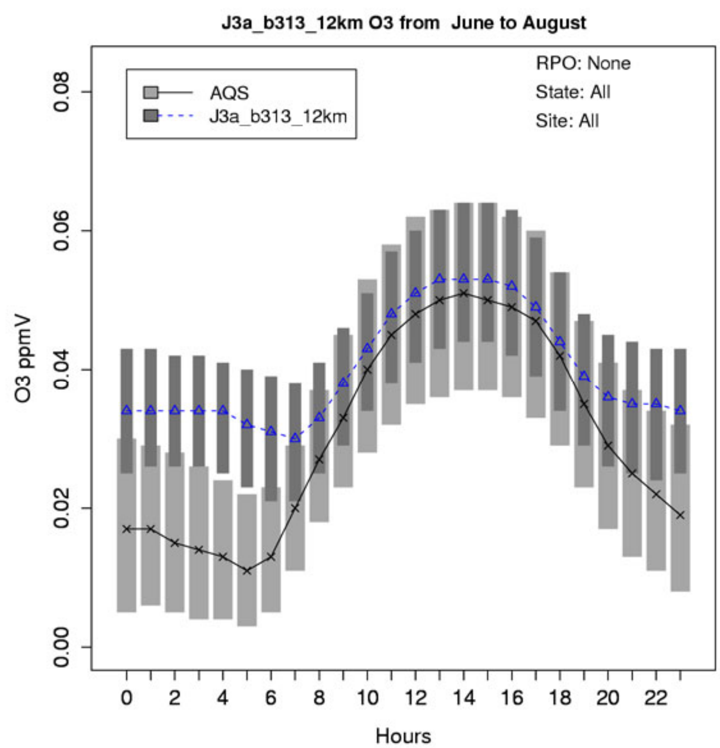
Scatter Plot – CMAQ v4.5 12 km



Diurnal Box Plot – CMAQ v4.5 36 km



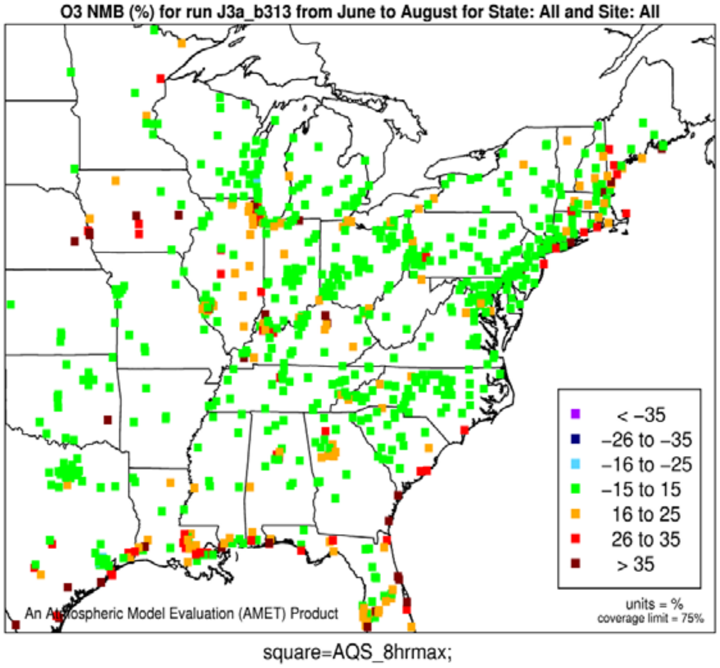
Diurnal Box Plot – CMAQ v4.5 12 km



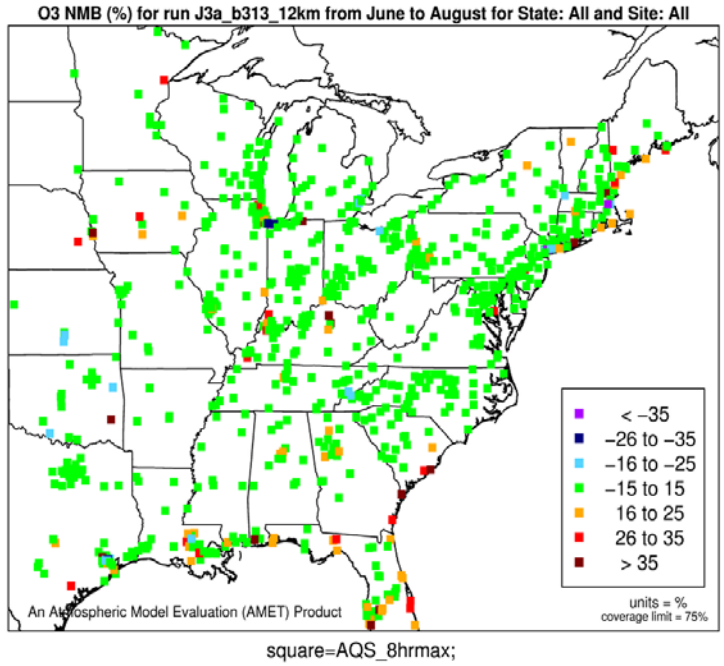
Network	# Obs	Mean Obs	Mean Model	SDEV Obs	SDEV Model	R	RMSE	NMB (%)	NME (%)
AQS (36 km)	71558	0.052	0.057	0.018	0.014	0.74	0.013	8.94	19.0
AQS (12 km)	71284	0.052	0.053	0.018	0.013	0.74	0.012	1.62	17.4

