



# **Overview of DOE-EPRI-TVA PM<sub>2.5</sub> Model Study**

**Elizabeth M. Bailey (TVA)**

**Robert E. Imhoff (MCNC)**

**Stephen F. Mueller (TVA)**



# Initial Objectives of DOE-EPRI-TVA PM<sub>2.5</sub> Model Study

**Conduct simulations with equivalent inputs using these models:**

**Models-3/CMAQ (Community Multiscale Air Quality)  
MADRID 1 and MADRID 2 versions of CMAQ (Model for  
Aerosol Dynamics, Reaction, Ionization and Dissolution)  
REMSAD (REGional Modeling System for  
Aerosols and Deposition)  
UAM-VPM (Urban Airshed Model with variable grid  
and particulate matter module).**

**Compare the performance of these models with emphasis on  
results relating to PM<sub>2.5</sub>.**

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**Additional participants: ICF Consulting/SAI, AER**

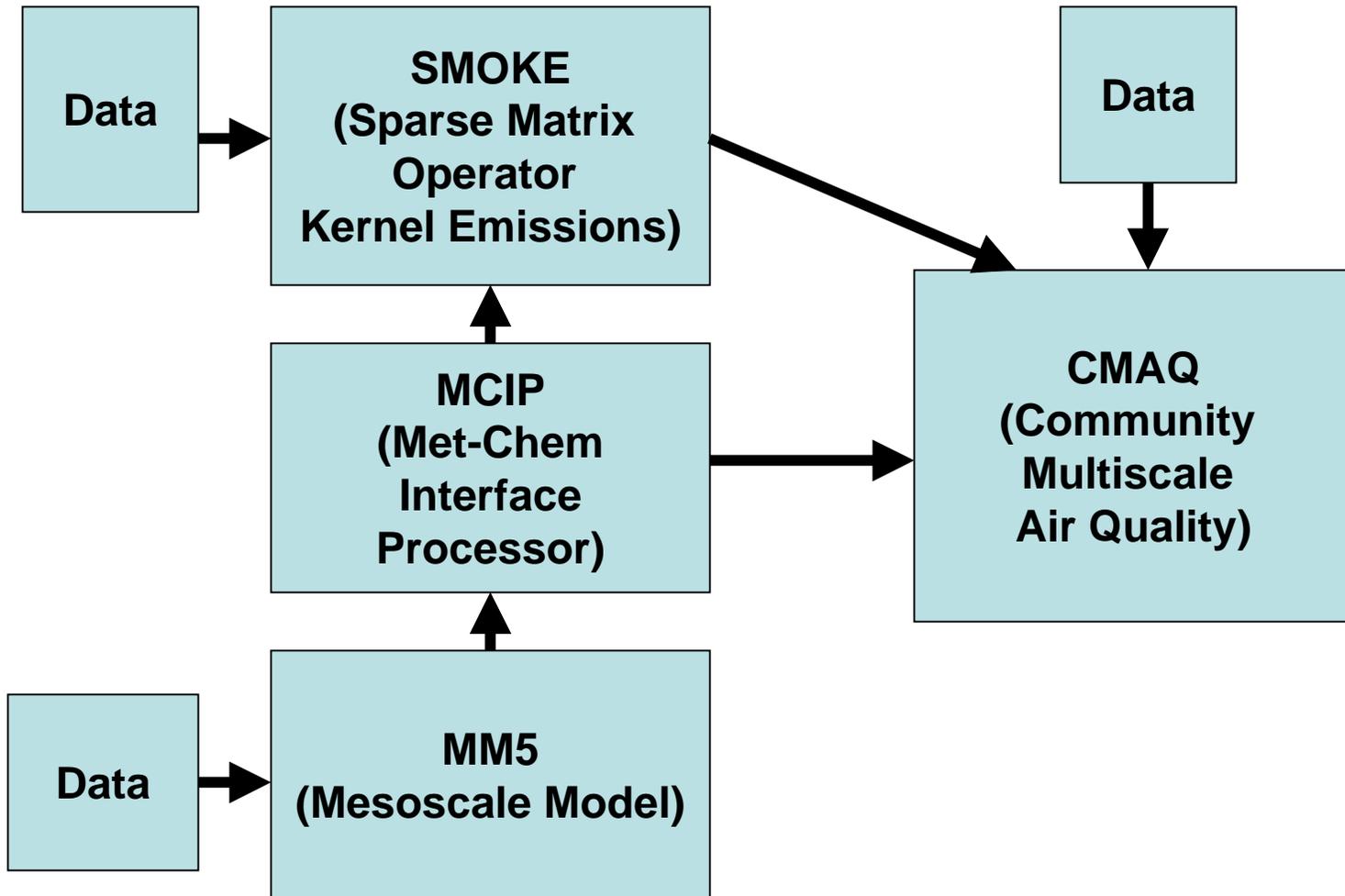


# **Initial TVA Objectives in DOE-TVA-EPRI Study**

- Develop emissions and meteorological inputs for Models3/CMAQ for the period July 1-10, 1999.**
- Conduct basecase simulation using these inputs.**
- Compare model results for  $PM_{2.5}$  to observations from monitoring networks and SOS 1999 Nashville study.**



# Partial Schematic of Steps Required to Run Models3/CMAQ





# MM5 Grids

- **Nested 32 and 8 km grids**
- **Coarse grid: 181 X 127 X 31**
- **Fine grid: 125 X 125 X 31**
- **Vertical grid extends to 15700 meters with 31 sigma levels**
- **Lambert conformal projection with center latitude and longitude of (40 N, 100 W)**



# MM5 Configuration

- **MM5 version 3**
- **NCEP/NCAR Global Reanalysis & NCEP Global Surface and Upper Air Observations data used for model initialization and boundary conditions as well as surface nudging**
- **Kain-Fritsch cumulus parameterization**
- **Reisner's mixed-phase moisture scheme**
- **NCEP's MRF PBL, and Rapid Radiative Transfer Model longwave radiation scheme**
- **OSU/Eta Land-Surface scheme used for predicting soil moisture and temperature**

