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

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Presented by Wyat Appel
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CMAQ v4.5: Major Updates

1) Aerosols
- Added sea salt (fine equilibrium; non-interactive coarse mode) -- aero4
- Updated aerosol dry deposition algorithm
- Updated ISORROPIA to v1.5 (25 Oct 2003) and fixed some discontinuities
- Modified SO_4 used in ISORROPIA call
- Corrected inconsistency in MINL2SG (aerodepv)
- Corrected the EMSULF (H_2SO_4 emissions) unit conversion bug

2) Chemistry
- Added CB4/chlorine chemistry and associated EBI solver
- Added CB4/air toxics and SAPRC99/air toxics chemistry and associated EBI solvers

3) PBL modeling
- Updated to use PURB (% urban) for setting minimum K_z

4) Clouds
- Added new sub-grid cloud mixing algorithm/module (based on ACM)

Model Characteristics for Evaluation Simulation

- 2005 Release of CMAQ (v4.5)
- 12km × 12km Eastern U.S. domain
- 14 vertical layers
- CB-IV gas-phase chemistry, EBI solver and AE4 aerosol module
- ACM cloud module, EBI solver
- Mass continuity scheme
- MM5 meteorology (2001) processed with MCIP v3.0

Model Simulation - Emissions

- EPA's 2001 NEI
- MOBILE6 of mobile emissions
- BEIS 3.13 for biogenic emissions
- Seasonality of NH_3 estimated by inverse modeling
  - Gilliland et al., available in Atmos. Env. special issue on model evaluation
- Emissions processed using SMOKE

Three Additional Evaluation Simulations

1. Annual simulation with 36km × 36km grid resolution using CMAQ v4.5 (parent domain for 12-km simulation)
2. Annual simulation with 36km × 36km grid resolution using CMAQ v4.4
3. 12km × 12km domain simulation using CMAQ v4.4 for winter and summer seasons only

Evaluation Report

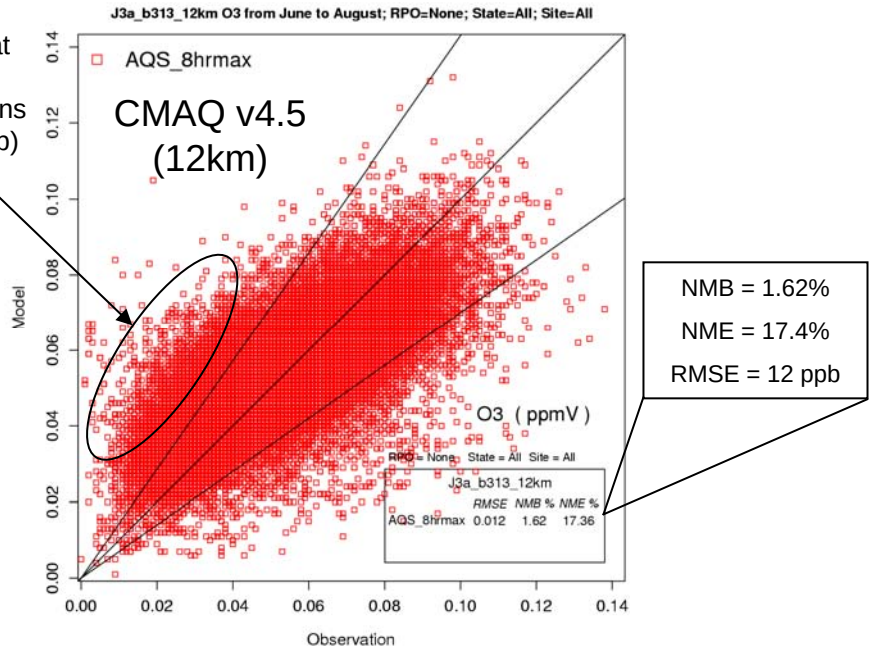
- Comprehensive evaluation of CMAQ v4.5 at 12-km grid resolution was performed
  - Seasonal analysis (winter (DJF), spring (MAM), summer (JJA) and fall (SON))
  - Ozone, organic and inorganic aerosols, total $PM_{2.5}$ mass and precipitation chemistry
  - 36-km versus 12-km performance comparison
  - CMAQ v4.4 versus v4.5 performance comparison
- Model to Observation pairing accomplished using Site Compare (available with 2005 release)
- Statistics and plots generated using AMET (information available during poster session)
- A very small portion of the complete report is shown here
  - Full evaluation report available through CMAS at http://www.cmascenter.org/docs/CMAQ/v4.5/CMAQv.5_EvaluationDocument-Final2005.pdf

Observation Networks

- AQS (majority urban)
  - O_3
- IMPROVE (rural)
  - SO_4, NO_3, EC, OC and $PM_{2.5}$
- STN (urban)
  - SO_4, NO_3, NH_4, EC, OC and $PM_{2.5}$
- CASTNet (sub-urban and rural)
  - SO_4, NO_3, NH_4, HNO_3 and TNO_3
- NADP (rural)
  - Wet deposition SO_4, NO_3, NH_4; precipitation

8-hr Maximum Ozone

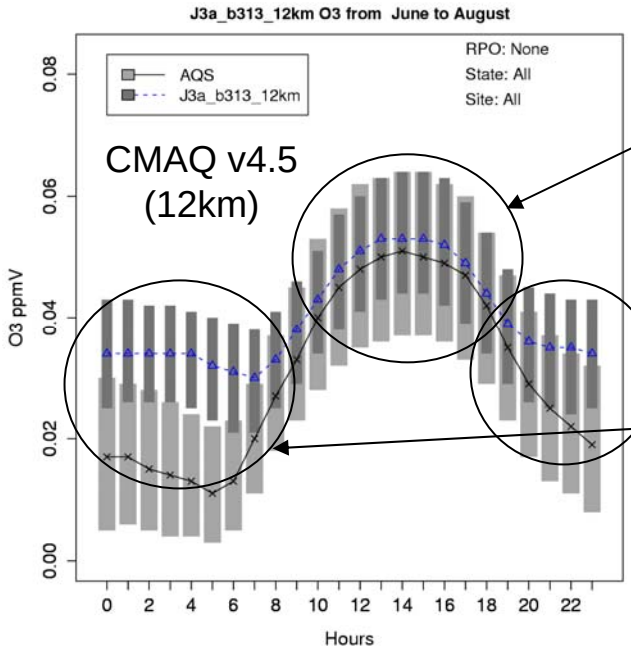
High bias at low concentrations (10 – 50 ppb)



NMB = 1.62%

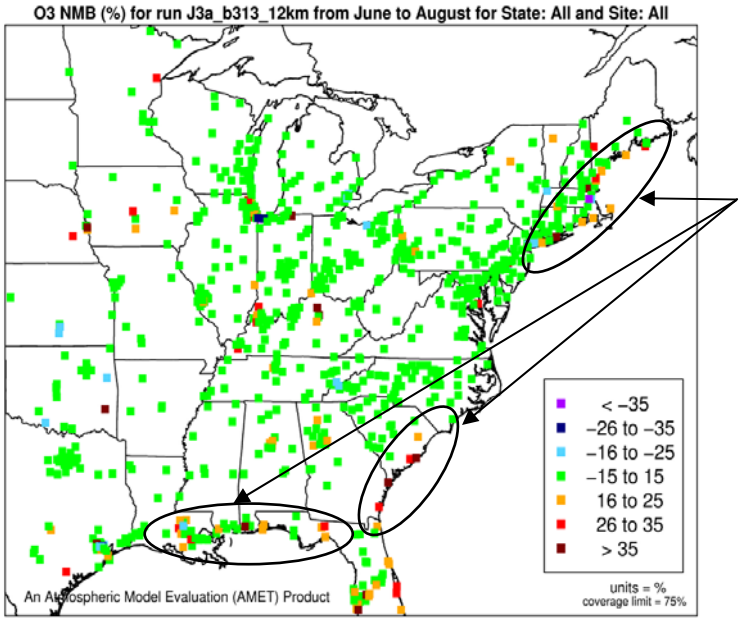
NME = 17.4%

RMSE = 12 ppb



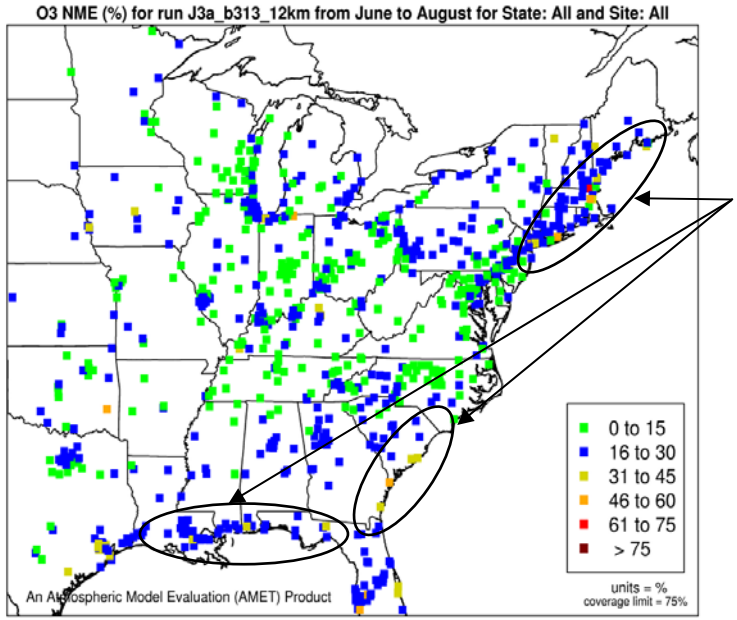
Good agreement during the day

Model not capturing overnight lows



square=AQS_8hrmax;

Higher biases along the coast



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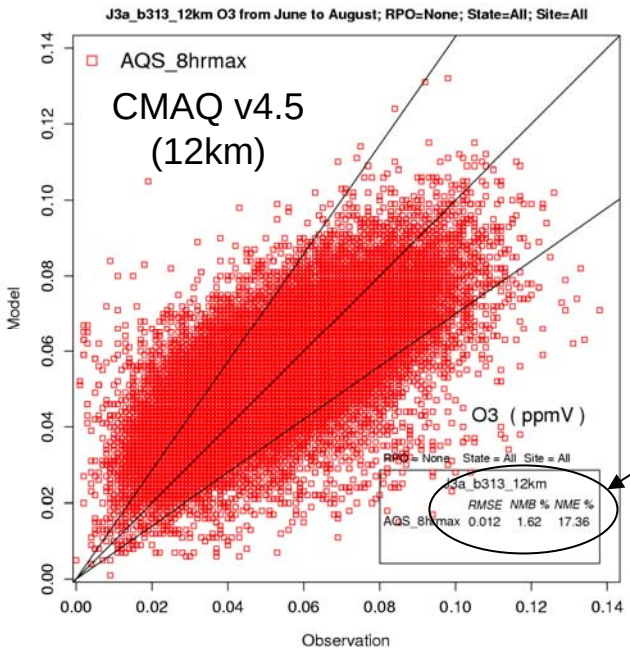
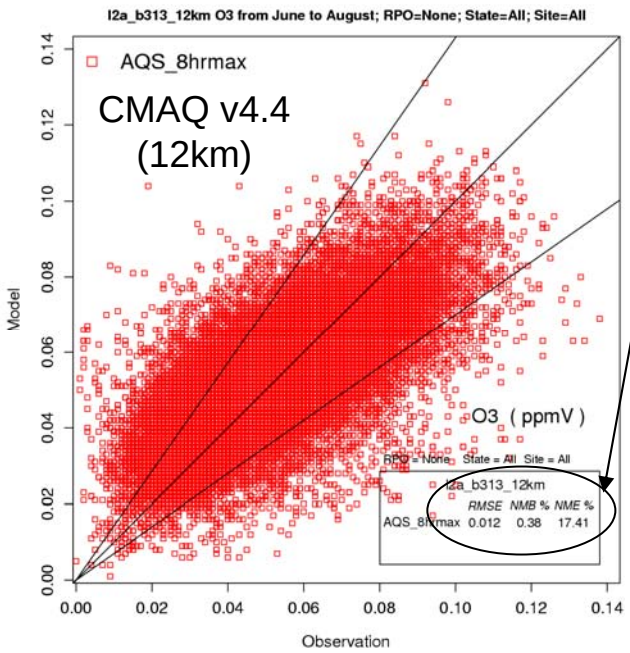
Higher errors along the coast

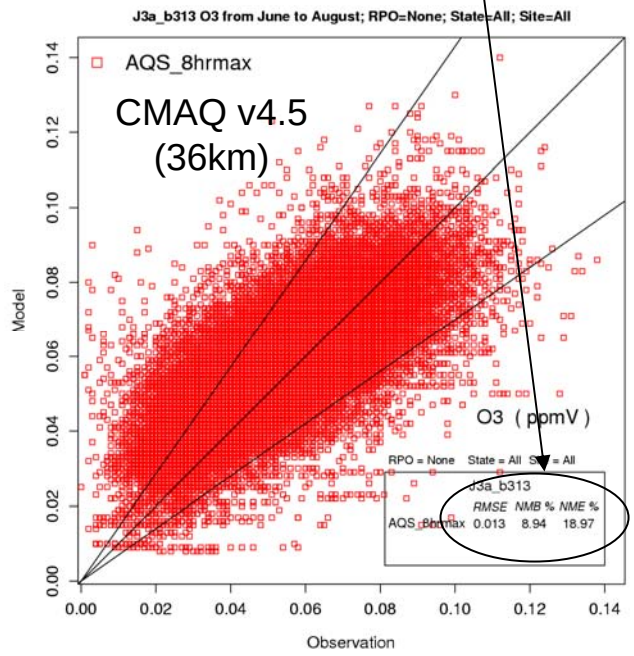
O_3 performance: v4.4 versus v4.5, 12km versus 36km



