Particulate Matter Forecasts with the Eta-CMAQ Modeling System: Towards Development of a Real-time System and Assessment of Model Performance

Rohit Mathur[1], Daiwen Kang[2], Shaocai Yu[2], Kenneth L. Schere[1], Jonathan Pleim[1], Jeff Young[1], George Pouliot[1], and Tanya Otte[1]

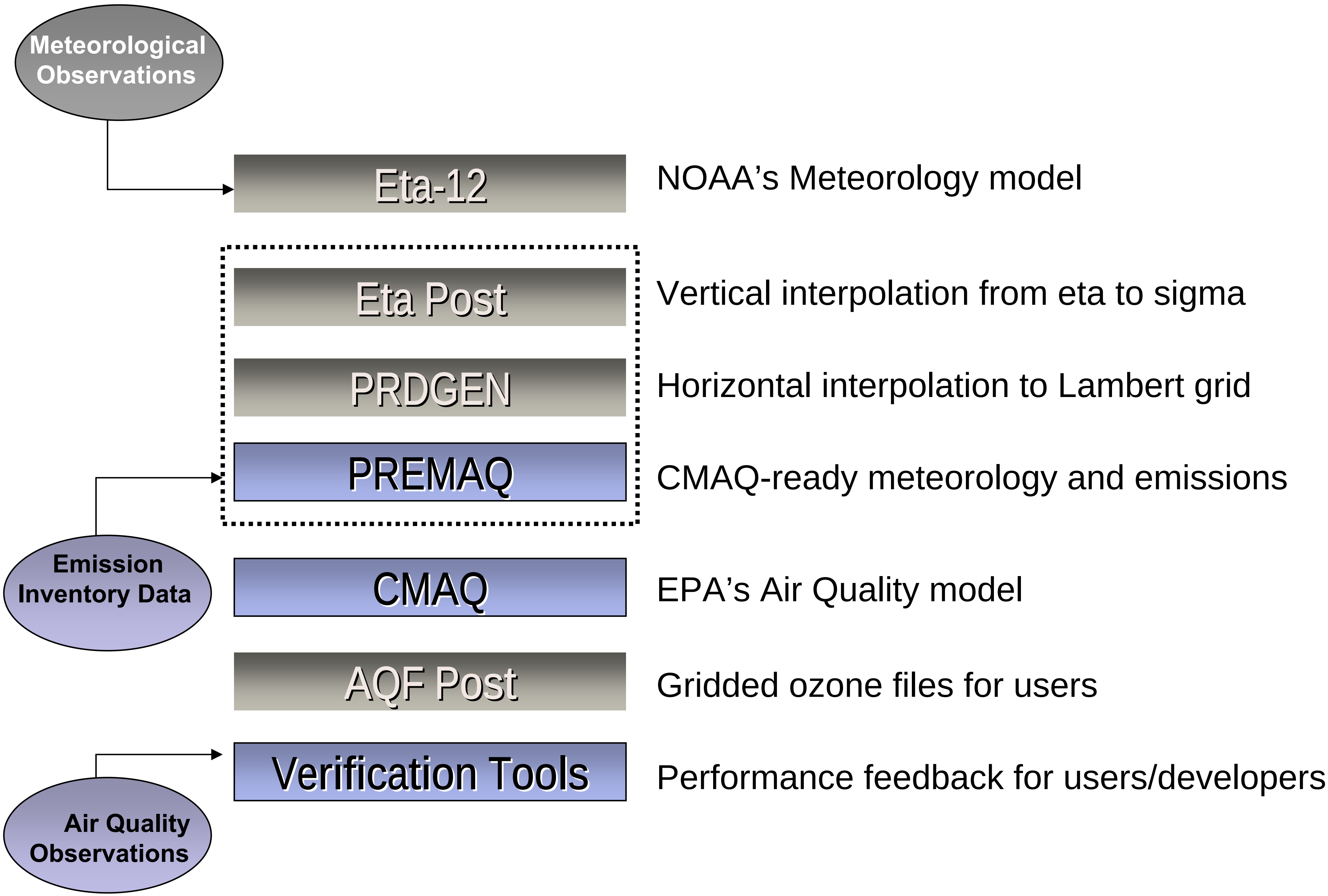
[1]Atmospheric Sciences Modeling Division, ARL/NOAA, NERL/U.S. EPA

[2]Science and Technology Corporation

Objectives

- Assess the ability of current air quality modeling systems to provide forecasts of particulate matter distributions (spatial and chemical)
  - Can/should we expect performance similar to hind-cast applications?
  - Assess model performance behavior for $PM_{2.5}$
    - Identify strengths/weaknesses of the overall system
  - Develop guidance for further model development to improve PM forecast capability

Eta-CMAQ AQF System



CMAQ Configuration

- **Advection**
  - Horizontal: *Piecewise Parabolic Method*
  - Vertical: *Upstream with rediagnosed vertical velocity to satisfy mass conservation*
- **Turbulent Mixing**
  - K-theory; PBL height from Eta
  - Minimum value of K_z allowed to vary spatially depending on urban fraction (f_{urban})
    - K_z = 0.1 m^2/s, f_{urban} = 0
    - K_z = 2.0 m^2/s, f_{urban} = 1
  - allows min. K_z in rural areas to fall off to lower values than urban regions during night-time
  - prevents precursor concentrations (e.g., CO, NOx) in urban areas from becoming too large at night; reduced mixing intensity) in non-urban areas results in increased night-time O3 titration

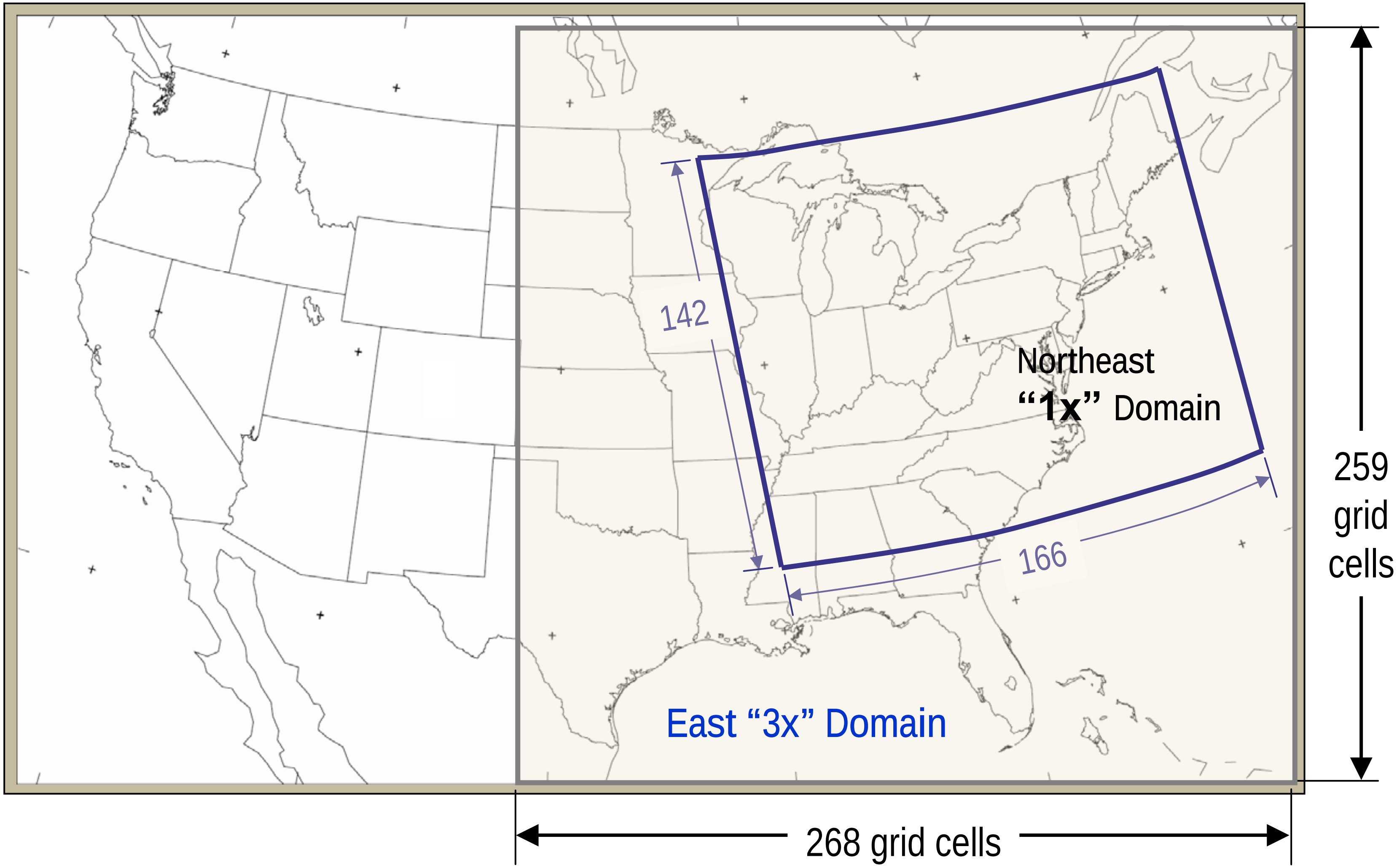
CMAQ Configuration (contd.)