AQS 8-hr Max Ozone - Summer

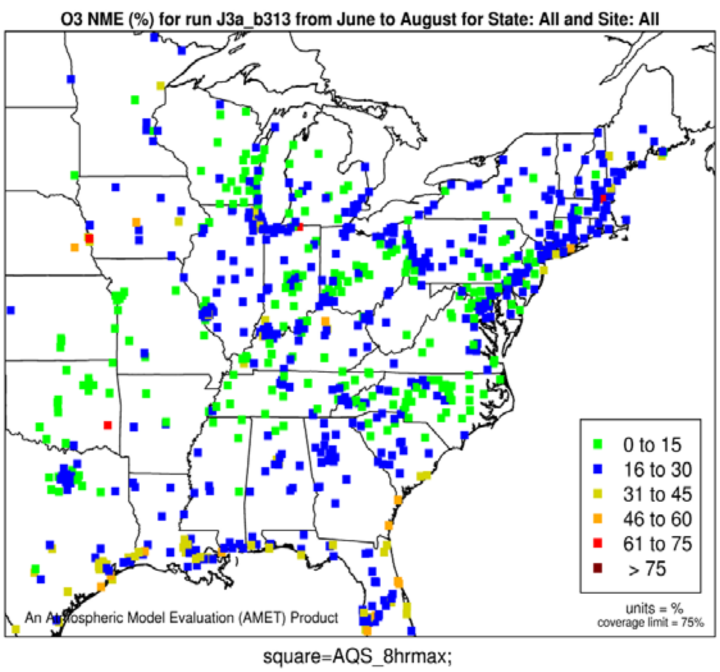
NMB (%) – CMAQ v4.5 36 km



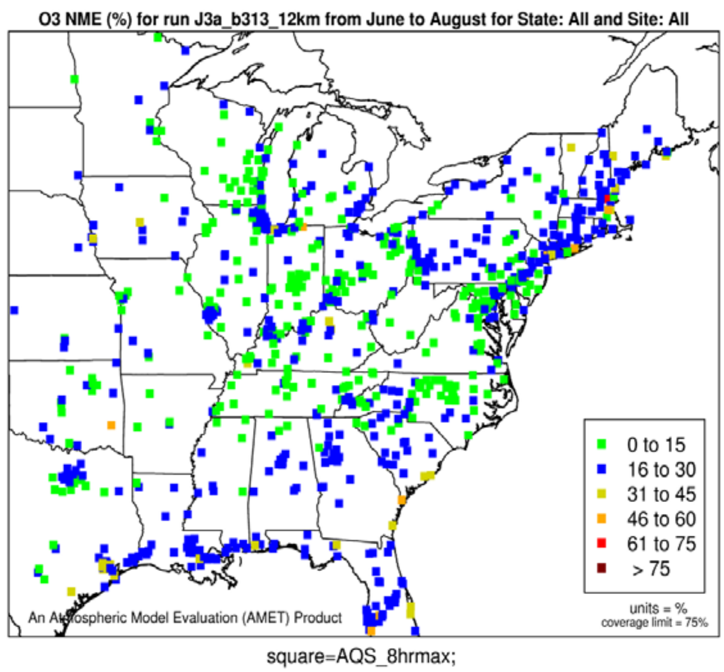
NMB (%) – CMAQ v4.5 12 km



NME (%) – CMAQ v4.5 36 km

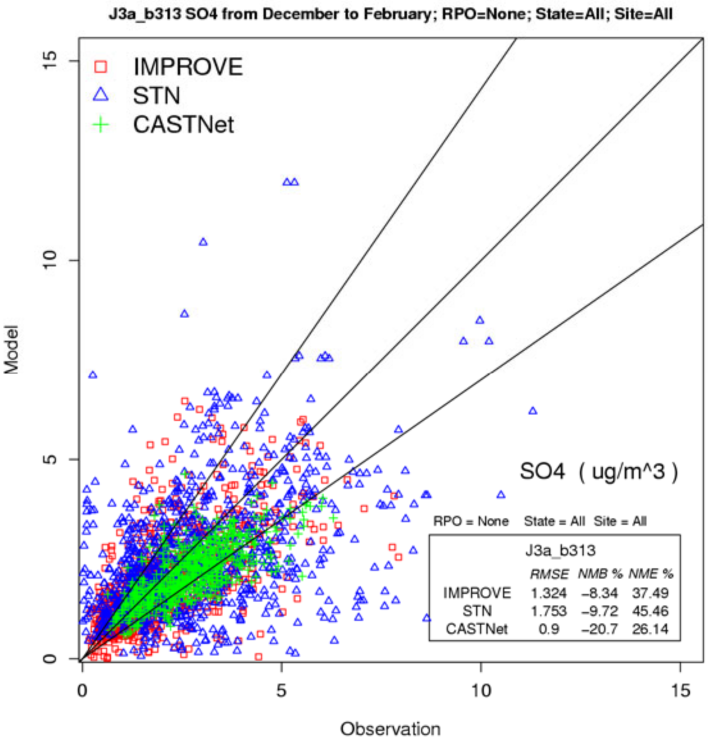


NME (%) – CMAQ v4.5 12 km

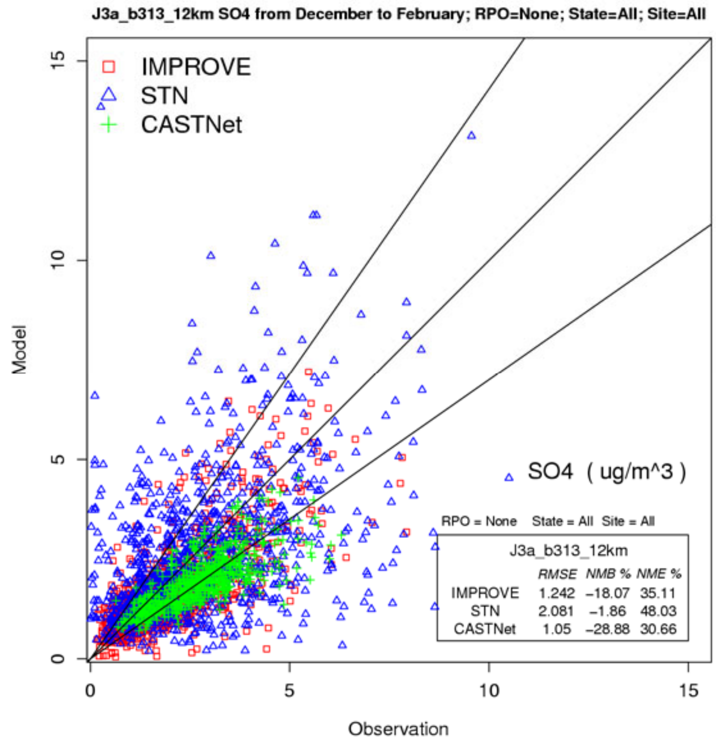


Sulfate (µg/m³) – Winter

Scatter Plot – CMAQ v4.5 36 km

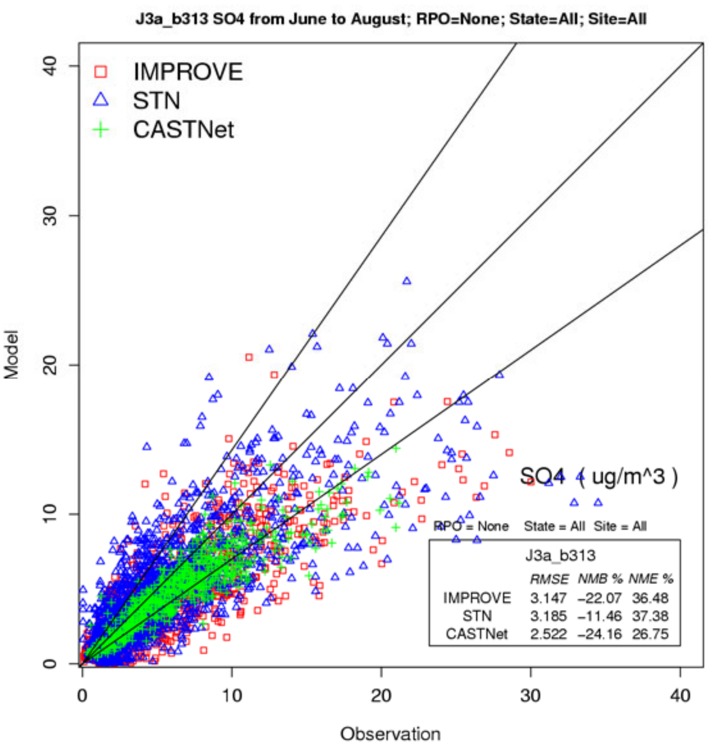


Scatter Plot – CMAQ v4.5 12 km

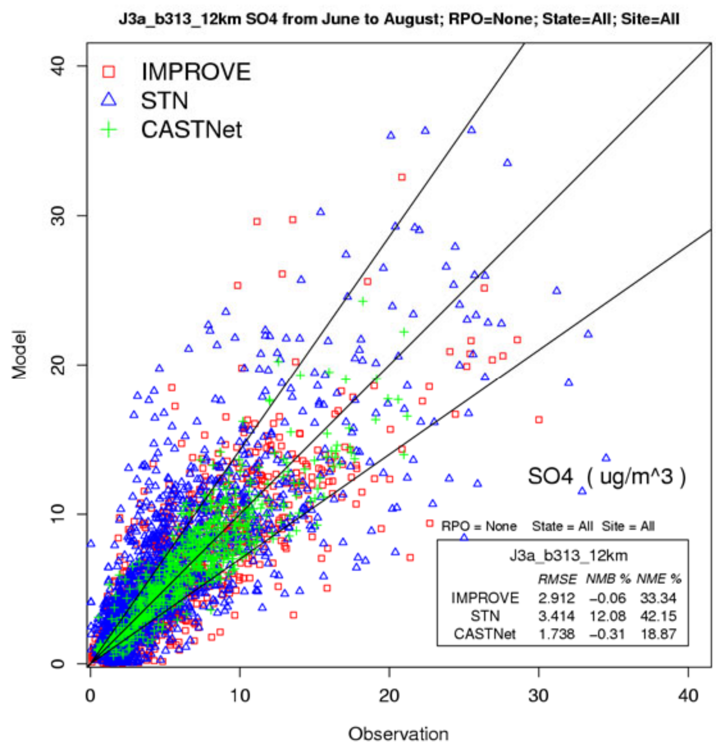


Sulfate (µg/m³) - Summer

Scatter Plot – CMAQ v4.5 36 km

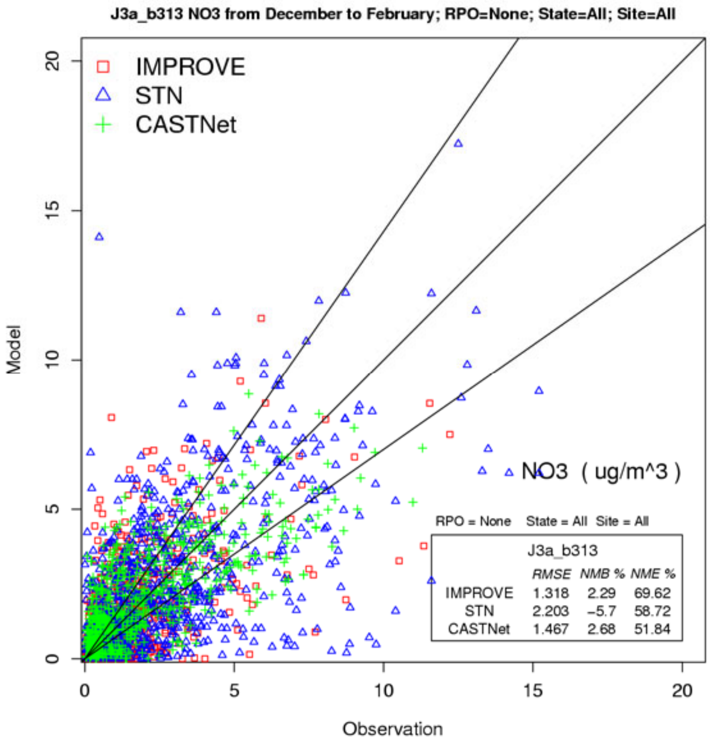


Scatter Plot – CMAQ v4.5 12 km

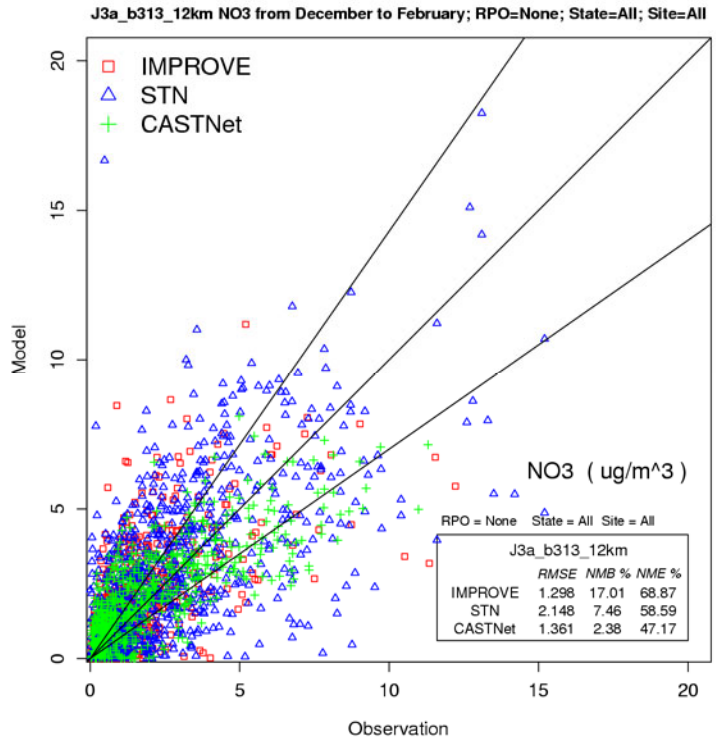