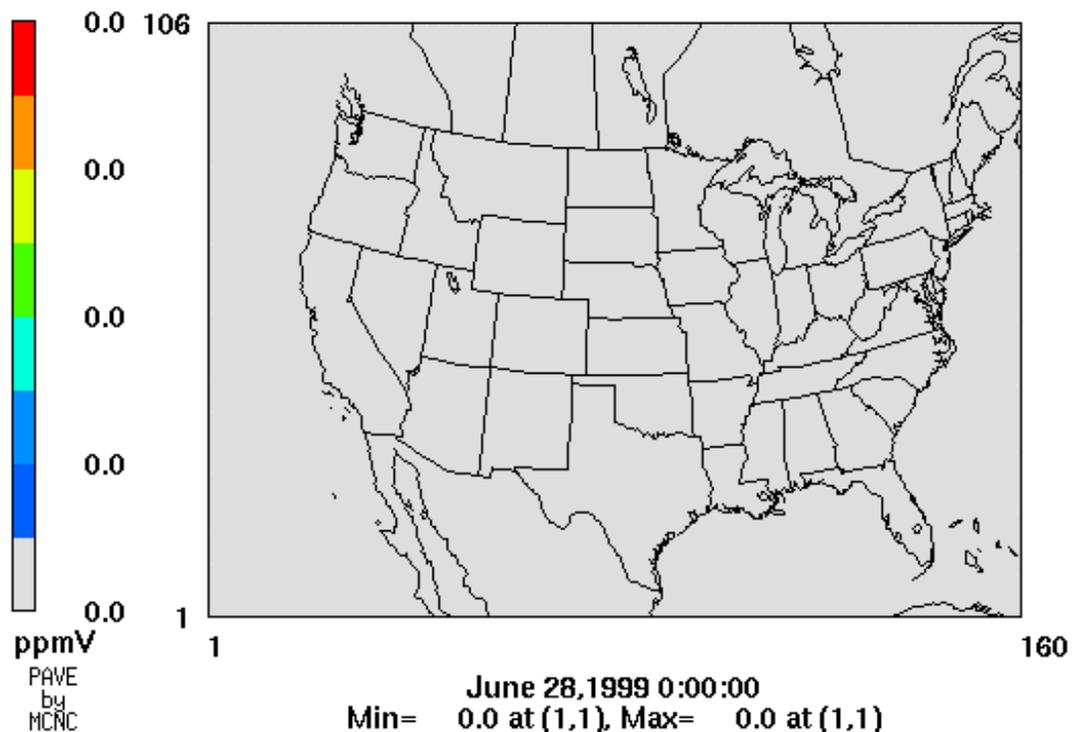


# **Grids Used in SMOKE and CMAQ**

- **Nested grids of 32 and 8 km**
- **32 km grid dimensions: 160 X 106 X 19**
- **8 km grid dimensions: 100 X 100 X 19**
- **Lambert conformal grids with cone latitudes of 30 and 60 degrees, coordinate system center of 40 deg N, 100 deg W**
- **Vertical grid extends to 15700 m with 19 sigma levels**

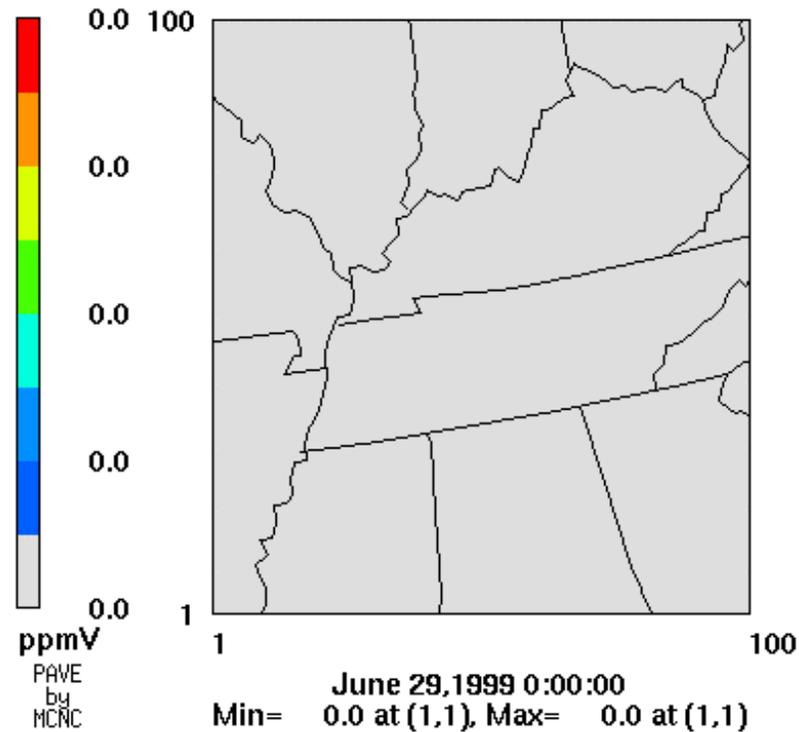


## Domain of Coarse Grid



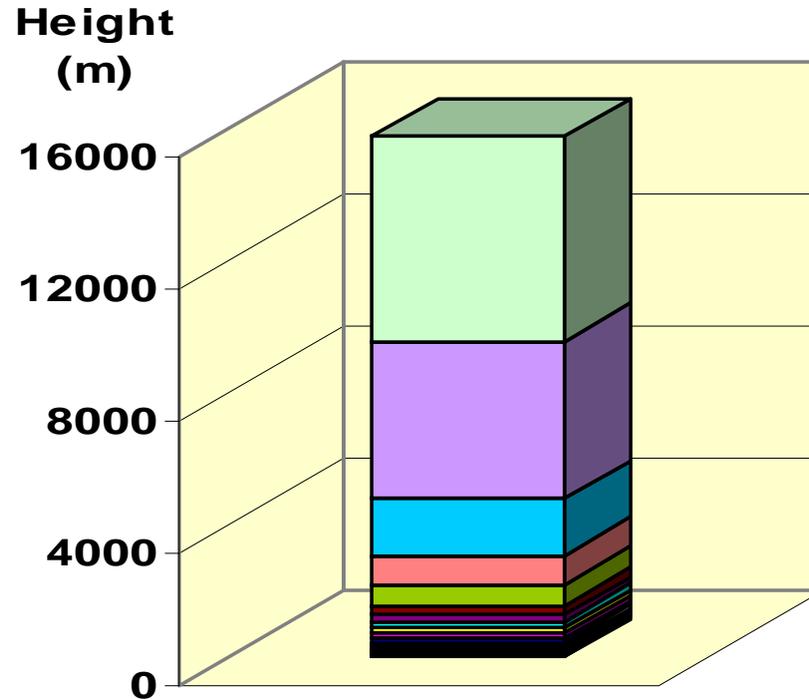


## Domain of Fine Grid





## Vertical Layers Used in MM5 and CMAQ



**MM5: 31 vertical layers; CMAQ: 19 vertical layers**



## **Emissions: Sparse Matrix Operator Kernel Emissions (SMOKE)**

- Ozone seasonal emissions from NET96 inventory were used except VMT data were used for 8 km mobile sources.**
- Biogenic emissions were provided by EPA.**
- RADM speciation profile was used.**
- Emissions from EDGAR global inventory were used to fill in for regions not covered by the NET96 inventory.**
- Hourly point source emissions were substituted for TVA and Southern Company sources (close to Nashville).**



# **Some Challenges Encountered in Running SMOKE**

- **Written for Sun, some executables failed to run on Compaq Alphas.**
- **VMT data could not be used for coarse grid because mobile processor failed for days with large variations in temperature.**
- **California VMT data not accurate.**
- **Hourly source data in IDA (Inventory Data Analyzer) format could not be included.**
- **Merge at matrix level gave flawed results; merge at grid level was required.**
- **Consistency check of units at merge did not catch difference between moles/h and moles/s.**