- **Gas phase chemistry**
  - *CB4 mechanism with EBI solver*
- **Cloud Processes**
  - Mixing and aqueous chemistry: *following the scheme in RADM*
- **Deposition**
  - Dry : M3dry modified to use Eta land surface parameters
  - Wet
- **Aerosols**
  - Lognormal size distribution (σ_g and D_g)
    - Aitken mode (0-0.1 µm)
    - Accumulation mode (0.1-2.5 µm)
    - Coarse (PM10 - PM2.5)
  - *2004 release version; Binkowski and Roselle, JGR, 2002*

CMAQ Modeling Domains

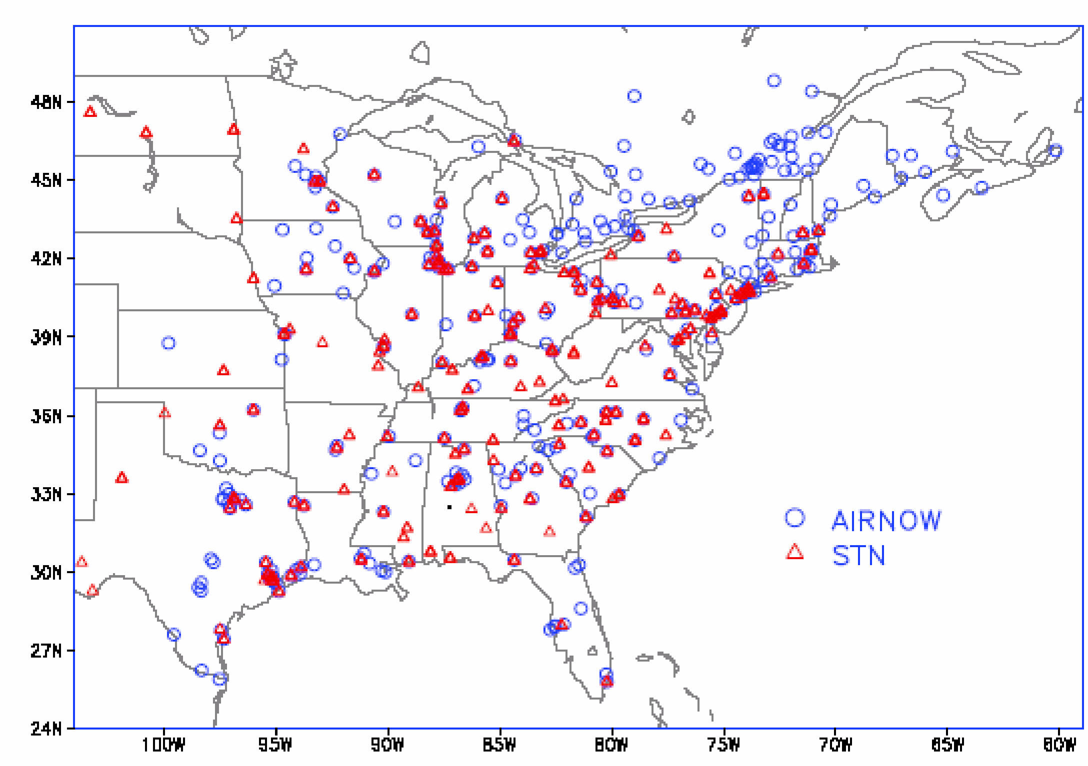
Experimental PM forecasts on 3x
Seasonal BCs from prior CMAQ simulations

Ozone forecasts on 3x and 1x



12 km resolution

PM Surface Network Measurements



AIRNOW: ~300 sites; Hourly total $PM_{2.5}$ measurements

- Available in near real time (1-day lag)

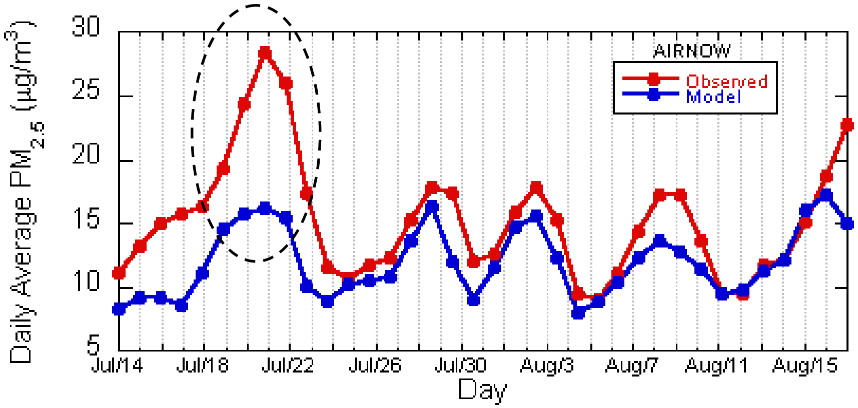
STN: ~130 sites; Speciated PM measurements every 3rd day: SO_4^{2-}, NO_3^-, NH_4^+, OC, EC, $PM_{2.5}$

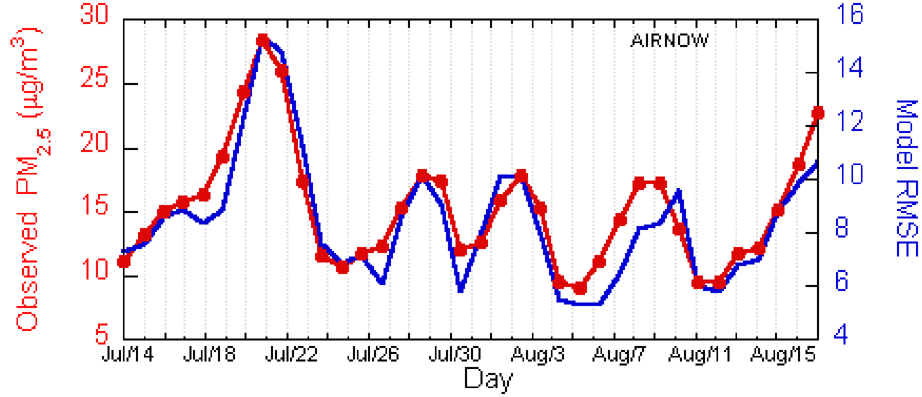
- Typically available after several months

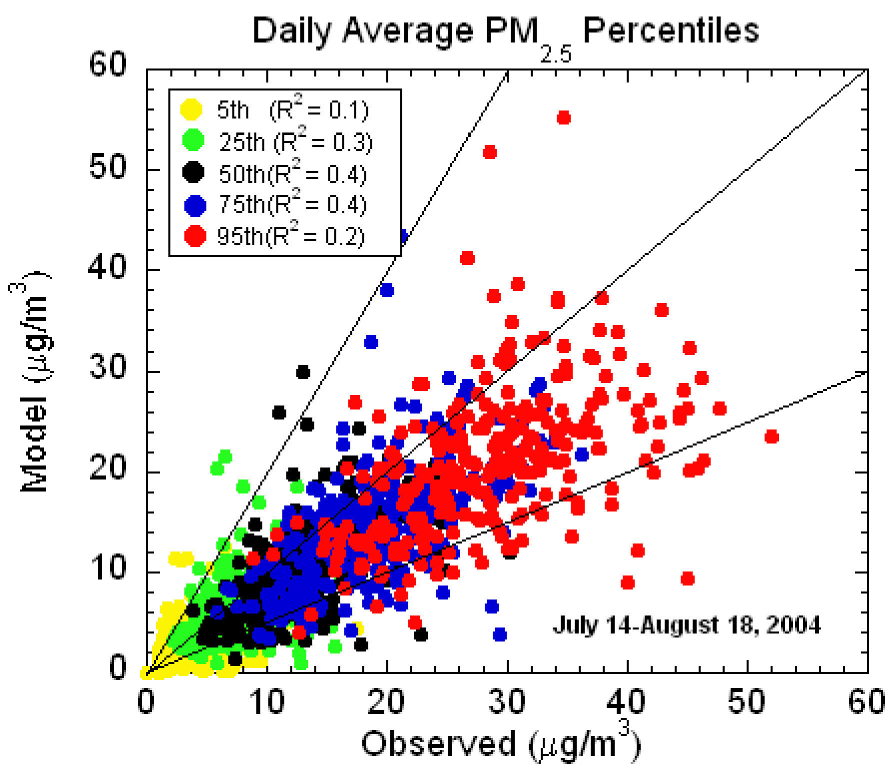
Compared modeled and measured daily mean values