Nitrate (µg/m^3) – Winter

Scatter Plot – CMAQ v4.5 36 km

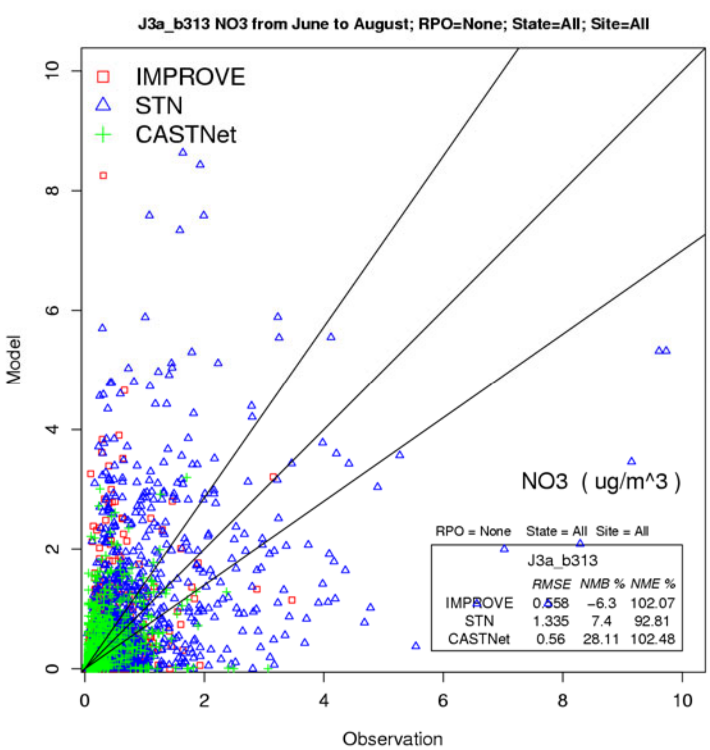


Scatter Plot – CMAQ v4.5 12 km

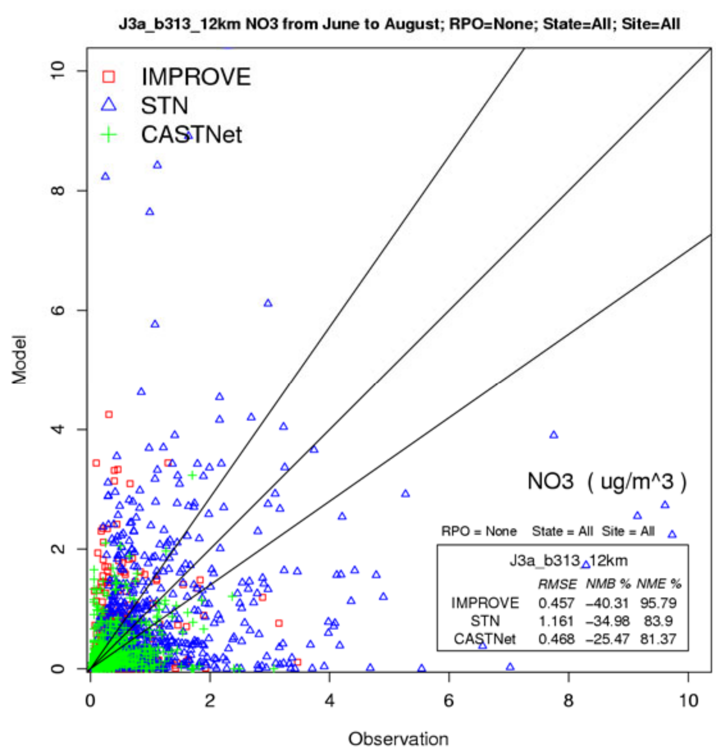


Nitrate (µg/m^3) - Summer

Scatter Plot – CMAQ v4.5 36 km

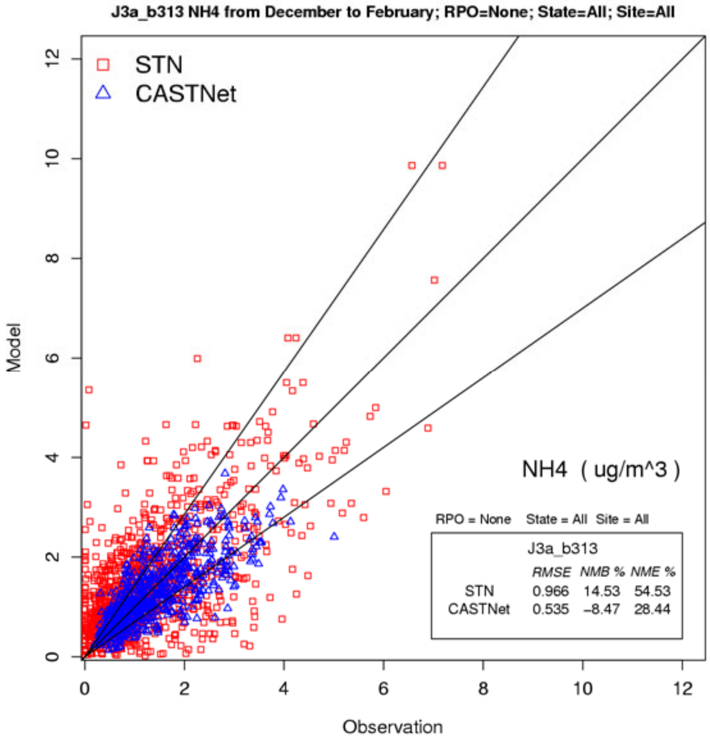


Scatter Plot – CMAQ v4.5 12 km

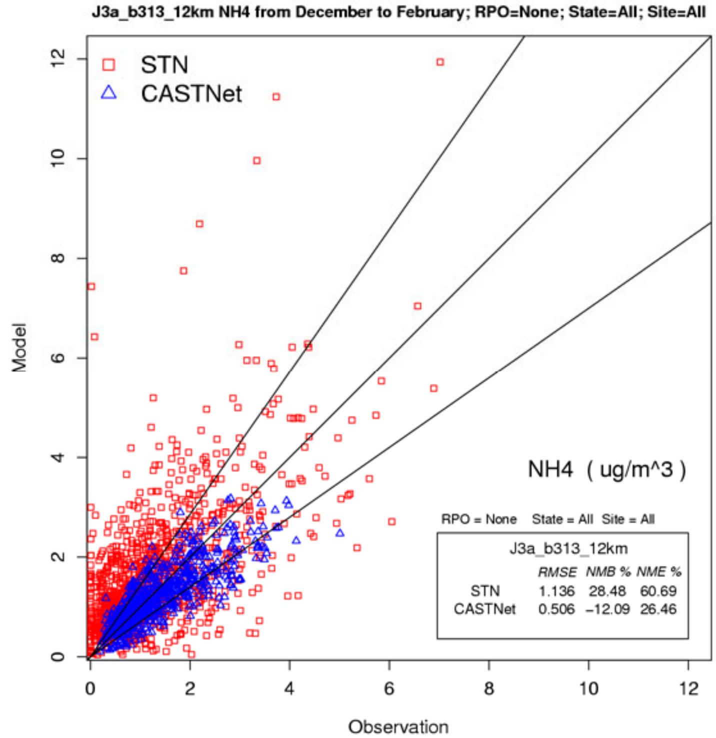


Ammonium (µg/m^3) – Winter

Scatter Plot – CMAQ v4.5 36 km

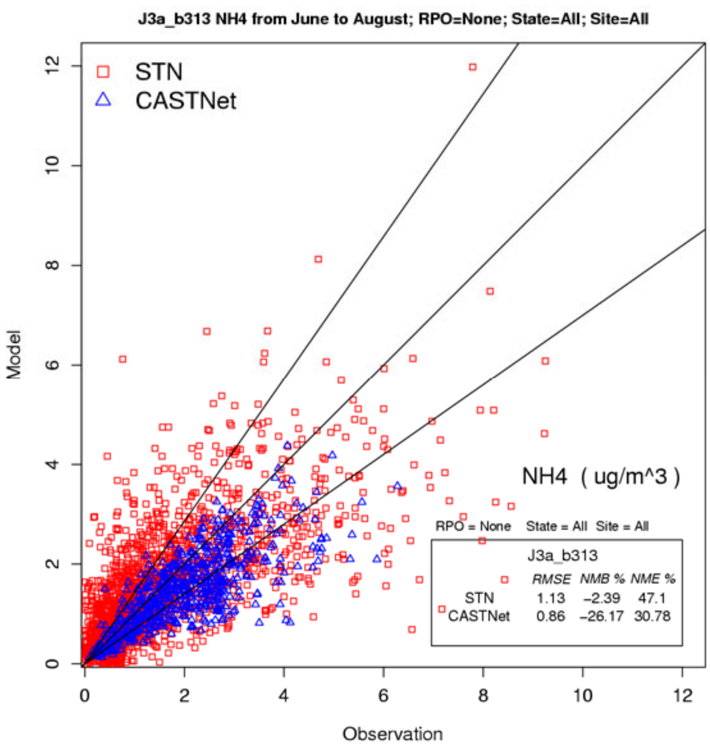


Scatter Plot – CMAQ v4.5 12 km

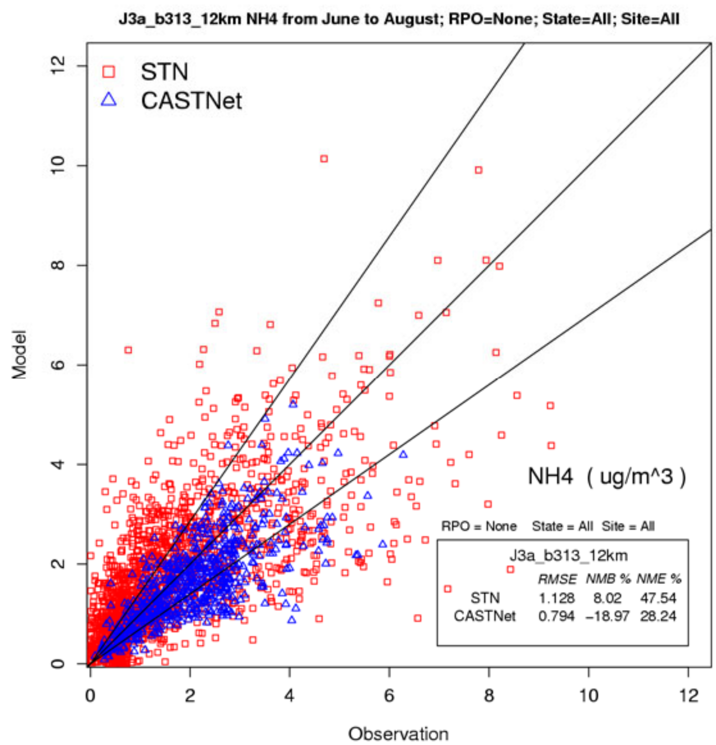


Ammonium (µg/m^3) – Summer

Scatter Plot – CMAQ v4.5 36 km

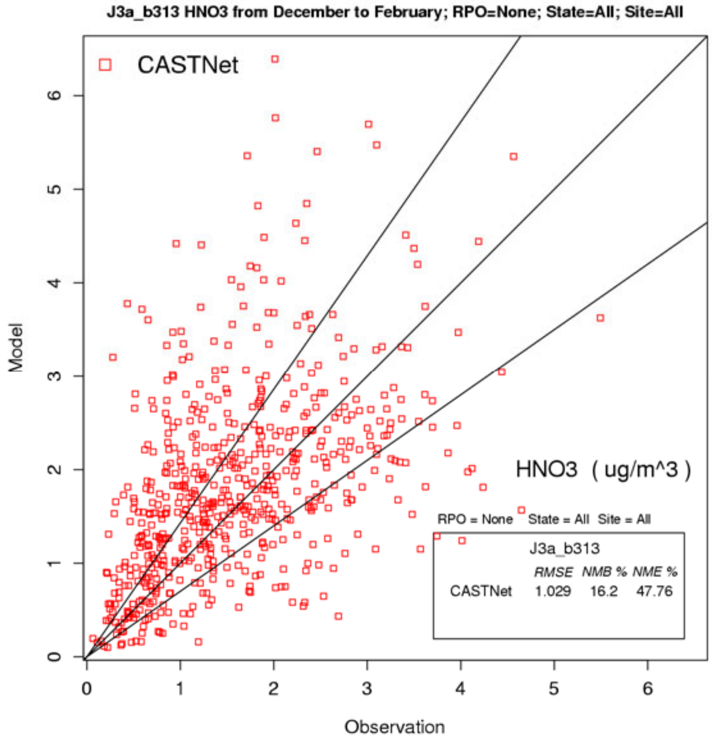