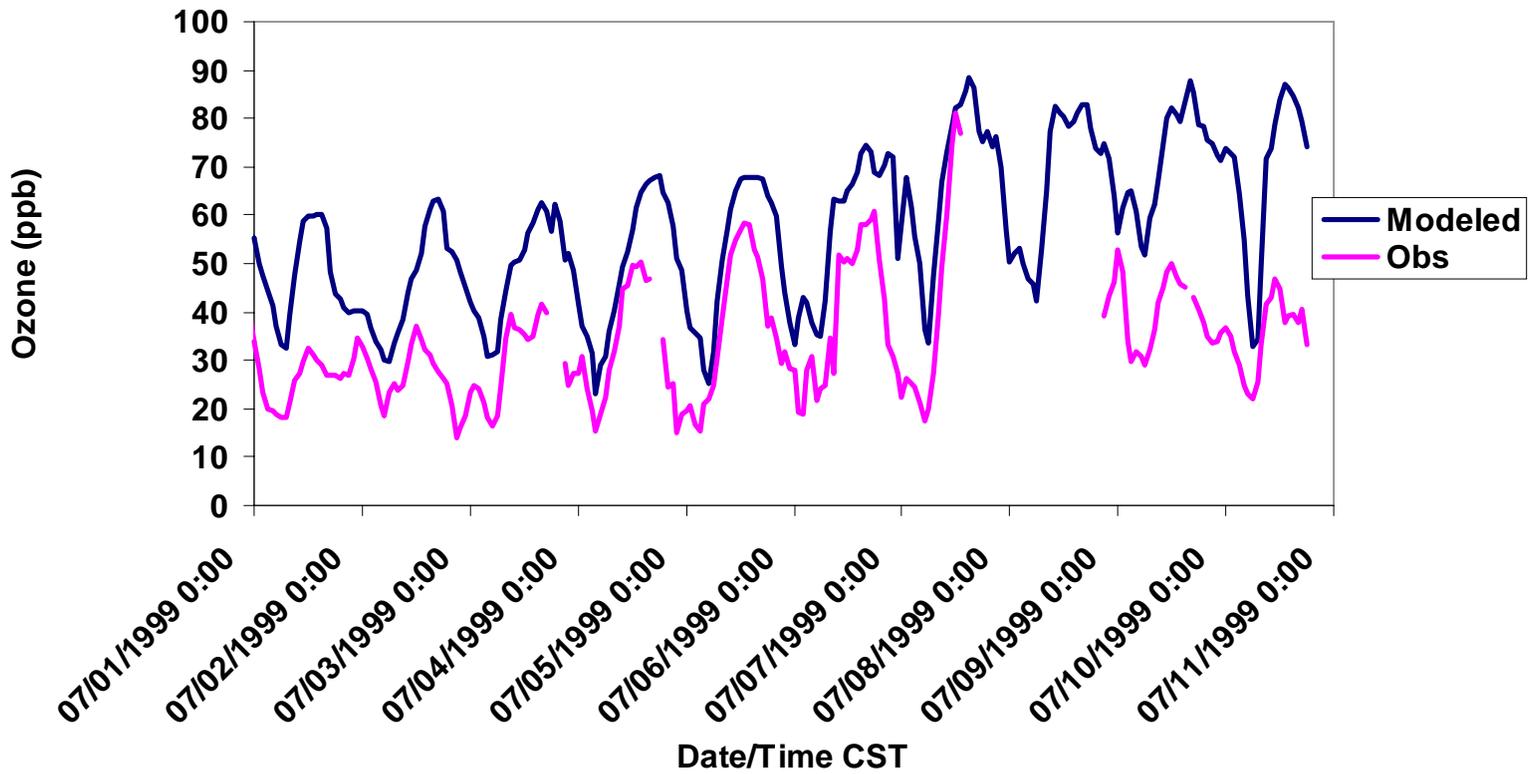


# CMAQ Configuration

- **Standalone models-3 version 4.1**
- **Ramp days: coarse grid: 3; fine grid: 2**
- **Clean air used for initial conditions and coarse-grid boundary conditions**
- **Chemistry: RADM2 with 4-product isoprene chemistry**
- **Fast solver supplied by EPA was used**
- **Piecewise Parabolic Method advective scheme was used**