$PM_{2.5}$ Model Performance Characteristics: Summer 2004

Comparisons with AIRNOW Data



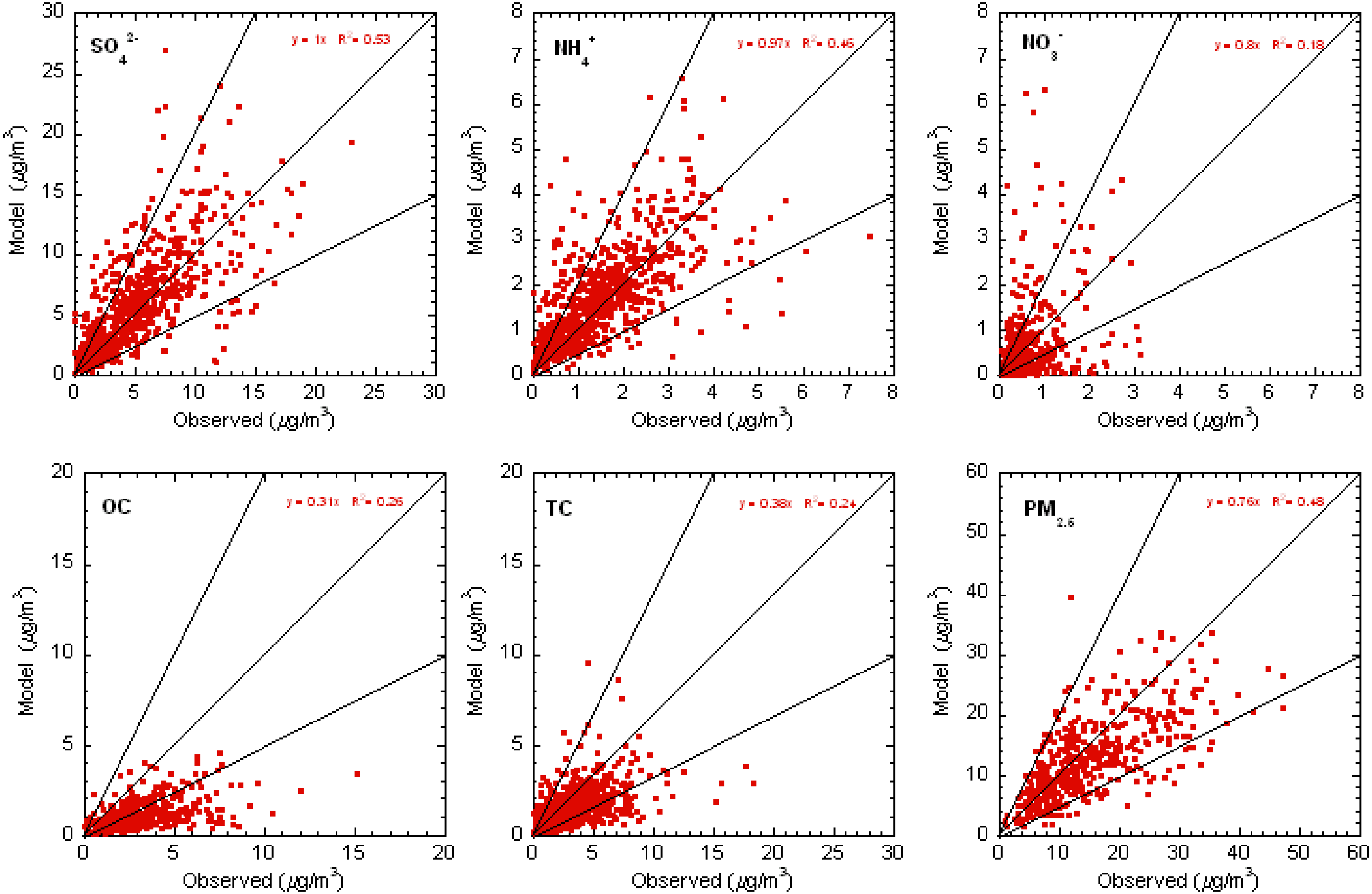




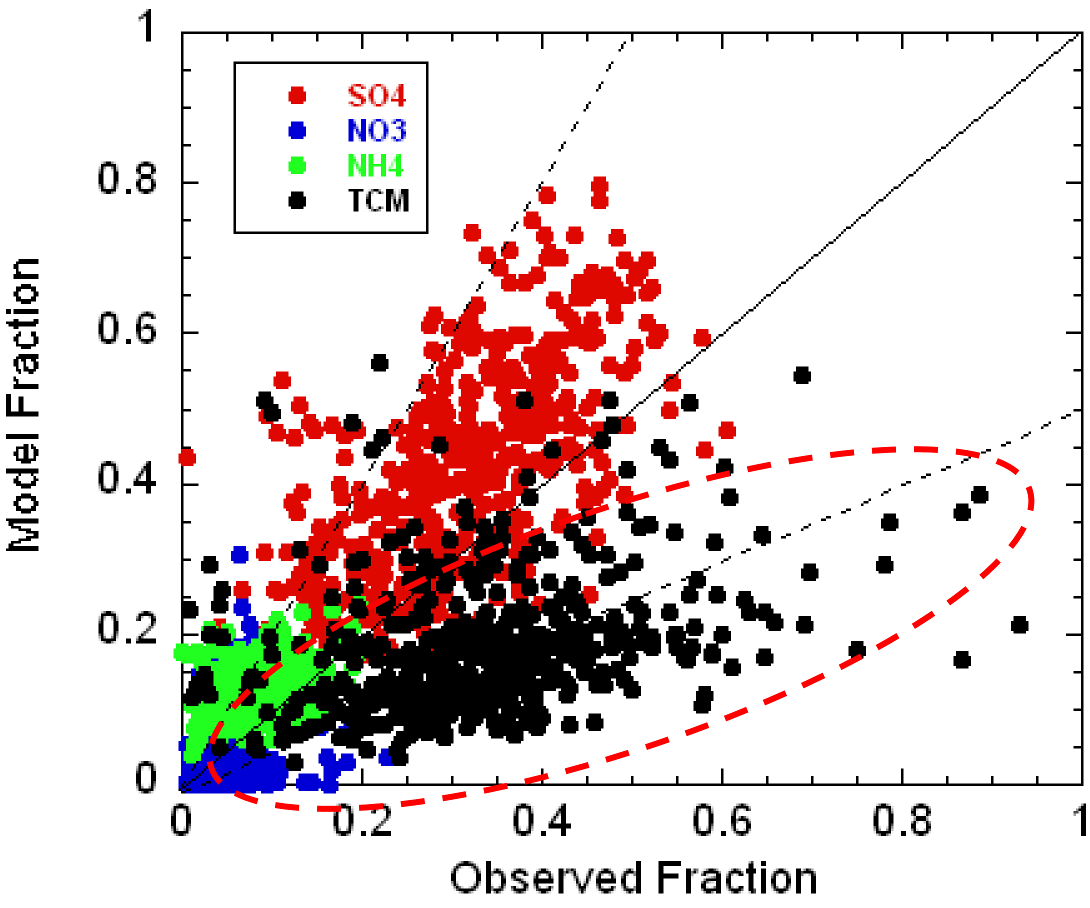
Larger error (under-predictions) at higher concentrations

