



CMAQ Modeling for the CRPAQS 2000-2001 winter PM Episode: Part II

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Collaborators

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 - Kathleen Fahey
 - Luis Woodhouse
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 - Karen Magliano
 - Kasia Turkiewicz
- **UCD:**
 - Michael Kleeman
 - Anthony Wexler
 - Max Zhang
- **CRPAQS Technical Committee**
- **EPA:**
 - Prakash Bhave
 - Frank Binkowski
- **STI:**
 - Neil Wheeler
- **Future:**
 - Christian Seigneur - AER
 - Yang Zhang - NCSU
 - Kim Prather - UCSD
 - Steven Reynolds, Envair



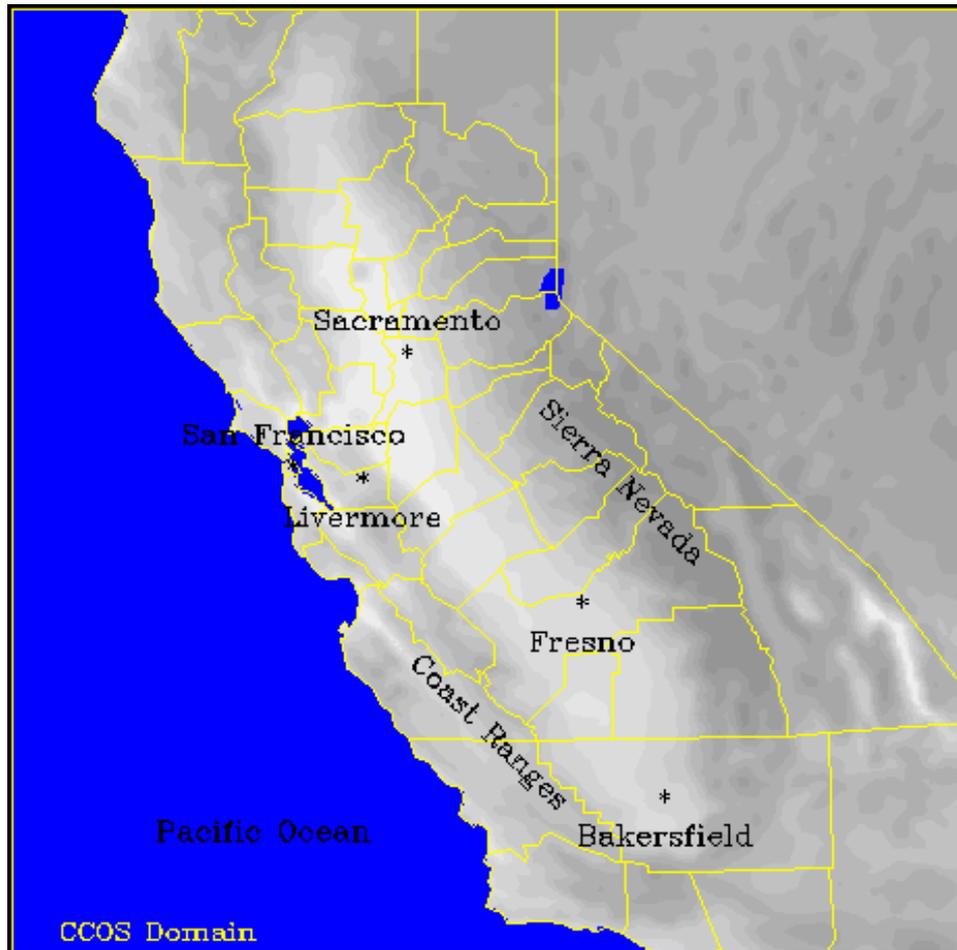
Overview

- Summary of previous presentation
- Progress since last September
- Corroborative Analysis
- Summary
- Future directions



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185 x 185 horizontal grids, 4km x 4km size



11 km ASL

7 km

Layer 15



**CMAQ
Model
Domain**

38 m

Layer 2

30 m

Layer 1



Previous Presentation

- CMAQ PM model was updated for CRPAQS winter study
- 24 simulations were conducted at ARB to understand the processes responsible for the 12/25/00-01/07/01 episode.
- Simulated PM_{2.5}, its components, and non-VOC precursors were compared with observations at surface and aloft.



Progress since last September

- 24 more runs using updated CMAQ
- VOC species evaluated with observations
- Corroborative analysis using an efficient PMF method
- FFT tool for time series analysis



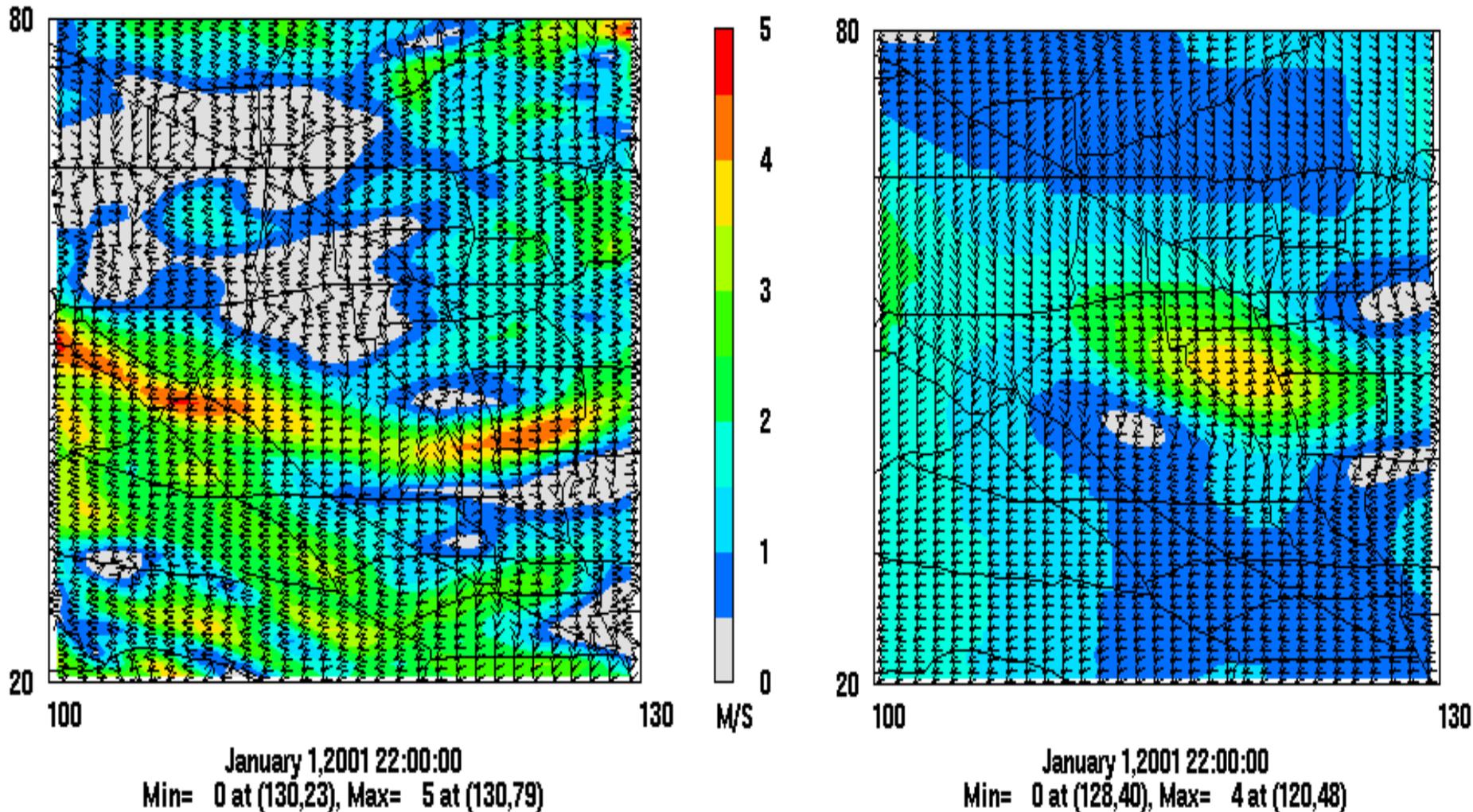
Progress: Sensitivity Runs

- 24 more simulations were conducted
- Additional issues investigated
 - Chemistry: $\text{OH} + \text{NO}_2 + \text{M}$, CH_4 , NaCl, MGLY
 - Emissions: NH_3 , NO_x , AVOC, precursor reduction scenarios, Terpene
 - Meteorology: RH, LWC, observed winds & T
- Model results look better, but no dramatic changes from September PM results



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MM5 vs. DWM





Progress: VOC Evaluation

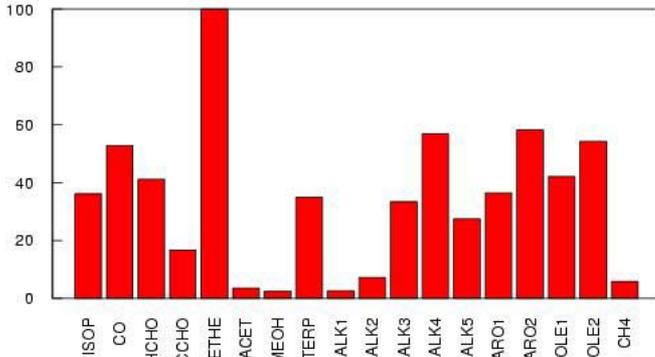
- Emissions
 - Approximately 600 VOC species in the inventory
- Measurements
 - Photochemical Assessment Monitoring Stations (**PAMS**) species + extra: 57 organic compounds with significant concentrations
 - Stations: ANGI, BODB, BTI, FSF, SNFH, OLW, YOY
- Model
 - SAPRC99: 5 Alkanes, 2 Aromatics, 2 Olefins, 1 monoterpene
 - 2km average; 14km radius, best match



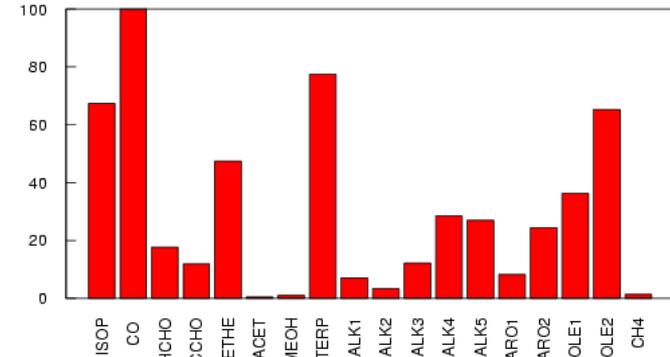
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VOC Reactivity in San Joaquin Valley