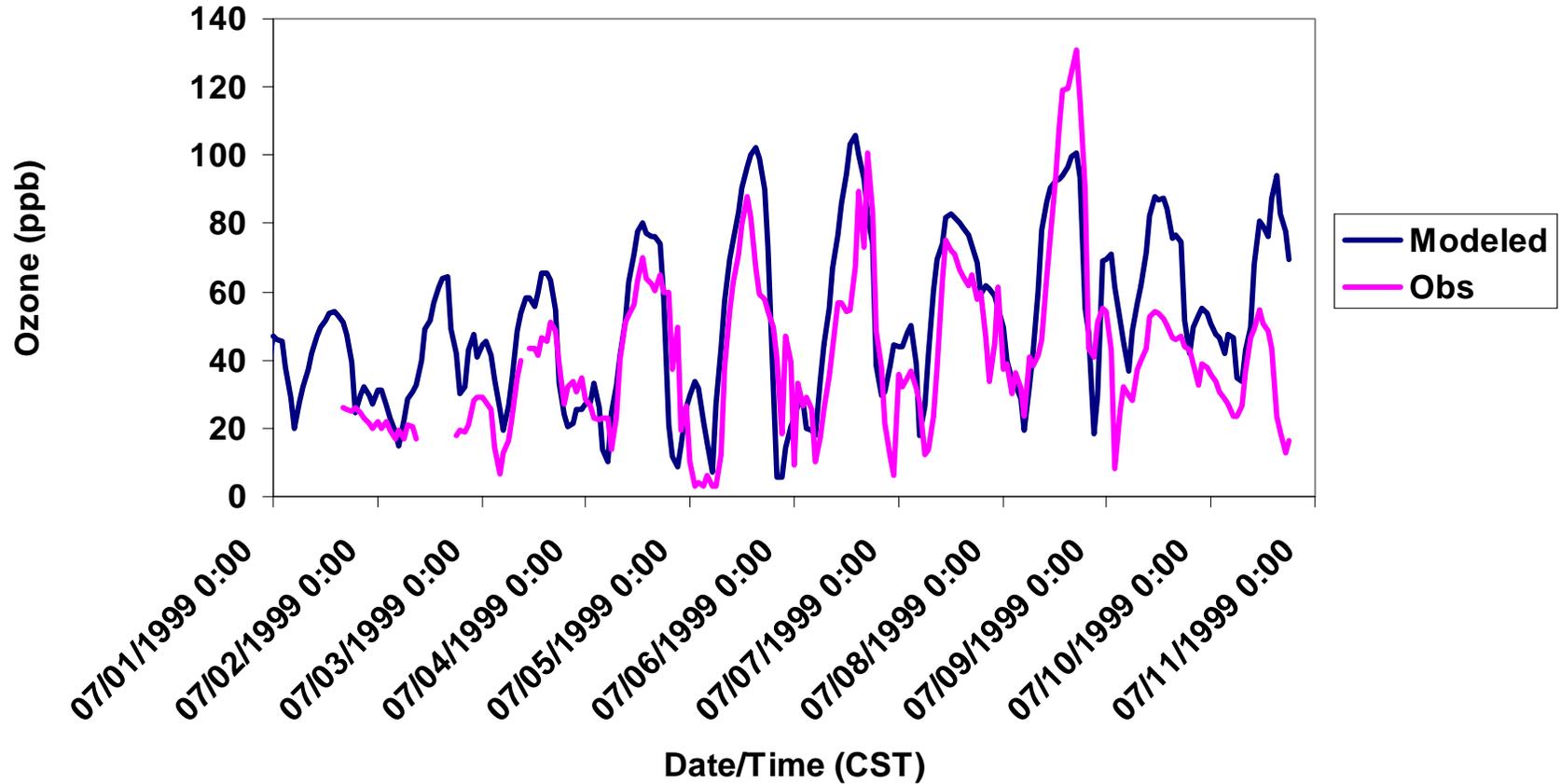


# Observed vs Modeled Ozone SOS 1999 - Dickson





# Observed vs Modeled Ozone SOS 1999 - Downtown





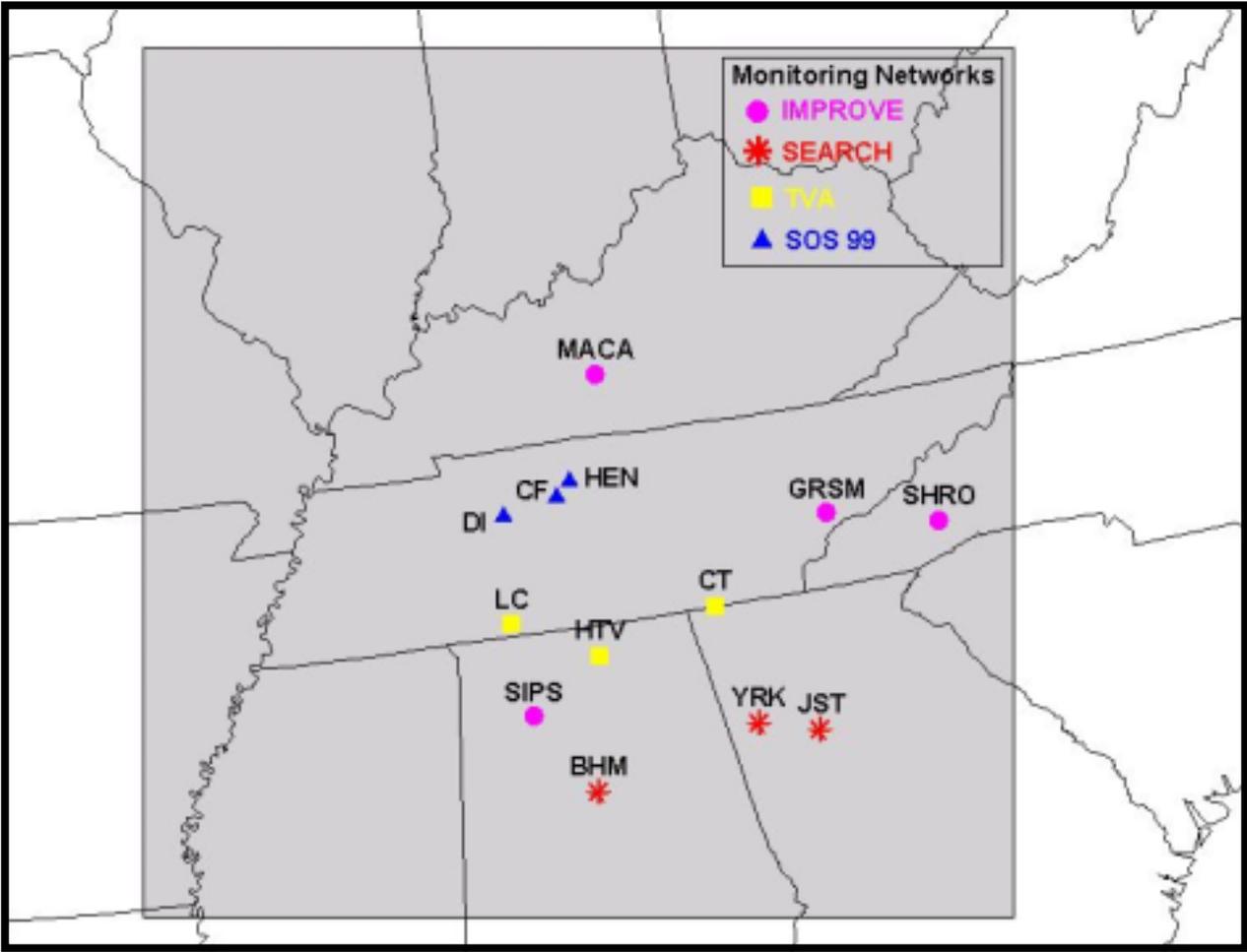
# Model Performance for Ozone at Dickson and Downtown Sites

Compute difference between modeled and observed maximum hourly  $O_3$  concentrations for days when the maximum observed  $O_3 > 40$  ppb.