Model Performance Characteristics: Summer 2004

$PM_{2.5}$ Constituents Against STN measurements, Daily averages



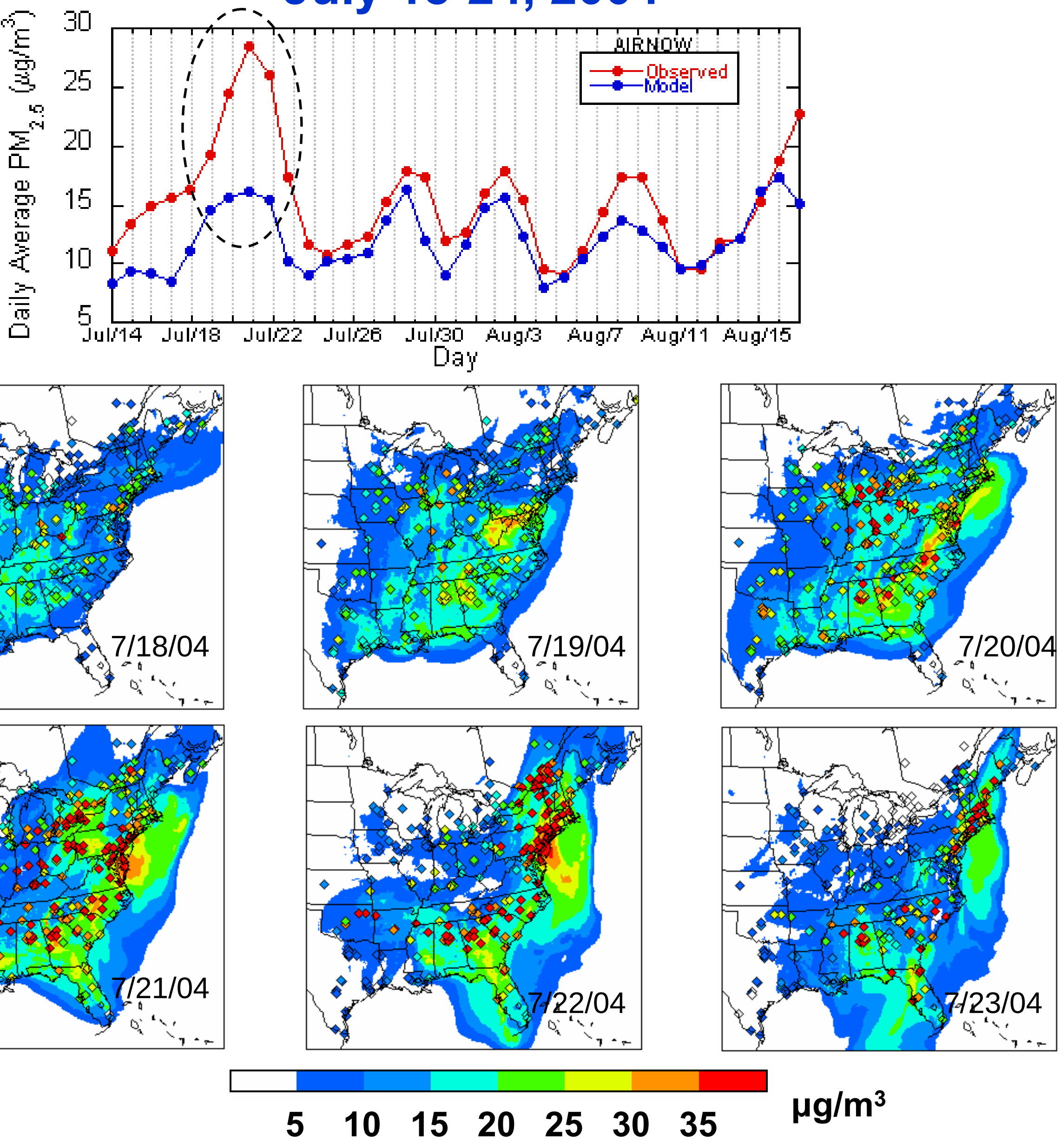
$PM_{2.5}$ Compositional Characteristics STN Measurements: Summer 2004



- Reasonable predictions for inorganic constituents
- Large under-predictions (often > 2x) in the organic contribution

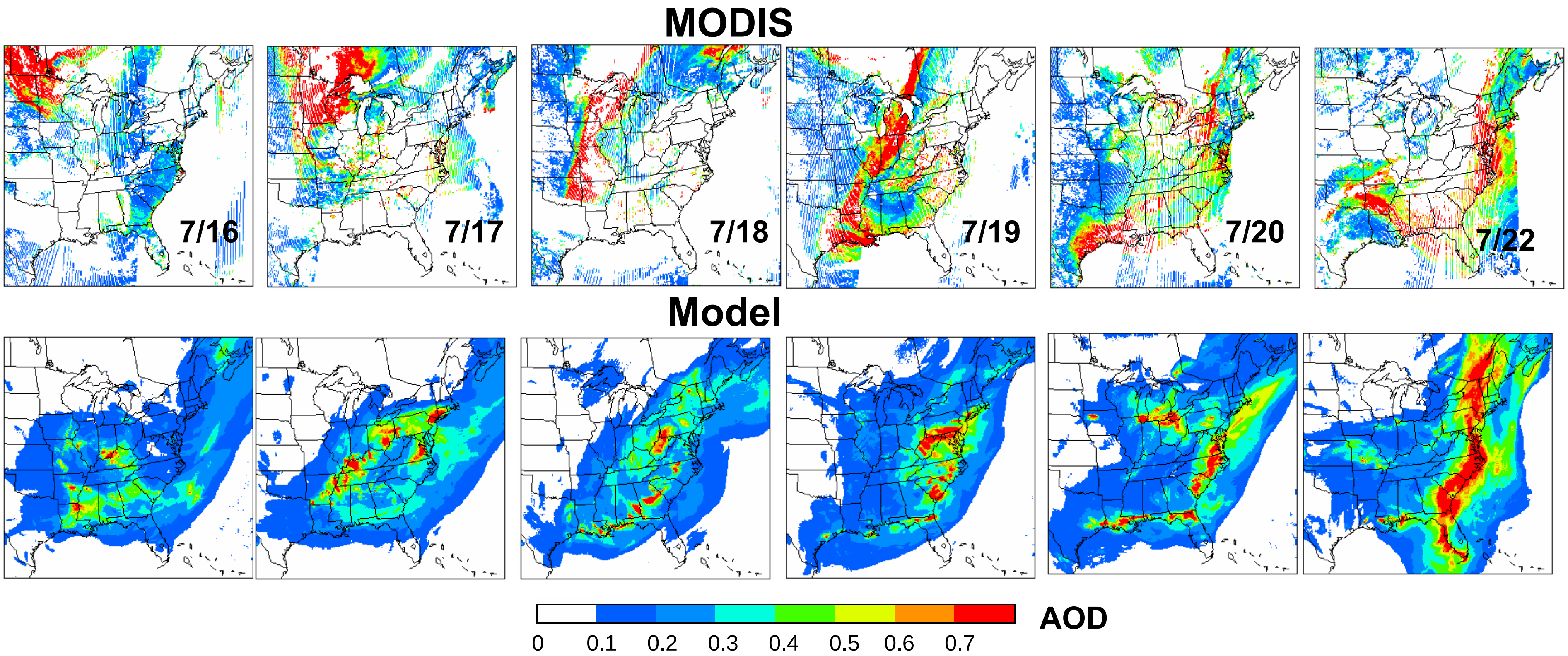
Reasons for Large Discrepancies in $PM_{2.5}$ Predictions

July 18-24, 2004



July 16-22, 2004: Evidence of Effects of Long Range Transport Originating from Outside the Modeled Domain

Evolution of Model and Observed Aerosol Optical Depth

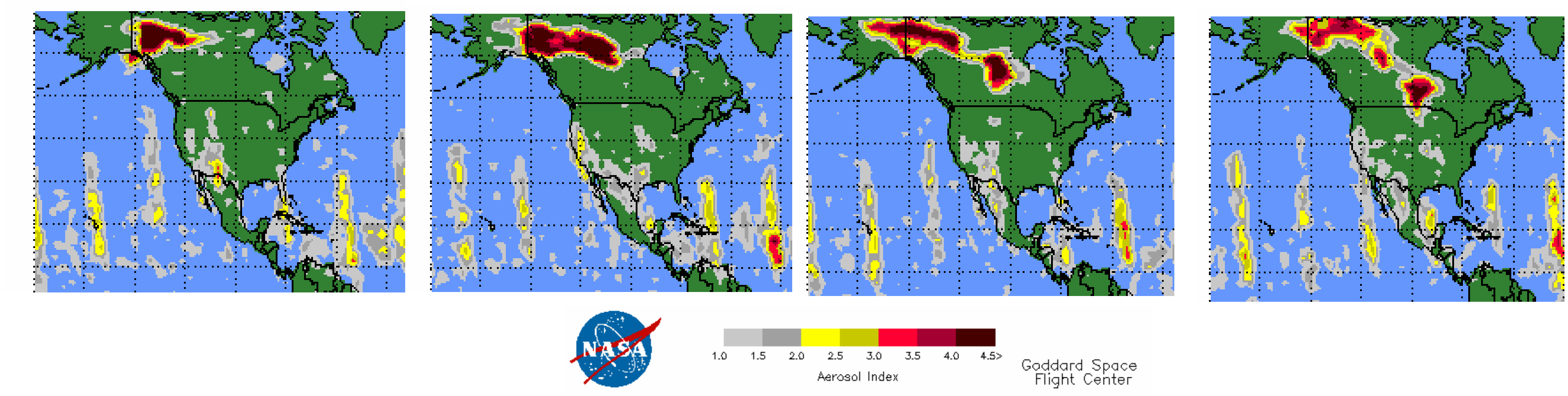


Transport from outside the domain influences observed PM concentrations which are grossly under-predicted during this period