Similar O_3 bias and error at 12km for v4.4 and v4.5

Bias at 12km is improved versus 36km





Organic and Inorganic Aerosols

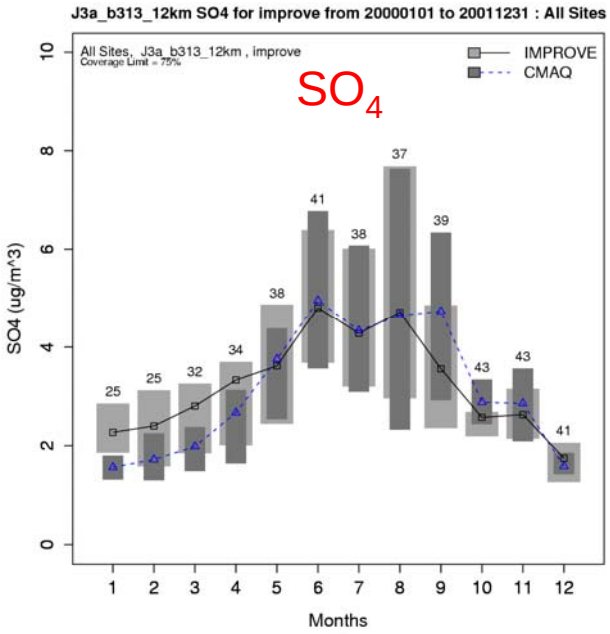
IMPROVE, STN and CASTNet

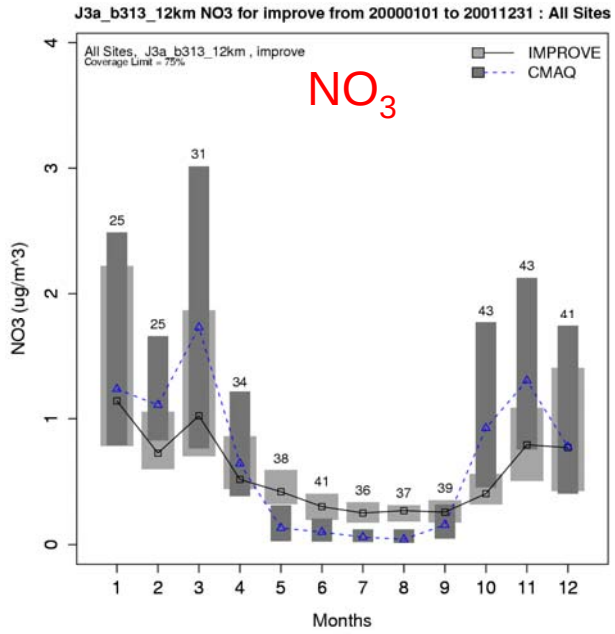
SO_4, NO_3 and NH_4, EC, OC, $PM_{2.5}$, HNO_3

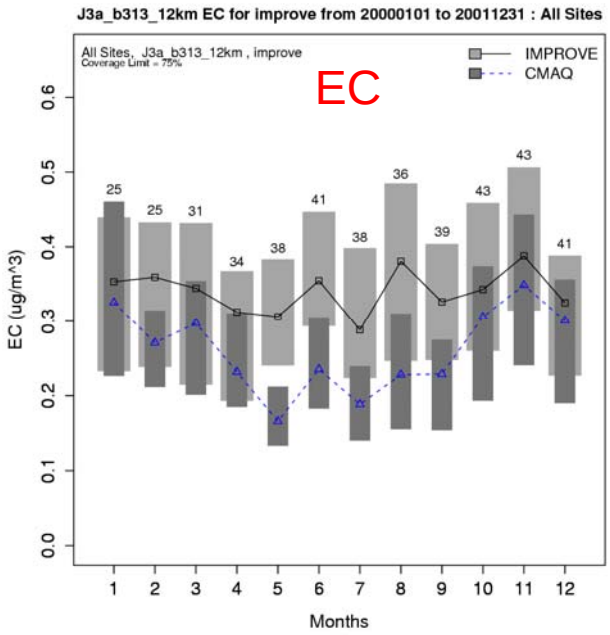
IMPROVE (v4.5, 12km)

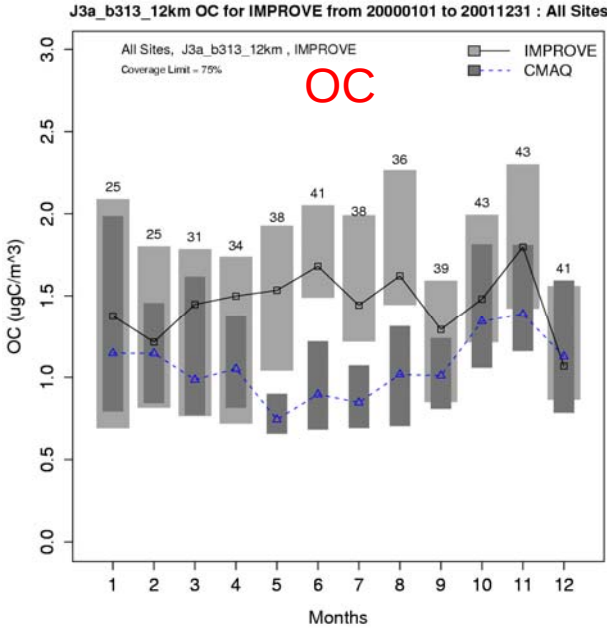
Under-predictions in SO_4, NO_3, EC and OC contribute to under-predictions in $PM_{2.5}$ in the spring and summer.

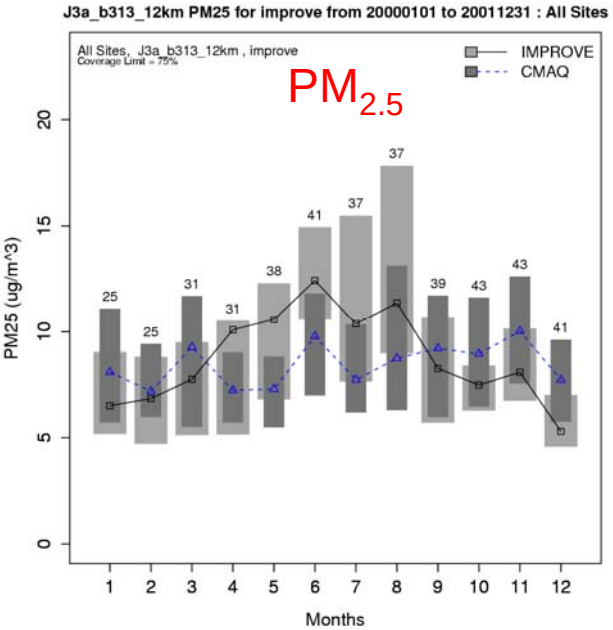
Over-predictions in SO_4 and NO_3 contribute to over-predictions in $PM_{2.5}$ in the fall.