Scatter Plot – CMAQ v4.5 12 km

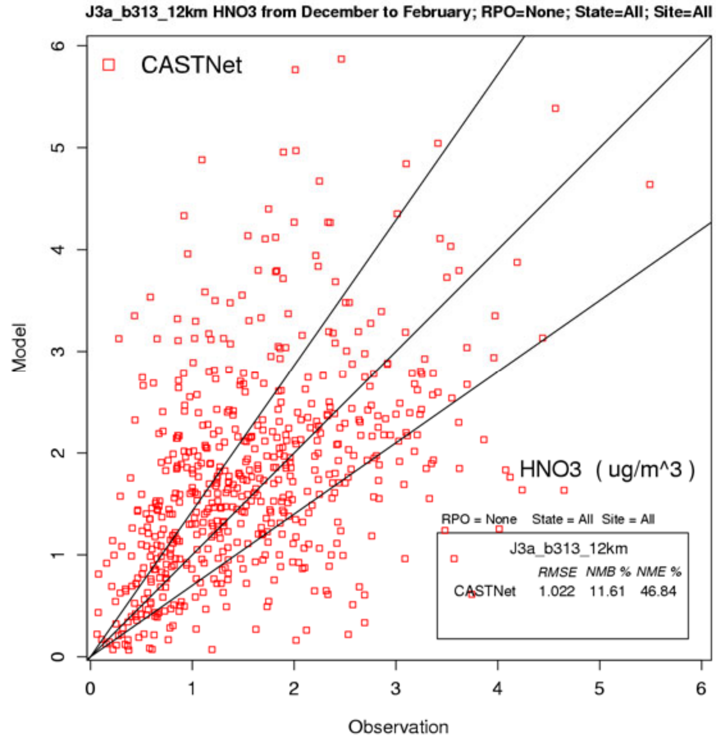


Nitric Acid (µg/m^3) – Winter

Scatter Plot – CMAQ v4.5 36 km

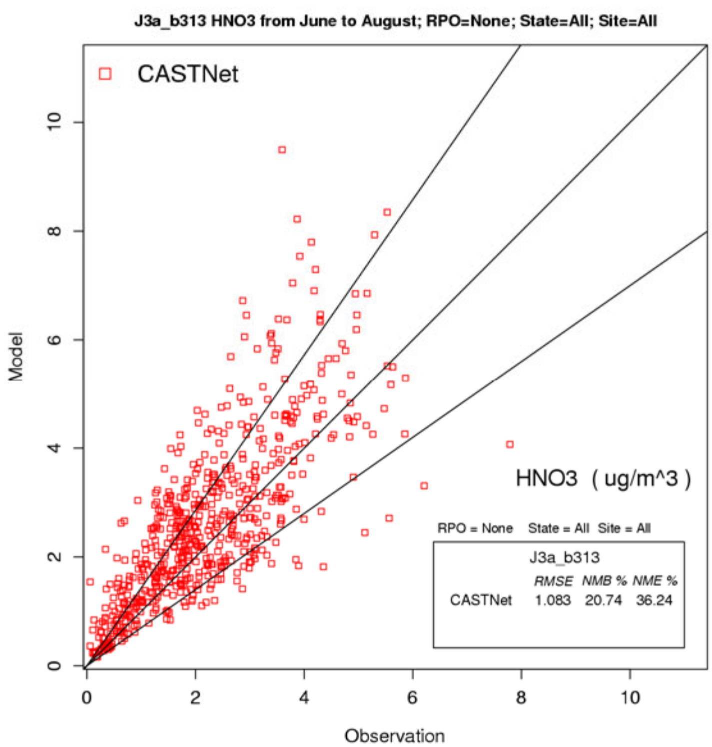


Scatter Plot – CMAQ v4.5 12 km

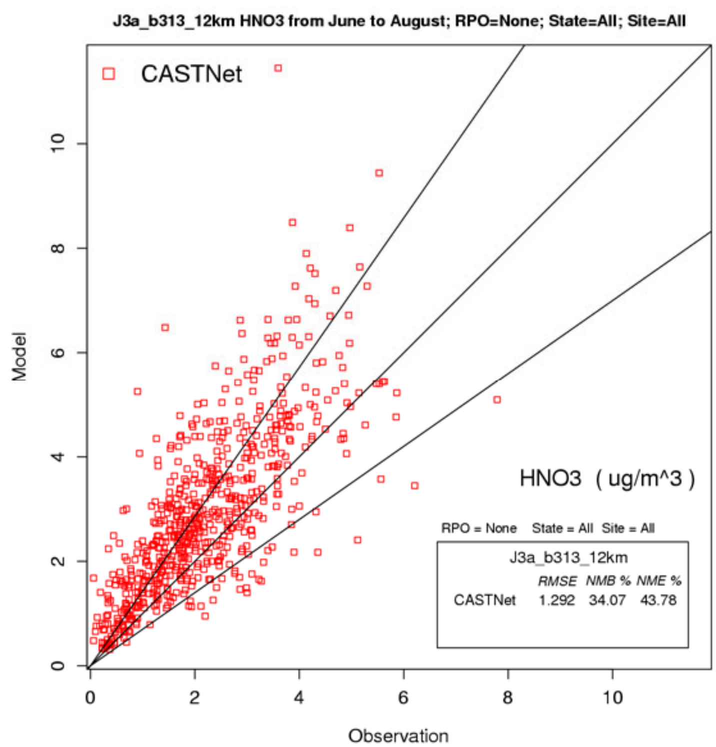


Nitric Acid (µg/m^3) – Summer

Scatter Plot – CMAQ v4.5 36 km

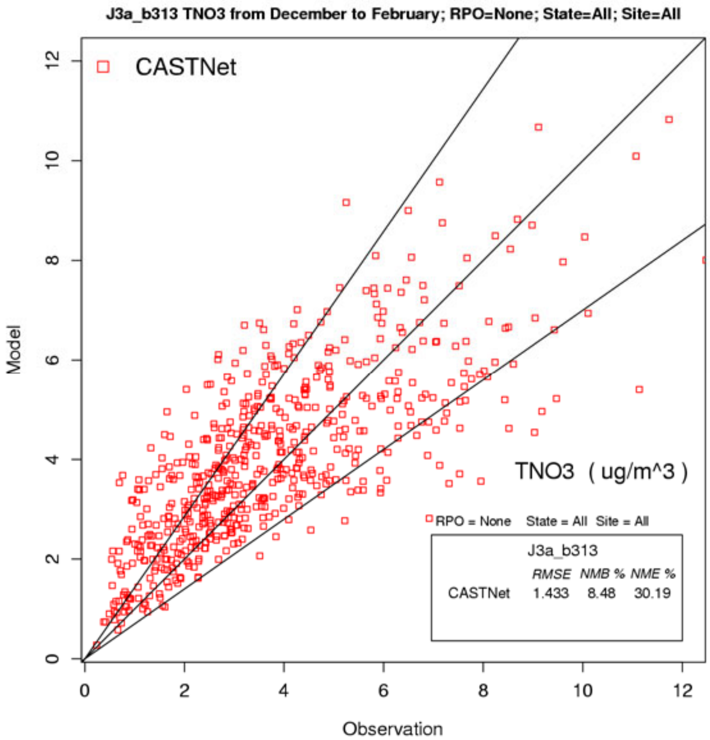


Scatter Plot – CMAQ v4.5 12 km

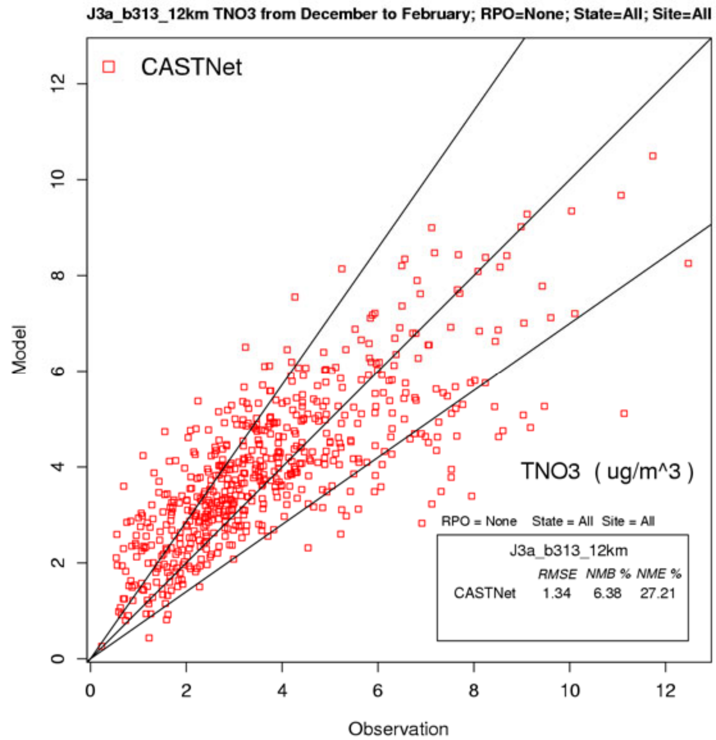


Total Nitrate (µg/m³) – Winter

Scatter Plot – CMAQ v4.5 36 km

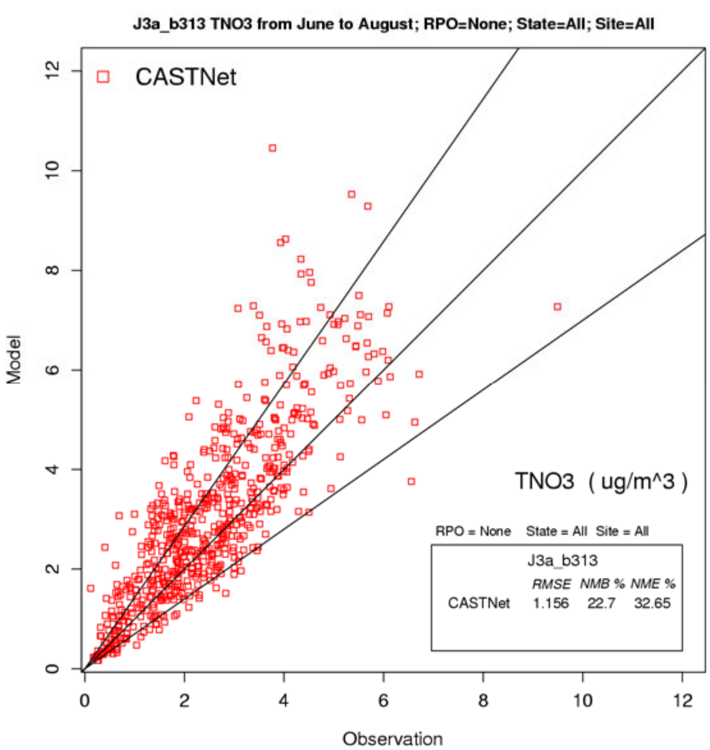


Scatter Plot – CMAQ v4.5 12 km

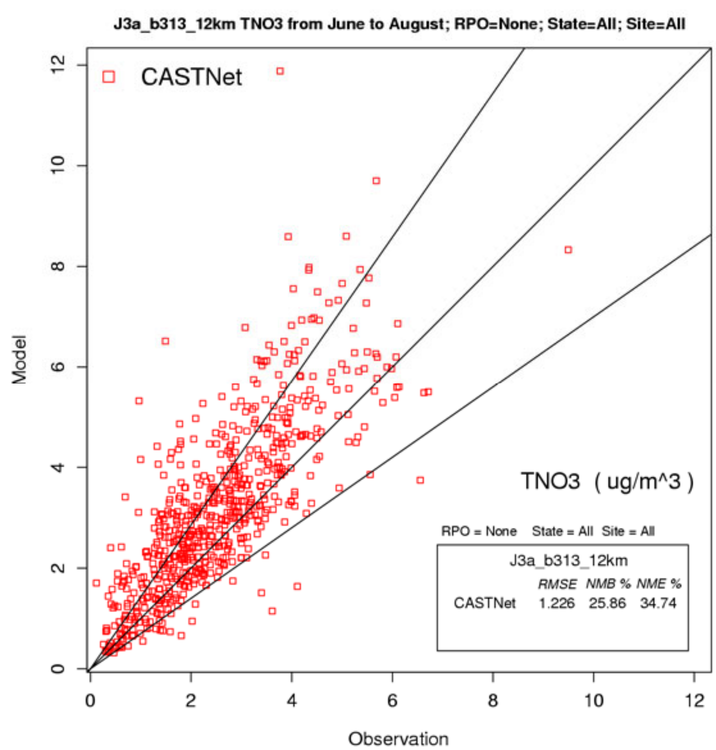


Total Nitrate (µg/m³) – Summer

Scatter Plot – CMAQ v4.5 36 km