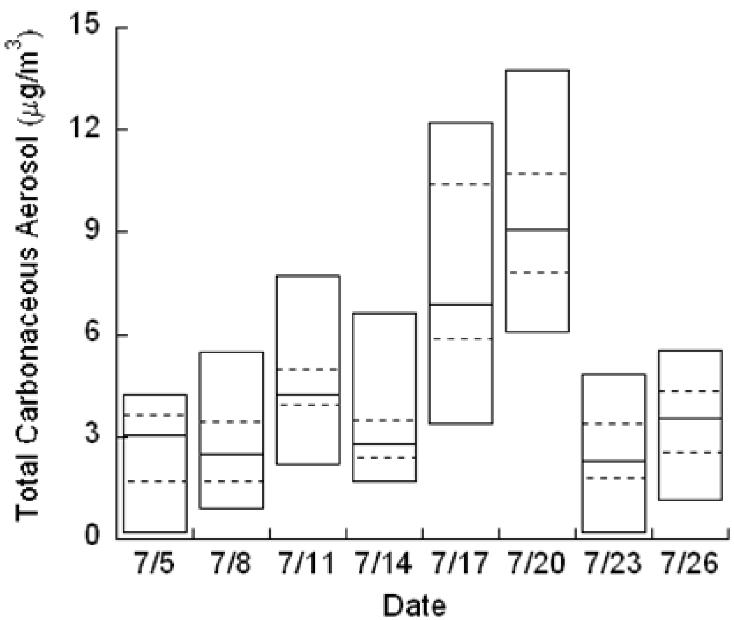
- Model picks up spatial signatures ahead of the front
- Under predictions behind the front (due to LBCs)

Further Evidence

7/13/04 7/14/04 7/15/04 7/16/04



Long Range Transport of Alaskan Plume

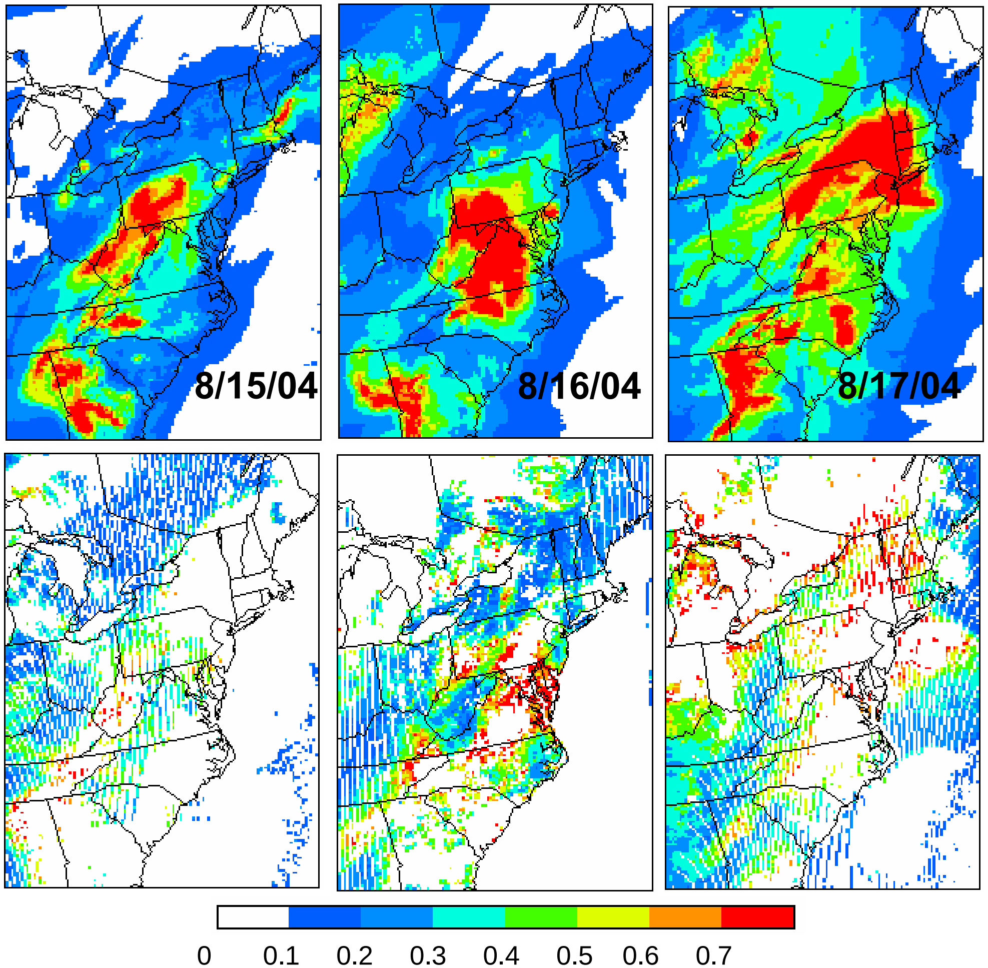


Distribution of measured carbonaceous aerosol at STN sites within domain

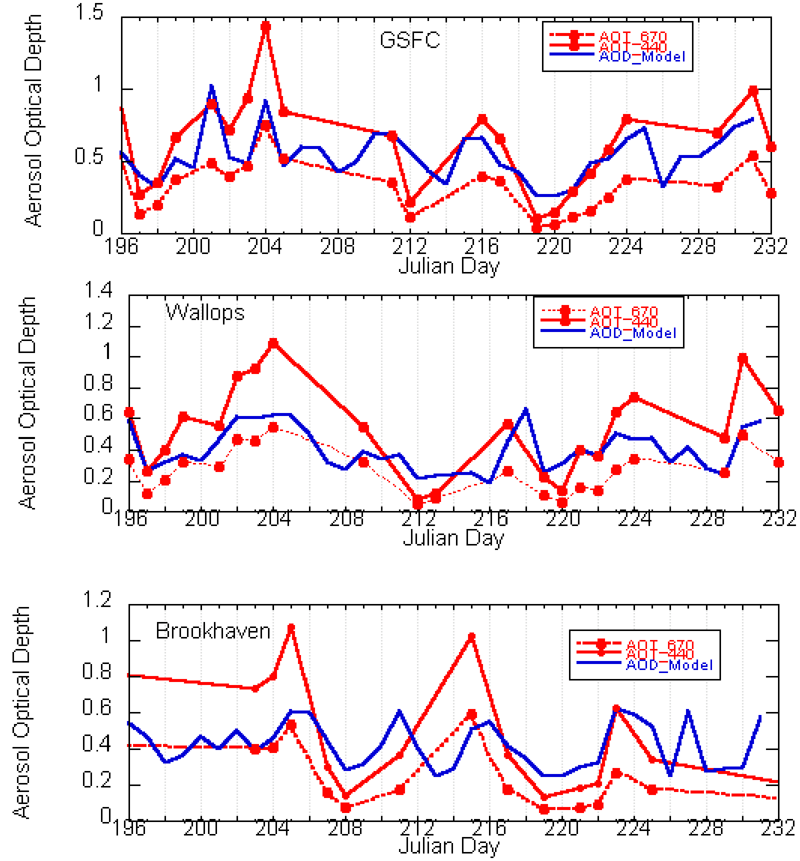
➡ Regional enhancement in TCM on July 17-20 suggests influence of wildfires on air masses advected into the domain

Model and Observed Aerosol Optical Depths (AOD)

Model (top panels) MODIS (bottom panels)



AERONET



Modeled AOD at 550nm
AERONET Data at 440 and 670nm

Reasonable model simulation of spatial and temporal variability in AOD is possible
➡ ***Can AOD assimilation improve model PM forecasts?***

Estimating the Impacts of Alaskan fires through Assimilation of Satellite AOD Retrievals

Methodology

1. **Model based correlation** between AOD and column PM burden (July-August, 2004 data):
   - **$[PM]_{Col.Burden} = f(AOD)$**
     - **linear relationship $r^2 = 0.9$**