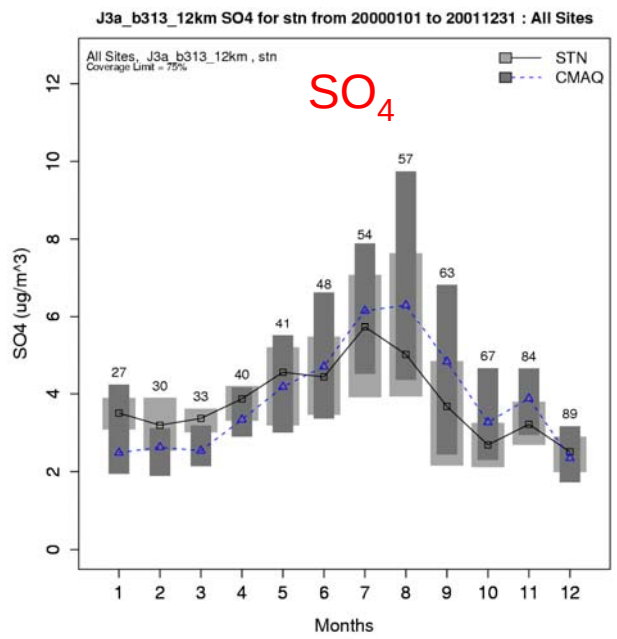


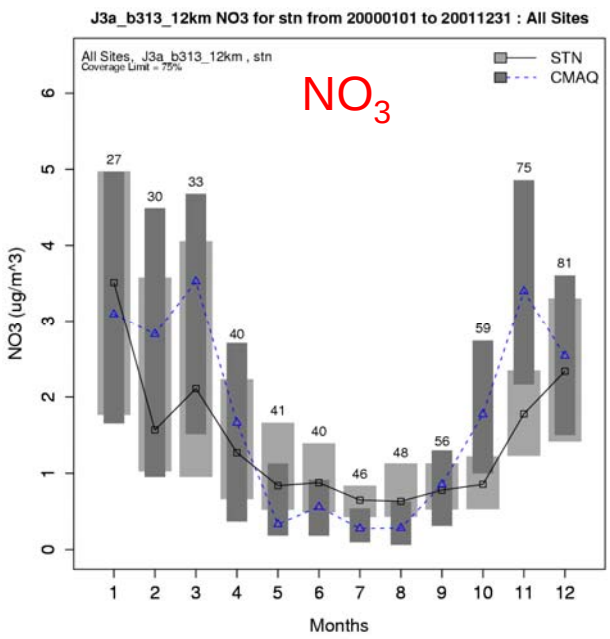


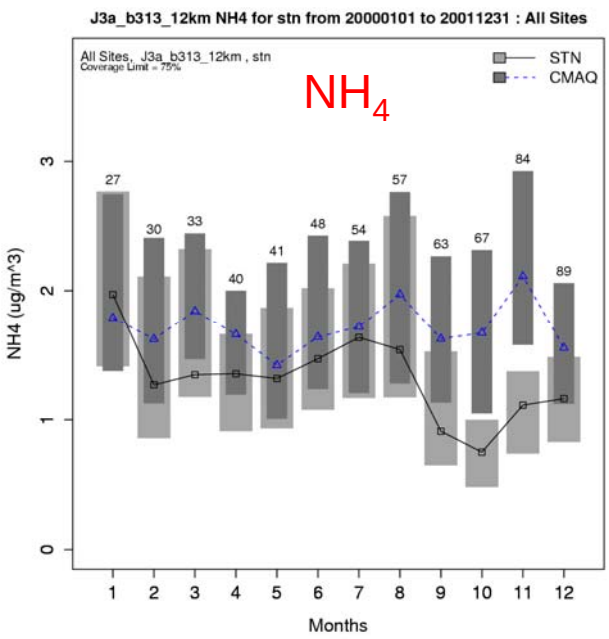


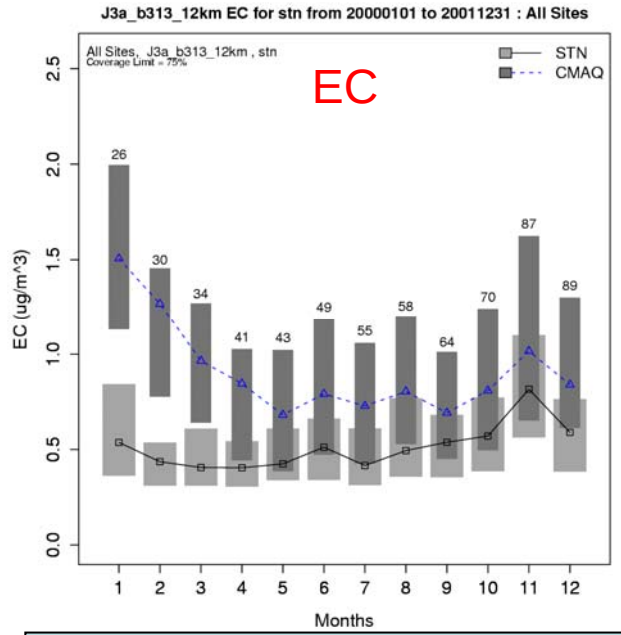


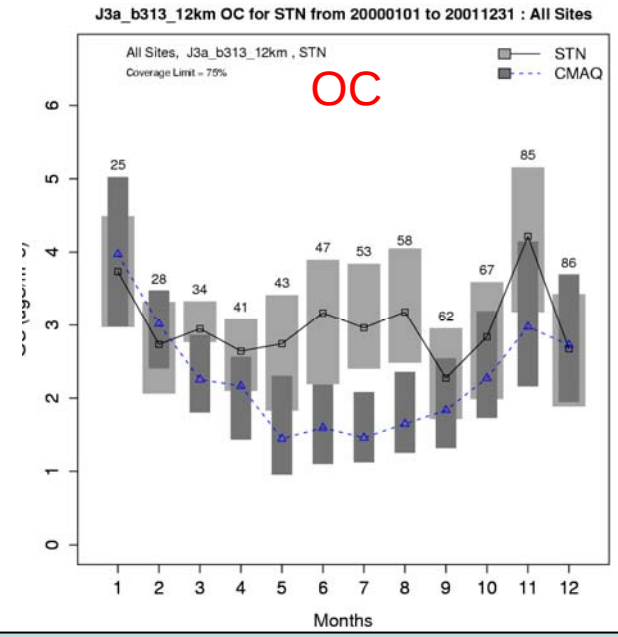


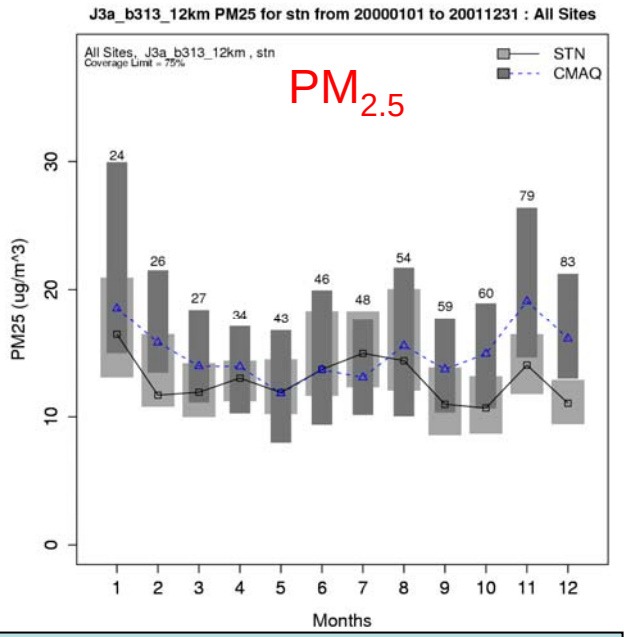












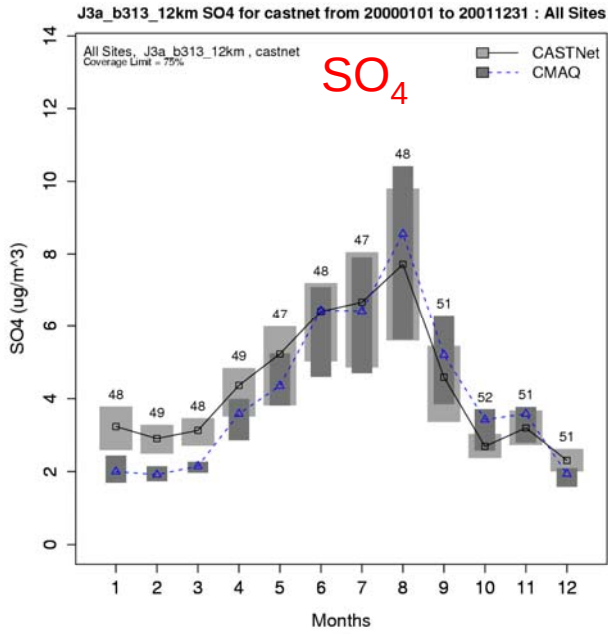
STN

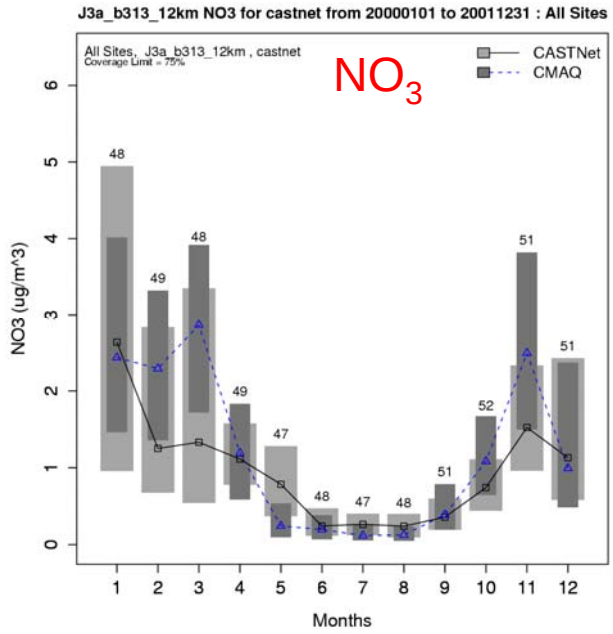
Total $PM_{2.5}$ mass is over-predicted for much of the year (other than summer). Due to the over-prediction in NO_3, NH_4 and EC.

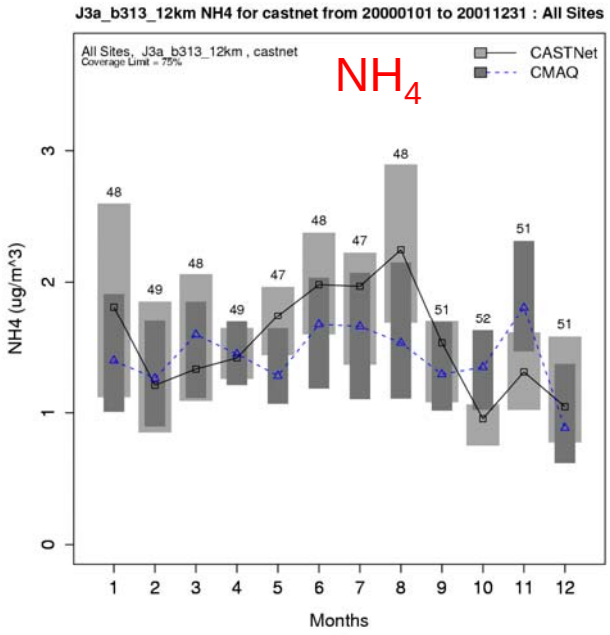
$PM_{2.5}$ performance during the summer is good, however, there appears to be compensating biases, with over-predictions in SO_4, NH_4 and EC and under-predictions in NO_3 and OC.

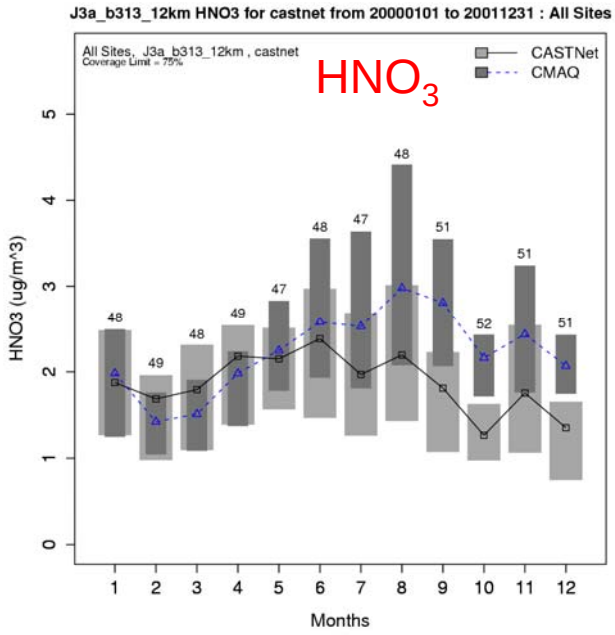
CASTNet (v4.5, 12km)

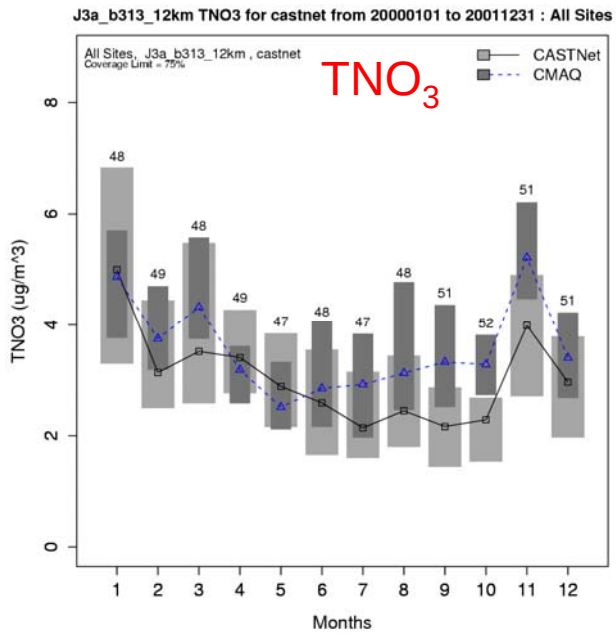
- SO_4 under-predicted in the winter
- NO_3 over-predicted in spring and fall
- NH_4 over-predicted in the fall, under-predicted in the summer
- HNO_3 and TNO_3 over-predicted for the latter half of the year
- NH_3 emissions adjustment may be needed in spring and fall