VOC MIR on 12/29/2000

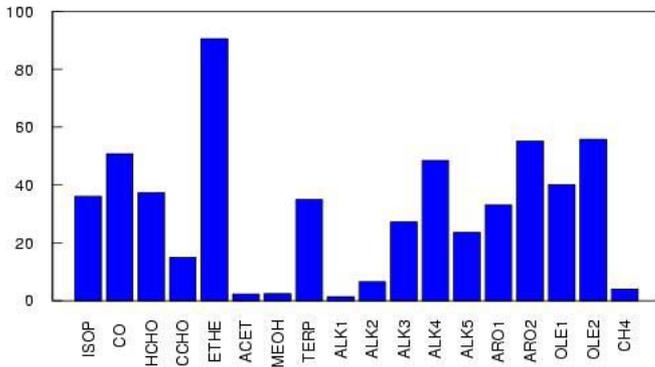


VOC OH Reactivity on 12/29/2000

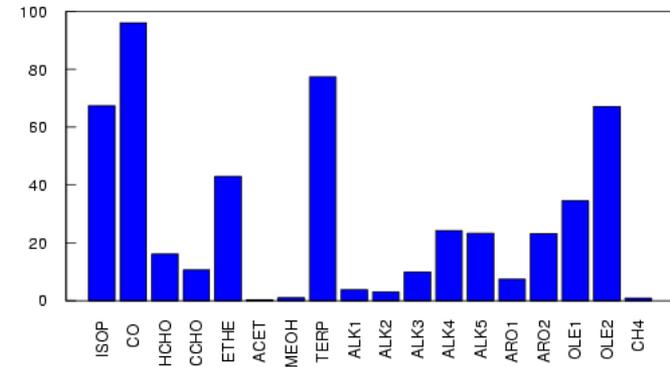


Friday

VOC MIR on 12/31/2000



VOC OH Reactivity on 12/31/2000



Sunday

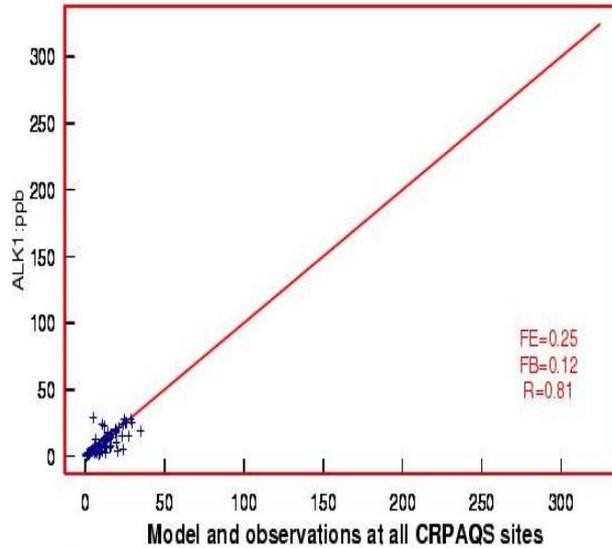
MIR-weighted VOC in San Joaquin Valley

VOC OH Reactivity in San Joaquin Valley

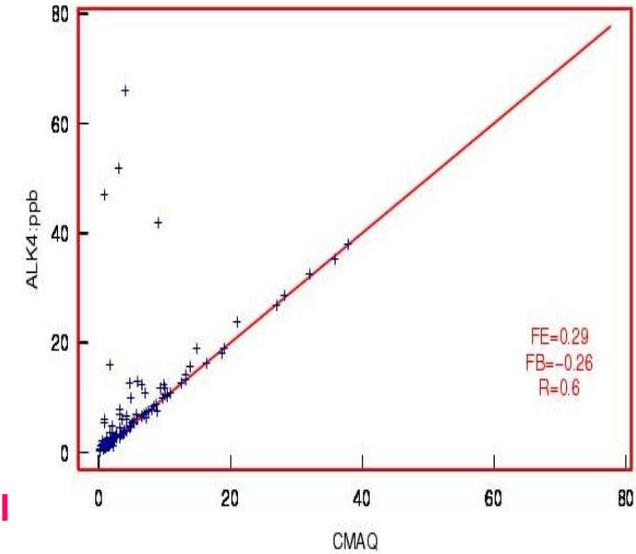
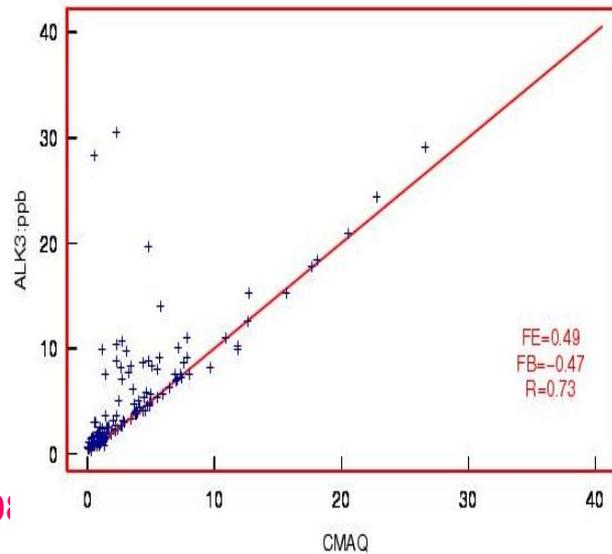
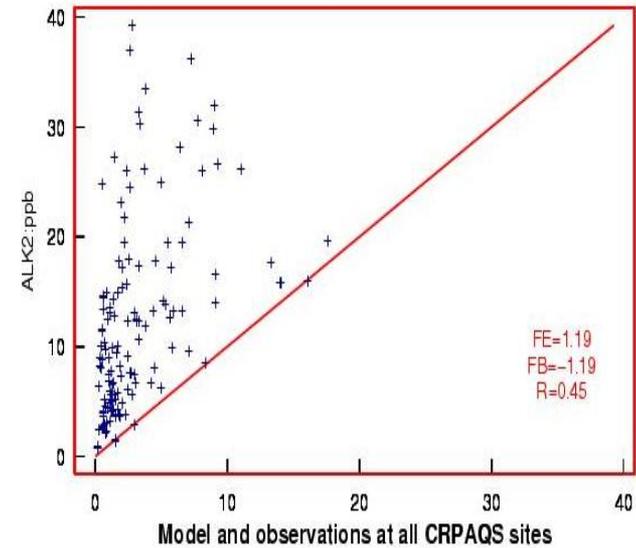


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Model and observations at all CRPAQS sites



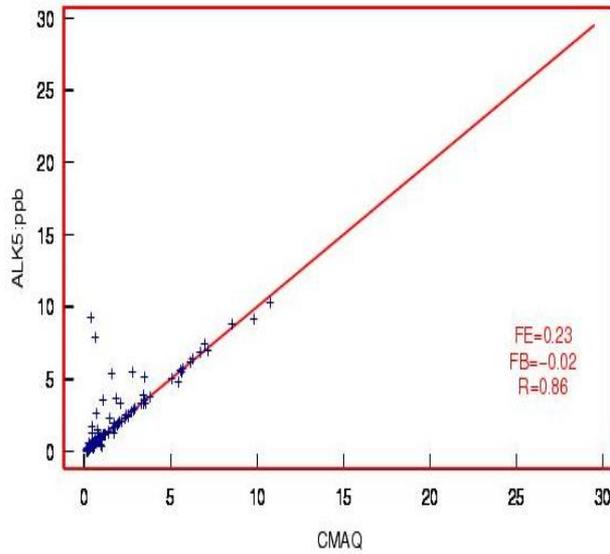
Model and observations at all CRPAQS sites



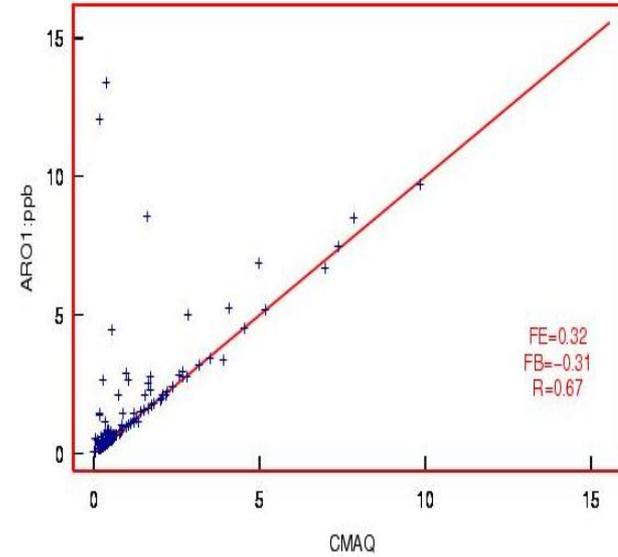


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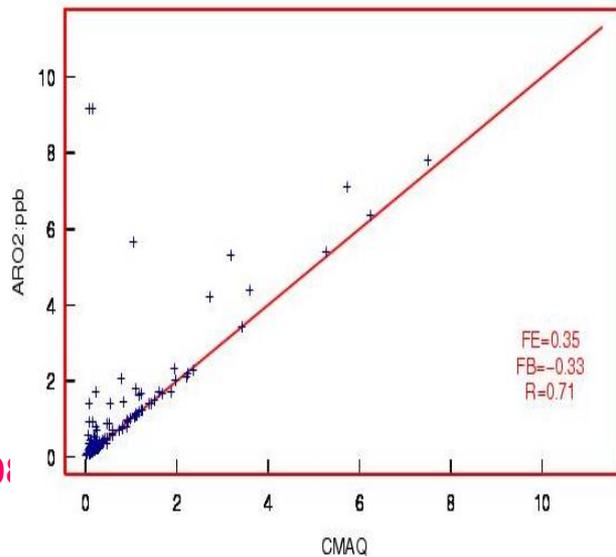
Model and observations at all CRPAQS sites



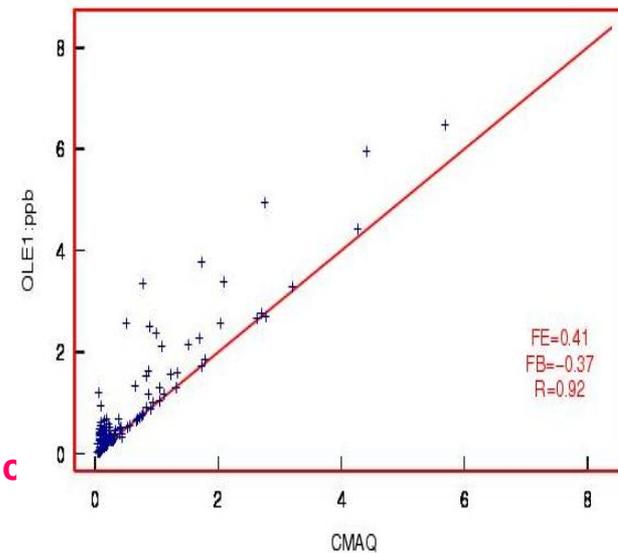
Model and observations at all CRPAQS sites



Model and observations at all CRPAQS sites



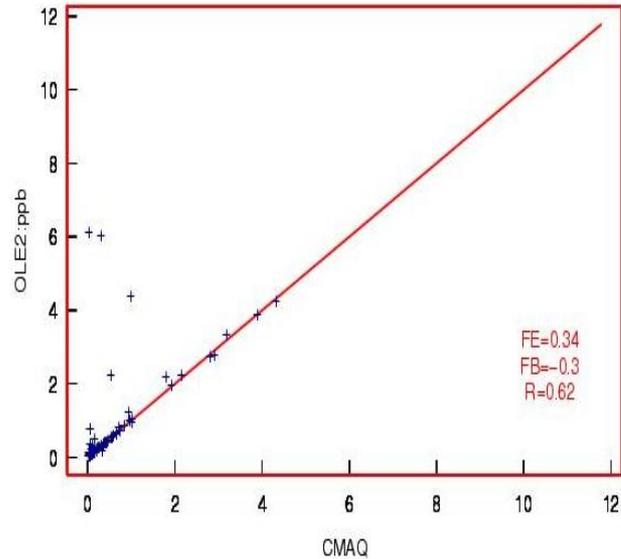
Model and observations at all CRPAQS sites



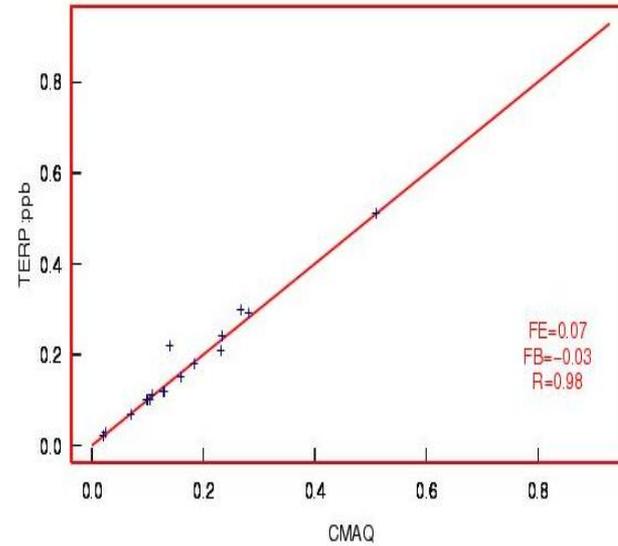


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Model and observations at all CRPAQS sites



Model and observations at all CRPAQS sites

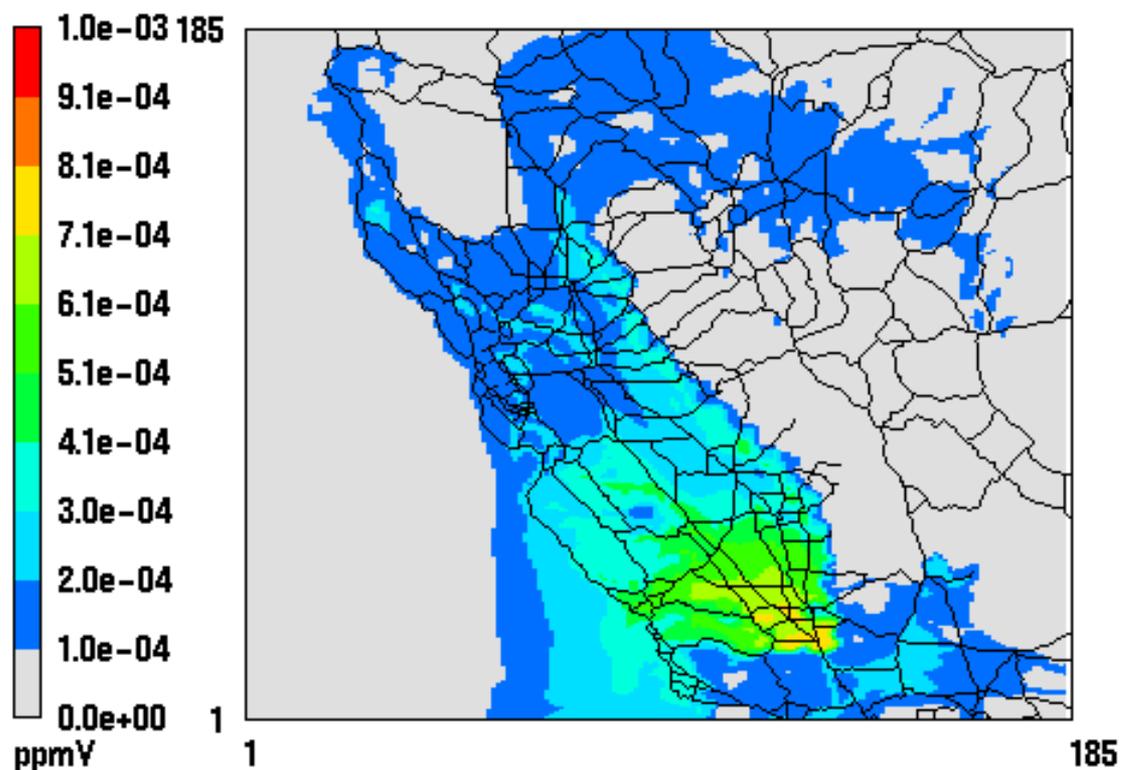




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Layer 1 PANd

d=ACONC.31.MGLY



December 31,2000 8:00:00

Min= 8.9e-07 at (185,185), Max= 7.8e-04 at (124,20)