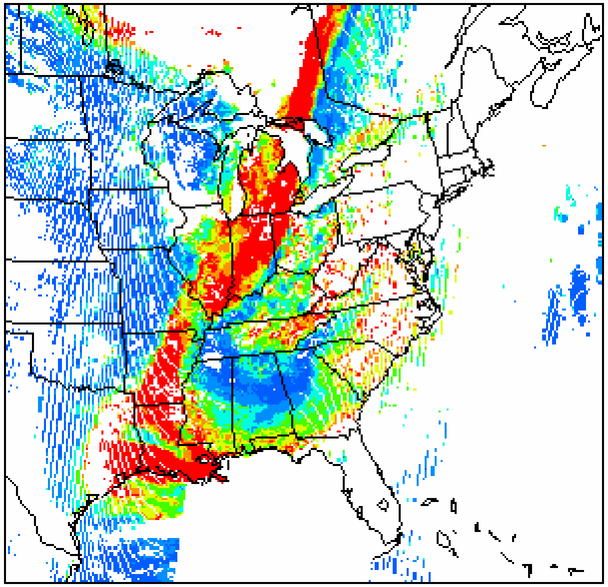
2. Estimate inferred PM burden:
   - **$[PM]_{infer} = f(AOD_{MODIS})$**

3. Estimate Difference in PM mass loading:
   - **$[PM]_{infer} - [PM]_{BaseModel}$**

4. Distribute PM mass difference vertically between predefined altitudes
   - Above BL: 2.2 – 4 km (*based on Regional East Atmospheric Lidar Mesonet (REALM) data*)

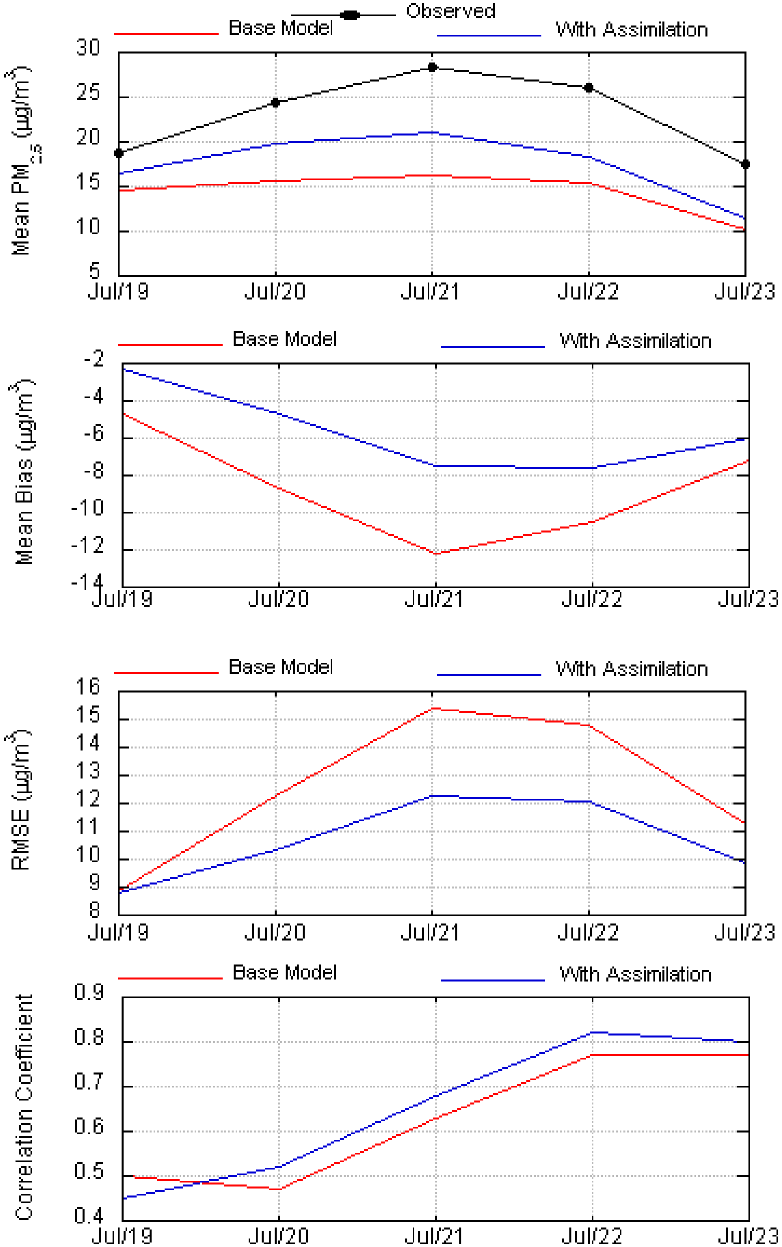
5. Speciation: ***OC (77%), EC(16%), SO_4^{2-} (2%), NO_3^- (0.2%), Other(4.8%)***

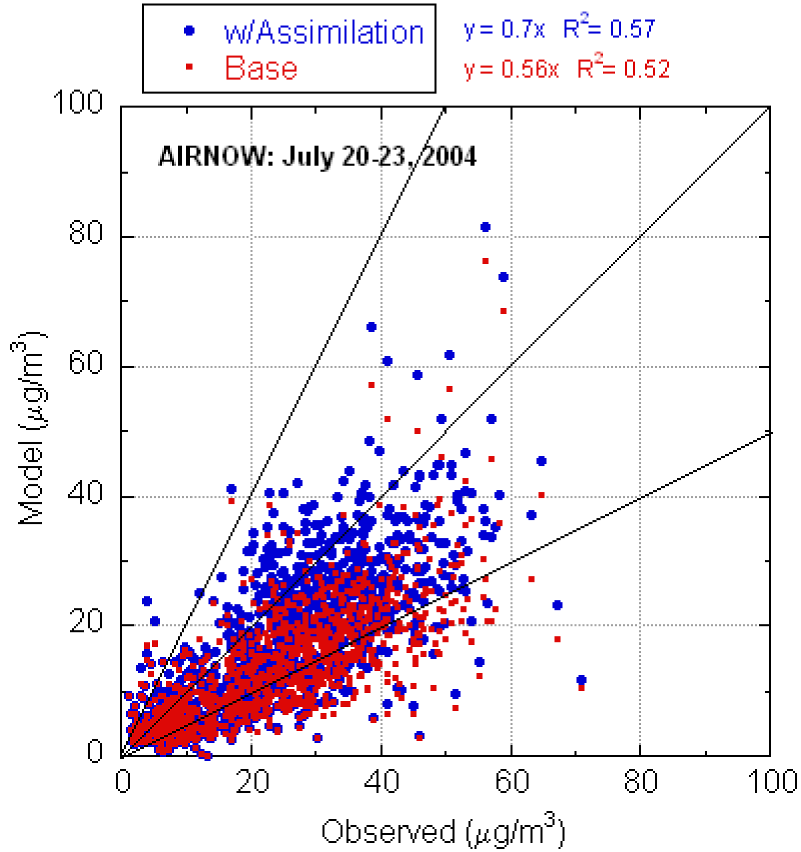
Adjust Model Initial Conditions
16Z on July 19, 2004