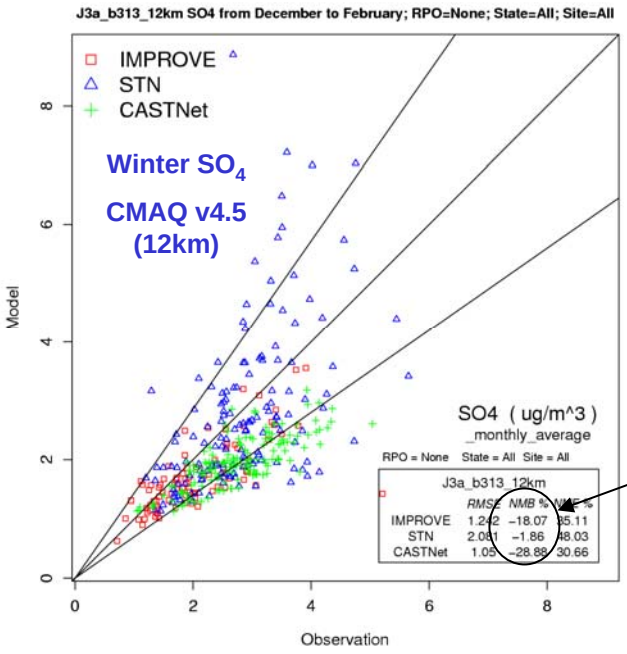


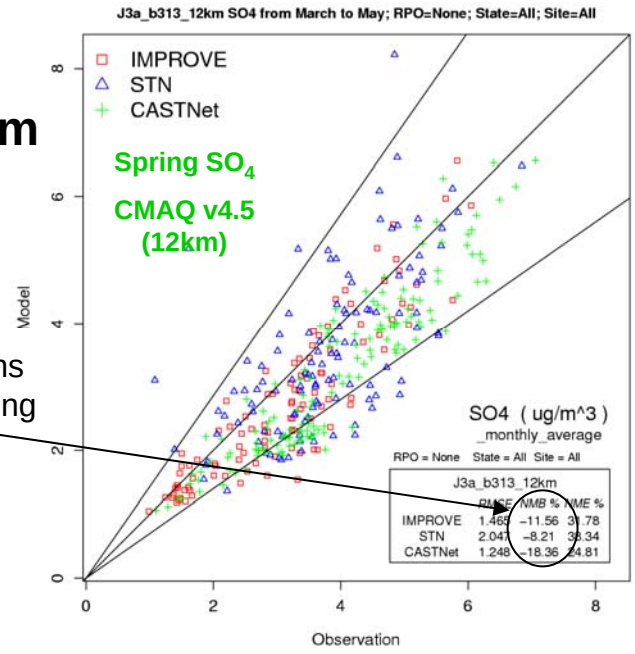




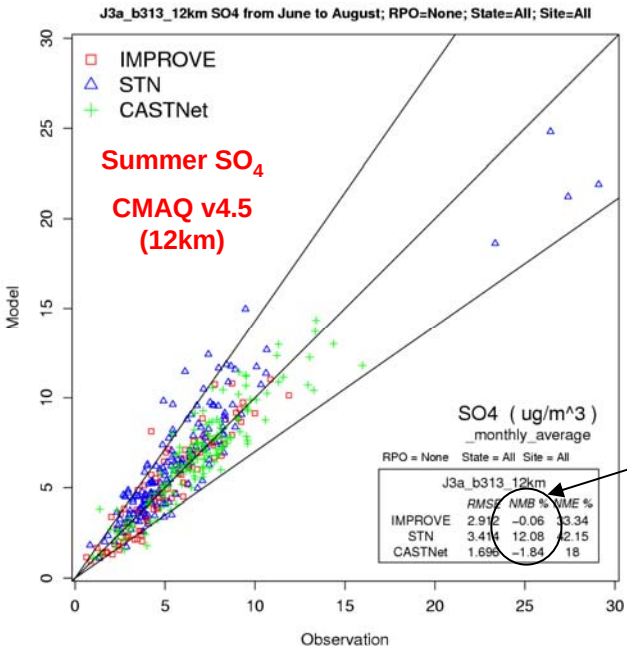


SO_4 v4.5, 12km

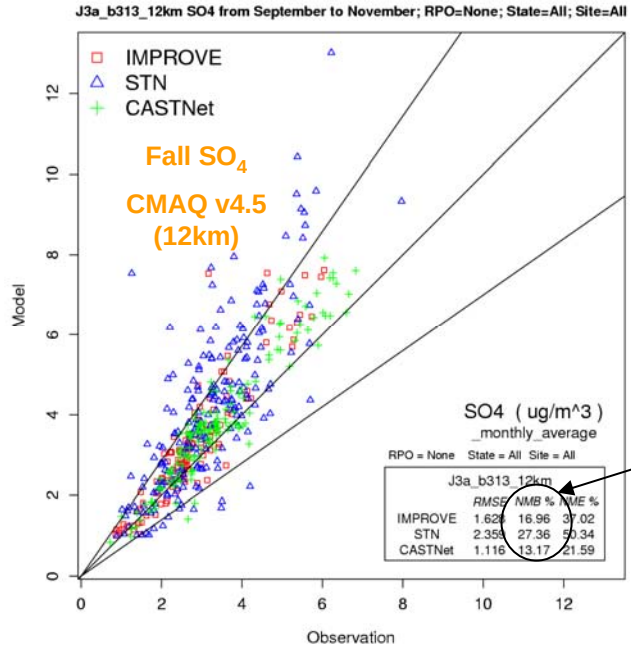




Under-predictions in winter and spring



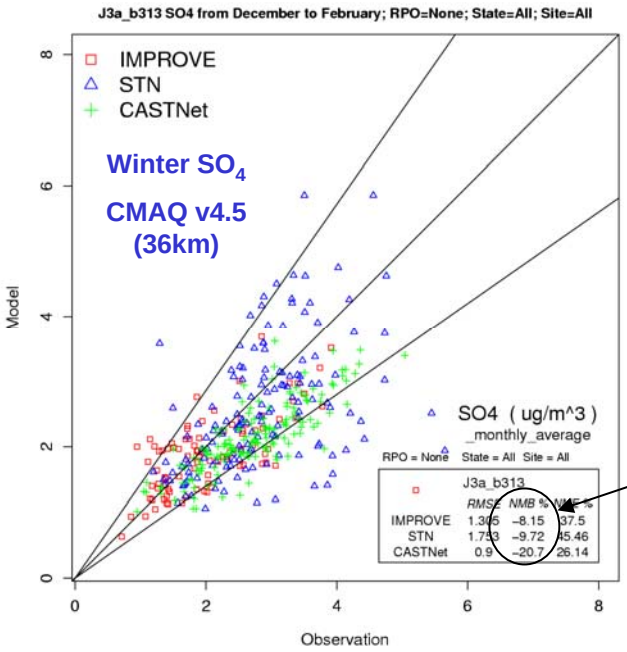
Nearly unbaised in the summer

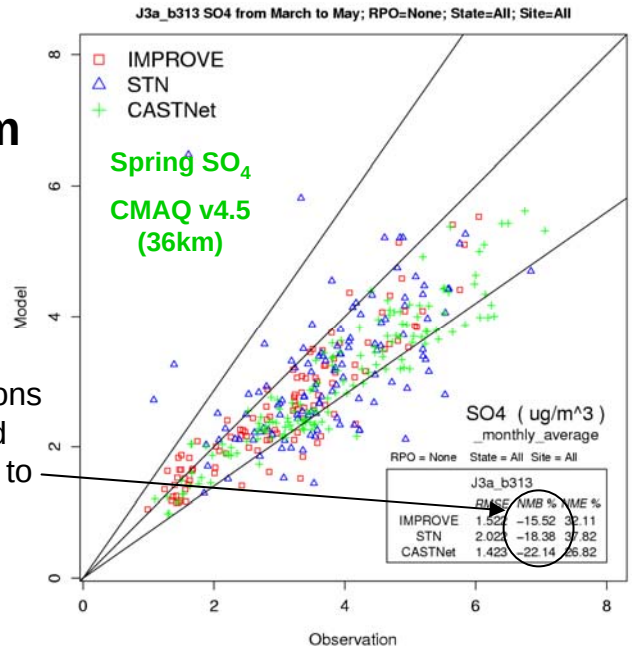


Over-predictions in the fall

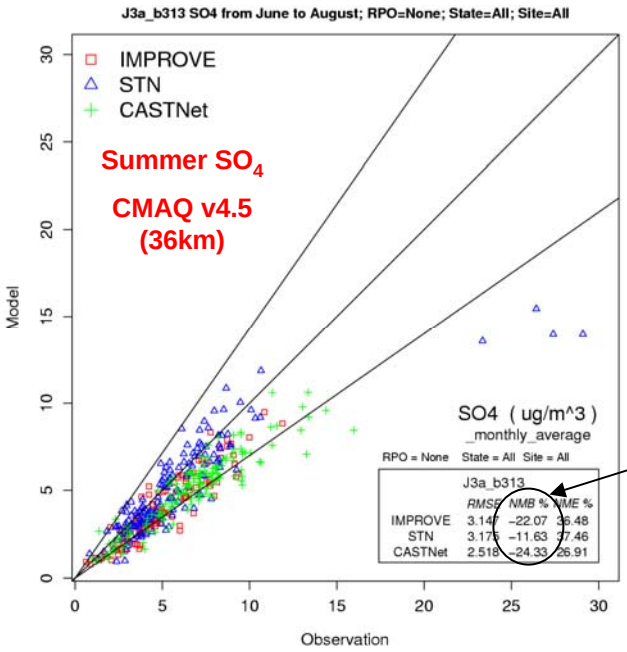
SO_4

v4.5, 36km

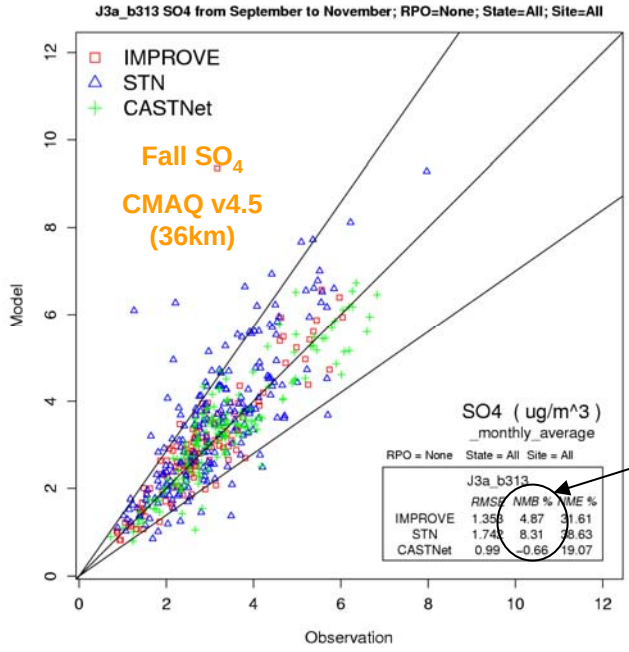




Under-predictions in winter and spring, similar to 12km



Large under-predictions in summer at 36km, versus nearly unbaised at 12km



Over-prediction in fall is larger at 12km

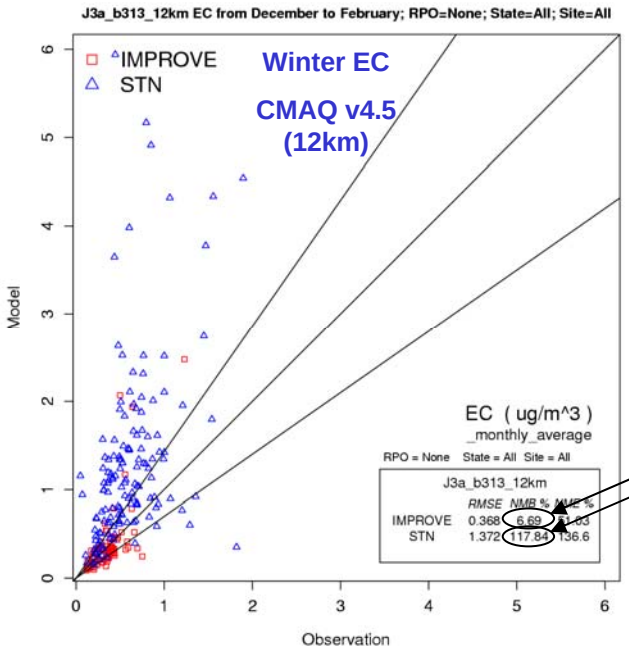
EC

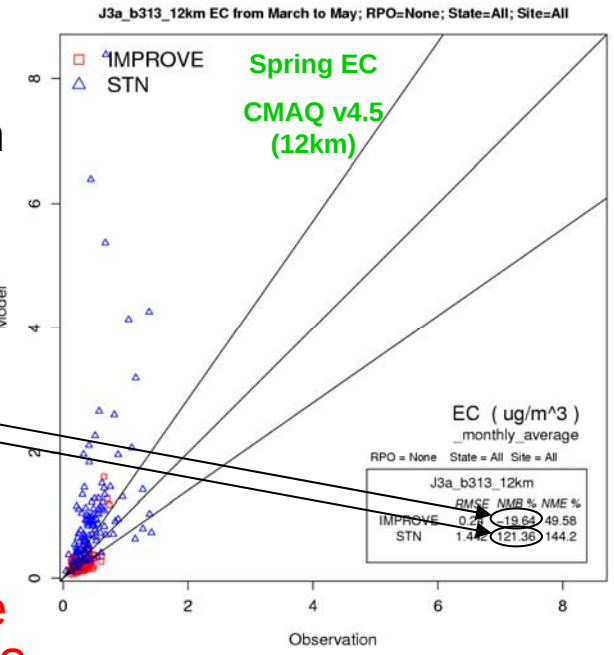
v4.5, 12km

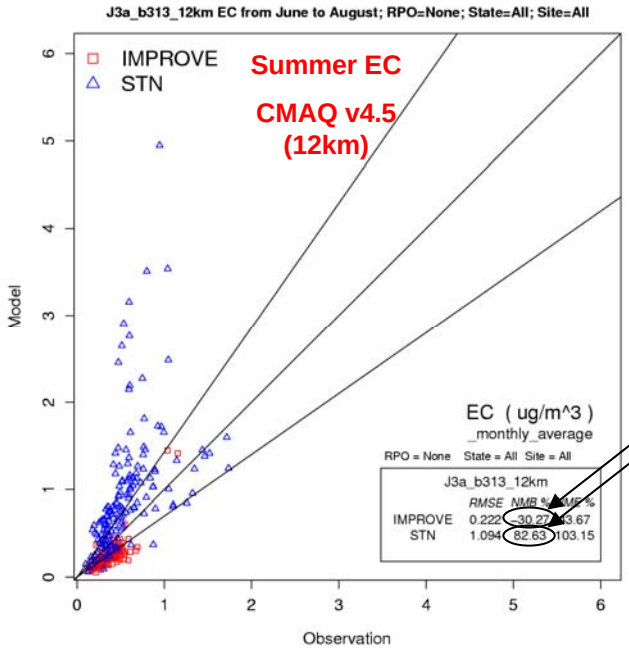
EC is generally under-predicted at rural IMPROVE sites

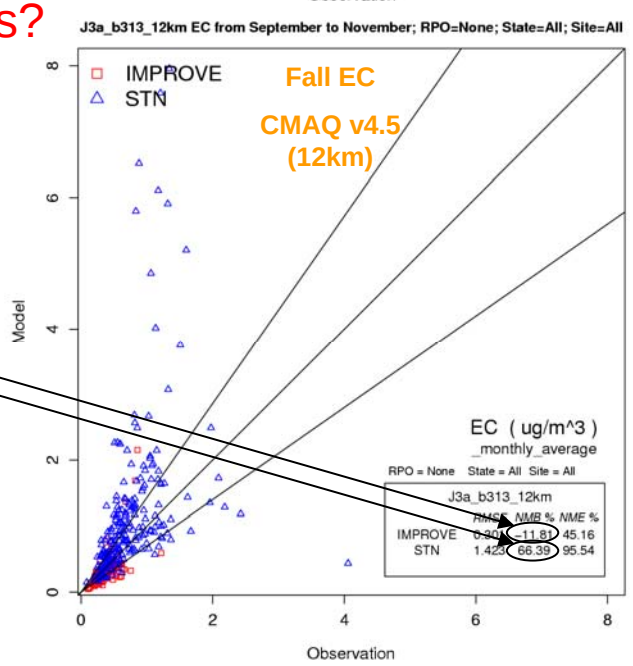
Large over-predictions of EC at urban STN sites

Issue in the urban areas?