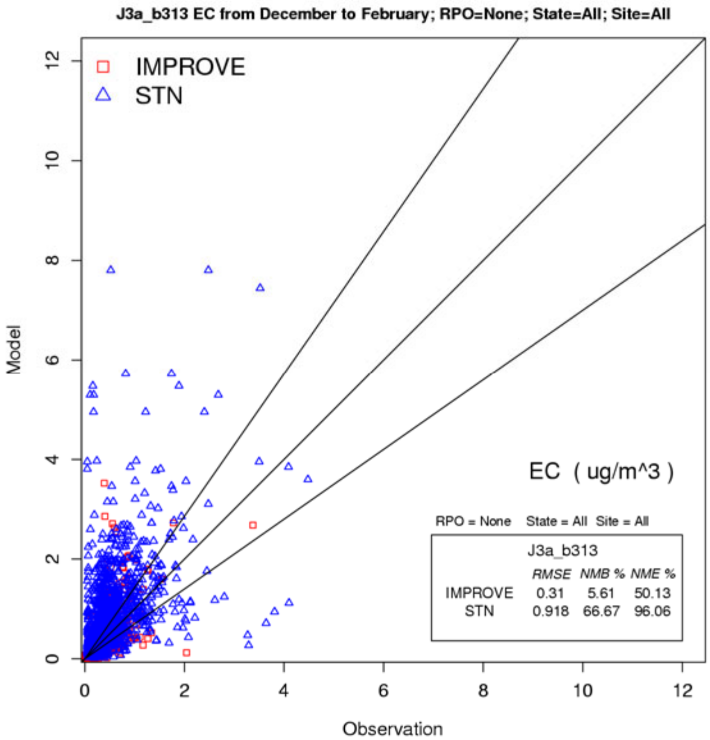


Scatter Plot – CMAQ v4.5 12 km

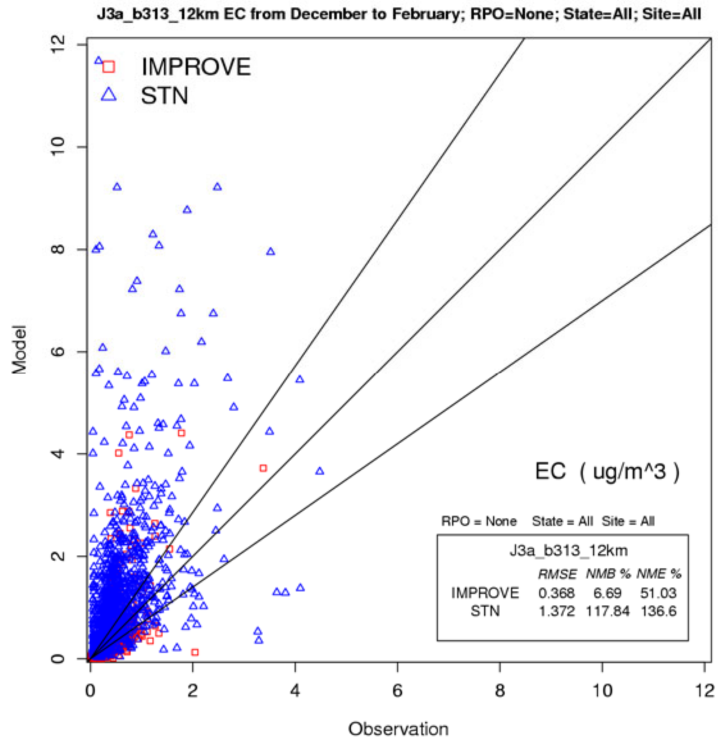


Elemental Carbon (μg/m³) – Winter

Scatter Plot – CMAQ v4.5 36 km

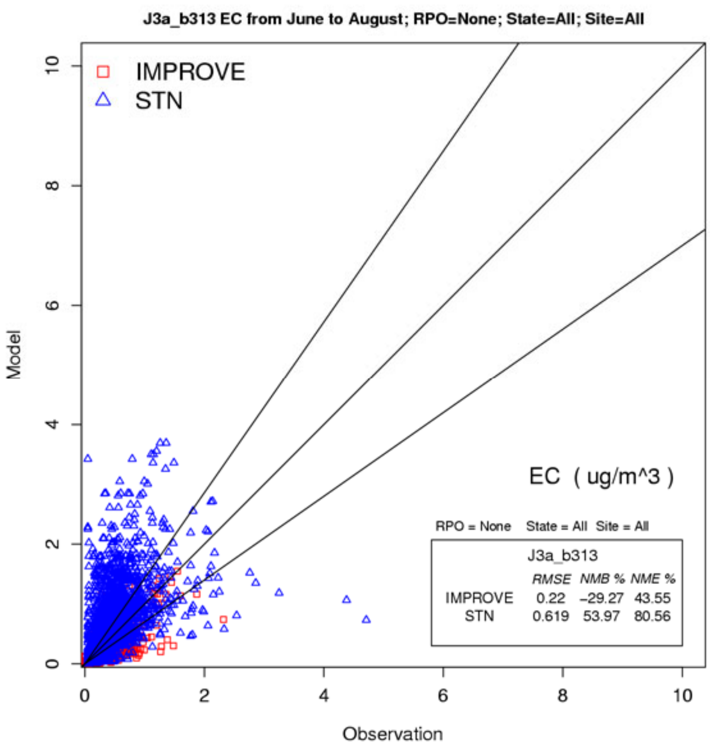


Scatter Plot – CMAQ v4.5 12 km

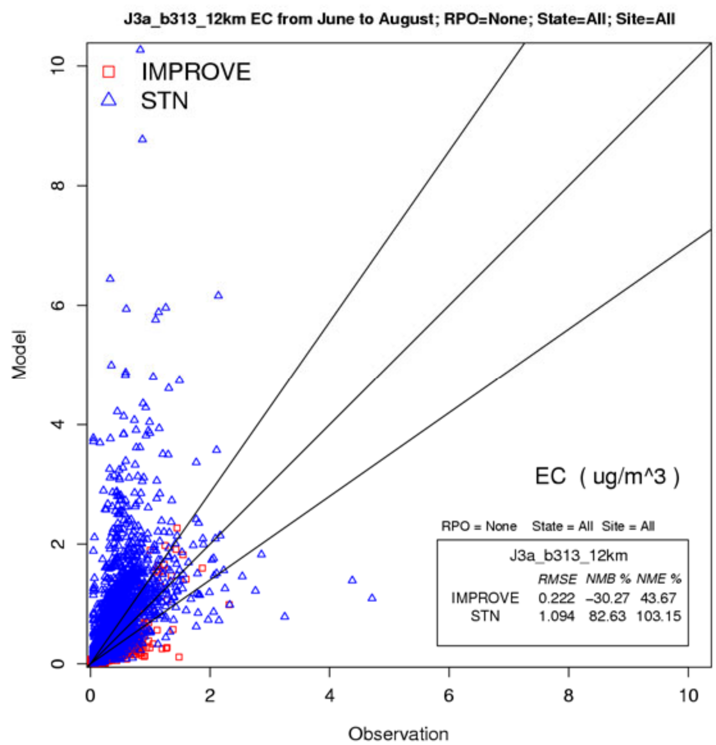


Elemental Carbon (μg/m³) – Summer

Scatter Plot – CMAQ v4.5 36 km

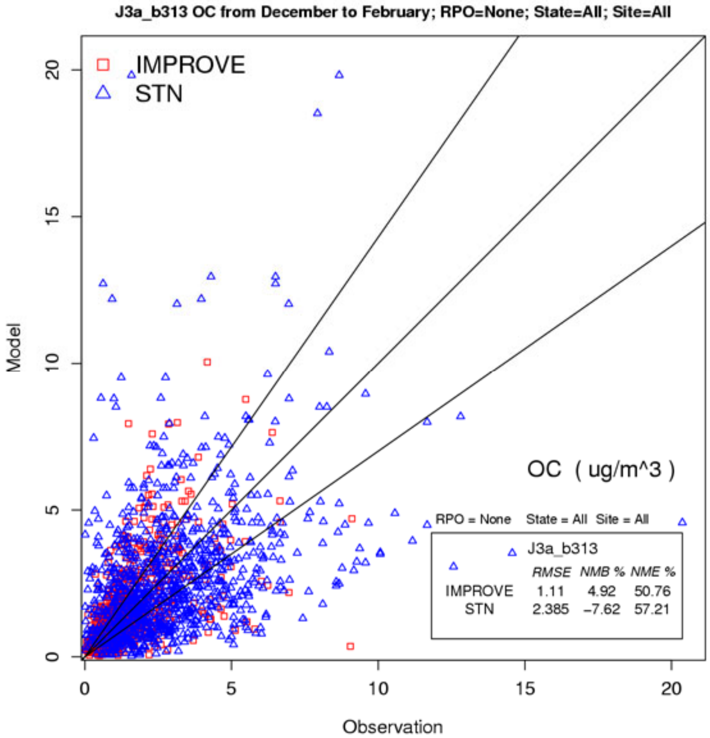


Scatter Plot – CMAQ v4.5 12 km

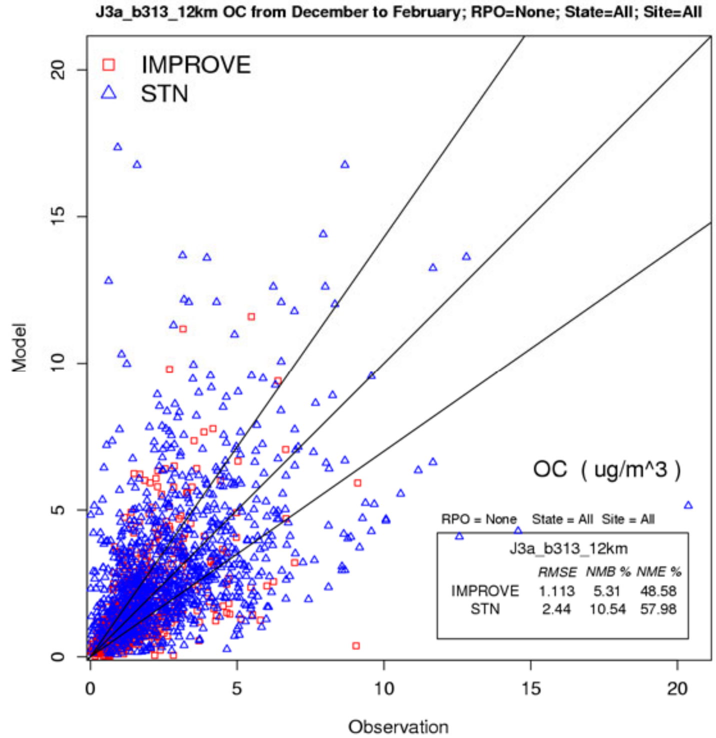


Organic Carbon (μg/m^3) – Winter

Scatter Plot – CMAQ v4.5 36 km

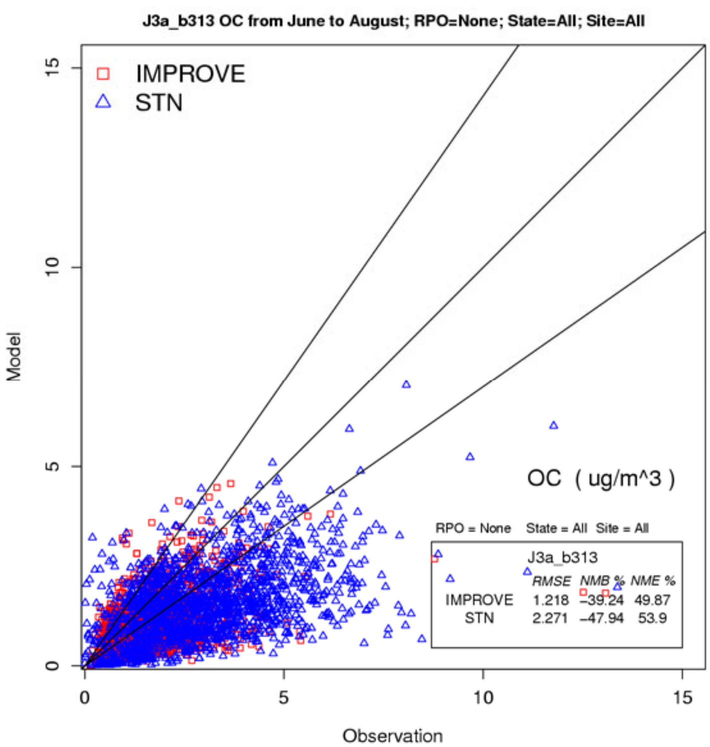


Scatter Plot – CMAQ v4.5 12 km