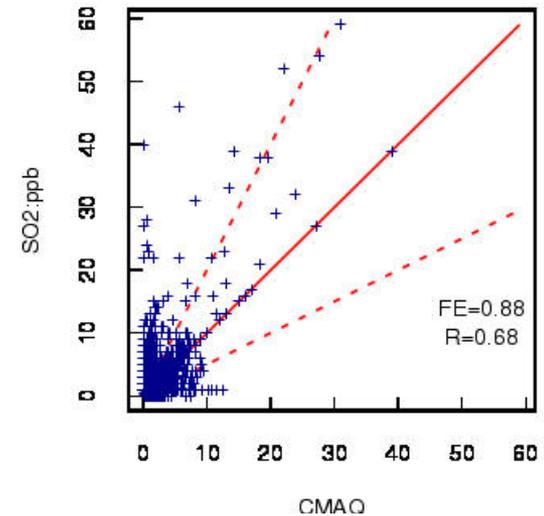
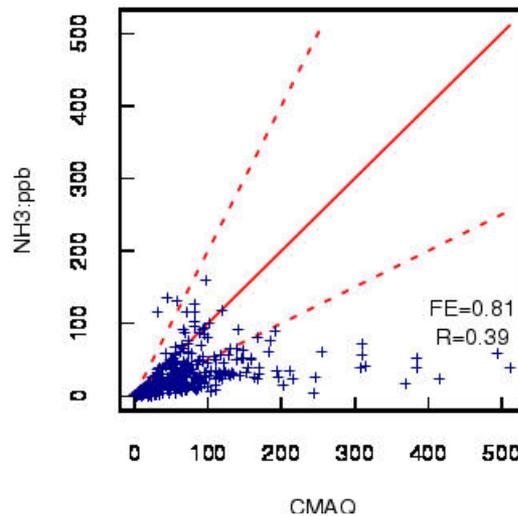
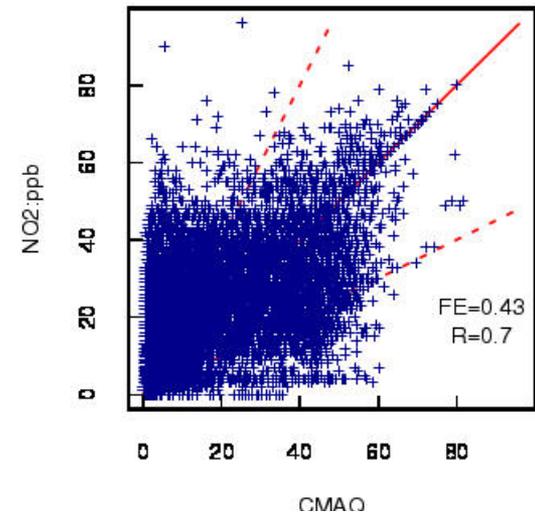
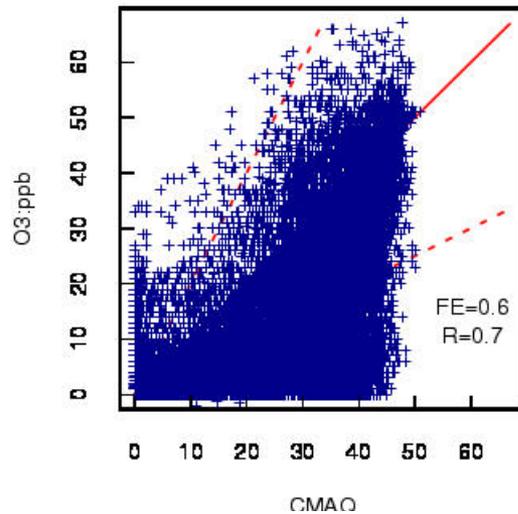


Current Case

- Domain-wide correlation plots
 - 4 km x 4km x 30m average vs. point
 - Gas (O_3 , NO_2 , NH_3 , SO_2)
 - PM ($PM_{2.5}$, NO_3 , SO_4 , OC)
- Time-history plots are shown for Angiola and Bakersfield (composite)
 - Gas (O_3 , NO_2 , NH_3 , SO_2)
 - PM ($PM_{2.5}$, NO_3 , SO_4 , OC)
- More graphics available at
orthus.arb.ca.gov/SIP_Modeling/PM_Modeling/

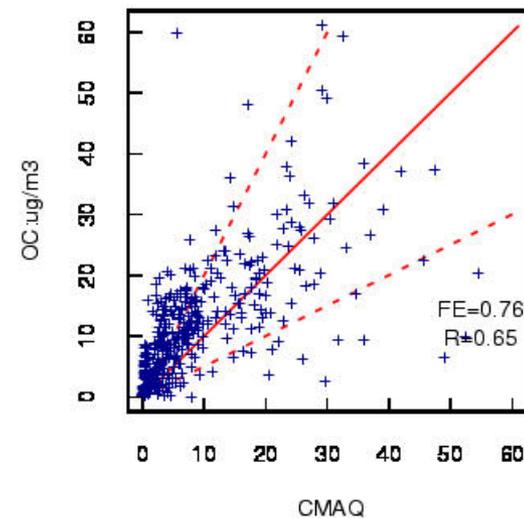
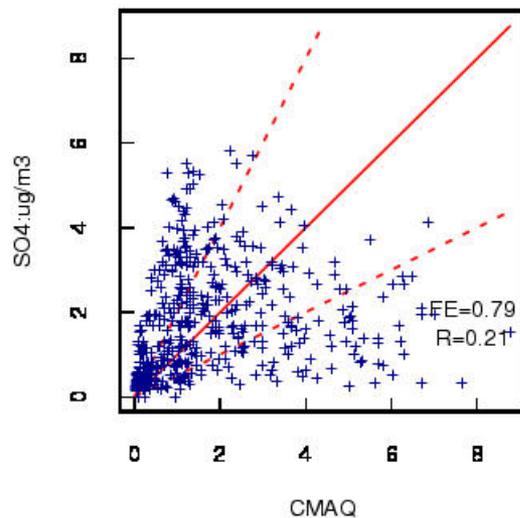
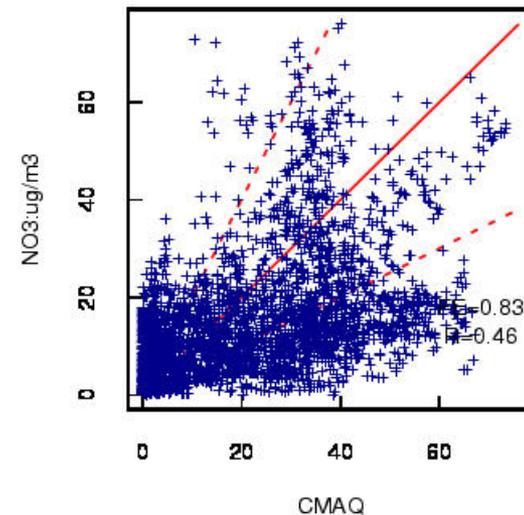
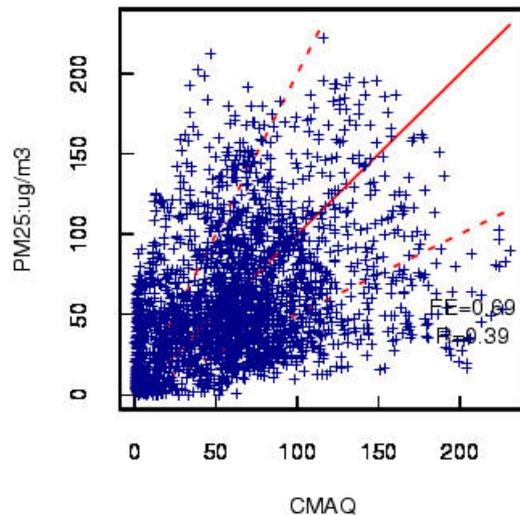