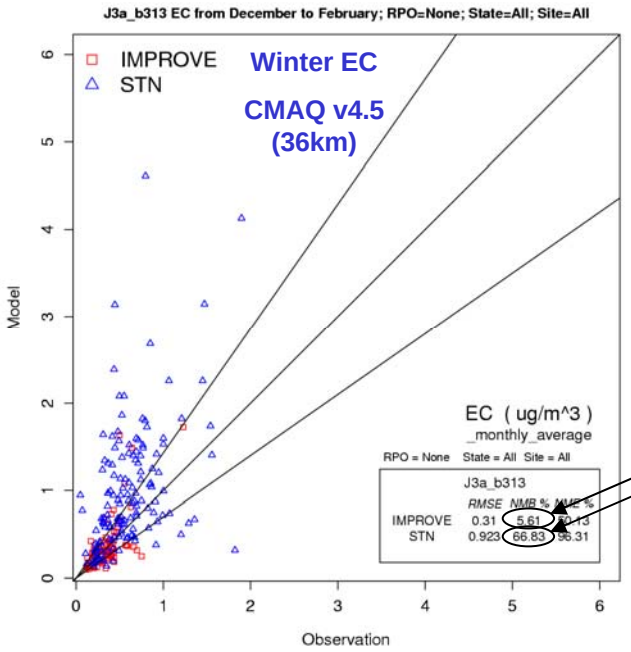


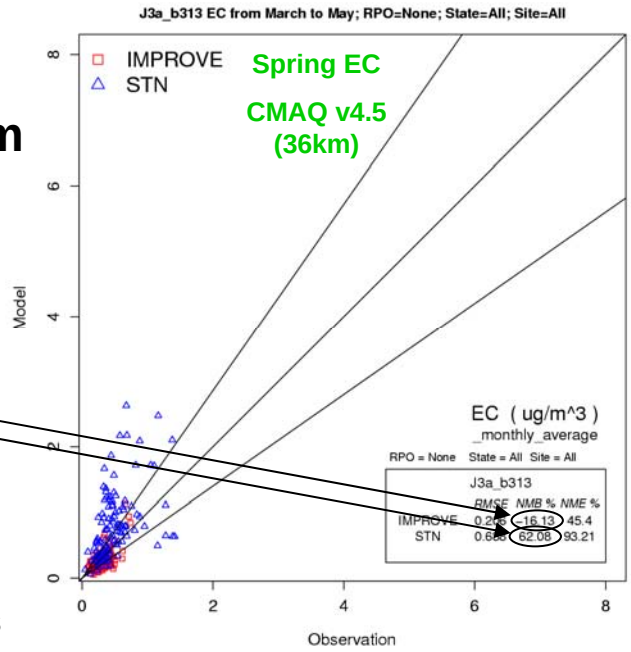


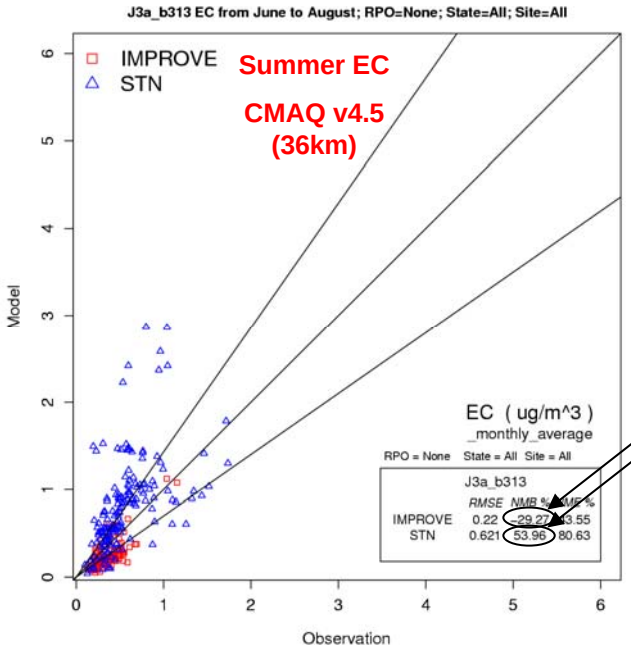


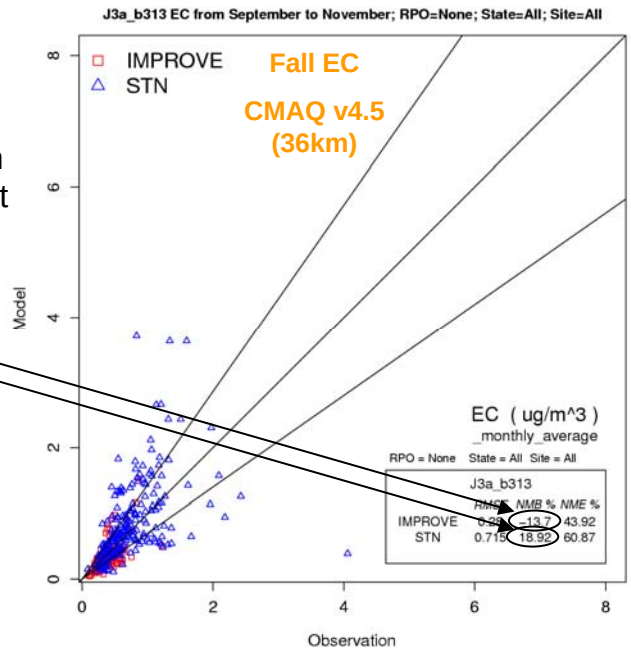
EC

v4.5, 36km









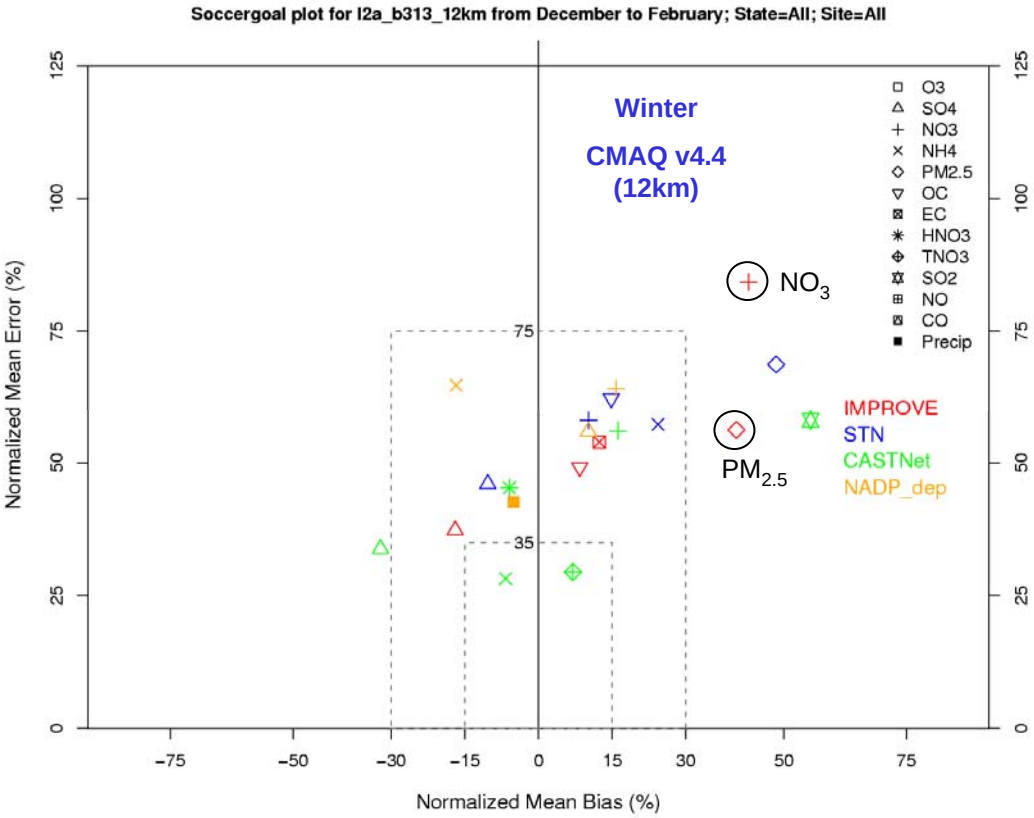
36km EC performance at IMPROVE sites is similar to 12km performance

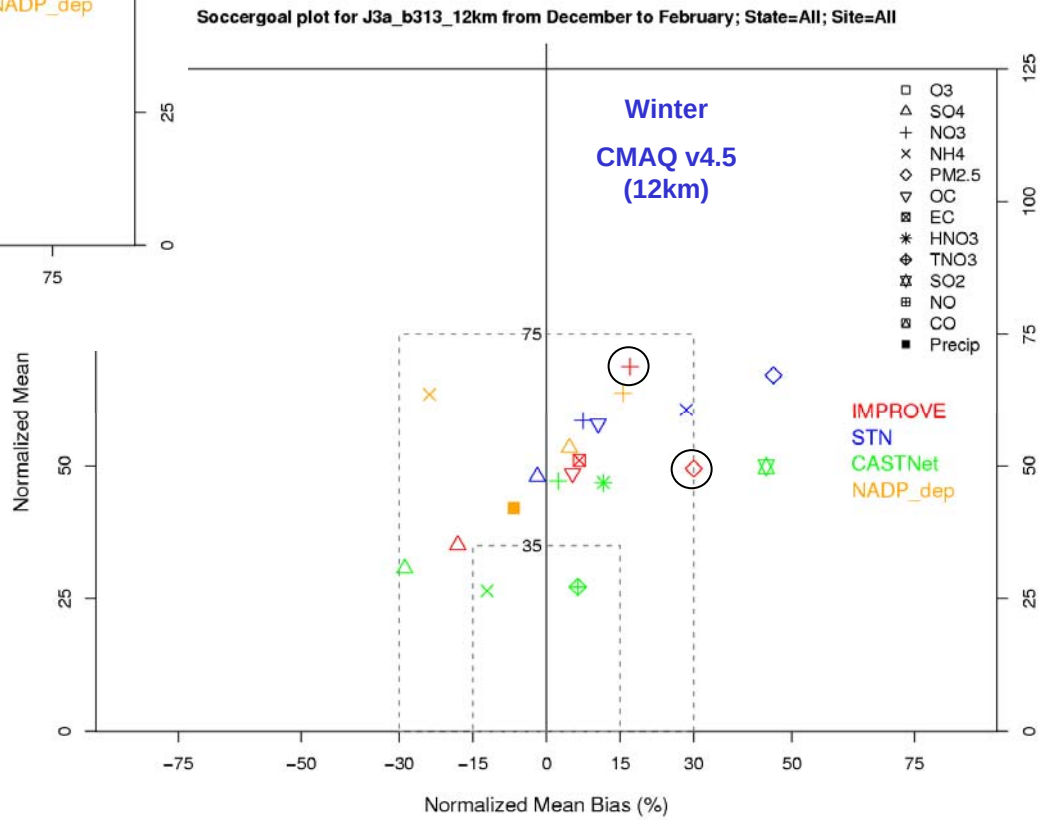
Over-prediction at STN sites not as large at 36km as 12km

CMAQ v4.4 versus v4.5

Soccer goal plot - Winter

v4.4 versus v4.5



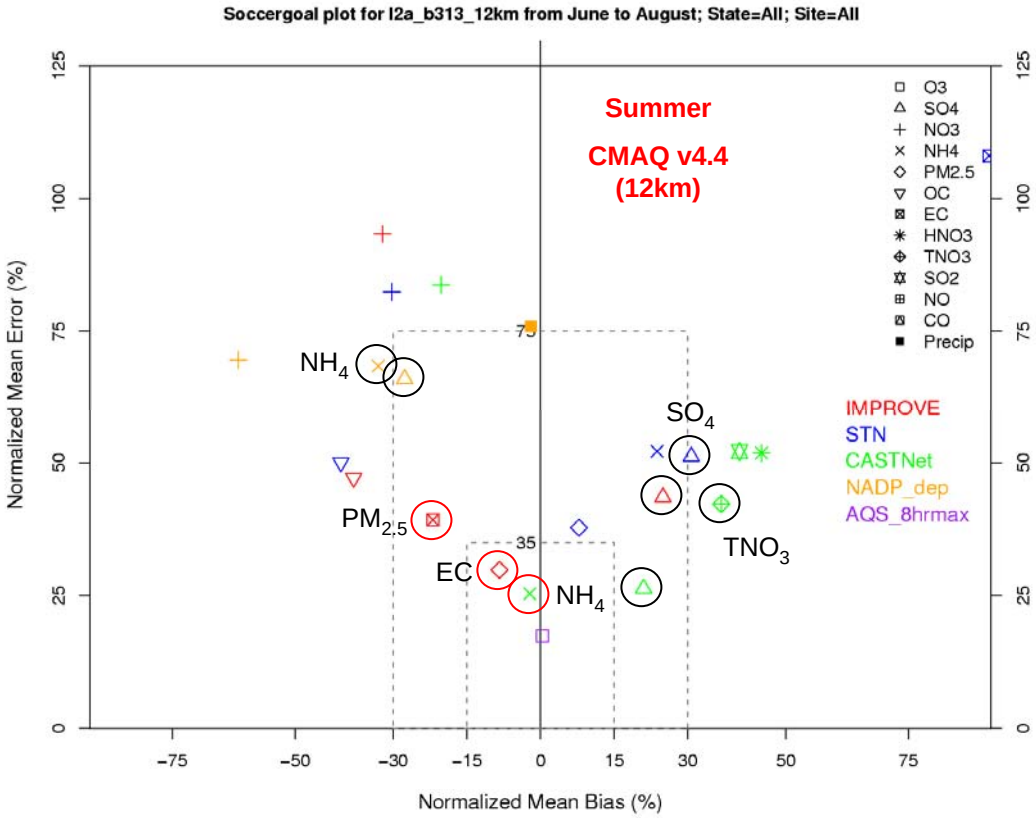


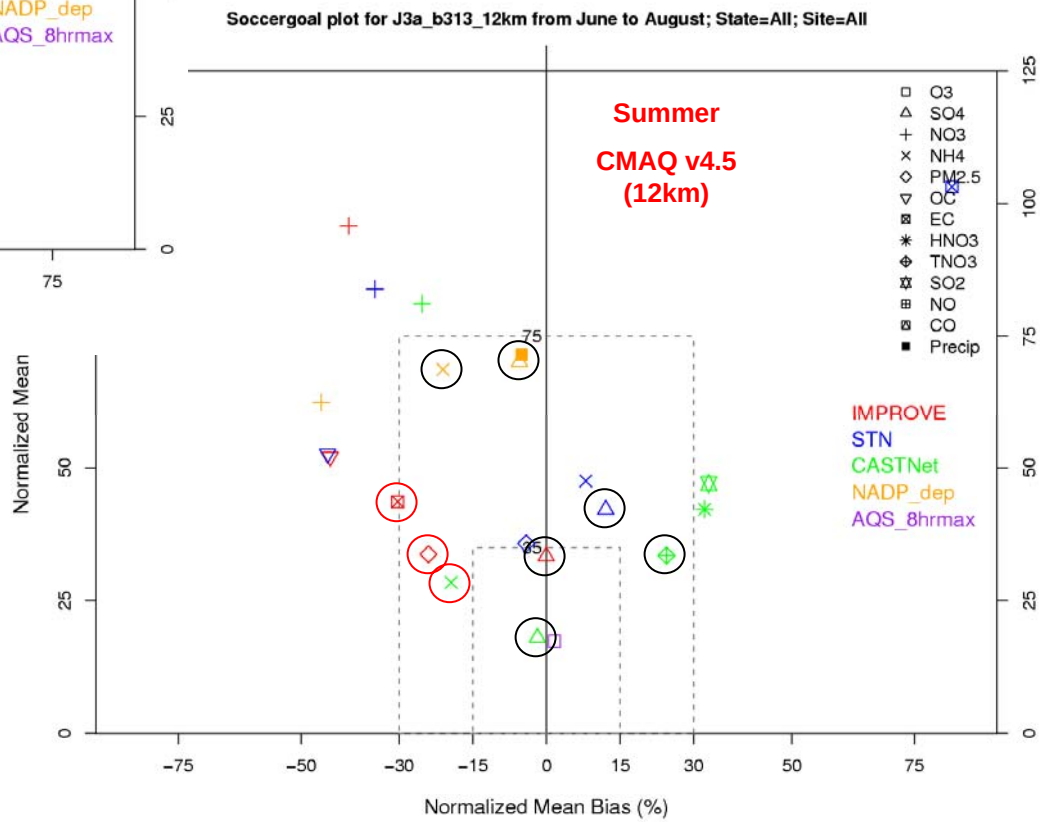
Better performance for IMPROVE NO_3 and $PM_{2.5}$