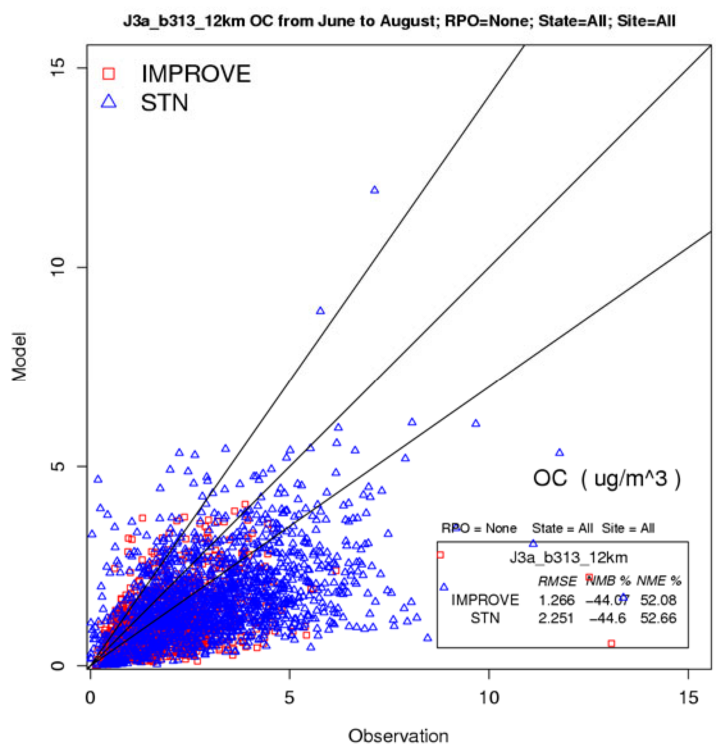


Organic Carbon (μg/m^3) – Summer

Scatter Plot – CMAQ v4.5 36 km

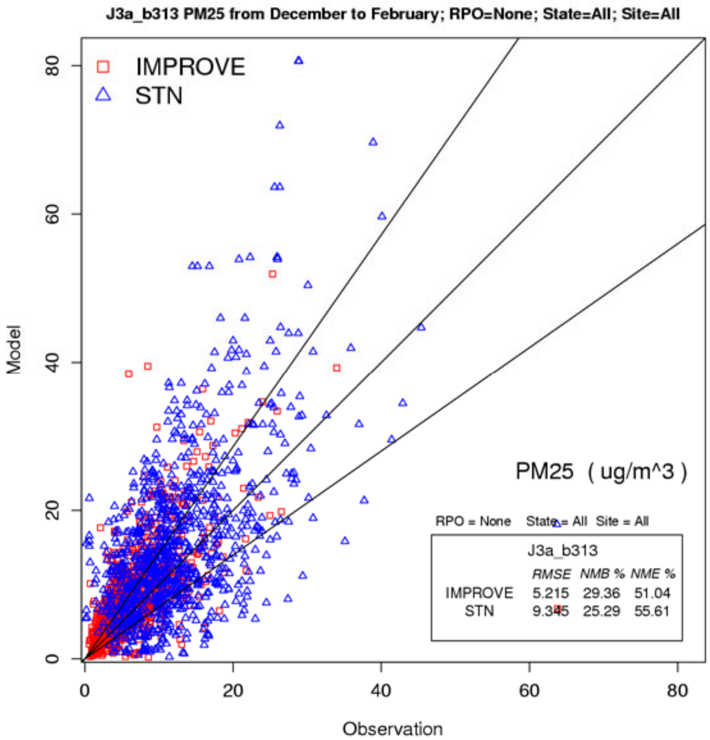


Scatter Plot – CMAQ v4.5 12 km

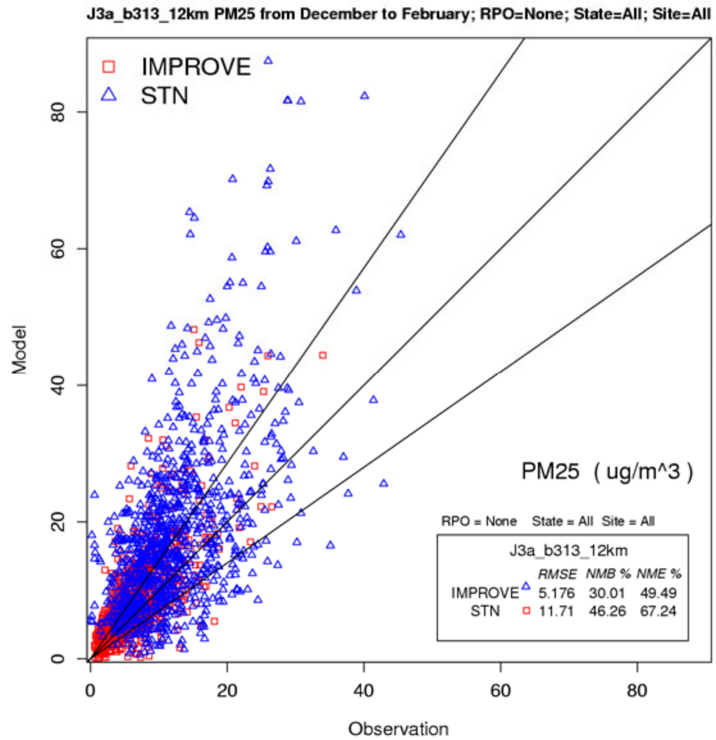


$PM_{2.5}$ ($\mu g/m^3$) – Winter

Scatter Plot – CMAQ v4.5 36 km

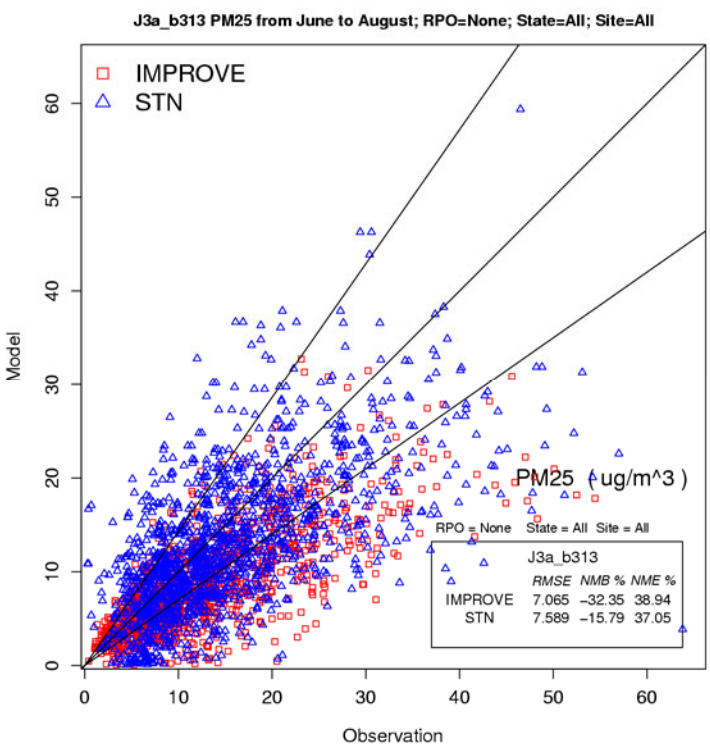


Scatter Plot – CMAQ v4.5 12 km

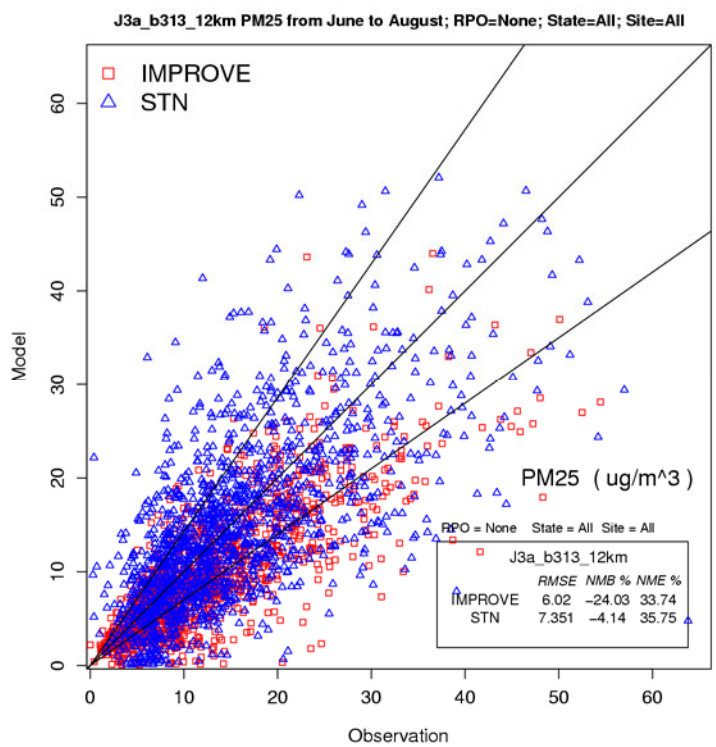


$PM_{2.5}$ ($\mu g/m^3$) – Summer

Scatter Plot – CMAQ v4.5 36 km

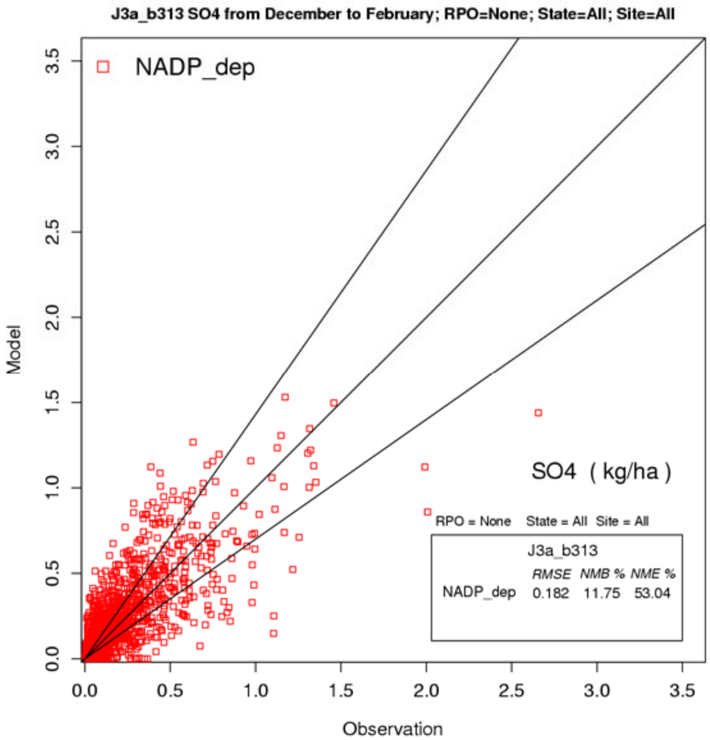


Scatter Plot – CMAQ v4.5 12 km

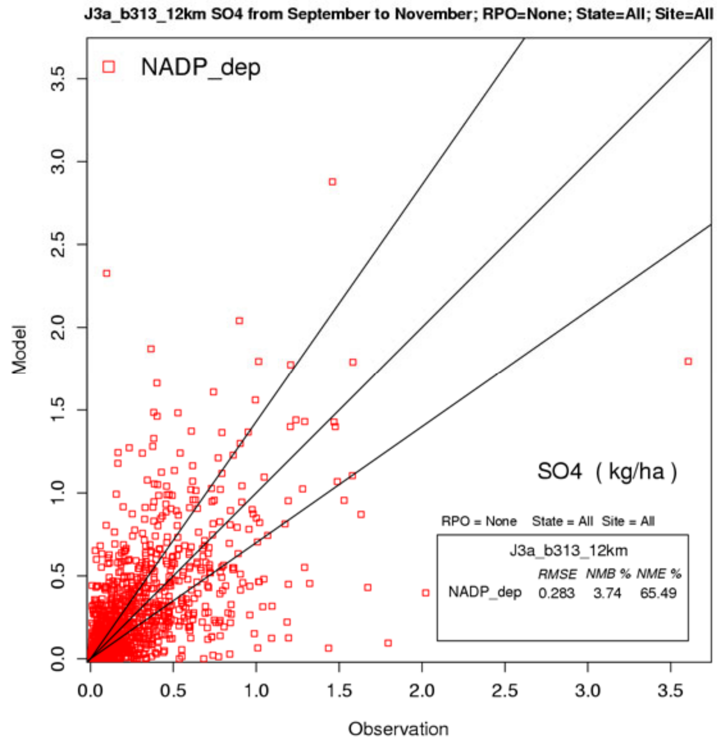


Wet Deposition Sulfate (kg/ha) - Winter

Scatter Plot – CMAQ v4.5 36 km