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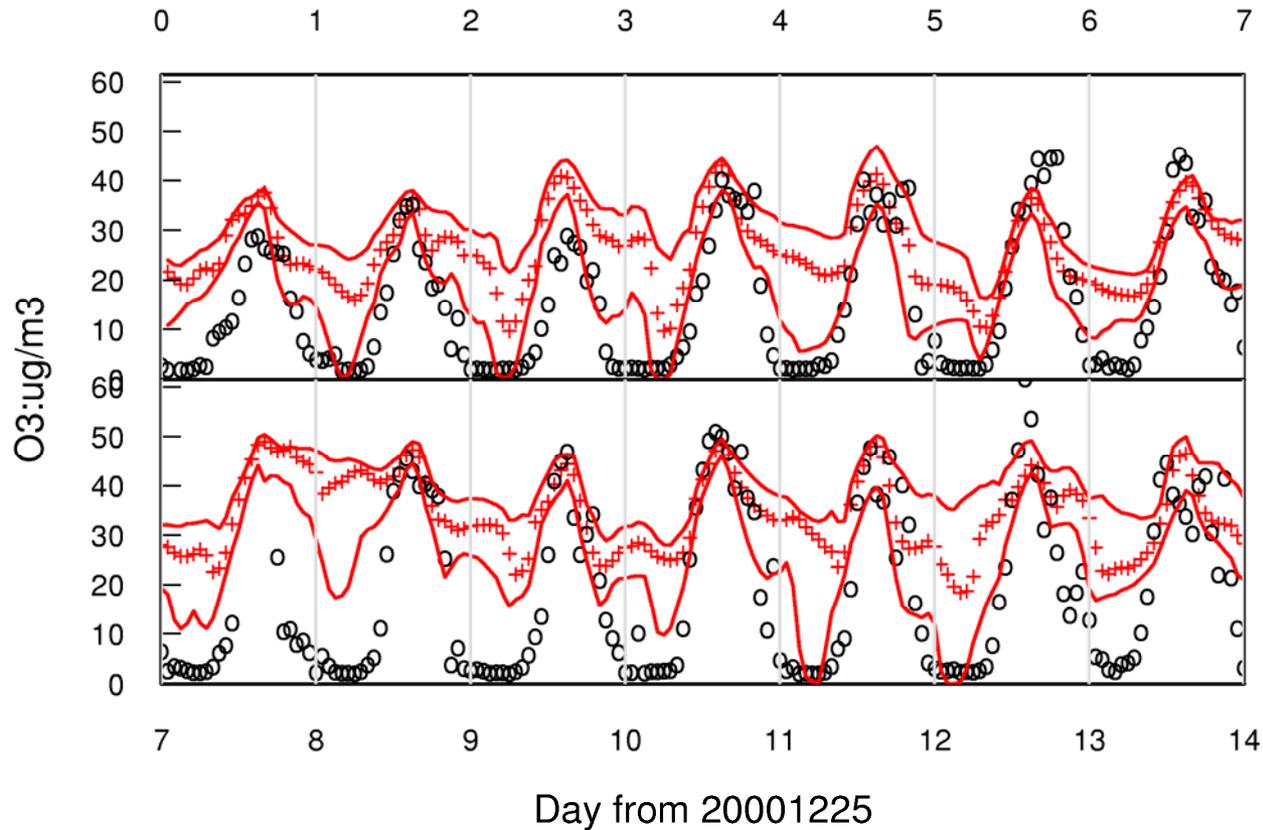
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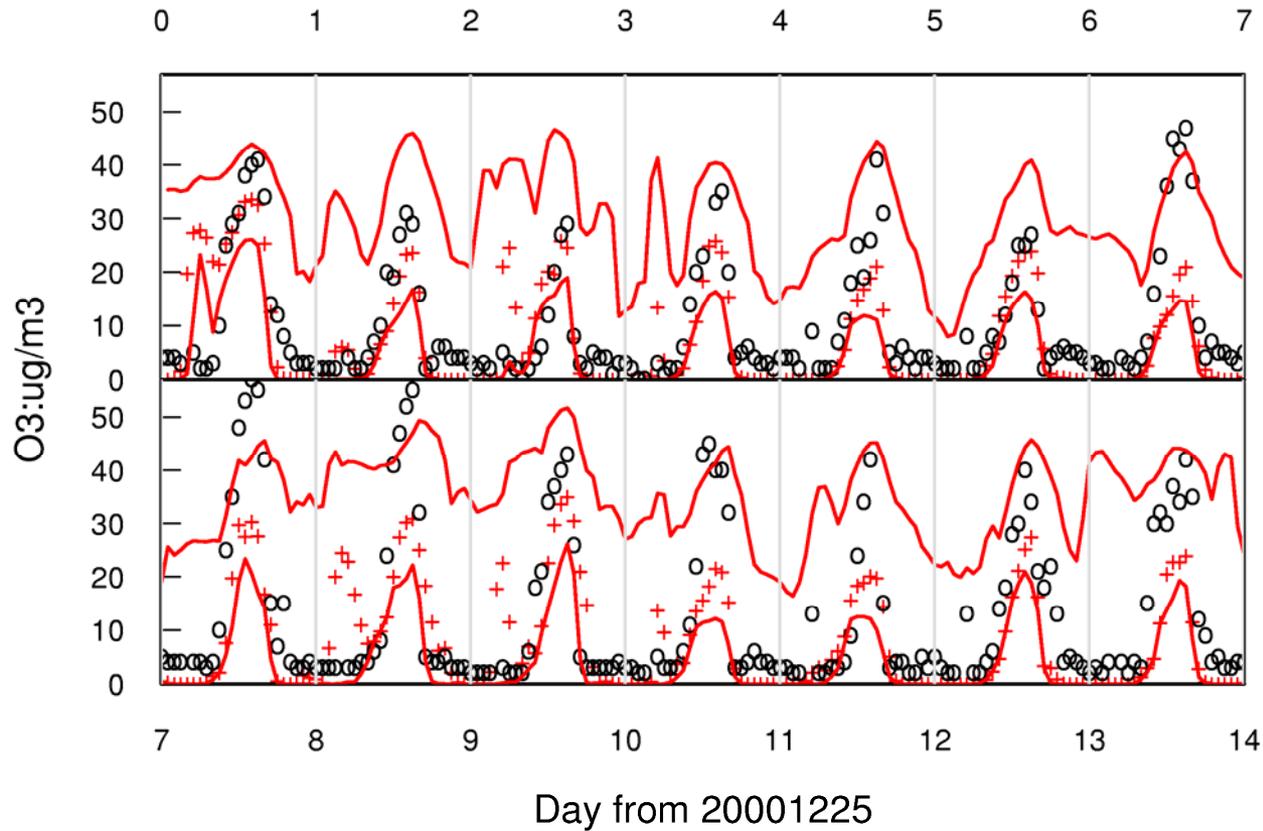
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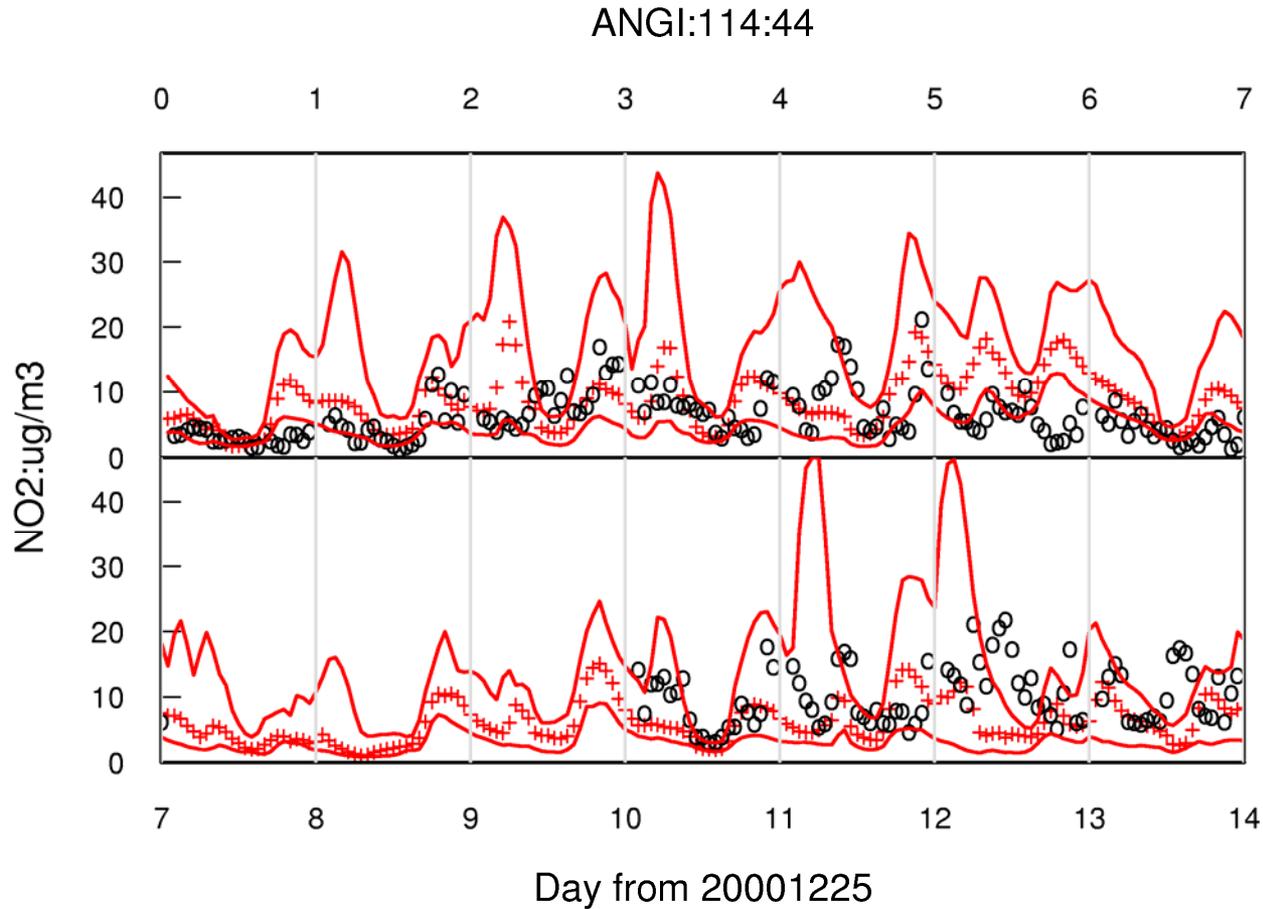
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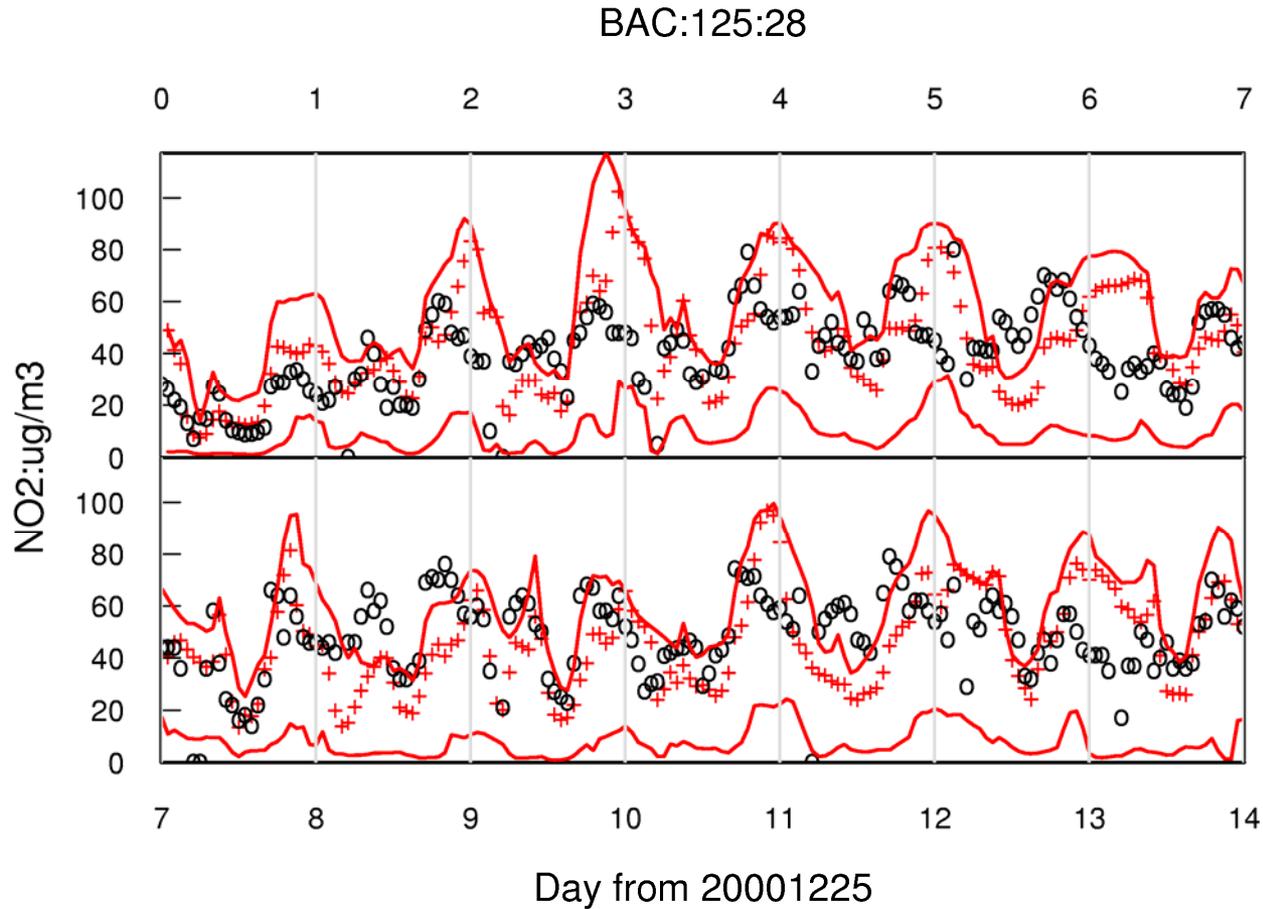


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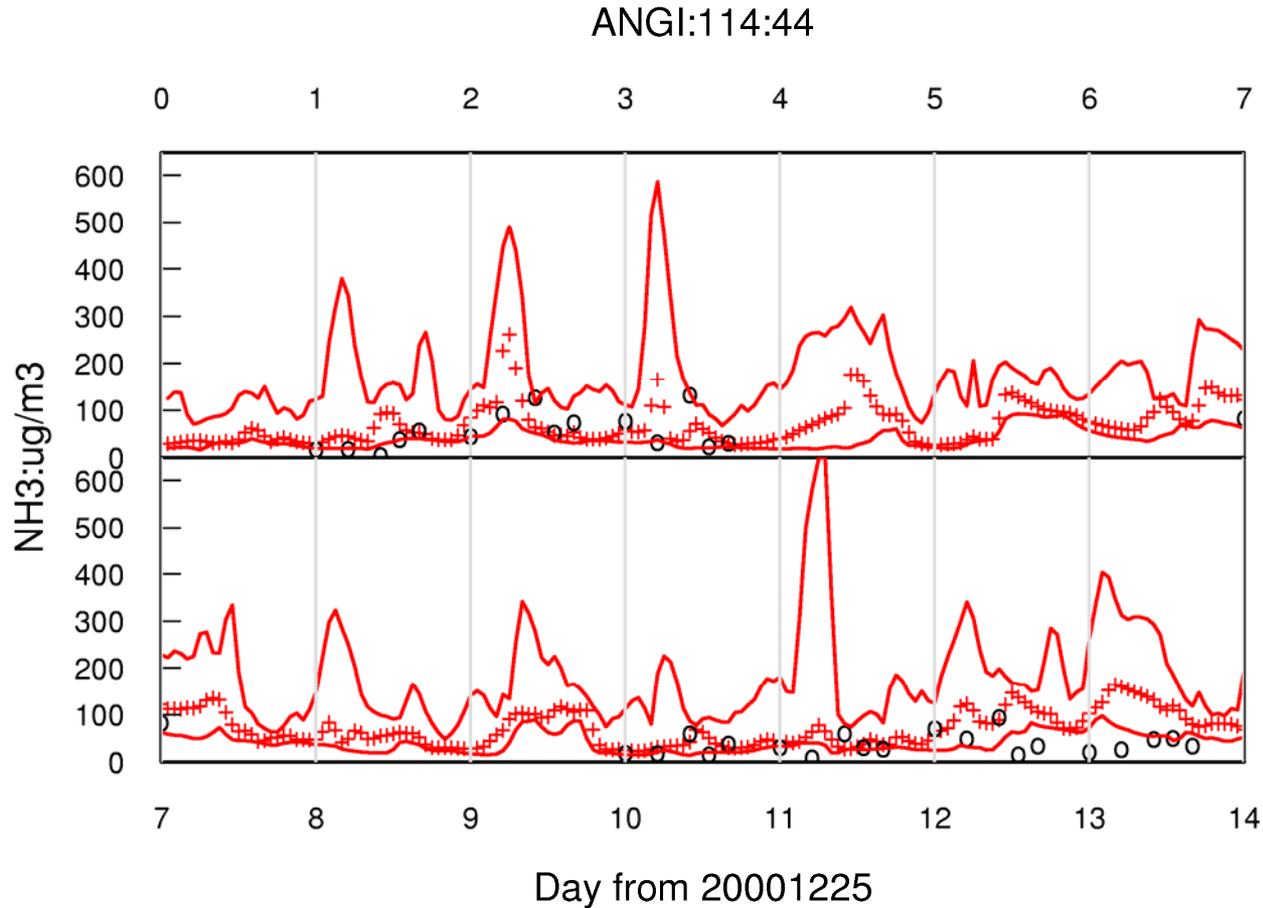