Little change in performance of other species

Soccer goal plot - Summer

v4.4 versus v4.5



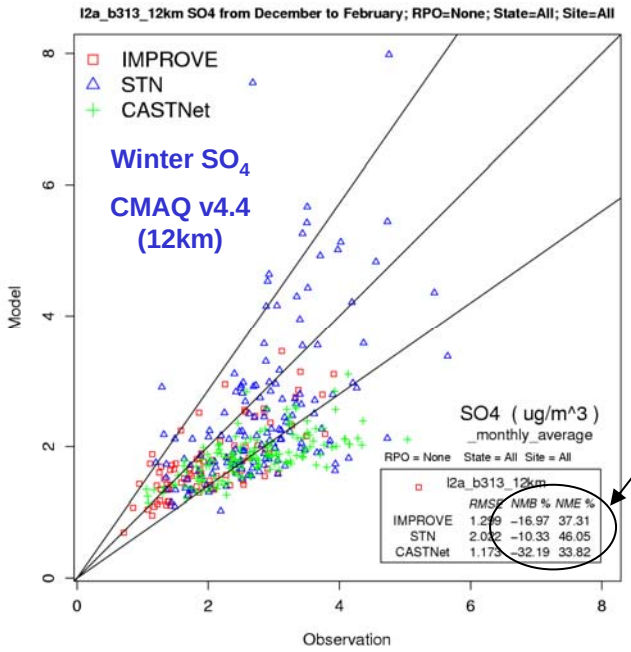


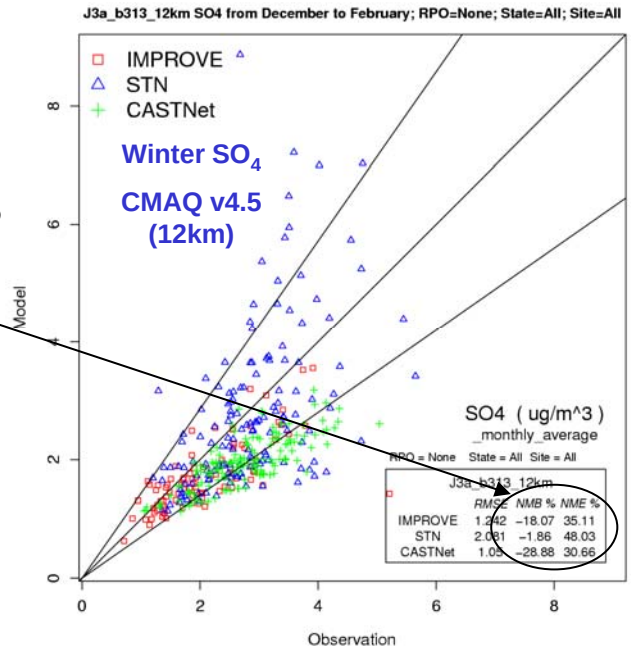
- Better performance for SO_4 (all networks)
- CASTNet TNO_3 and NADP NH_4 improved
- IMPROVE EC and $PM_{2.5}$ performance decreases
- CASTNet NH_4 performance decreases

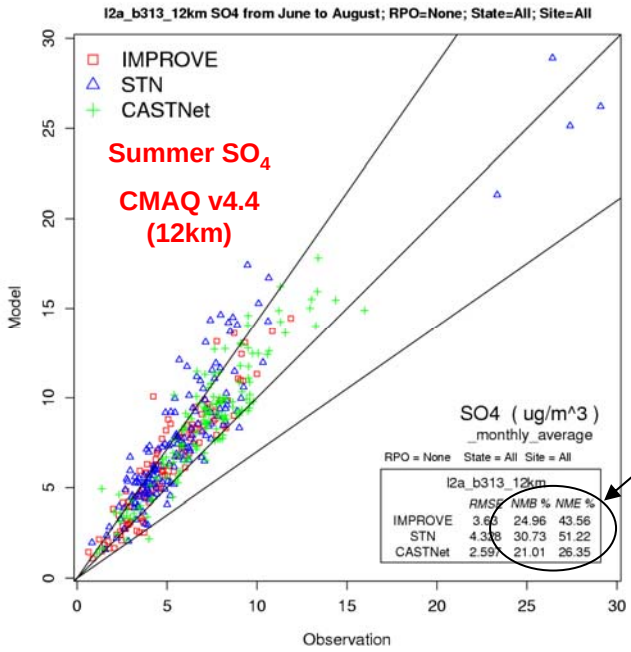
Sulfate

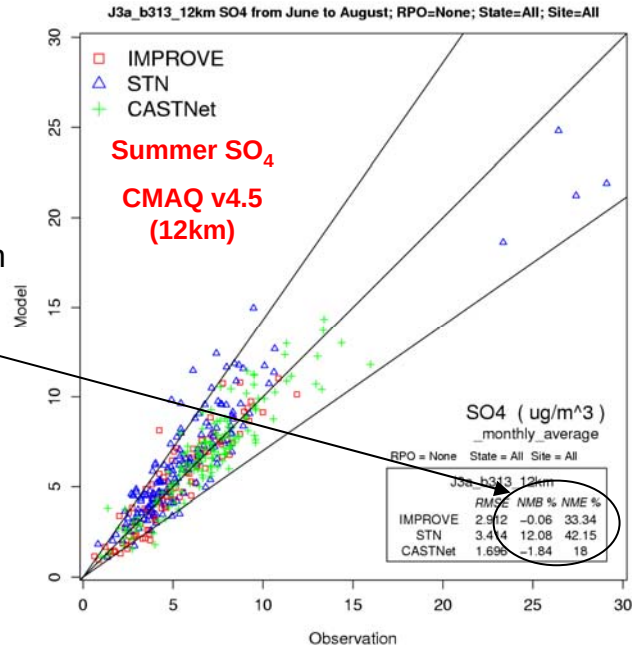
SO_4 bias in the winter is slightly improved in v4.5

SO_4 bias and error in the summer is much better in v4.5





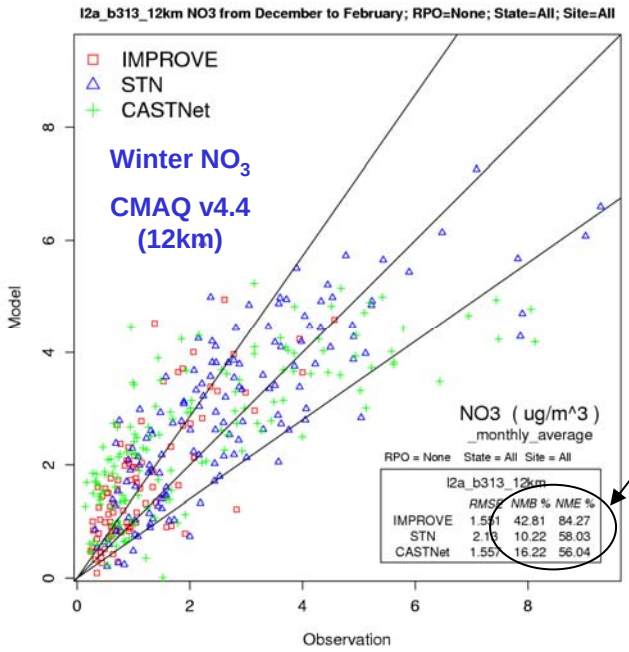


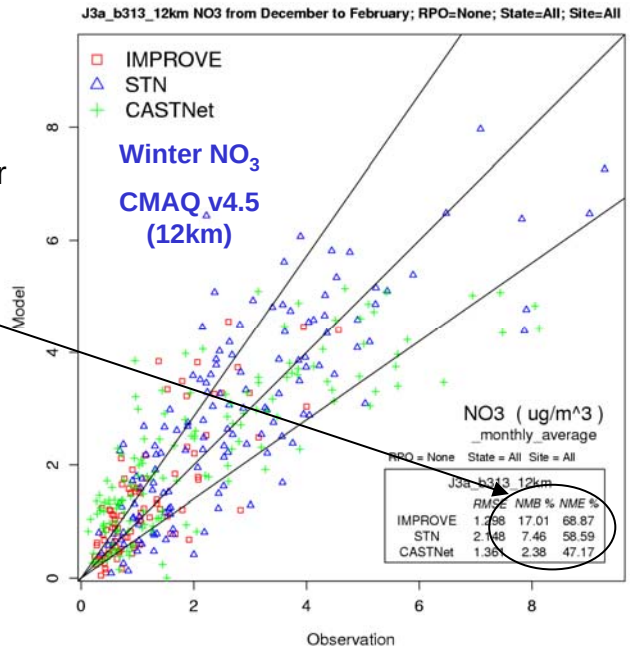


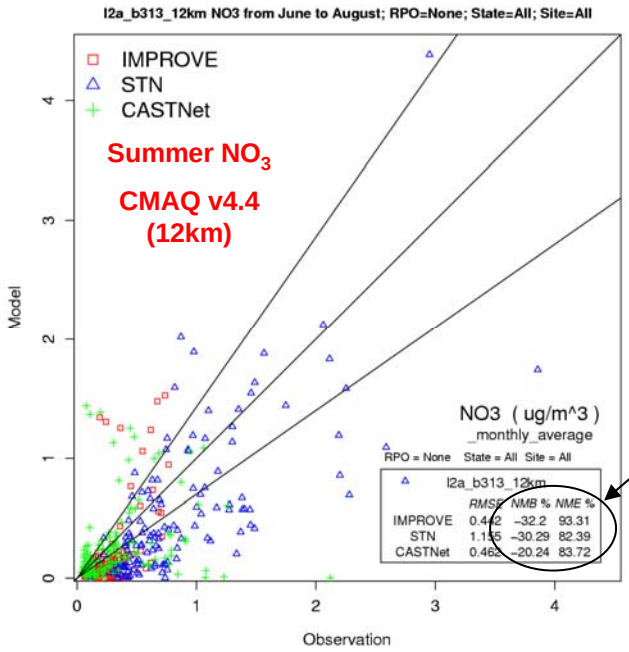
Nitrate

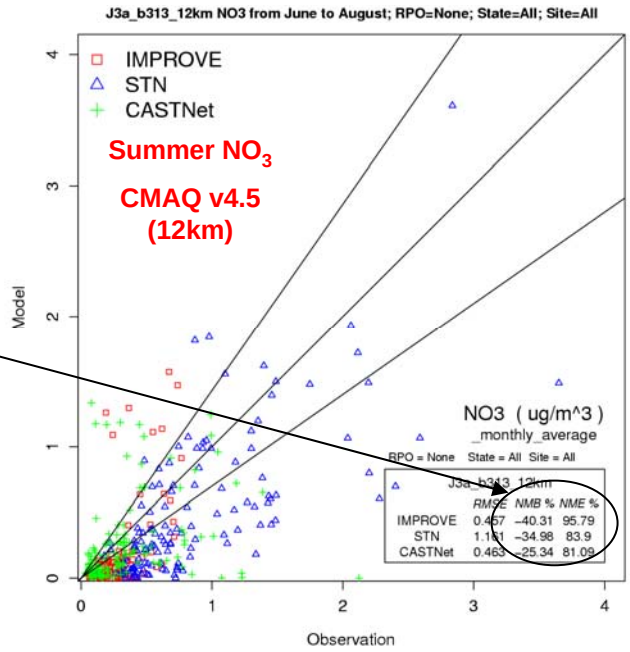
NO_3 bias and error in the winter is improved in v4.5