	Downtown	Dickson	Both
Mean Diff (ppb)	11.8	22.1	16.5
Standard Dev	21.0	12.2	18.1



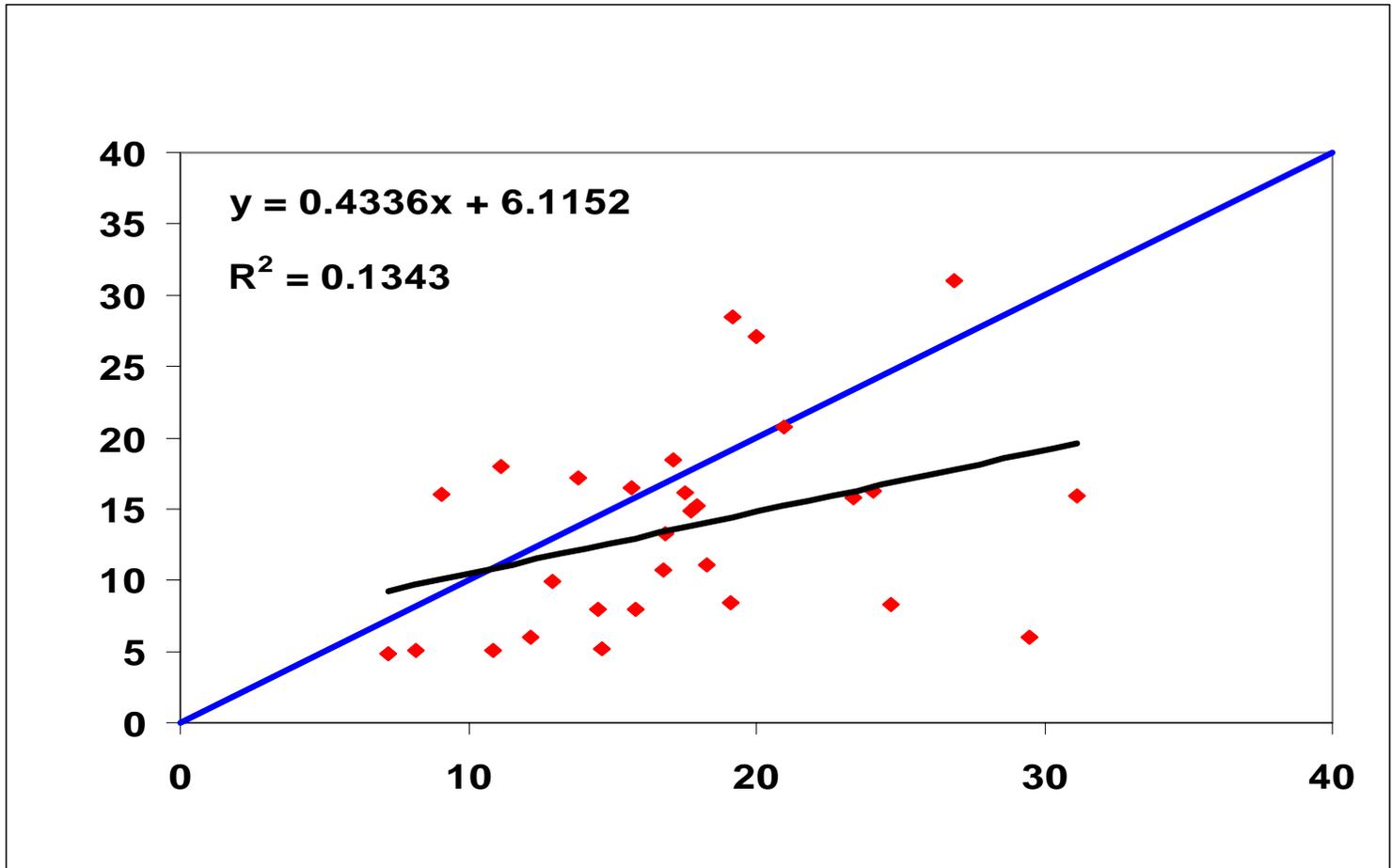
# Monitoring Networks on Fine Grid





# Relationship between Observed and Modeled Total PM<sub>2.5</sub> Data (24-Hour Averages) SEARCH, Improve and TVA Networks

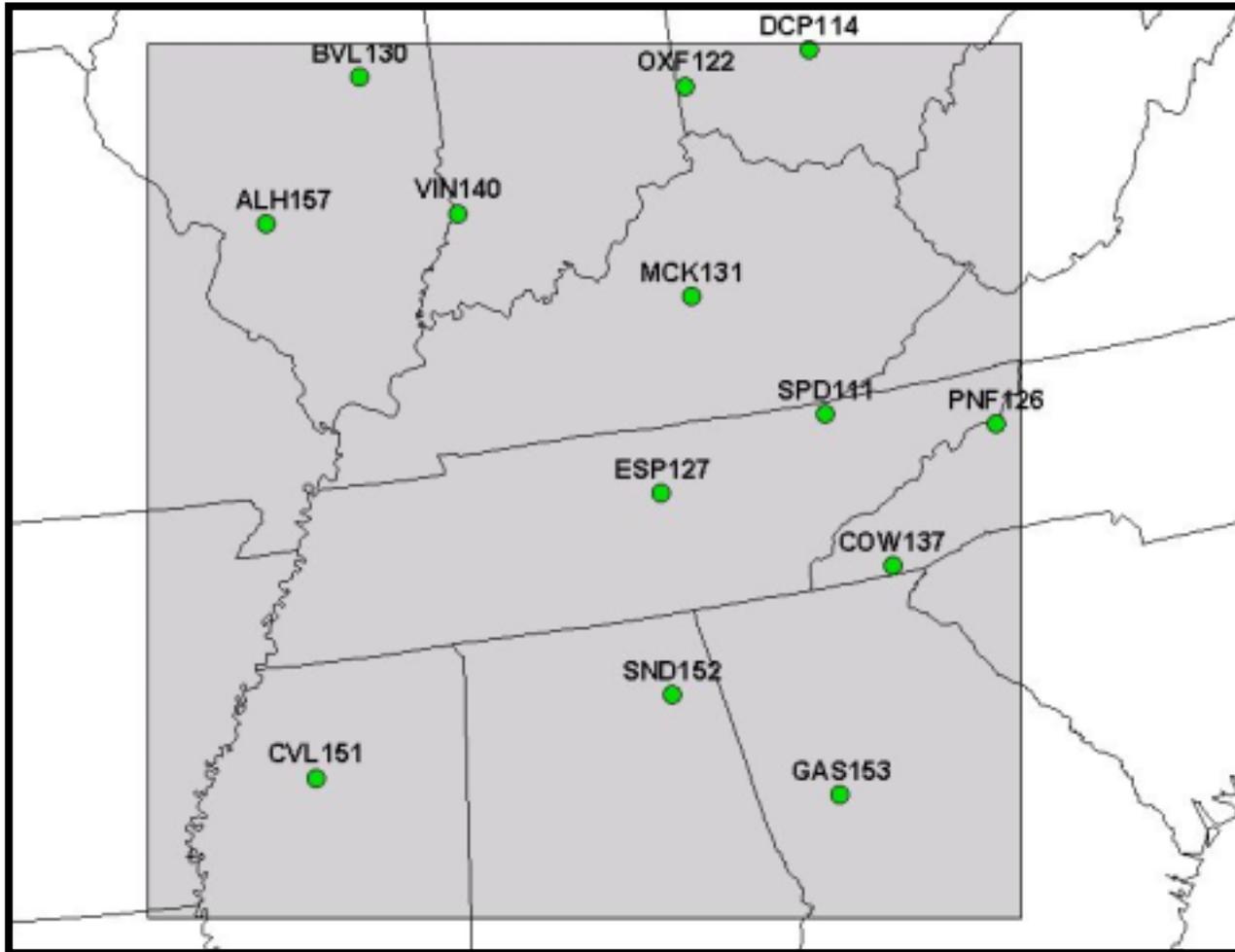
Modeled  
( $\mu\text{g}/\text{m}^3$ )



Observed ( $\mu\text{g}/\text{m}^3$ )