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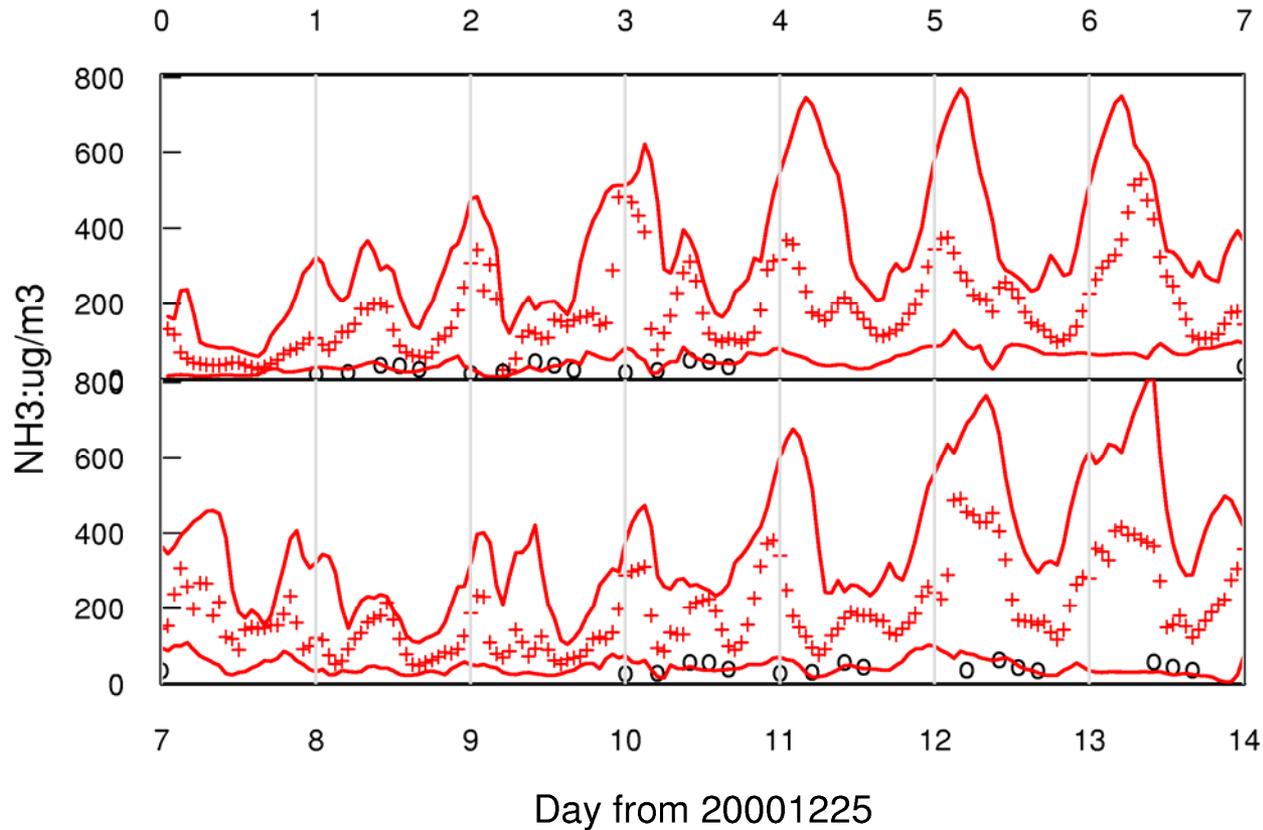
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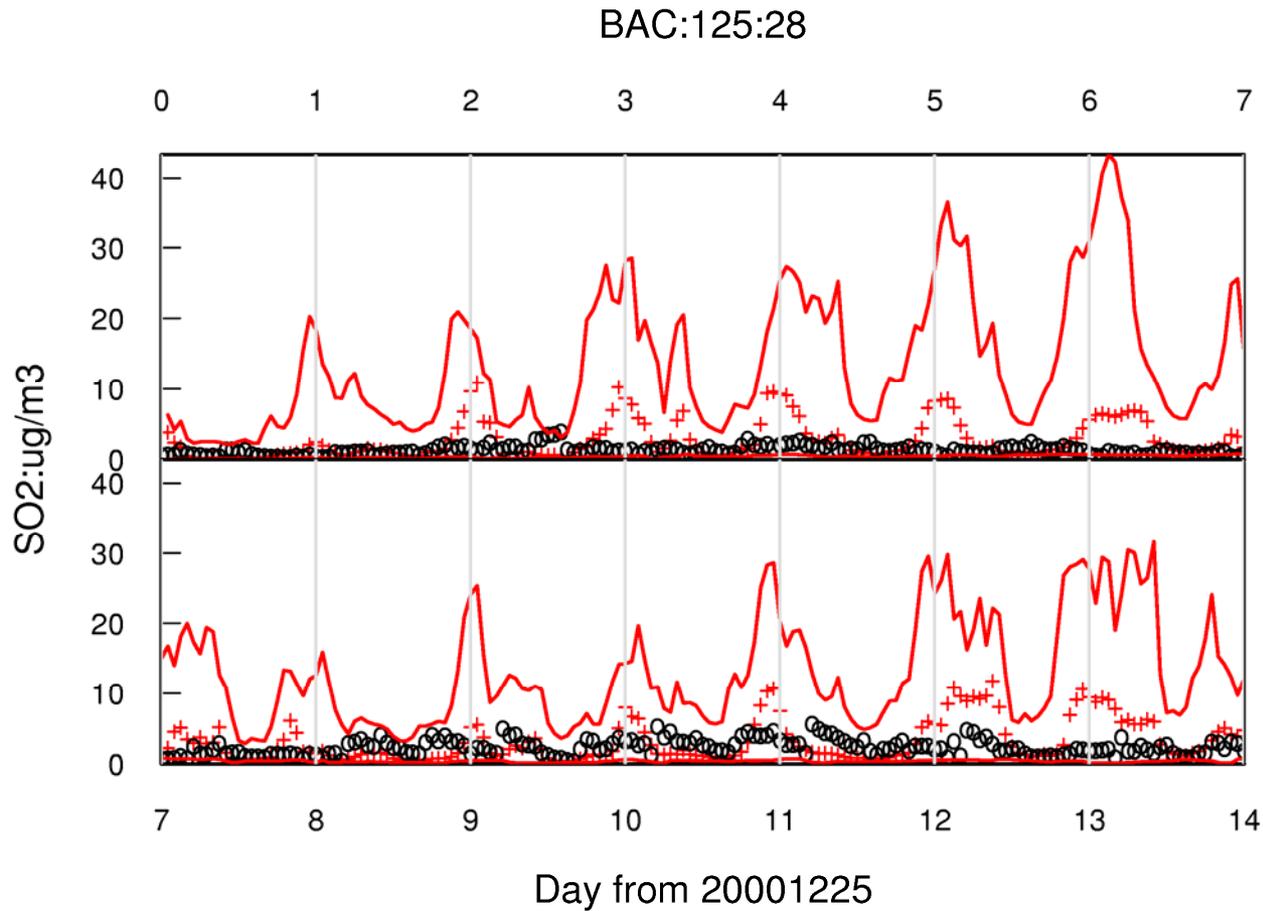
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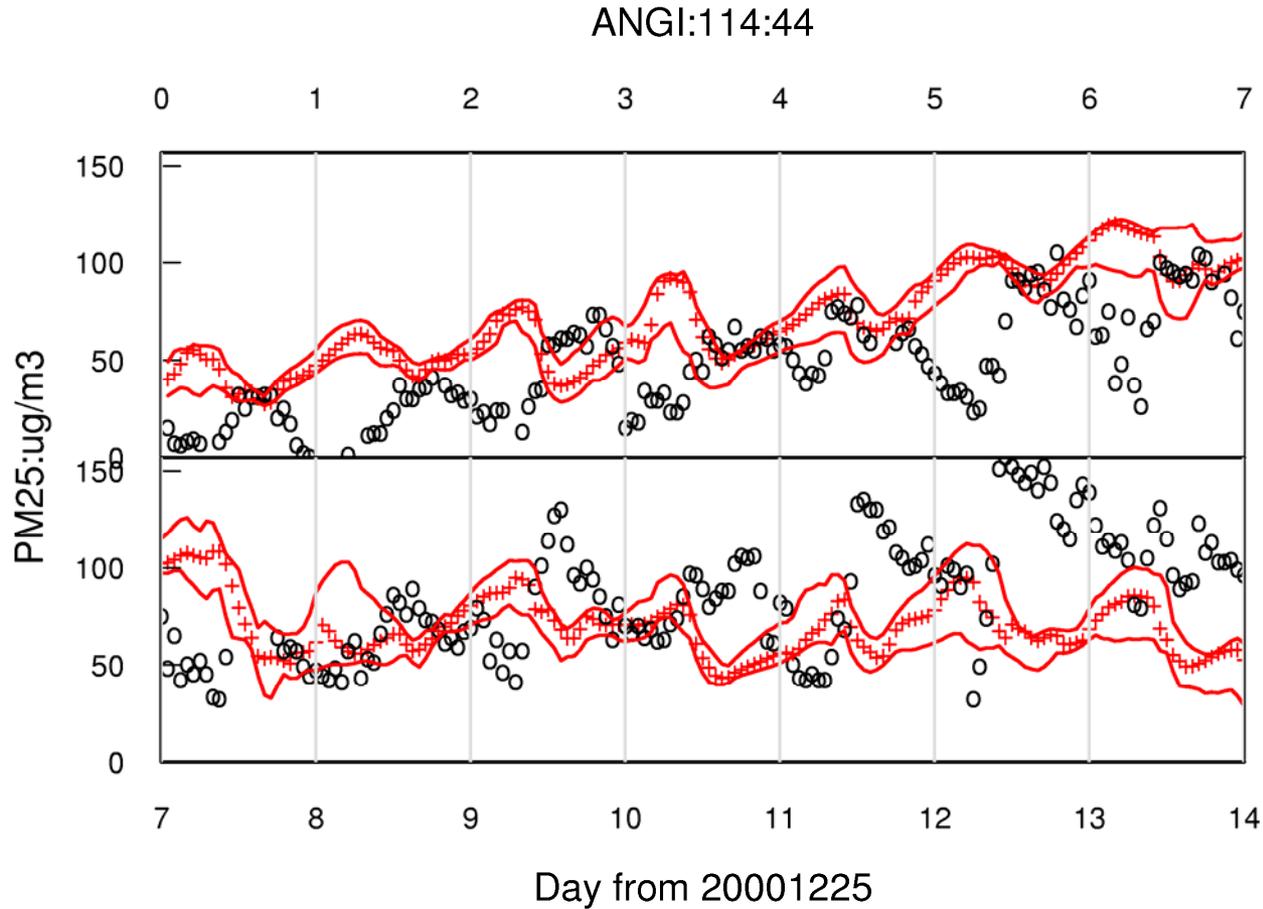


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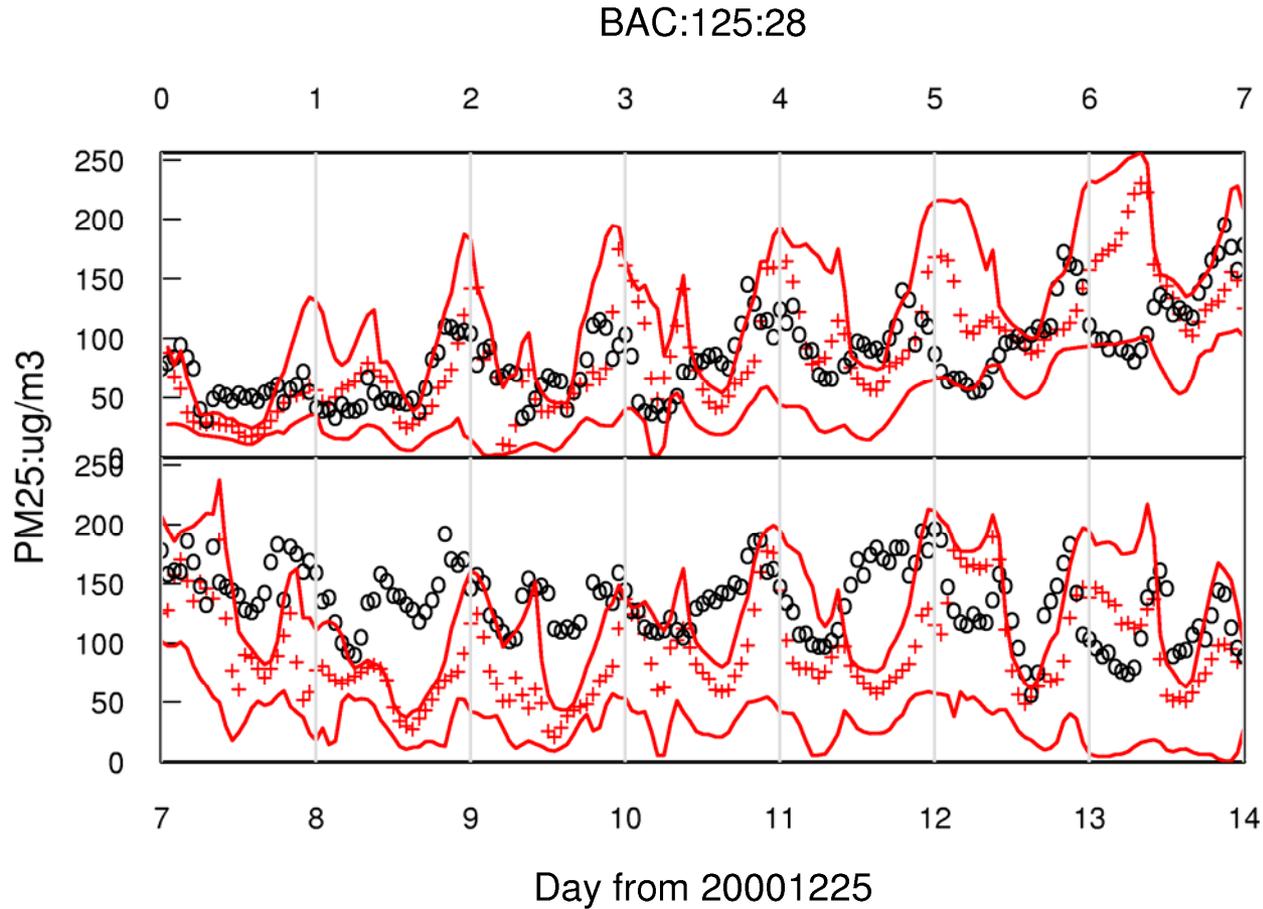