NO_3 bias in the summer is slightly worse in v4.5



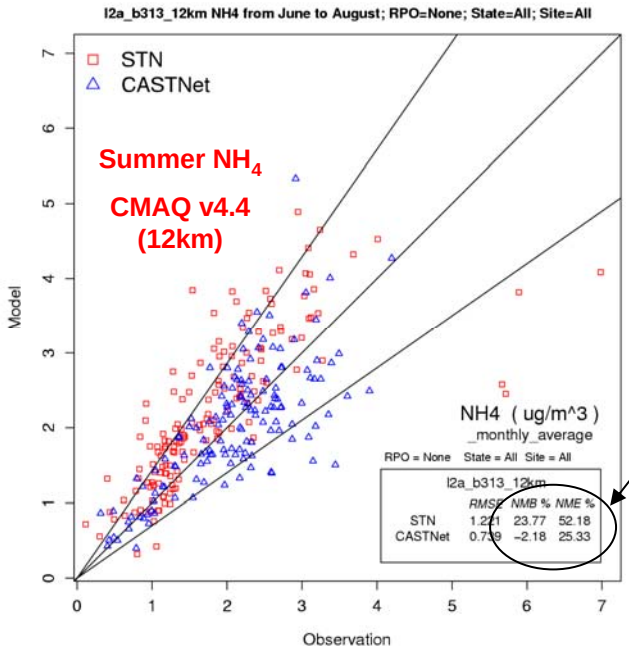


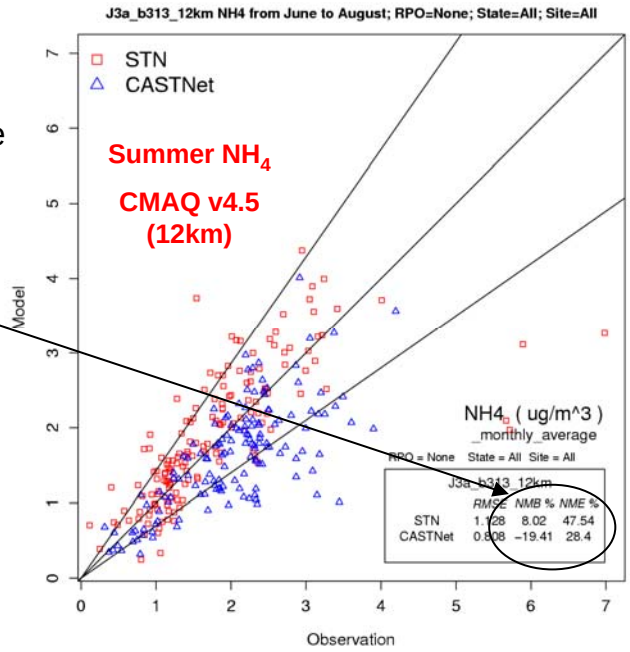




NH_4

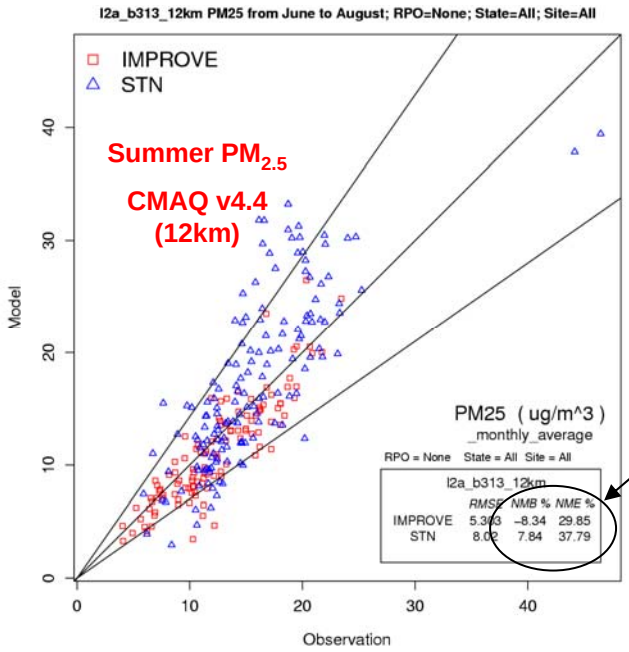
NH_4 performance in the summer is mixed

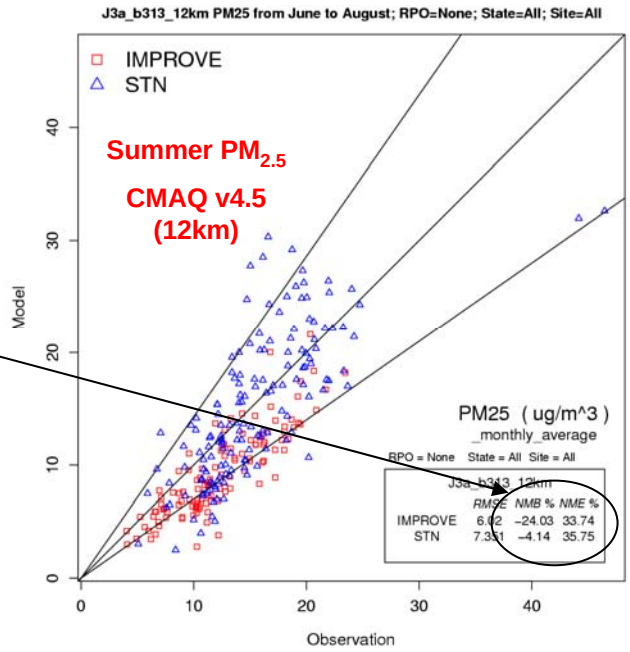




$PM_{2.5}$

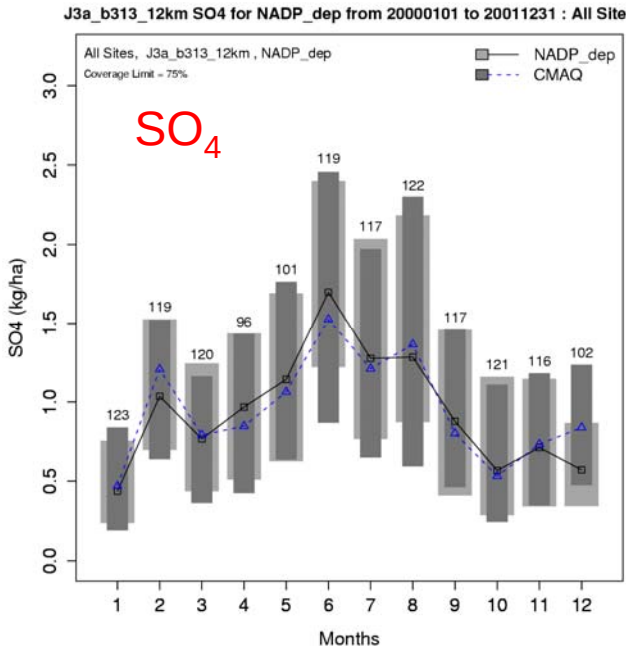
$PM_{2.5}$ under-predictions at IMPROVE sites are larger in v4.5

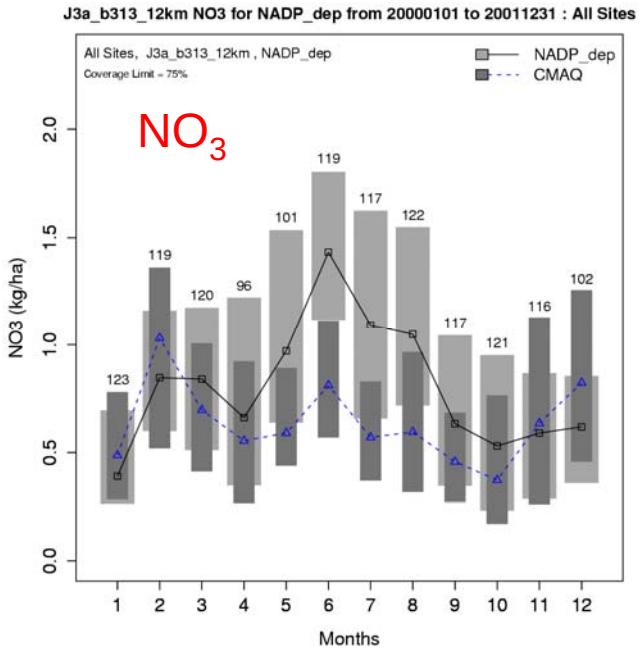


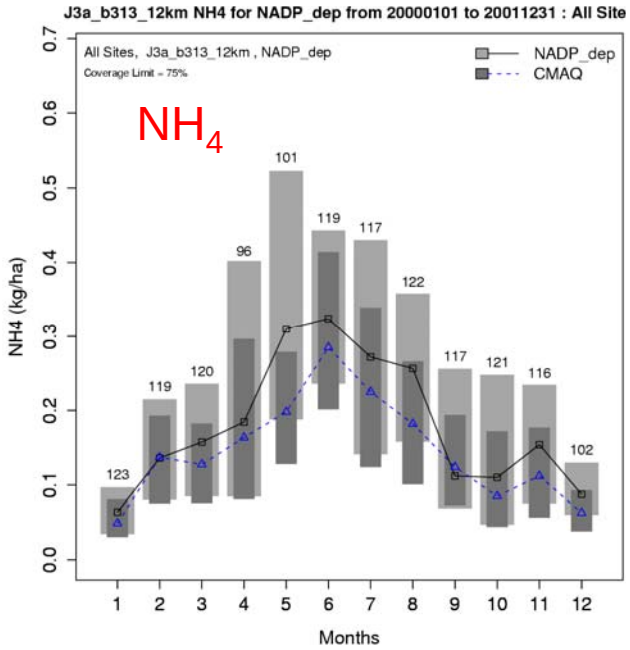


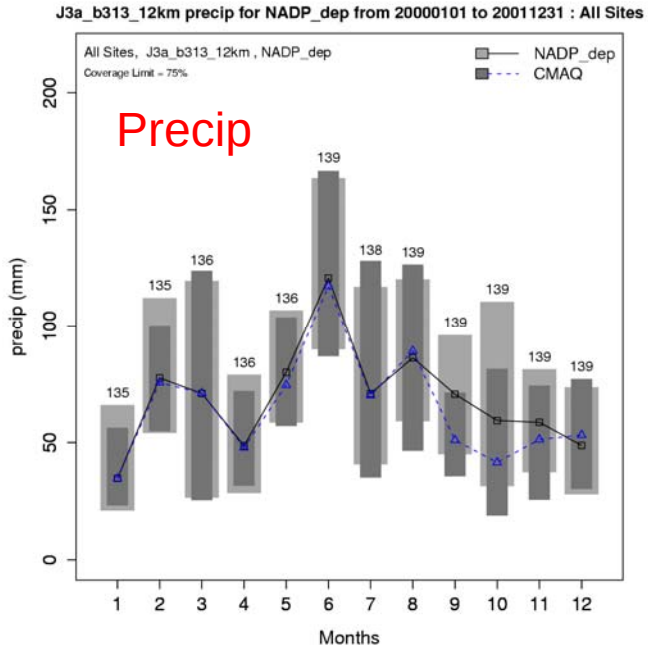
Precipitation Chemistry

NADP Wet Deposition SO_4, NO_3 and NH_4





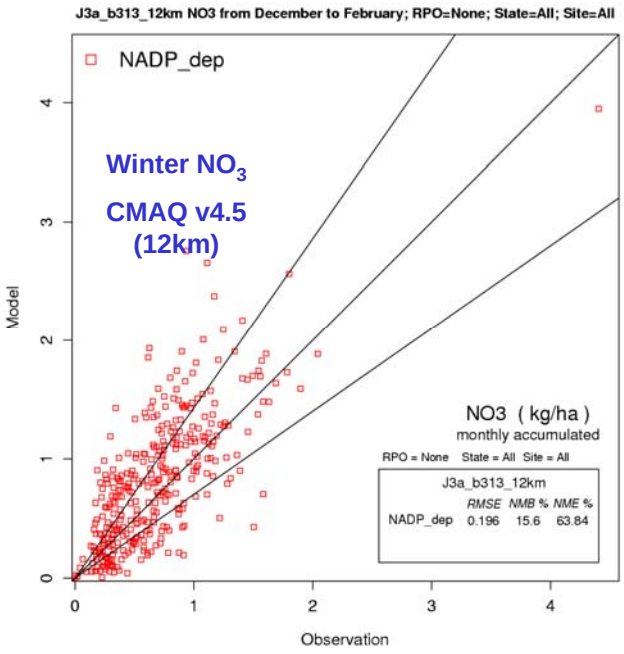


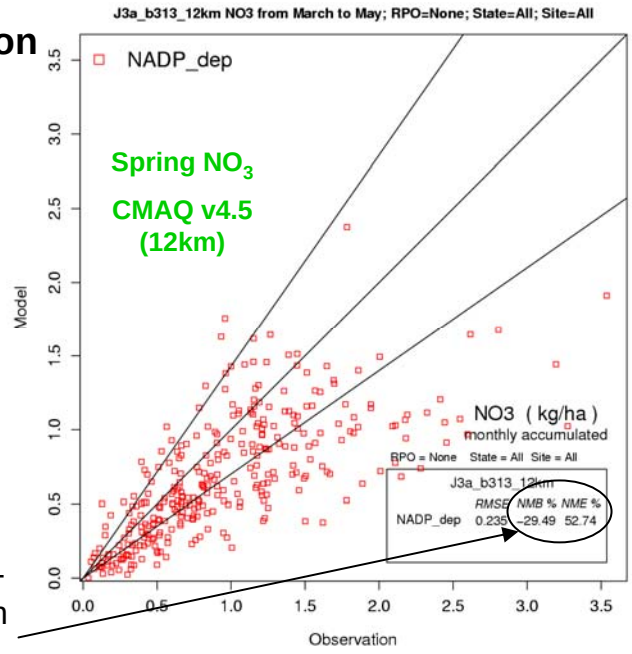


NADP

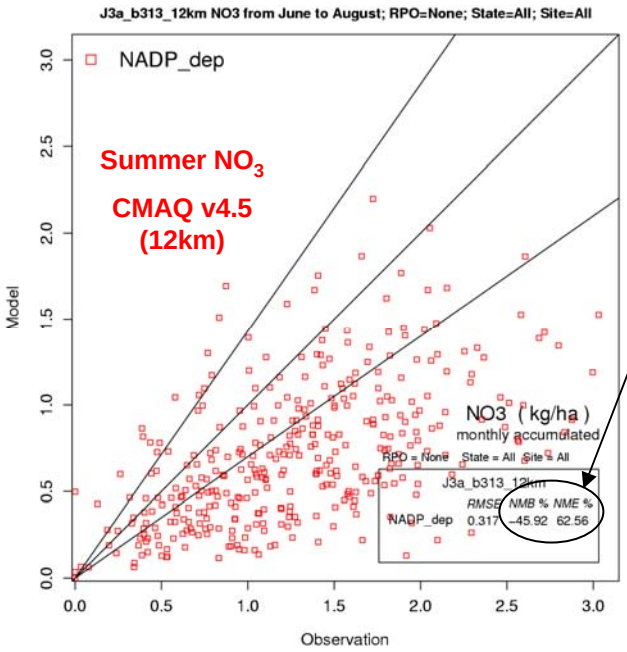
- SO_4 performance is relatively good throughout the year
- NO_3 is under-predicted in the spring, summer and fall and over-predicted in the winter
- NH_4 is generally under-predicted throughout the year
- Precipitation performance is relatively good, although there are issues in the fall