AOD Assimilation: Impact on $PM_{2.5}$ Model Performance Relative to AIRNOW

July 19-23, 2004



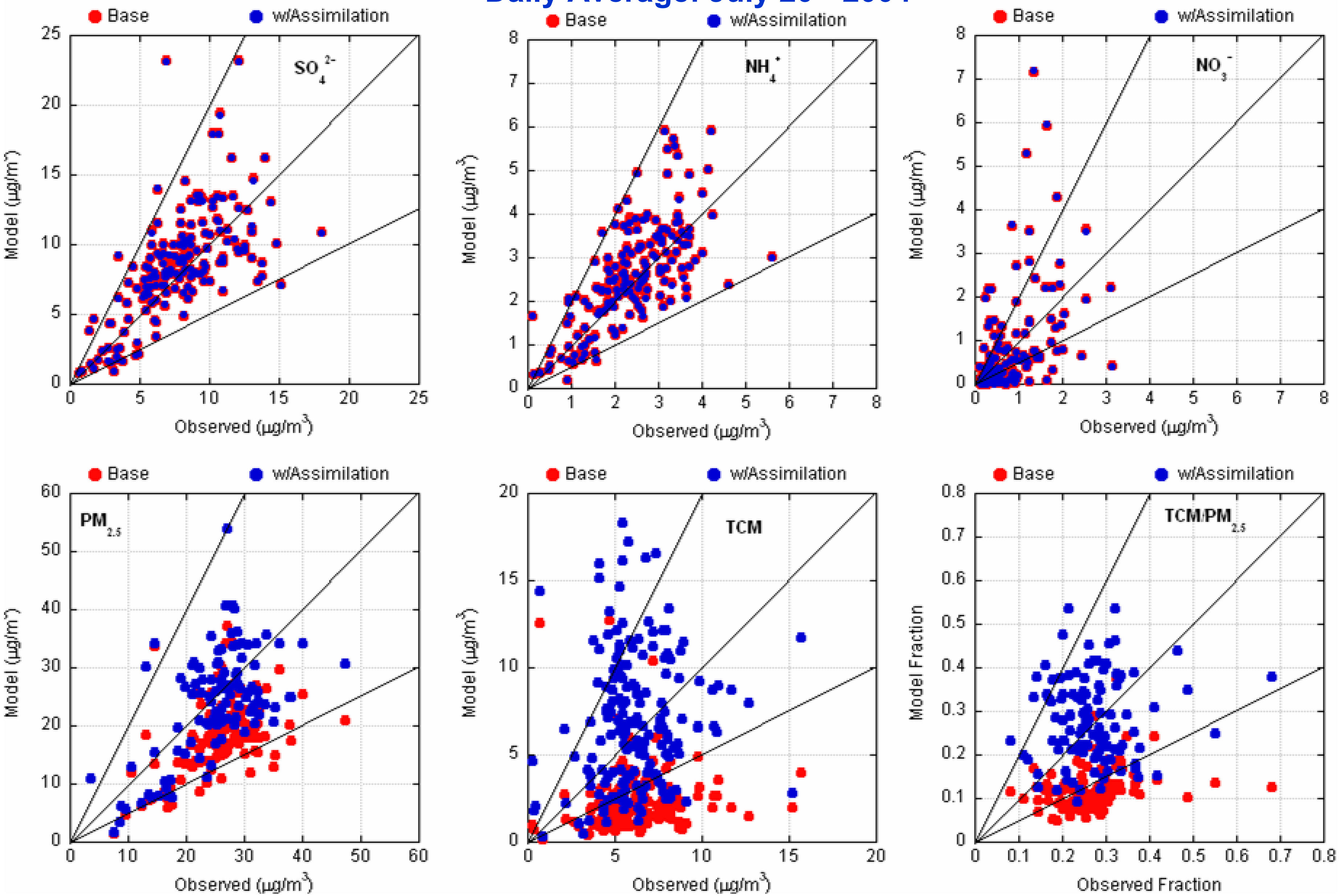


- Reduced Bias and Error
- Improved Correlation Coefficient

➡ **Domain median surface levels enhanced by 23 - 42% due to Alaskan fires on different days**

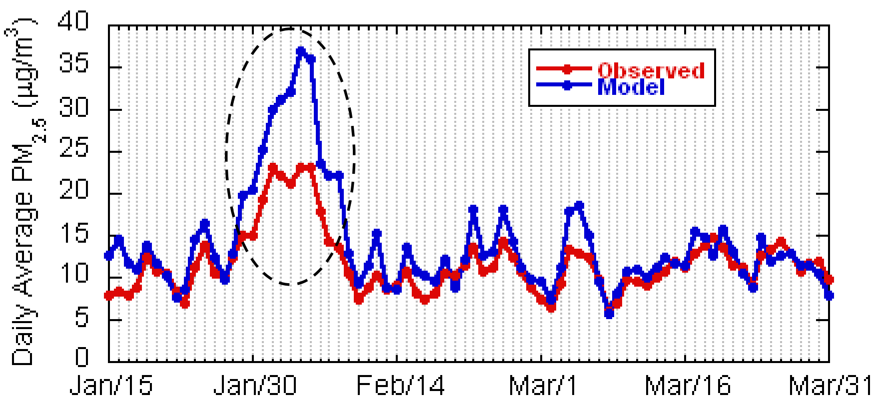
AOD Assimilation: Impact on $PM_{2.5}$ Model Performance Relative to STN