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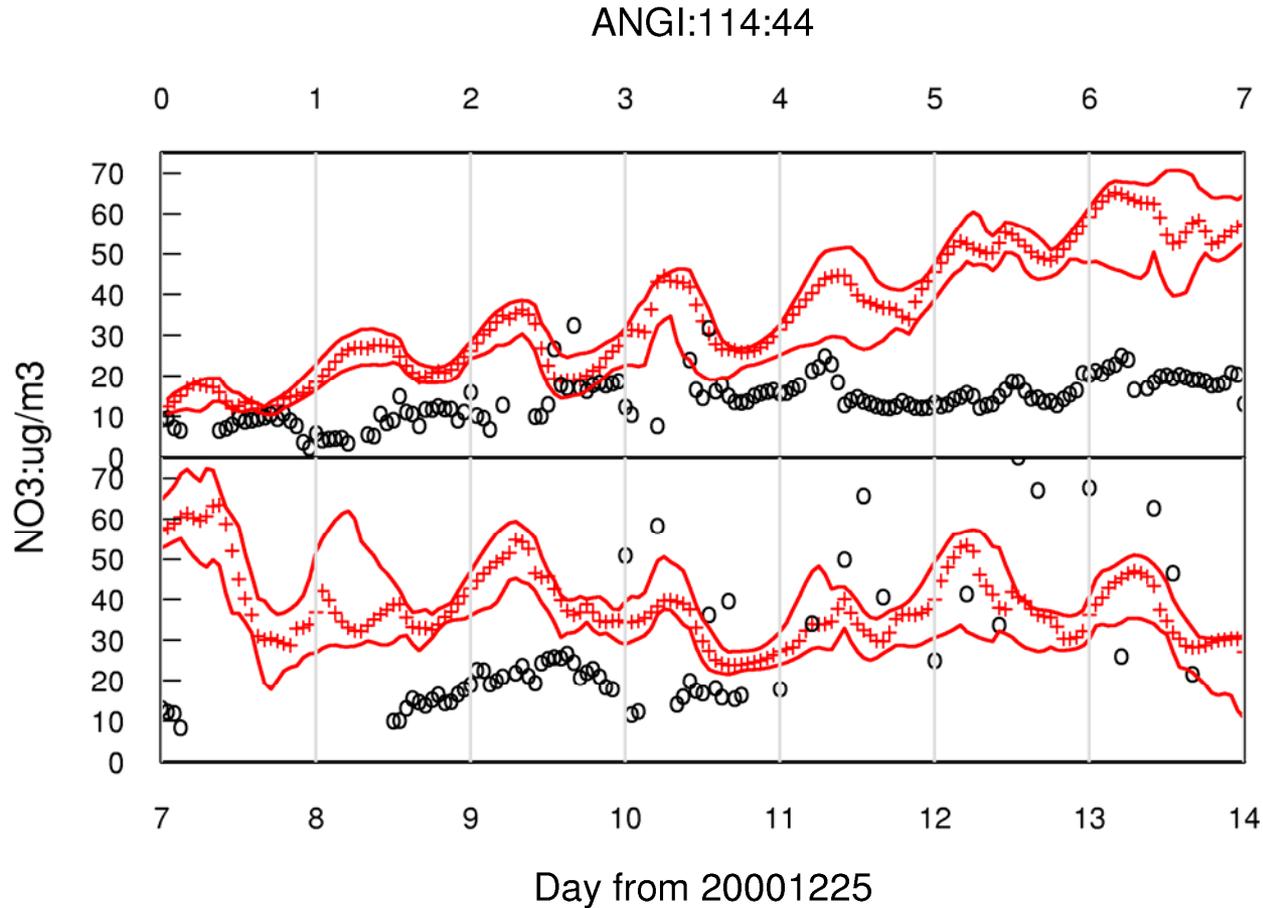


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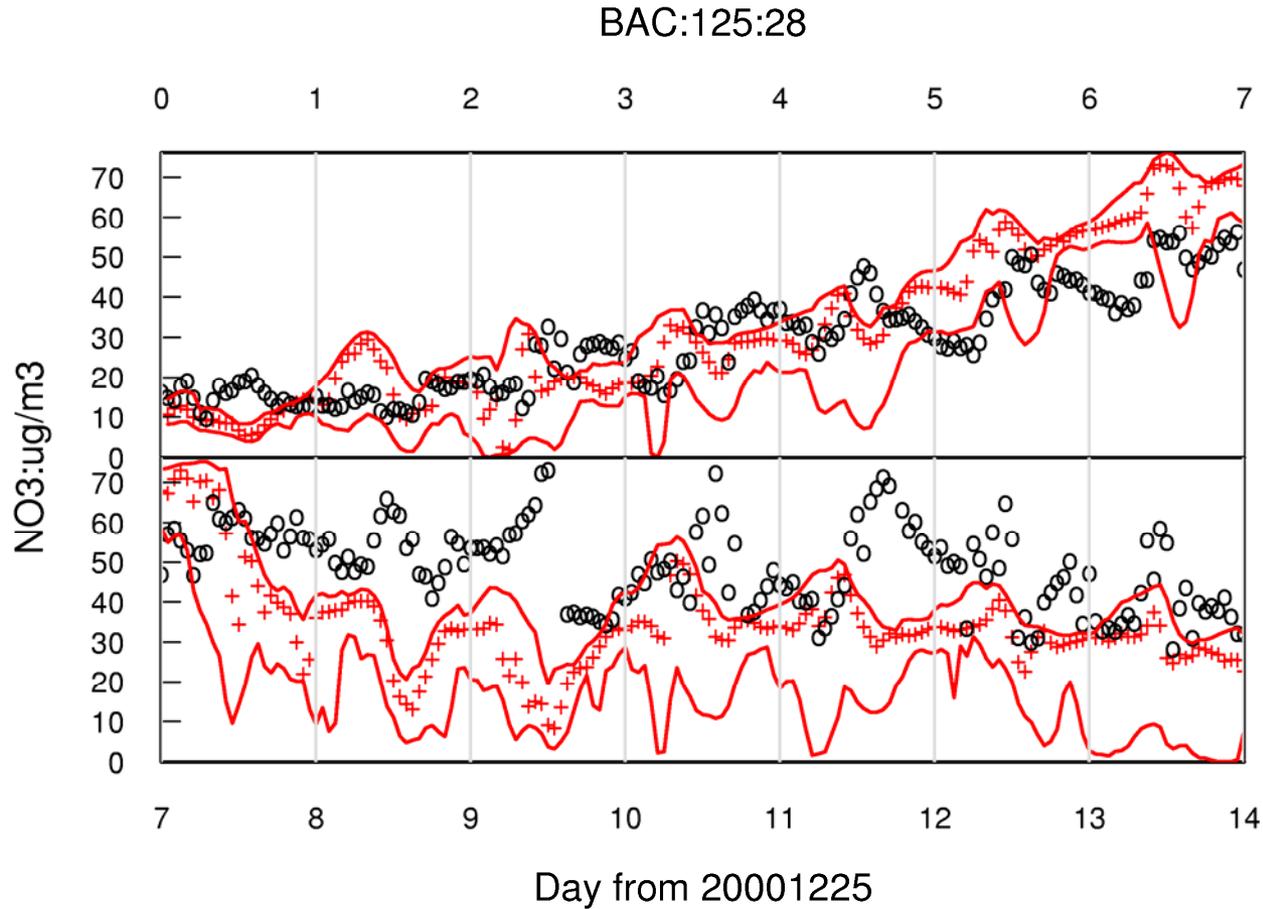