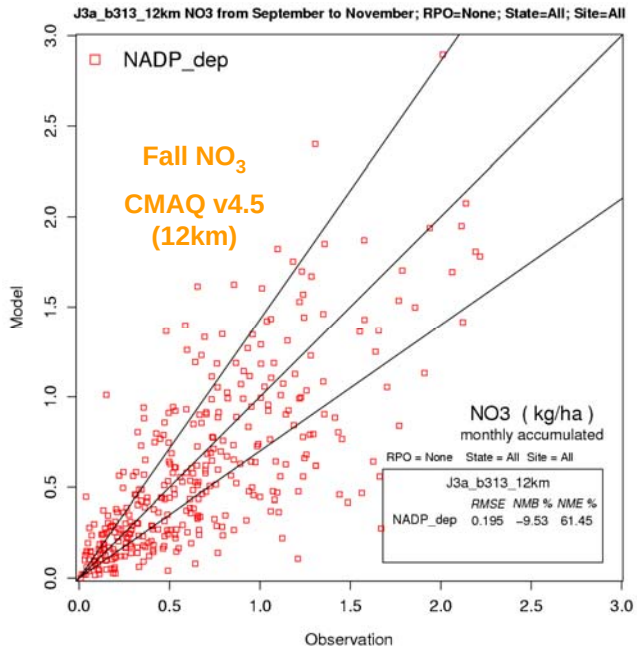
Wet Depostion NO_3



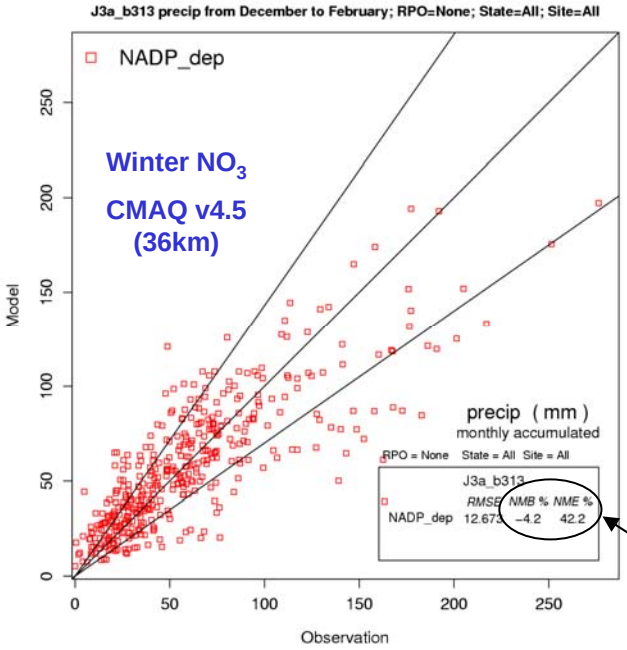


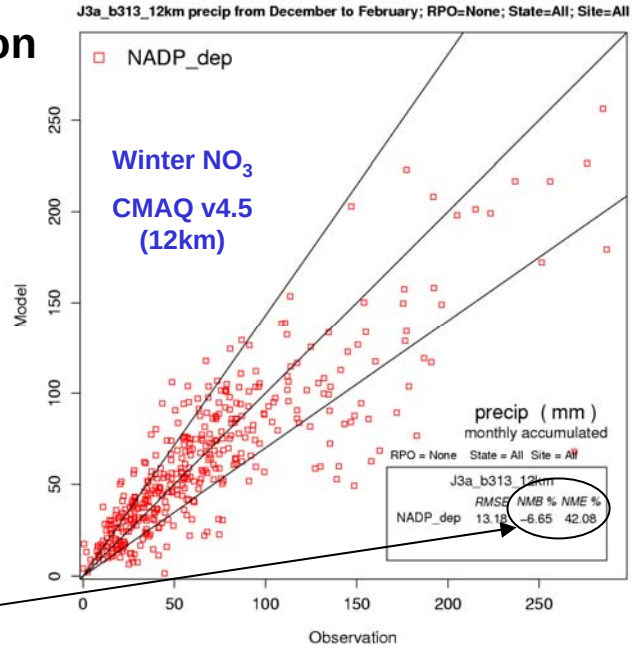
Large under-predictions in the spring and summer

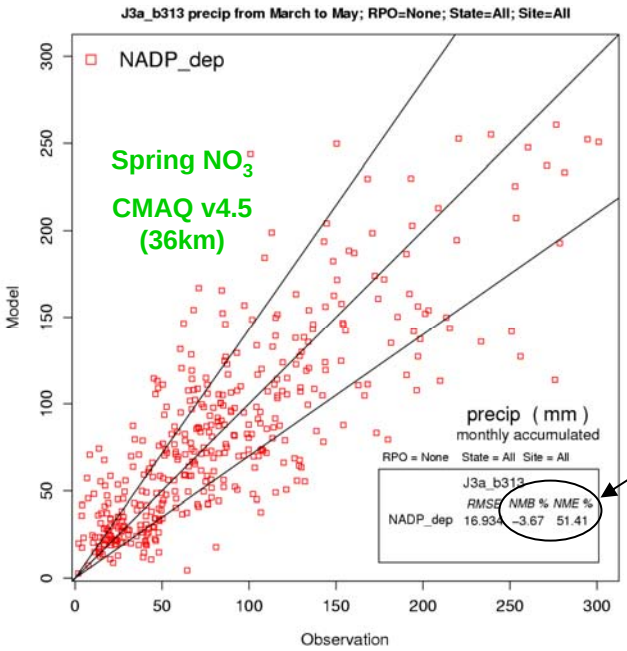




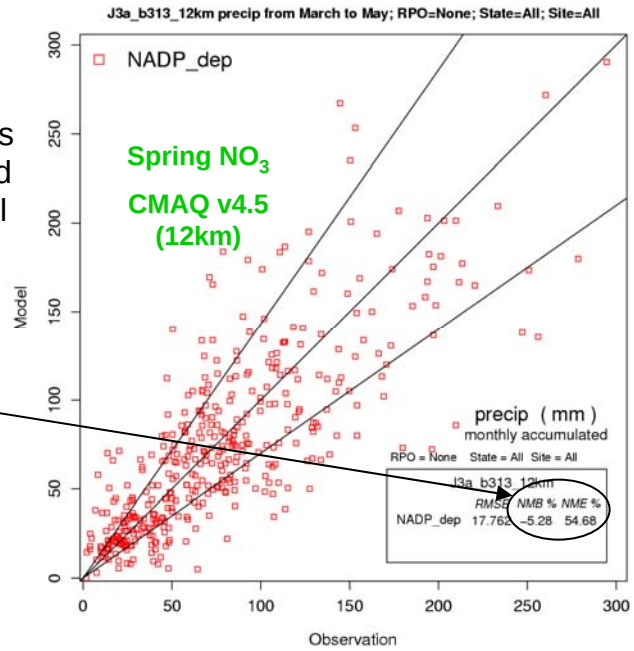
Precipitation



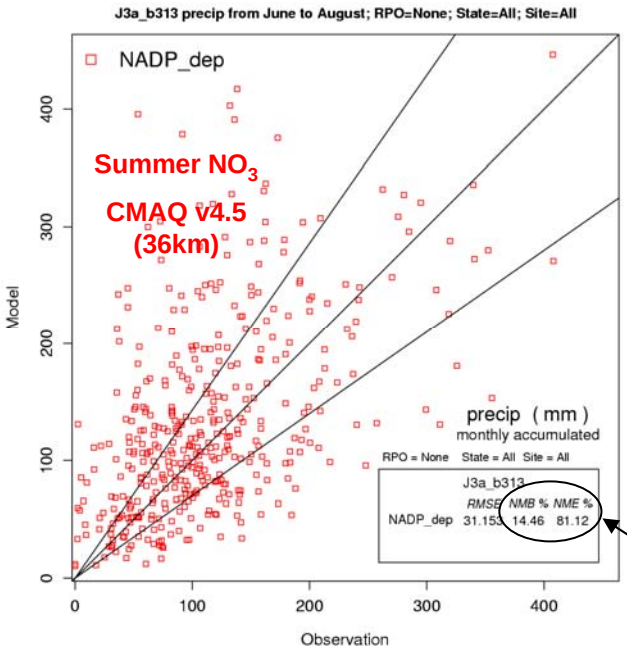


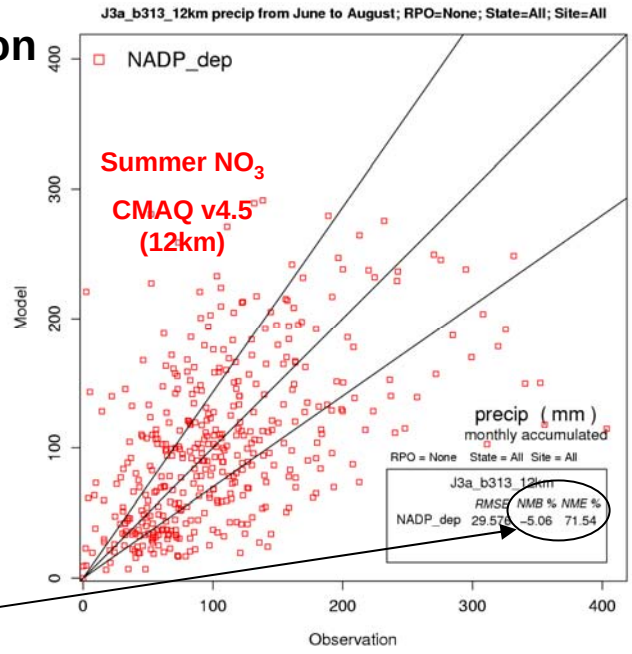


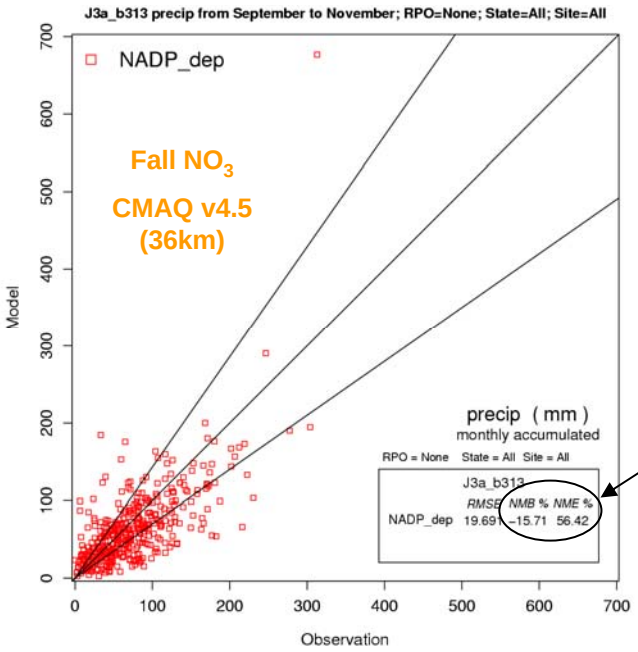
Differences in precipitation bias in the winter and spring are small

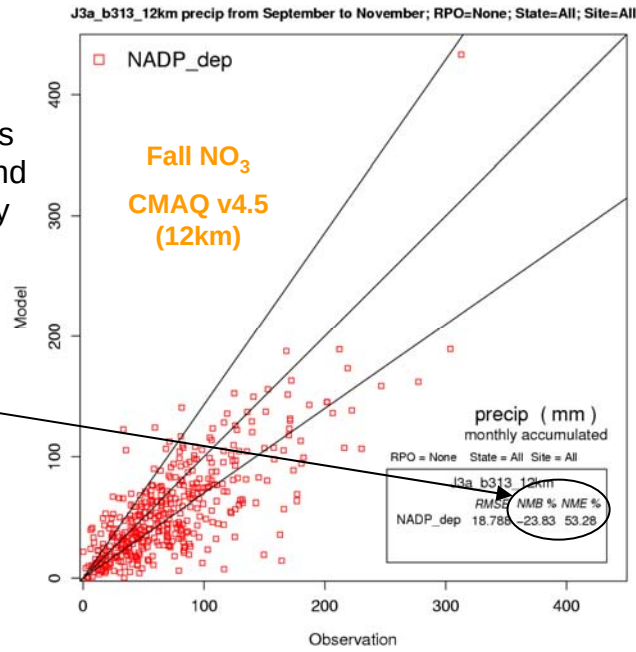


Precipitation









Differences in precipitation bias in the summer and fall are relatively large

Summary

- V4.5 O_3 bias and error similar to v4.4
- SO_4 bias and error is improved versus v4.4
- NO_3 bias is mixed between versions and grid resolutions
- EC bias and error is much higher at 12km than 36km
- Wet deposition SO_4 performance is relatively good
- Wet deposition NO_3 and NH_4 are generally under-predicted
- Precipitation bias and error values in the winter and spring are comparable at 36km and 12km
- Precipitation bias in the summer and fall is considerably different at 36km and 12km

Further Investigation

- O_3 overnight bias
  - K_z minimum?
- EC and OC under-predictions at IMPROVE
- Large EC over-predictions at STN
  - Comparison issues
  - Urban emissions issue?
- HNO_3 over-prediction in spring through fall
- Wet deposition NO_3 under-prediction
  - Needs investigating

Lastly

- **Complete evaluation report available through CMAS**
- The authors would like to acknowledge:
  - *Lucille Bender* with CSC
  - *Steven Howard* for his Site Compare code
  - *Alfreida Torian* for help with data management
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