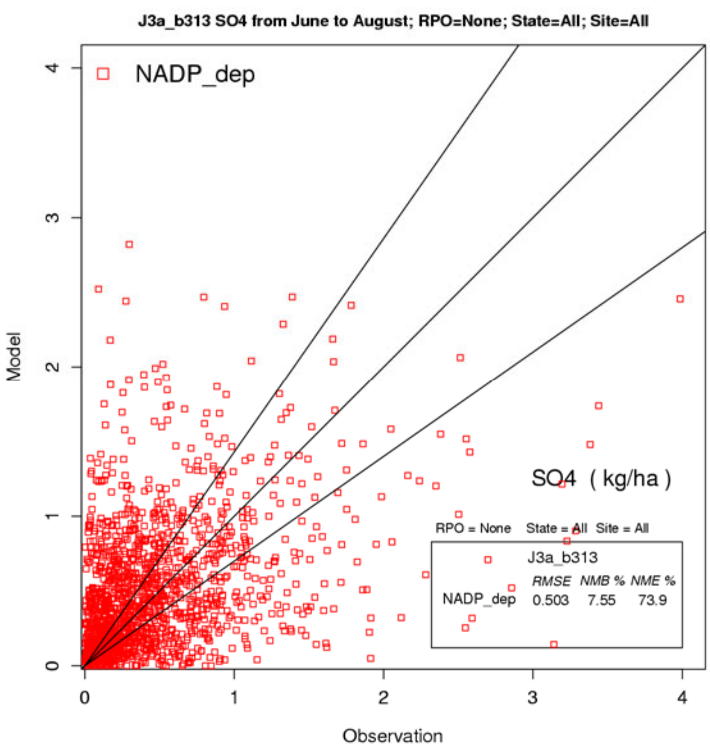


Scatter Plot – CMAQ v4.5 12 km

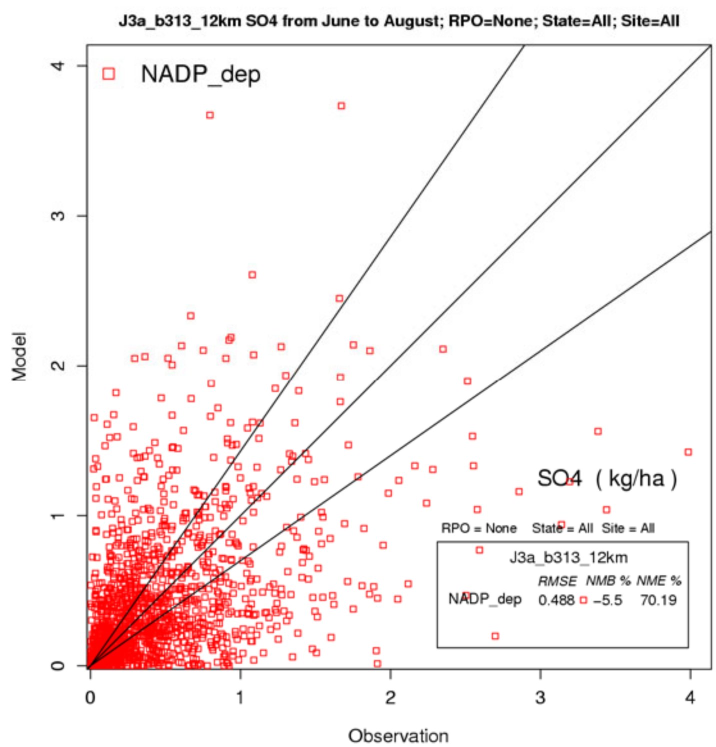


Wet Deposition Sulfate (kg/ha) - Summer

Scatter Plot – CMAQ v4.5 36 km

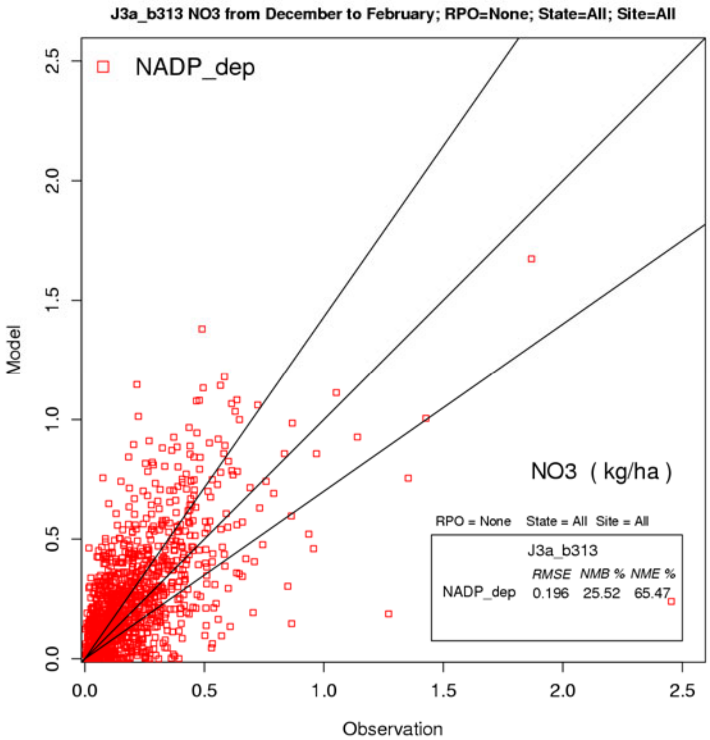


Scatter Plot – CMAQ v4.5 12 km

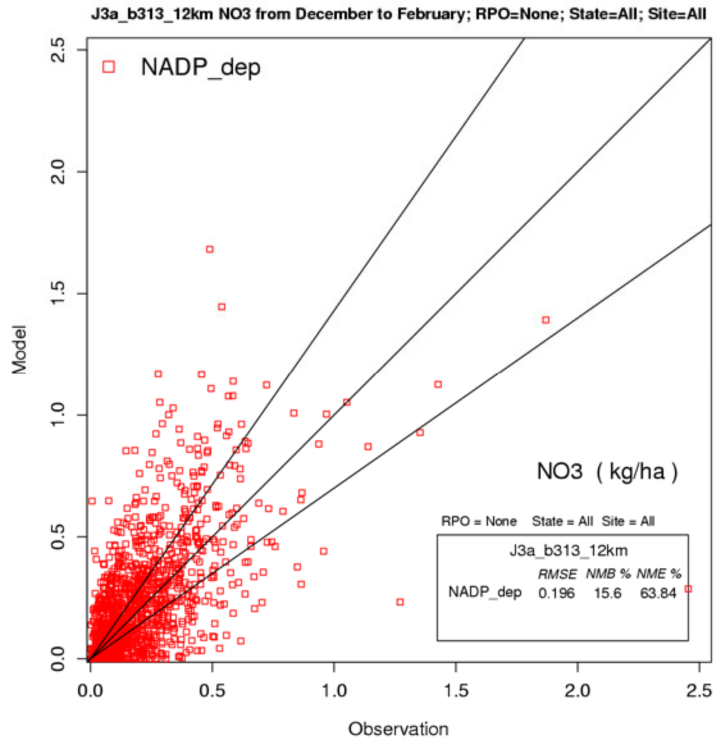


Wet Deposition Nitrate (kg/ha) - Winter

Scatter Plot – CMAQ v4.5 36 km

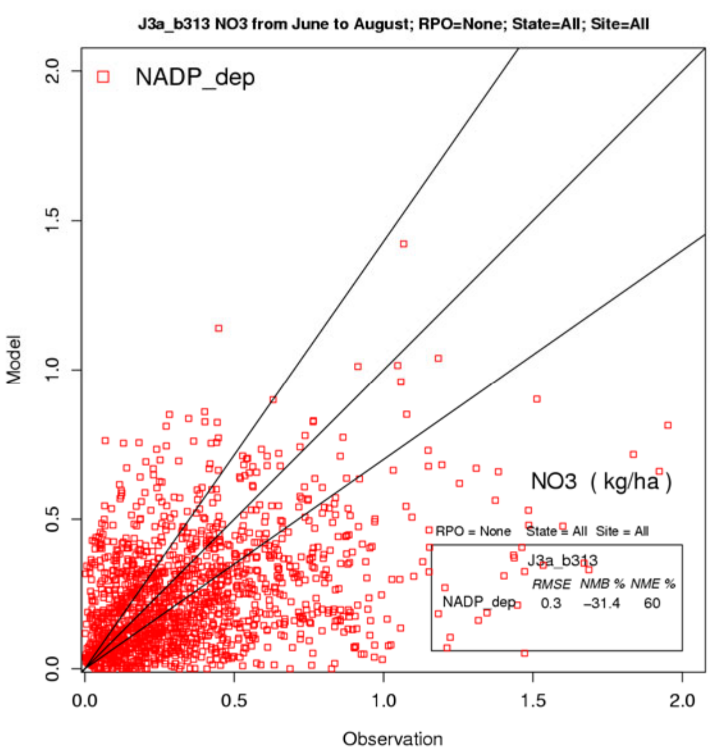


Scatter Plot – CMAQ v4.5 12 km

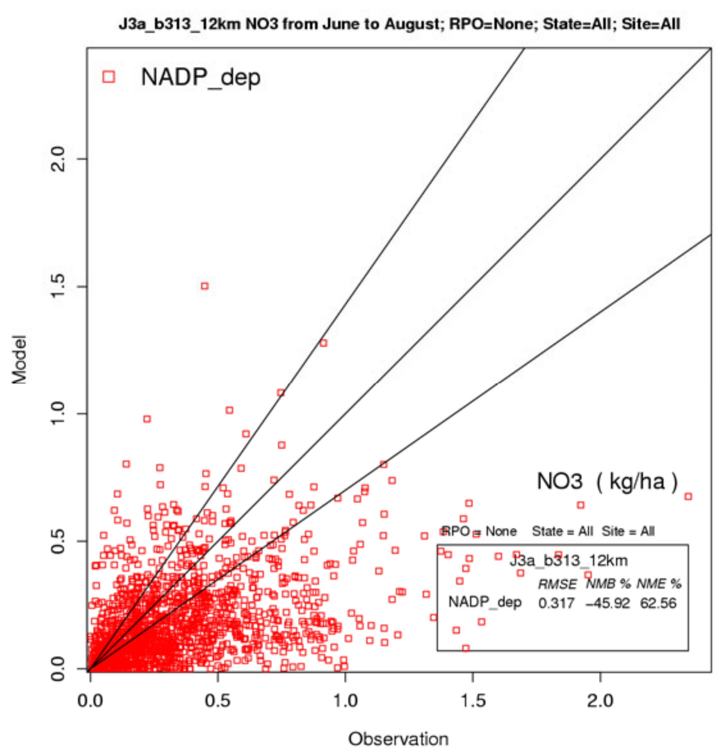


Wet Deposition Nitrate (kg/ha) - Summer

Scatter Plot – CMAQ v4.5 36 km

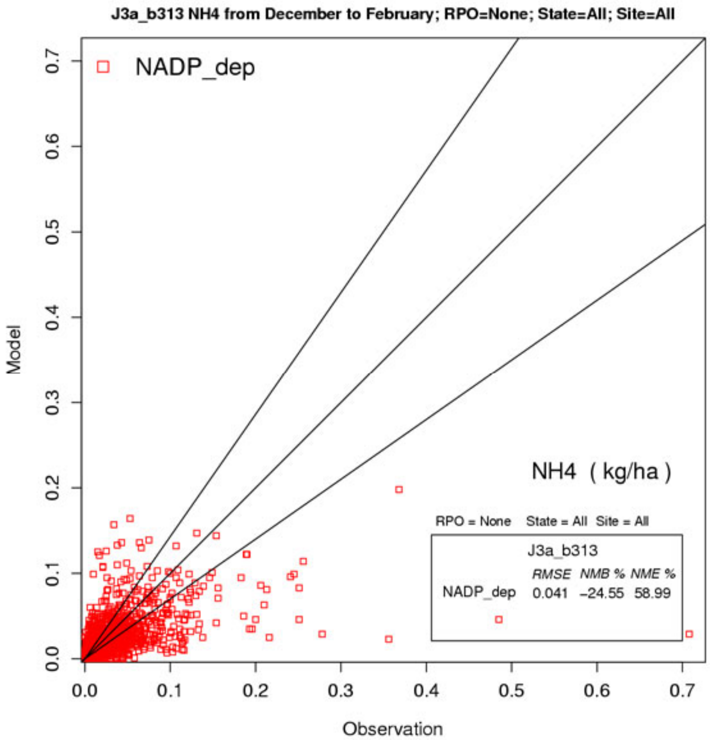


Scatter Plot – CMAQ v4.5 12 km