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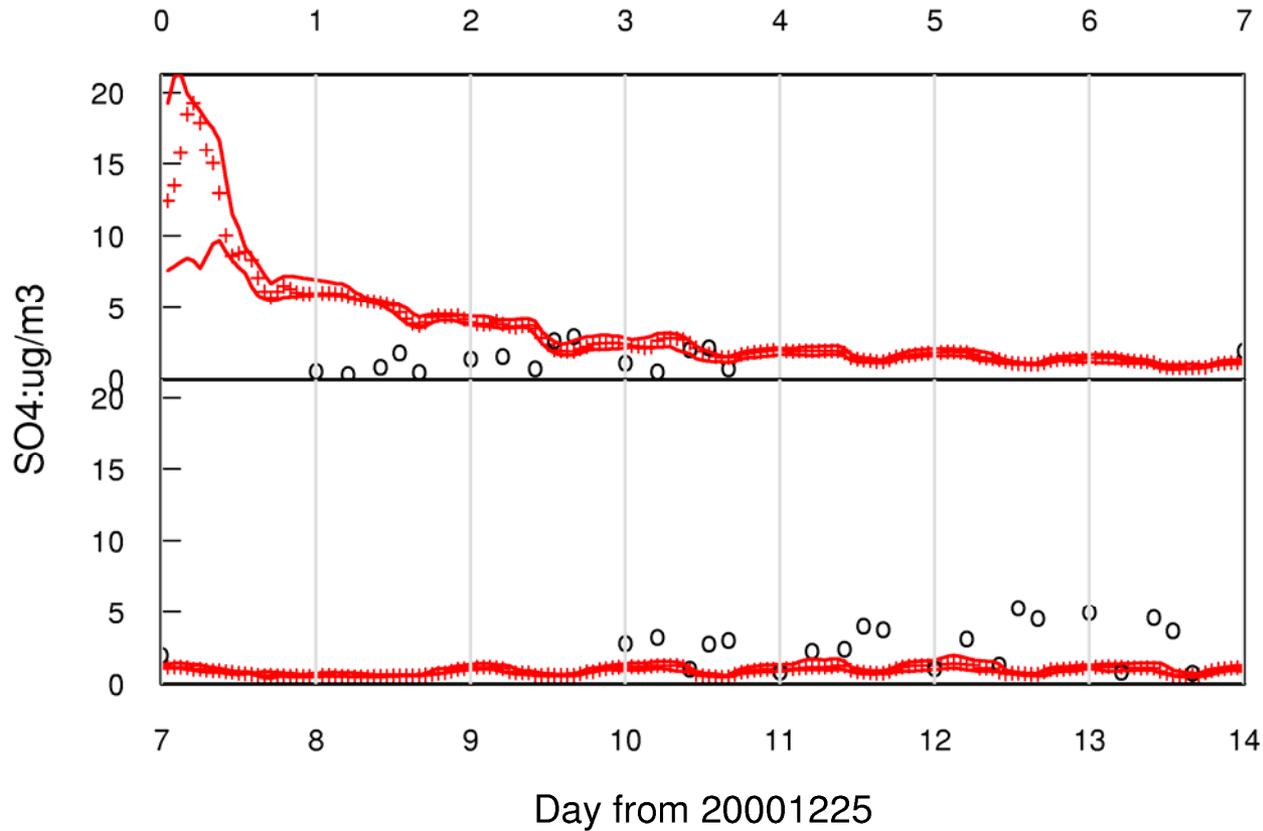
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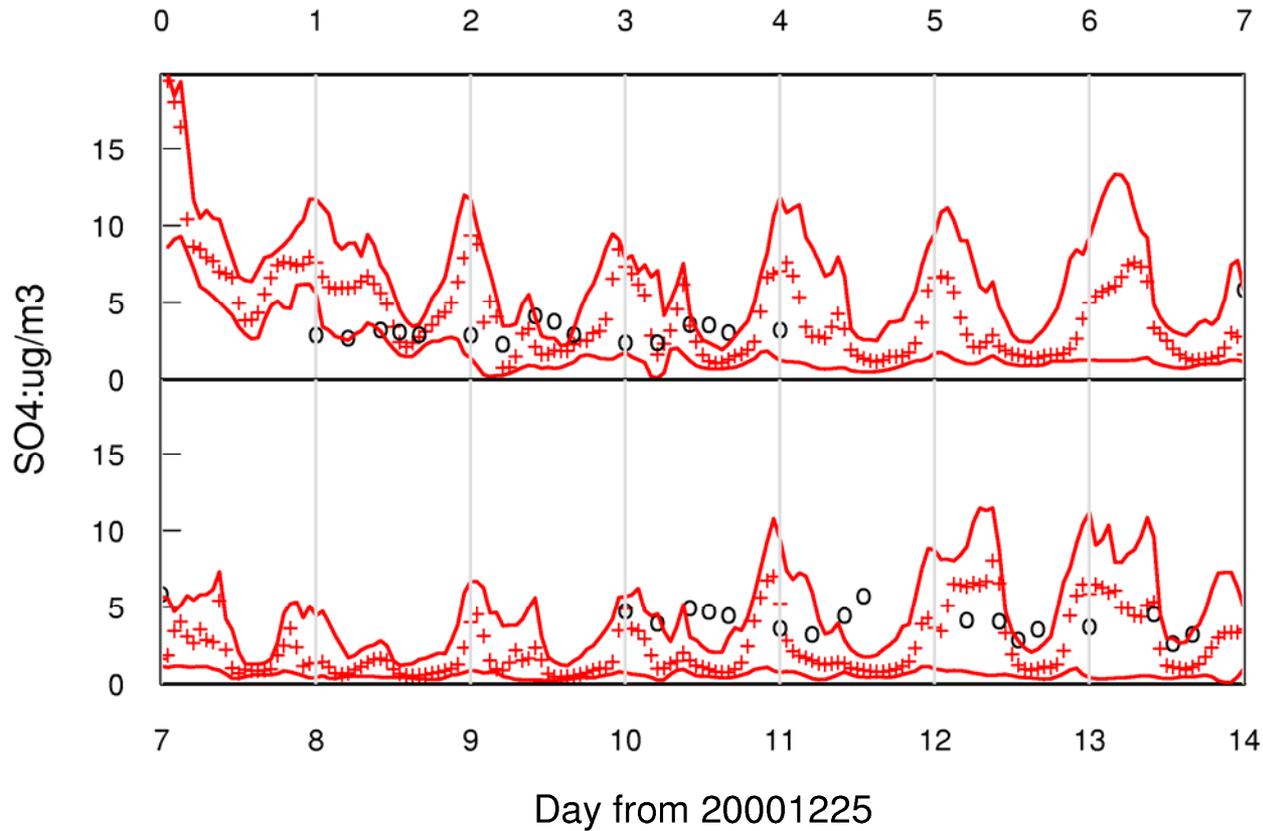
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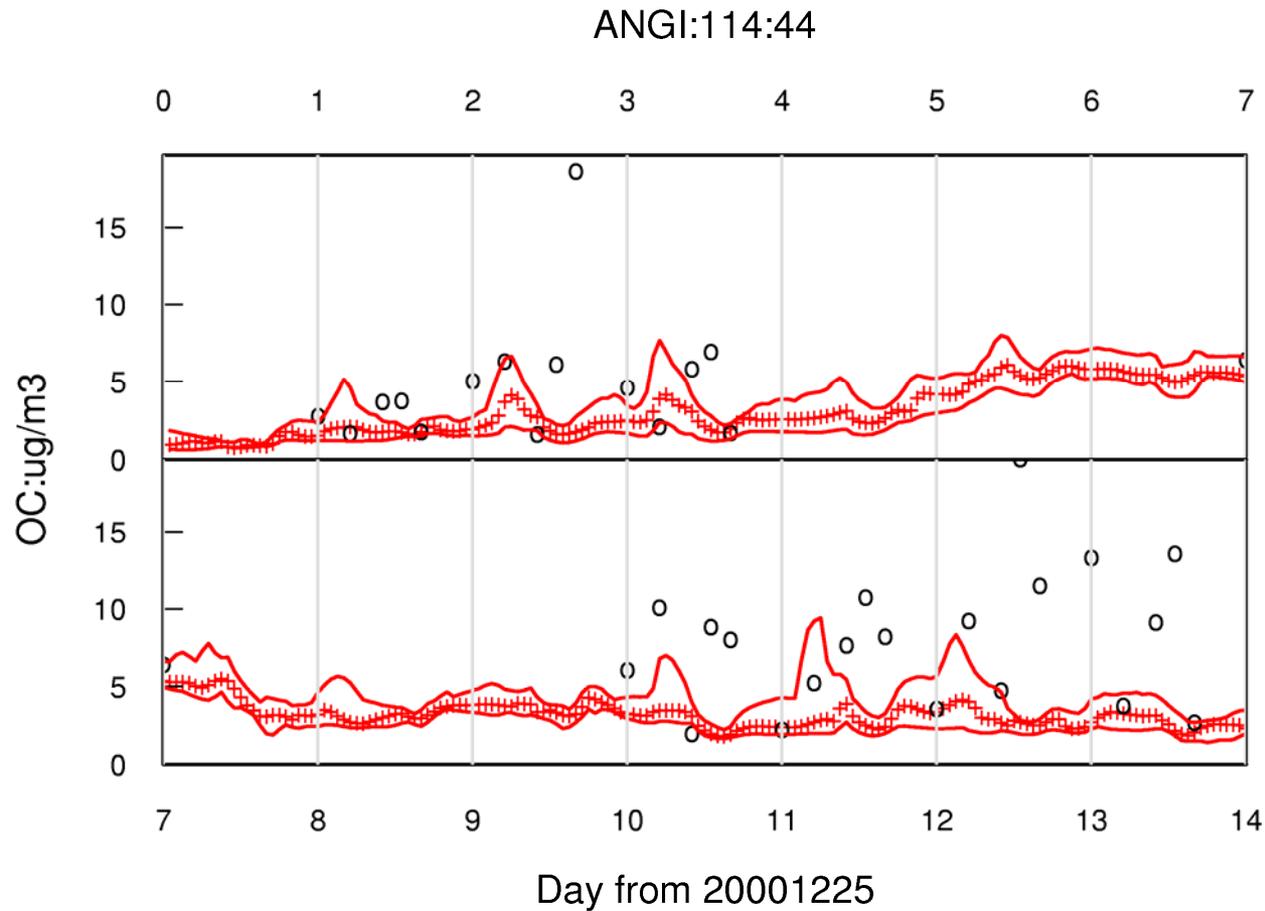
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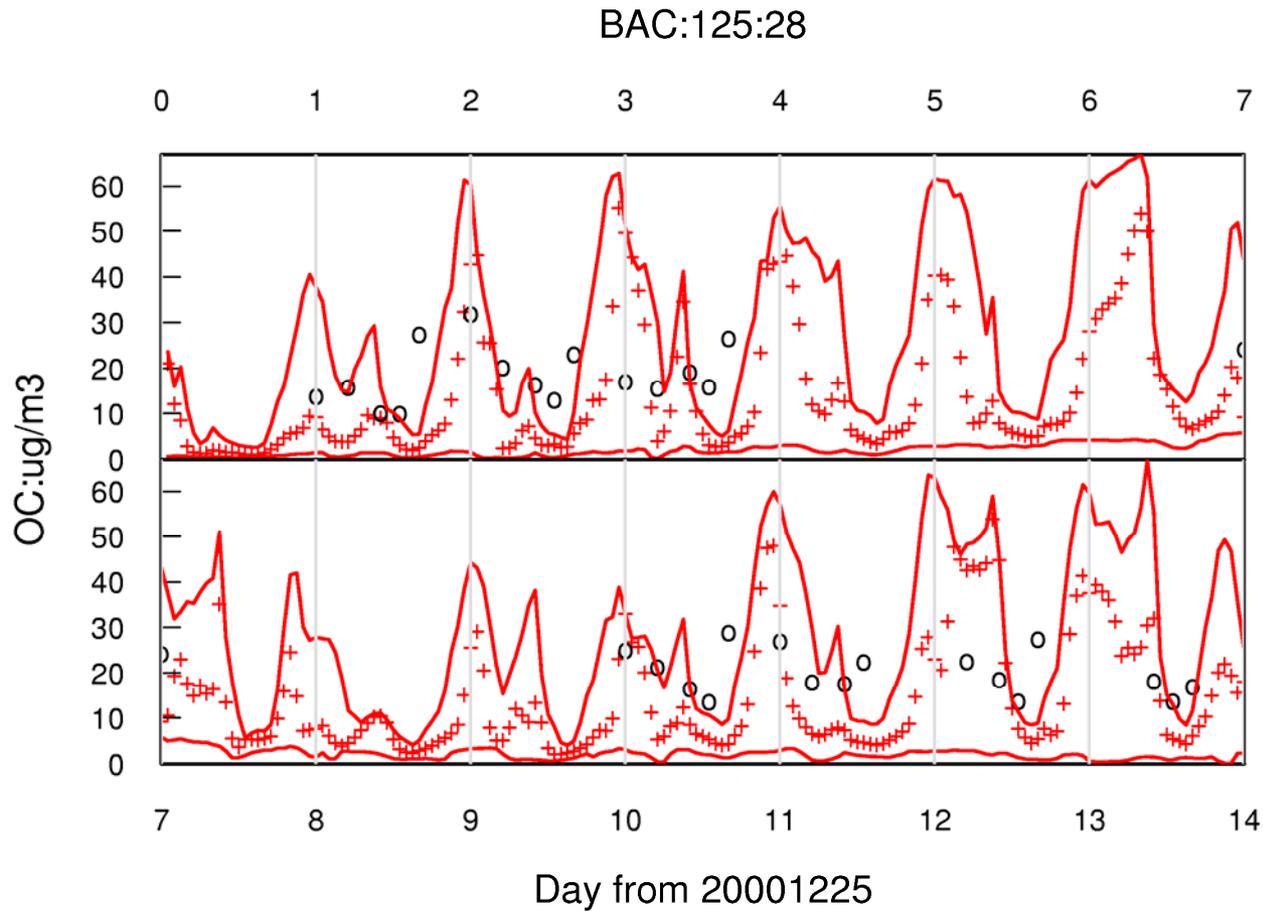


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Corroborative Analysis

- The NMFROC model
- A CMAQ case
- NMFROC diagnosis
- Improved results
- The efficiency of the NMFROC method



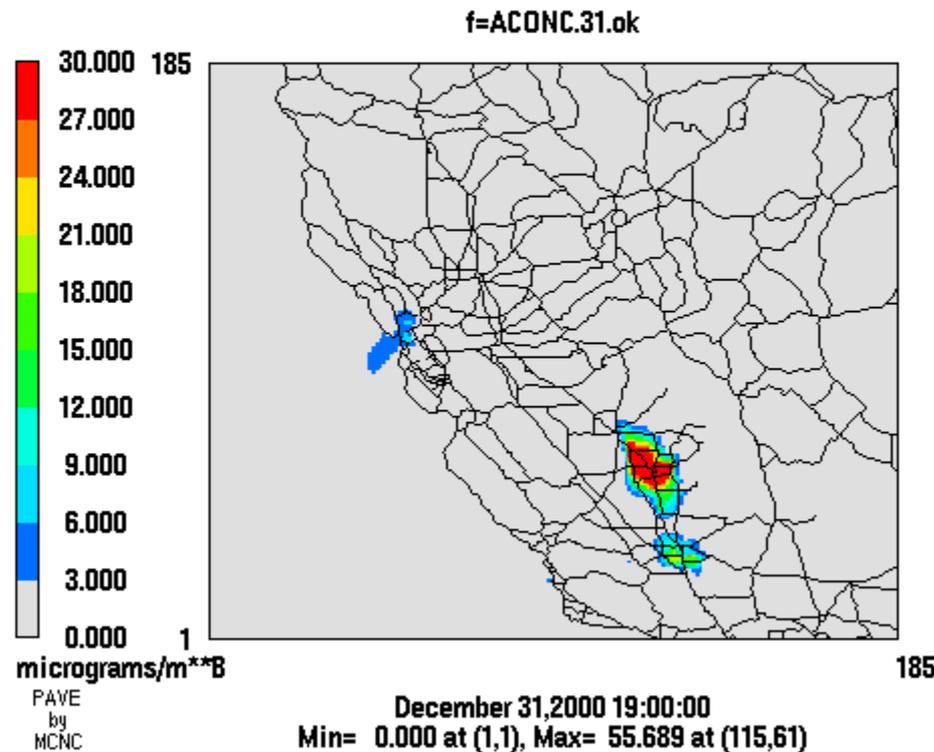
NMFROC Model: Functions

- $A [v, s] \rightarrow B [v, p] \times C [p, s]$; constraints
 - $A, B, C [i, j] \geq 0$;
 - $s > v > p$;
 - least squares error
- Features
 - Factorize large data matrix in a short time
 - Factors are as close to the interior of data set as possible
 - Input matrix must be non-negative, but no other assumption or inference



A CMAQ Case

Layer 1 ASO4Jf



Abnormally high
PM sulfate in
SJV



A CMAQ Case

- Symptom:
 - CMAQ sulfate was too high in Central Valley during CRPAQS 2000-2001 wintertime PM episode
- Possible causes
 - Emissions
 - Meteorology
 - H_2O_2 and/or O_3
 - Catalytic pathway
 - Others
- What can NMFROC tell us about it ?