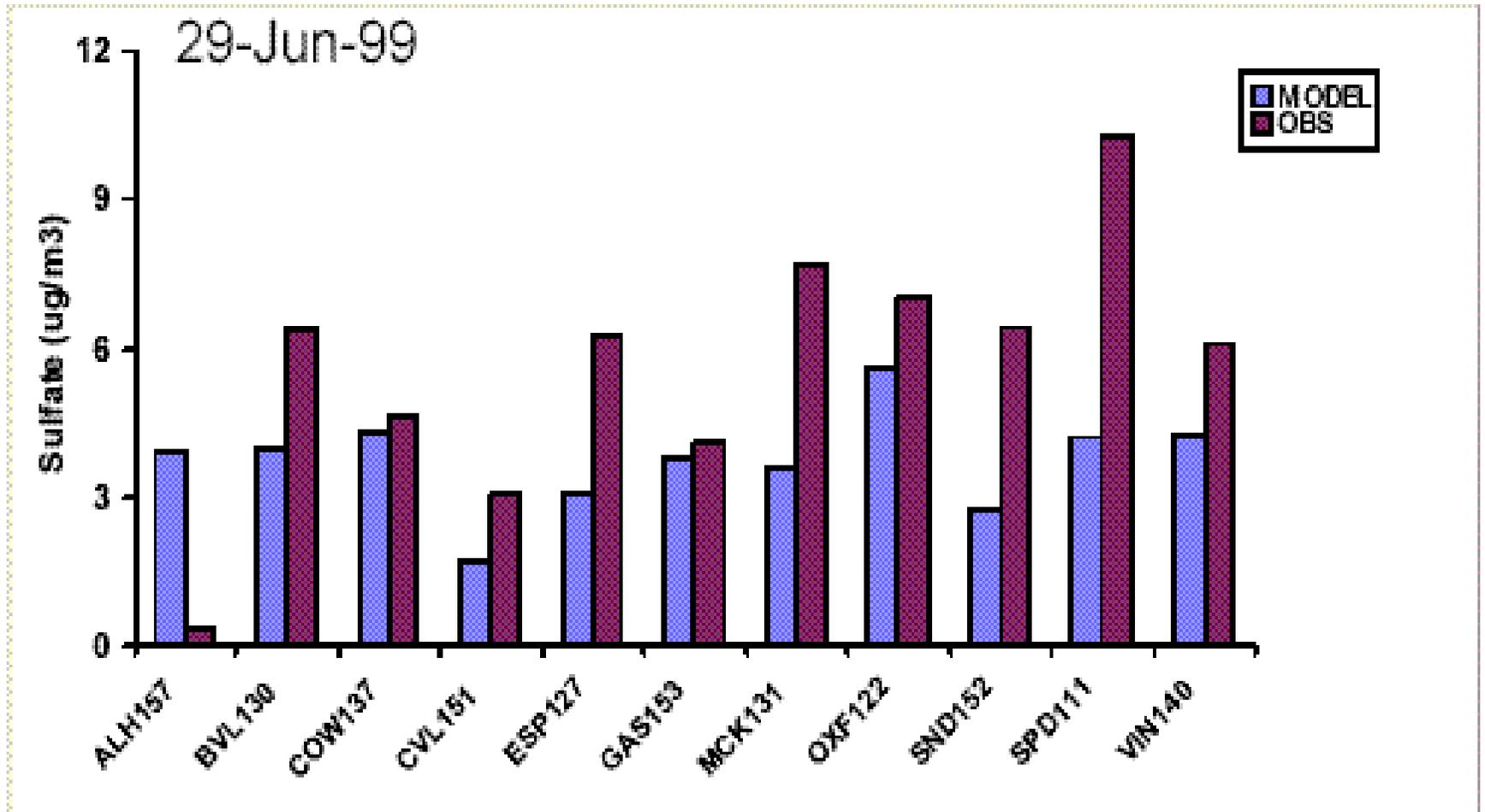


# CASTNet Sites on Fine Grid



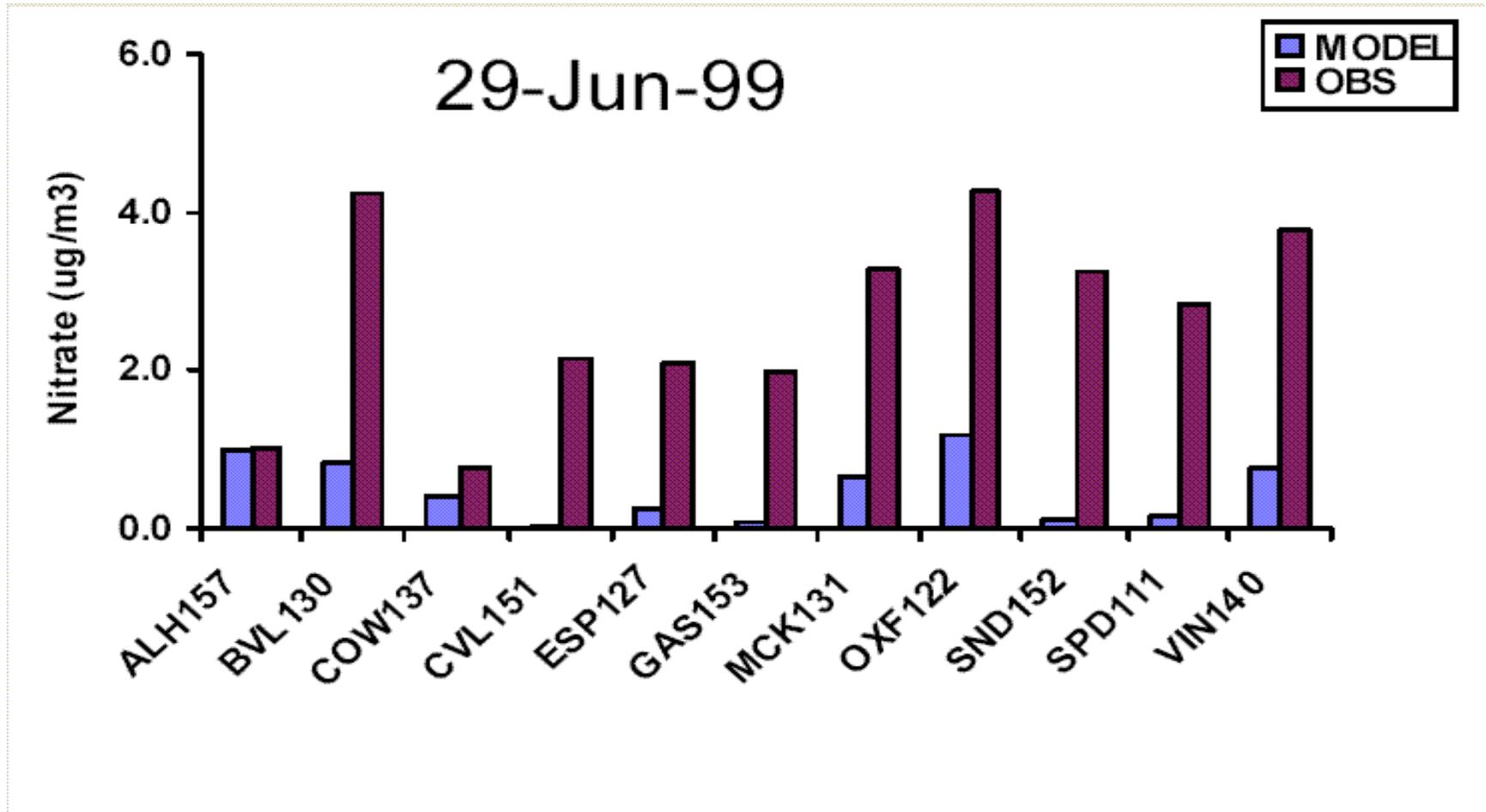


## Observed versus Modeled Sulfate CASTNet Sites on Fine Grid



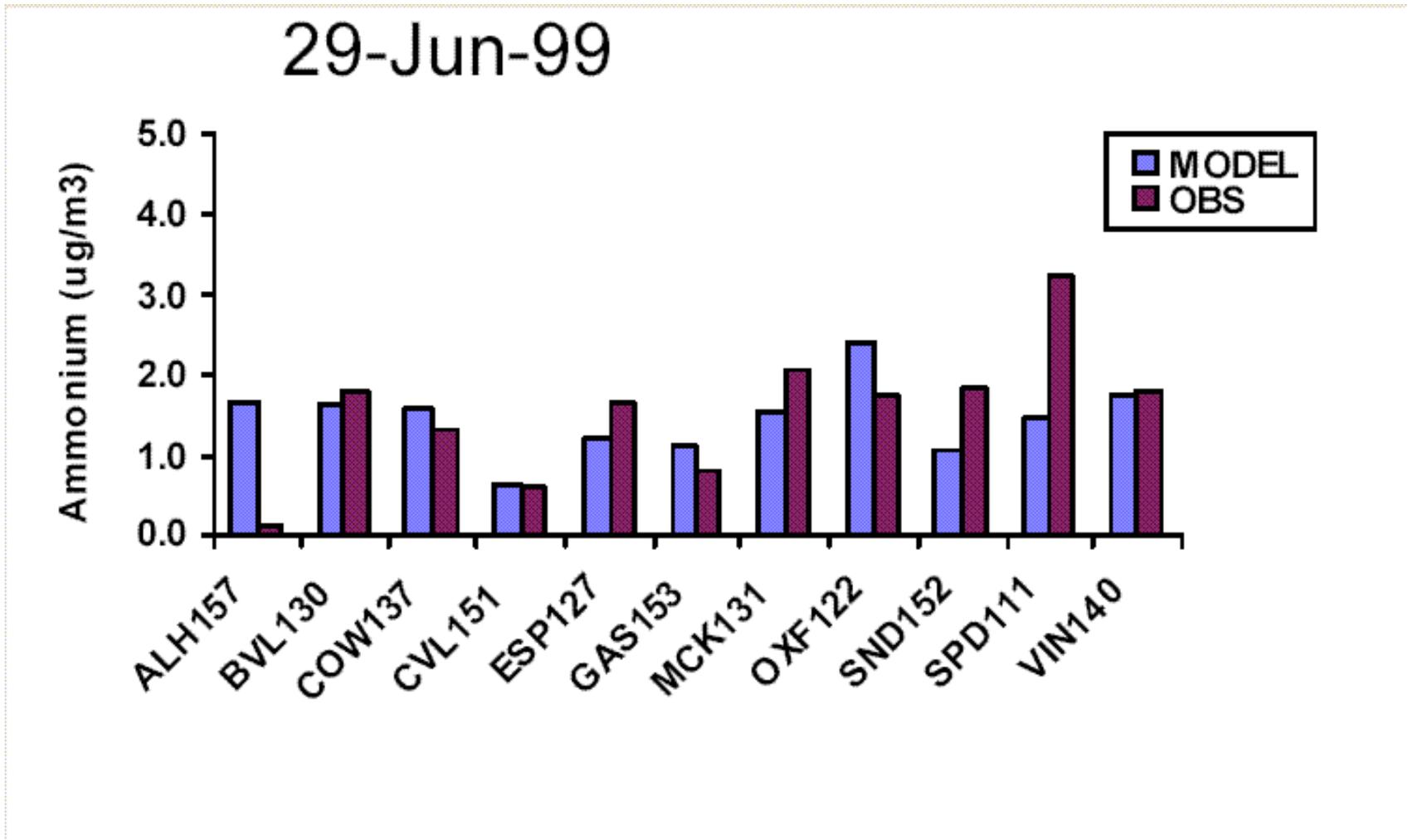


## Observed versus Modeled Nitrate CASTNET Sites on Fine Grid



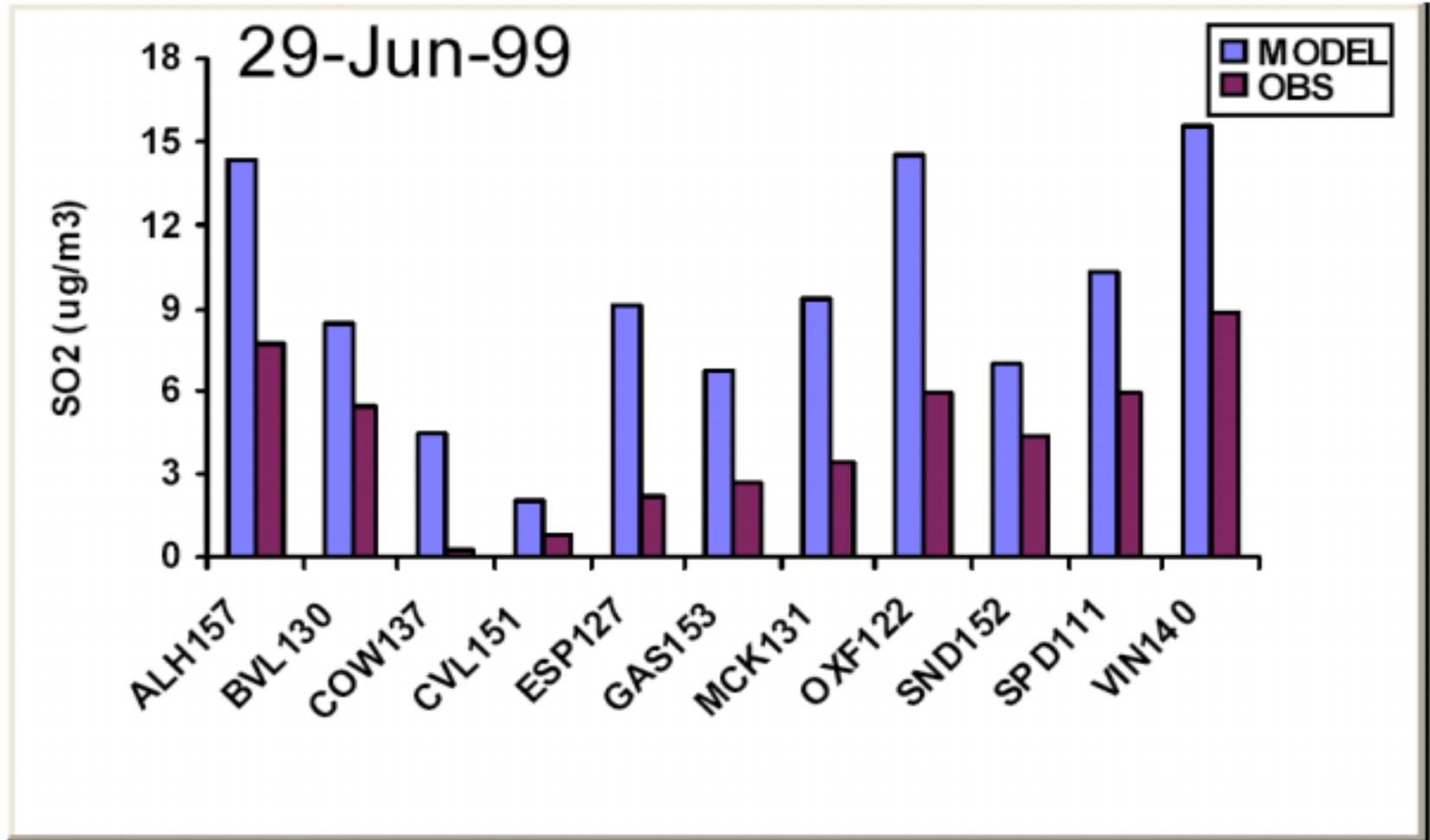


# Observed versus Modeled Ammonium CASTNet Sites on Fine Grid



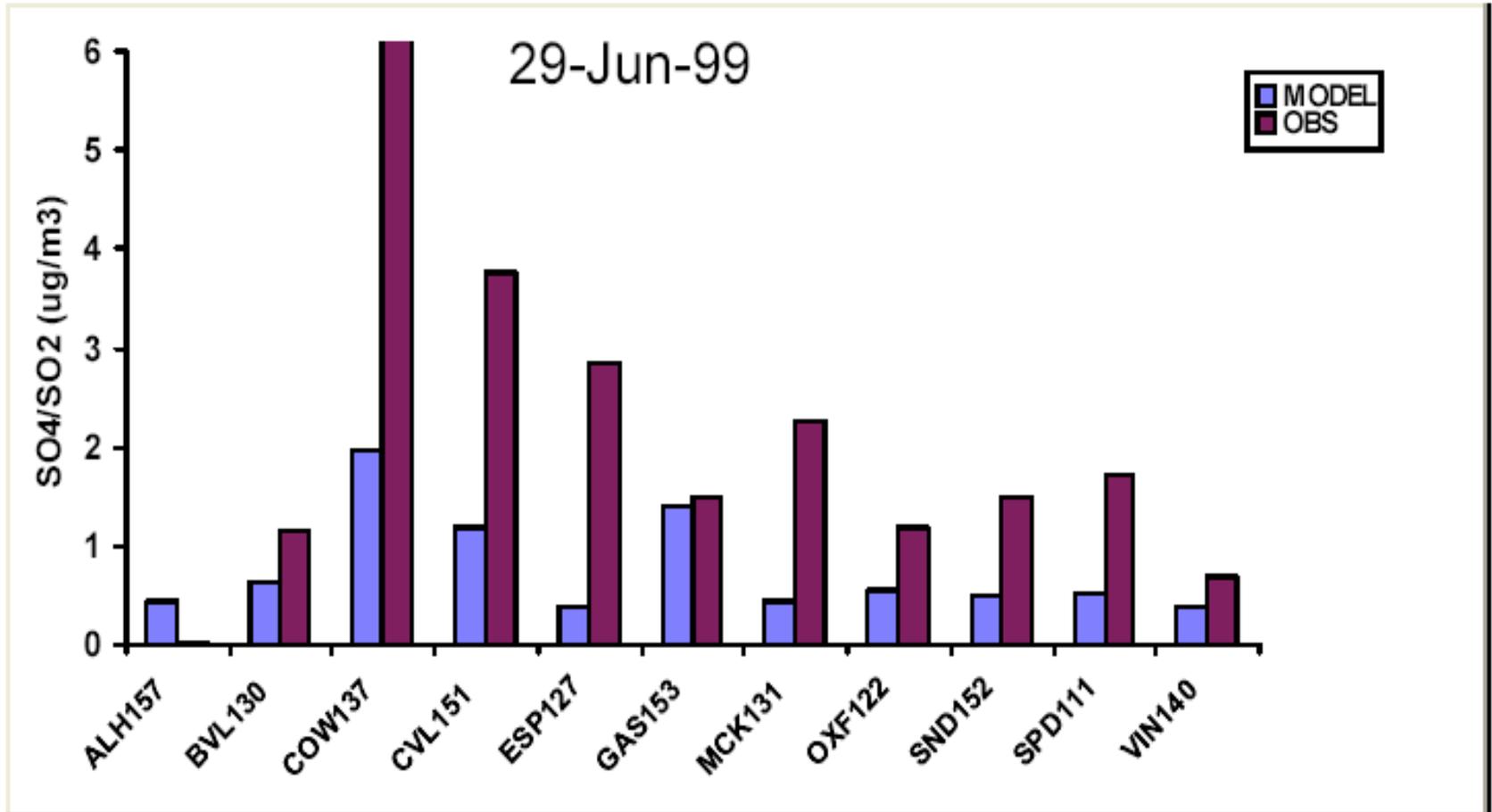


## Observed versus Modeled SO<sub>2</sub> CASTNet Sites on Fine Grid





# Observed versus Modeled Ratio of Sulfate/SO<sub>2</sub> CASTNet Sites on Fine Grid





# Model Performance for CASTNet Data

<b>CASTNet Sites (June 29 - July 06 1999)</b>					