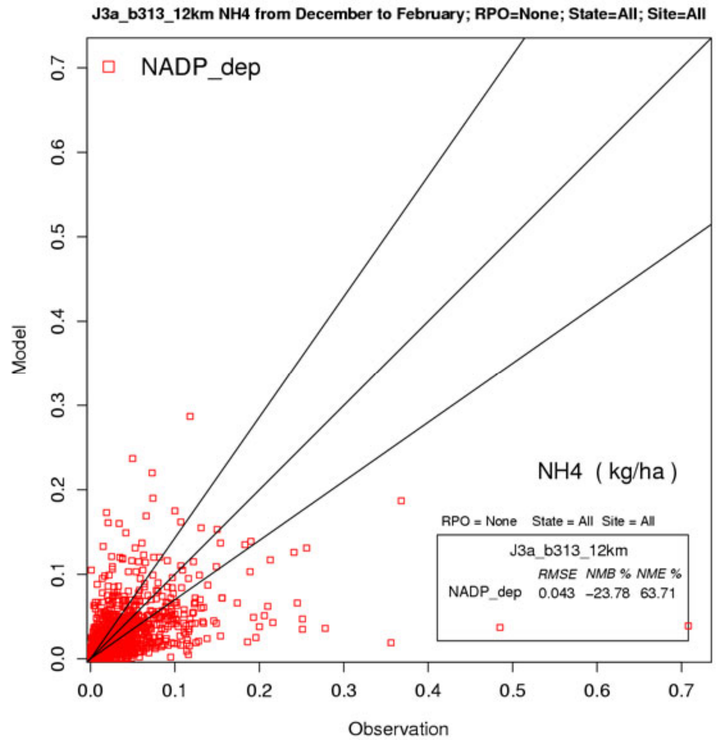


Wet Deposition Ammonium (kg/ha) - Winter

Scatter Plot – CMAQ v4.5 36 km

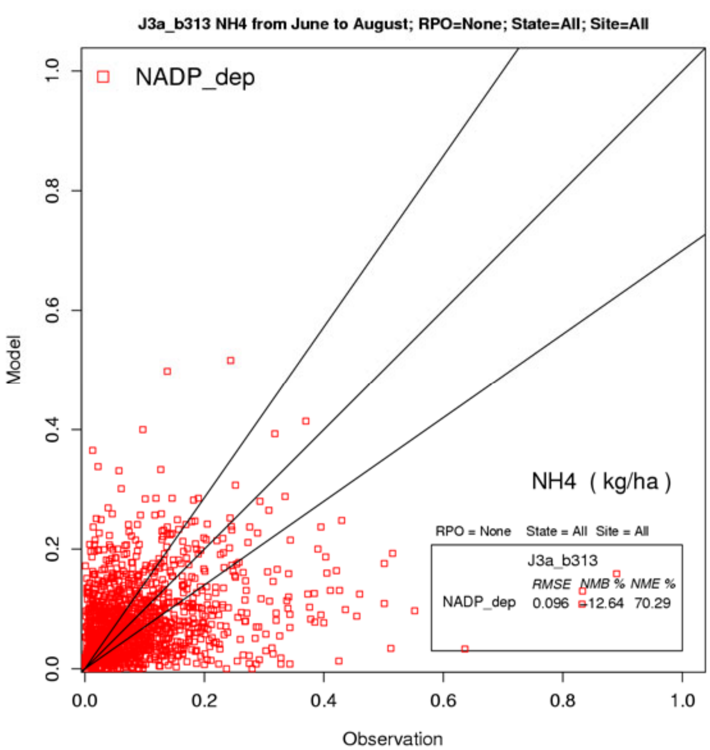


Scatter Plot – CMAQ v4.5 12 km

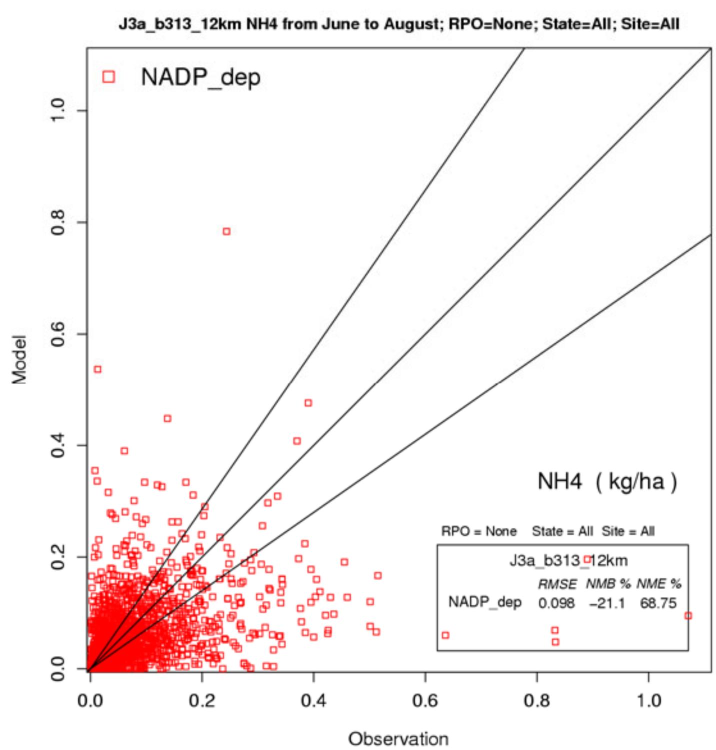


Wet Deposition Ammonium (kg/ha) - Summer

Scatter Plot – CMAQ v4.5 36 km

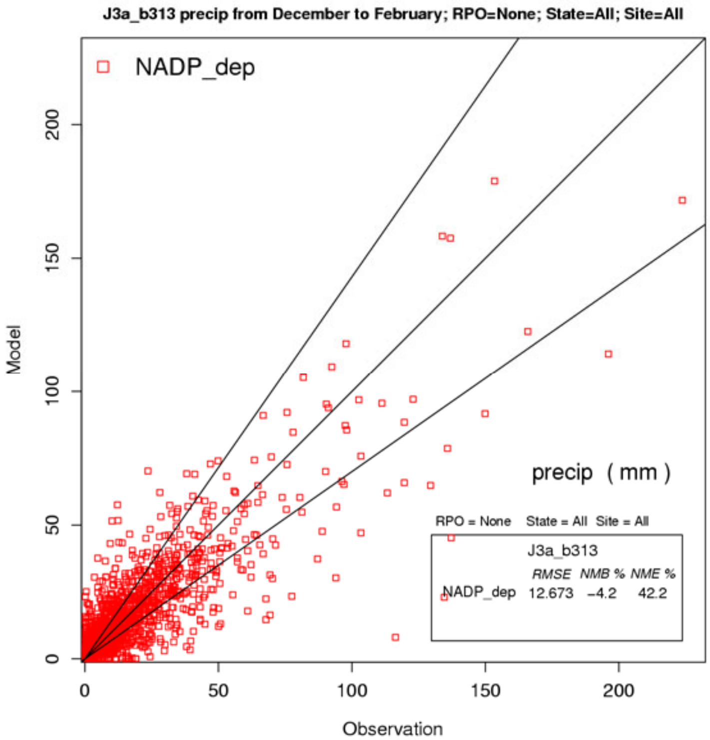


Scatter Plot – CMAQ v4.5 12 km

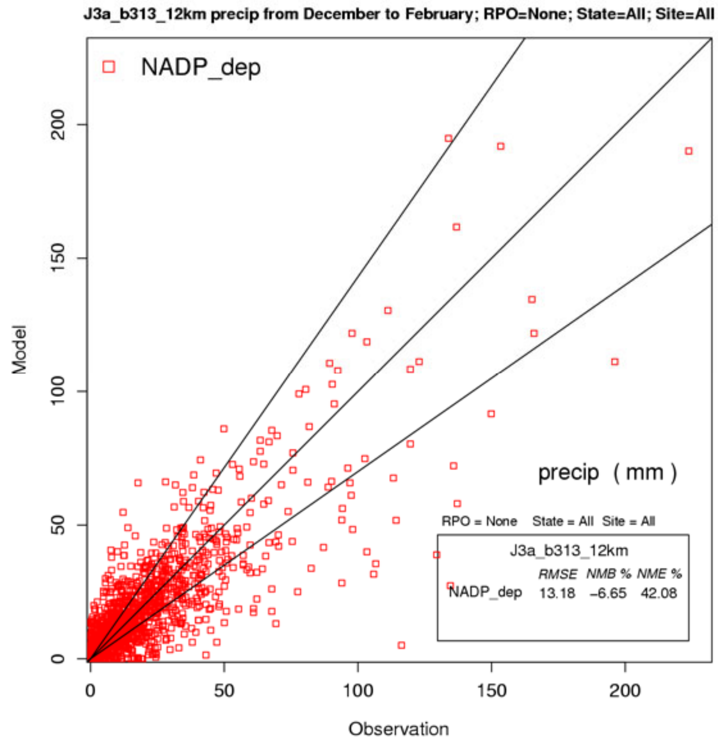


Precipitation (mm) - Winter

Scatter Plot – CMAQ v4.5 36 km

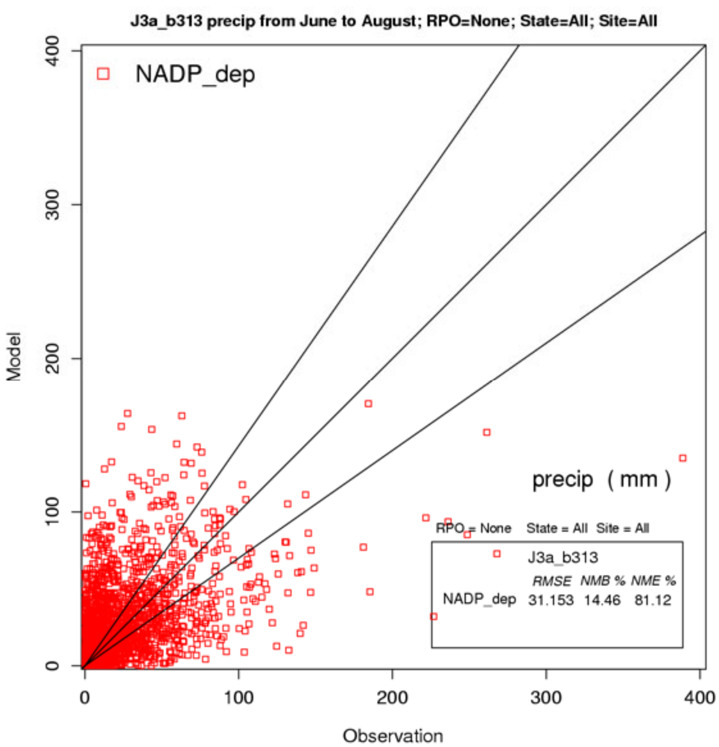


Scatter Plot – CMAQ v4.5 12 km



Precipitation (mm) - Summer

Scatter Plot – CMAQ v4.5 36 km



Scatter Plot – CMAQ v4.5 12 km