NMFROC Diagnostics

- CMAQ inputs and outputs
 - Emissions of gas and PM species (34)
 - Key meteorological parameters (10)
 - Outputs of CMAQ species (32)
 - Two-week hourly data at three anchor sites
- Size of input matrix
 - $V = 76$, $S=1008$
 - 76608 elements



NMFROC Diagnostics Input matrix formation

- Problem 1
 - U, V, MOLI have negative values
 - Solution: coordinate shift
- Problem 2
 - Different units for emission, conc., and met.
 - Solution: similarity theory to remove the unit

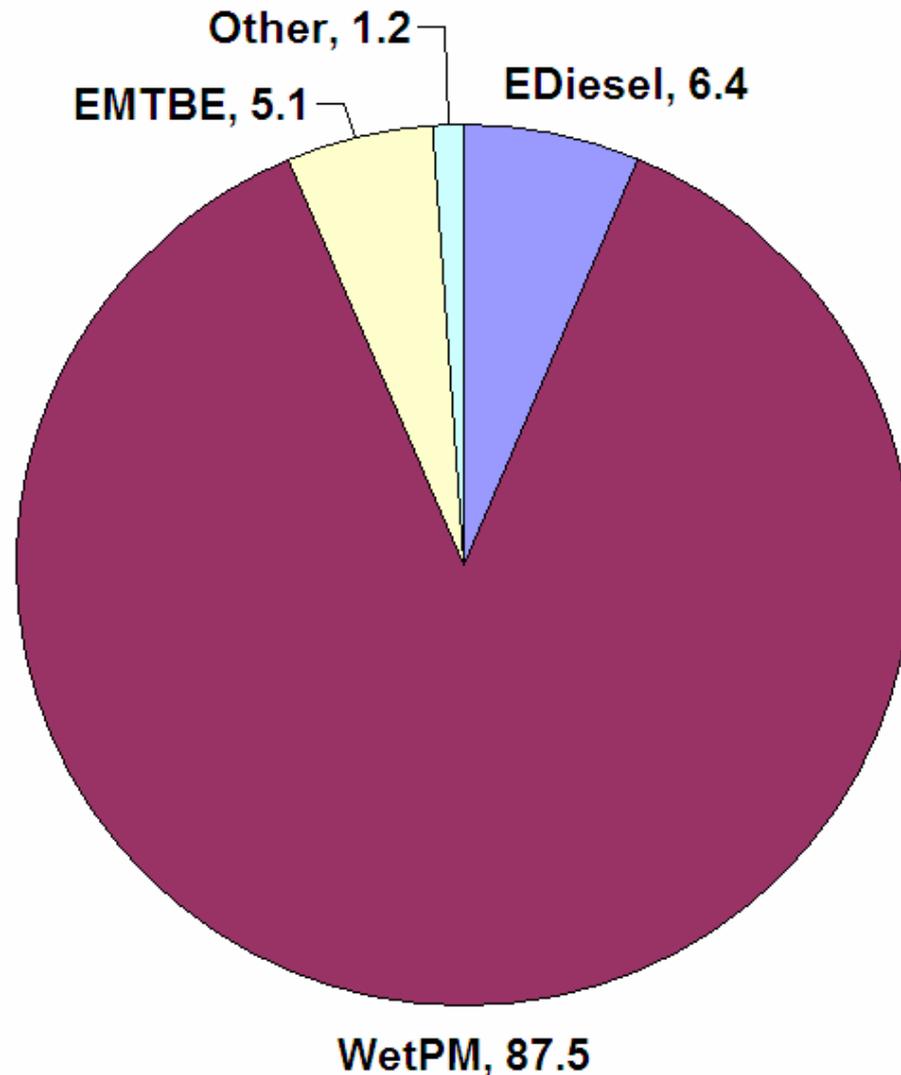


NMFROC Results: Factors

- Emission factors
 - (NO_x+PNO₃+PEC, MTBE+OLE2+SO₂)
- O₃ factors
 - Sunny (HNO₃, RGRND, PBL, ISOPRENE)
 - Rural (NH₃, D_m, σ)
 - Cloud aloft (CFRAC, PBL, PAN)
- Fog and rain factors (QC, CFRAC; QR)
- Wet PM factor (AH₂O, ASO₄)
- Plume factor (NO, SO₂, AORGPA)



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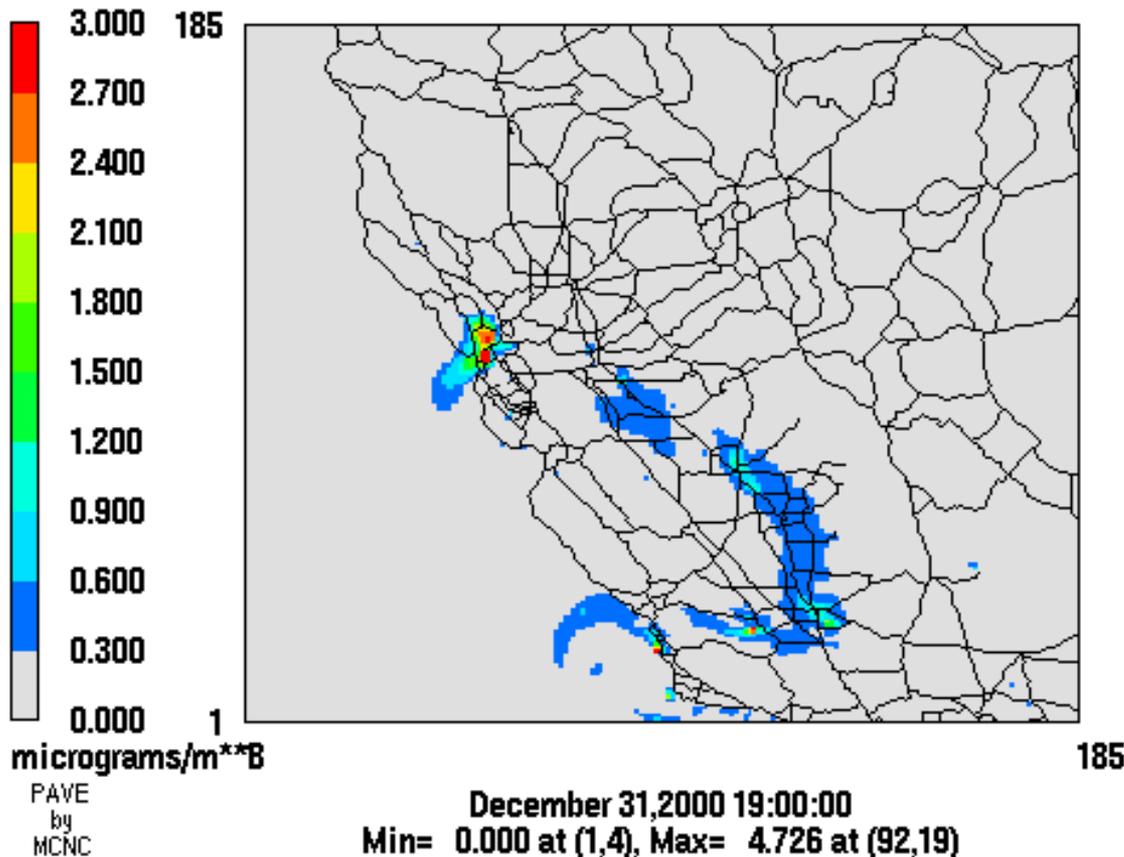
**Contributions
(%) to CMAQ
PM SO₄ in slide
6 at BAC site
(P/O=1.28)**



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Layer 1 ASO4Jy

y=ACONC.31.DMS

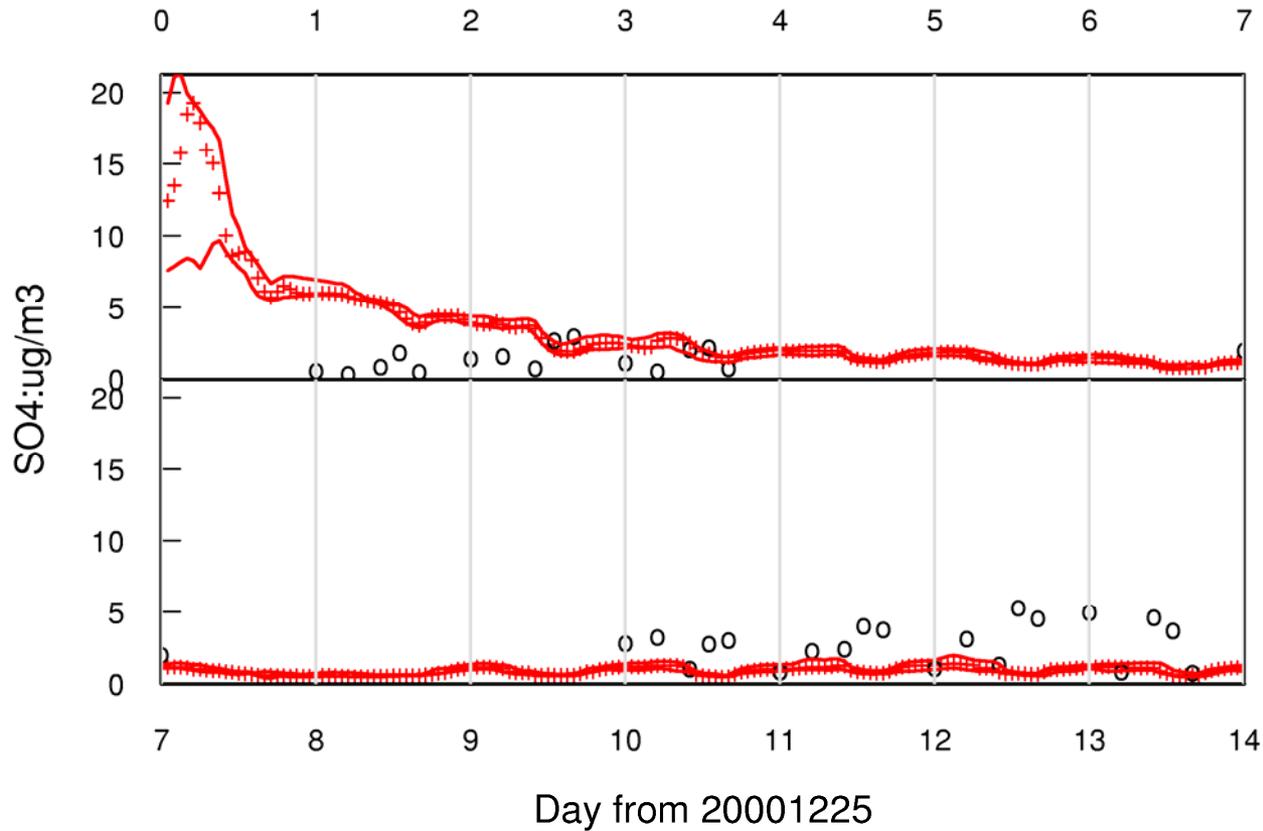


- Limit PM H₂O ≤ 0.1 g m⁻³
- Turn catalytic pathway off
- PM SO₄⁼ reduced by ~ 10 folds (≈ slide 11)



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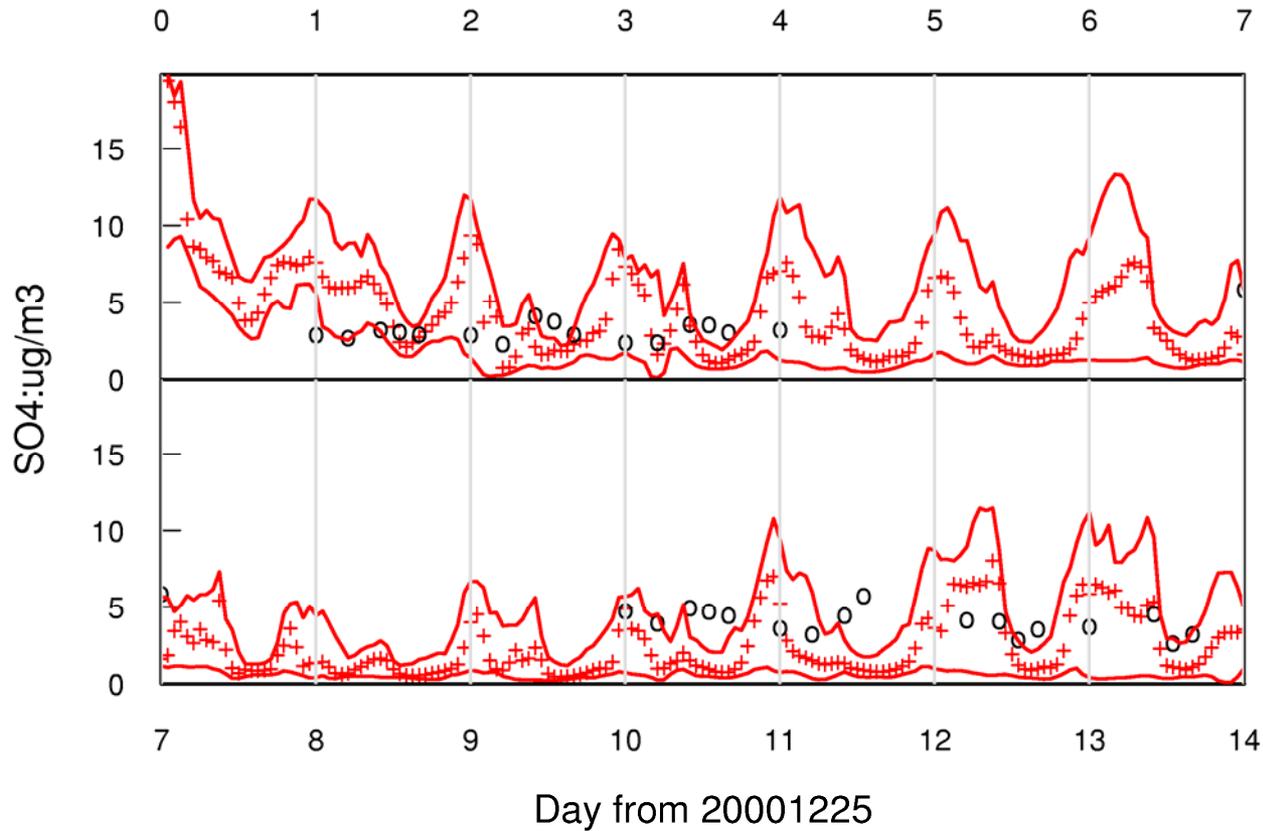
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Summary

- 48 winter simulations were conducted
- All PM components and precursors are evaluated against observations
- Corroborative analysis tools are employed
- More detailed look at input emissions, meteorological parameters, and observations



Future Directions

- Model improvements in (the) future
 - Boundary conditions from GEOS-CHEM
 - Alternate chemical mechanisms (e.g., CACM)
 - Internal+external mixing states, size bins
- Meteorology improvement and episode extension
- Quality assurance
 - Meteorological inputs
 - Emission inputs
 - Observed data



END of Presentation

- Question/Answer