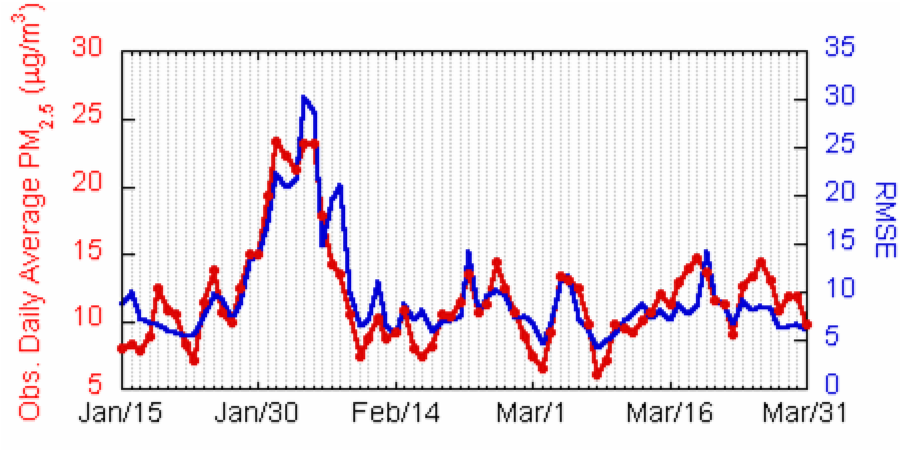
Daily Average: July 20th 2004

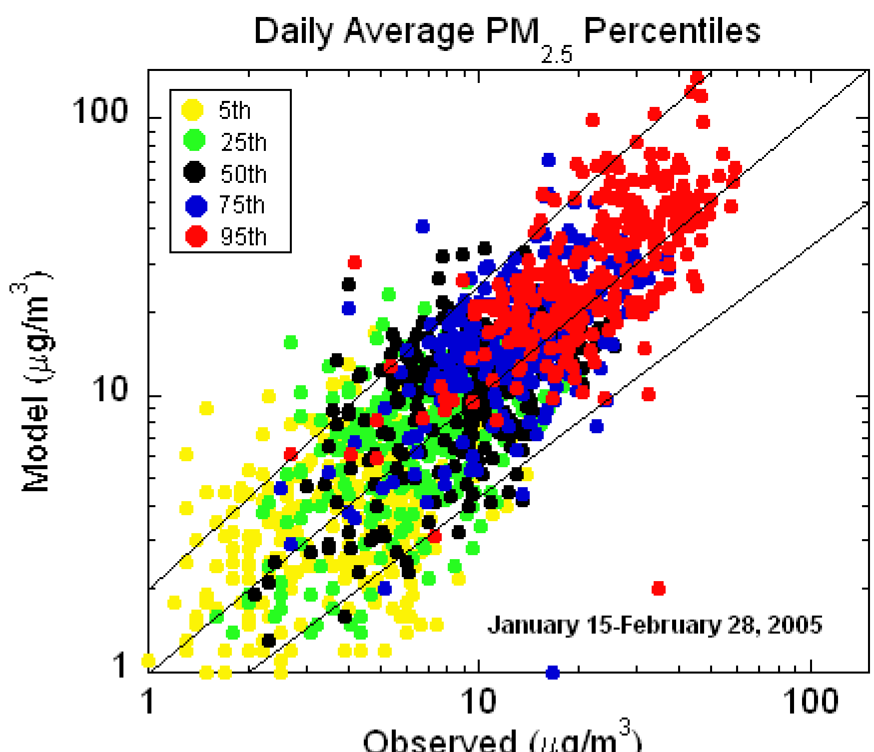


$PM_{2.5}$ Model Performance Characteristics: <u>Winter</u> 2005

Comparisons with AIRNOW Data



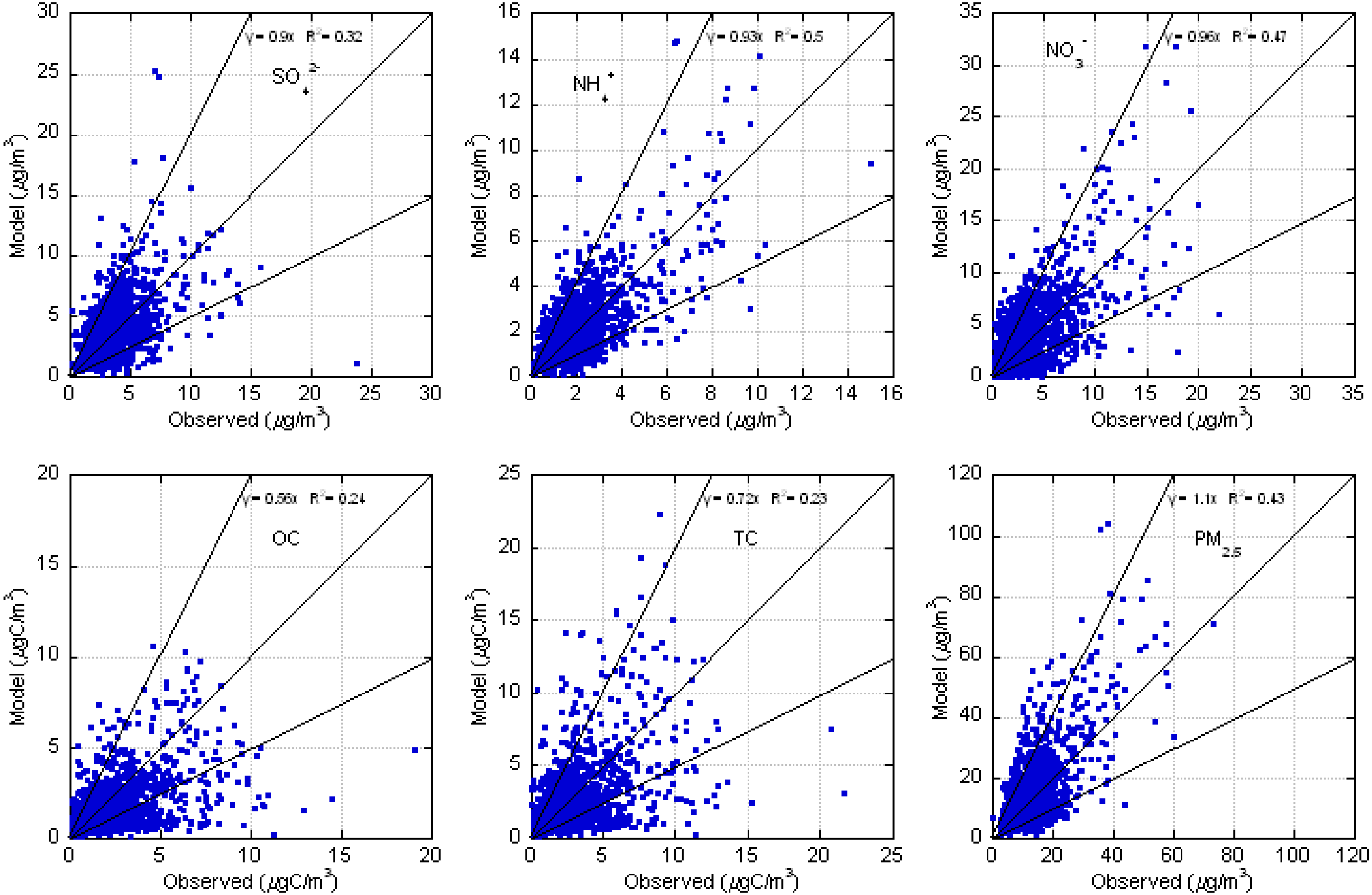




Larger error (over-predictions) at higher concentrations

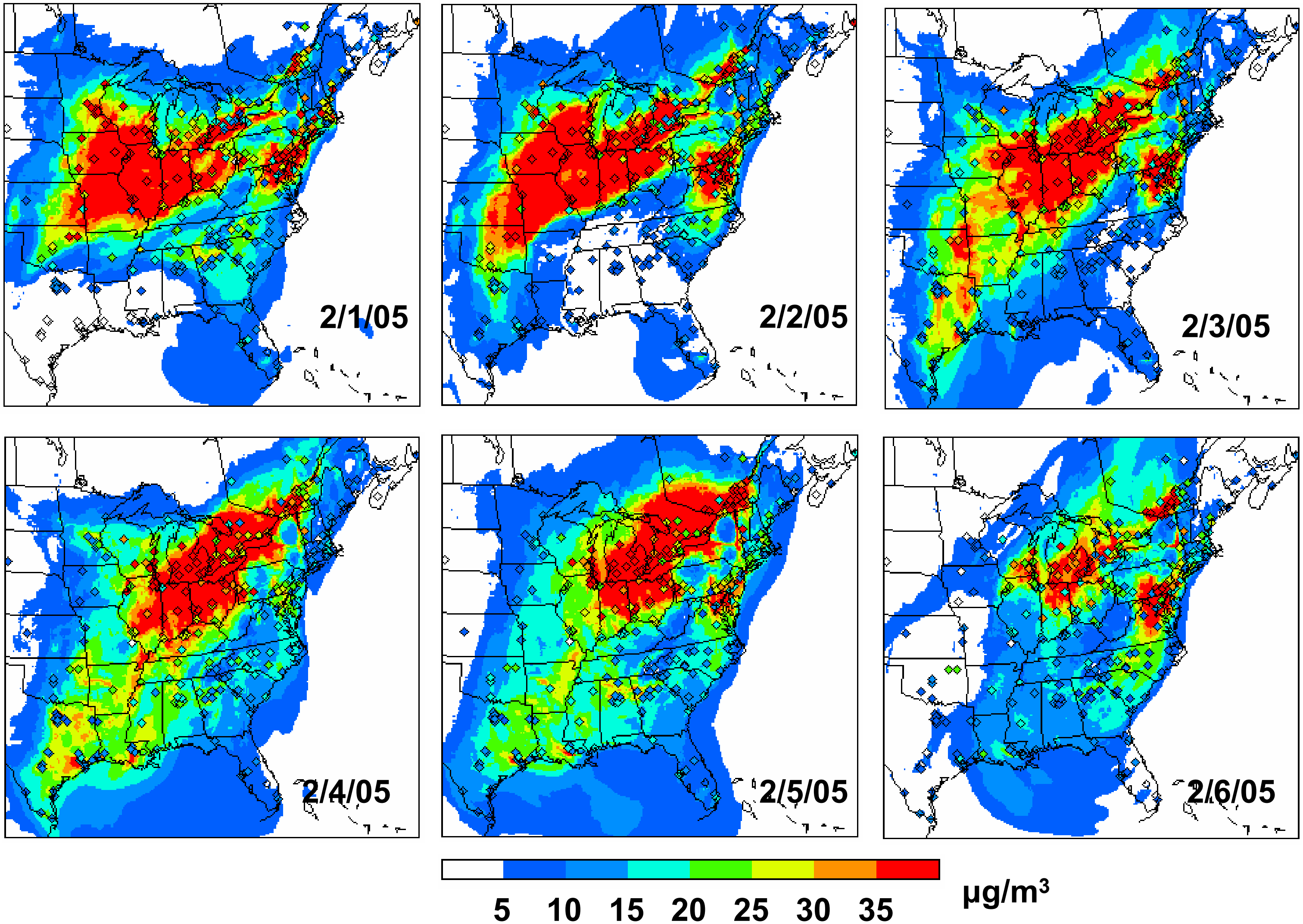
Model Performance Characteristics: Winter 2005

$PM_{2.5}$ Constituents Against STN measurements, Daily averages



Model Performance Characteristics: Winter 2005

Model and Observed Daily Average Surface $PM_{2.5}$



Capture hot-spots, tendency to over-predict

- *possible role of mixing; K_{zmin} and/or PBL height ?*

Summary

- **CMAQ-Eta was able to reproduce the day to day variations in regional surface $PM_{2.5}$ distributions**
  - Relative to AIRNOW measurements
    - Under-predictions in summer
    - Over-prediction in winter (possible role of mixing; K_{zmin} and/or PBL height)
  - The compositional characteristics of the inorganic aerosol constituents are forecast well; *Performance similar to hind-cast applications*

- **In the absence of extraneous forcing, the model is able to qualitatively capture the spatial distributions in aerosol optical depth**
  - Indirect assessment of predicted PM columnar distributions

- **Long-range transport of pollution originating from Alaskan wild fires have significant impact on PM distributions and levels in the east U.S.**
  - For the conditions examined, carbonaceous aerosol concentrations and fractional contributions to $PM_{2.5}$ are under-predicted
  - AOD assimilation helps improve representation of impacts of these fires on predicted PM levels and compositional characteristics
  - ***Model estimates of impacts on $PM_{2.5}$*** :
    - Cumulative PM burden in eastern U.S. due to fires on 7/19/04 = ***0.12 Tg***
      - (CONUS fine PM emissions = 5 Tg/year); ~***10 times the daily emissions***
    - Domain median surface concentrations enhanced by ***33%*** at STN sites (on 7/20) and ***23-42%*** at AIRNOW sites (July 20-23)
  - Highlights the need to **<u>forecast</u> the impacts of fire emissions**

Acknowledgements

- Jeff McQueen and Pius Lee
- Paula Davidson, program support and management
- James Szykman for providing MODIS data
- Dev Roy for assistance with processing/analyzing MODIS data
- Venkatesh Rao for providing STN data

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 views or policies.