<b>Species</b>	<b>Mean Observed (ug/m3)</b>	<b>Mean Bias (ug/m3)</b>	<b>Normalized Bias (%)</b>	<b>Mean Error (ug/m3)</b>	<b>Normalized Error (%)</b>
<b>Sulfate</b>	<b>5.66</b>	<b>-1.93</b>	<b>-34.10</b>	<b>2.58</b>	<b>45.66</b>
<b>Nitrate</b>	<b>2.70</b>	<b>-2.20</b>	<b>-81.46</b>	<b>2.20</b>	<b>81.46</b>
<b>Ammonium</b>	<b>1.55</b>	<b>-0.10</b>	<b>-6.31</b>	<b>0.59</b>	<b>38.32</b>
<b>SO2</b>	<b>4.33</b>	<b>4.94</b>	<b>114.16</b>	<b>4.94</b>	<b>114.16</b>



## **Future Plans for Models3/CMAQ**

**DOE-EPRI-TVA Project: Sensitivity simulations will be conducted using modified emissions.**

**Other: Simulations for 2 Southern Appalachian Mountain Initiative (SAMI) episodes will be conducted using Models3/CMAQ. Inputs will duplicate conditions used in SAMI so that the performance of Models-3/CMAQ and URM-1ATM for PM can be compared.**



# Conclusions

- **Modeled PM<sub>2.5</sub> concentrations were usually lower than observations.**
- **Compared to observations from CASTNet:**
  - **Modeled sulfate concentrations were lower.**
  - **Modeled nitrate concentrations were much lower.**
  - **Modeled ammonium concentrations agreed reasonably well.**
  - **Modeled SO<sub>2</sub> concentrations were much higher.**
- **Much valuable diagnostic information will be gained from the model intercomparison studies described in this presentation.**