A Seasonal Perspective on Regional Air Quality in Central California

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CCOS Technical Committee Meeting

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Team Members

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- <u>NOAA:</u> Jian-Wen Bao, Sara Michelson, Jim Wilczak

Research Objectives

- Use CMAQ with state-of-the-art emissions, meteorological, and chemical inputs to model ozone in Central California for summer 2000

- Estimate how regional control strategy options for both 1-hour, 120 ppb, and new 8-hour, 80 ppb ozone standards change with respect to time and location

Task Structure--Overview

- **Task 1 – Develop modeling protocol**
- **Task 2 – Prepare model inputs**
  - 2.1 Meteorological
  - 2.2 Emissions
- **Task 3 – Conduct AQ modeling**
- **Task 4 – Model results analysis**
  - Evaluate analysis methods
  - Diagnose pollutant responses to precursors

Task 2.2: Emissions Inventory Development

Emission files:

CARB (area, biogenic, point, fire)
UC Berkeley (motor vehicle, biogenic)

Provided on 190x190 grid with 4 km resolution

Hourly temporal resolution

Chemically speciated into SAPRC99

Emissions (for 7/24 - 8/8/2000)

Category	Date-specific	Day-of-week specific	Obtain from	Comment
Area		X	CARB	
Motor		X	UCB	
Biogenic	X		CARB UCB	Date-specific due to meteorology
Point	X		CARB	Date-specific due to Smoke 2.1 plume-rise
Fires	X		CARB	Only available for IOP2 five days. Smoke 2.1. Zeroed for current 15-day simulations

Task 3: Air Quality Modeling

- **CMAQ V4.5 air quality model**

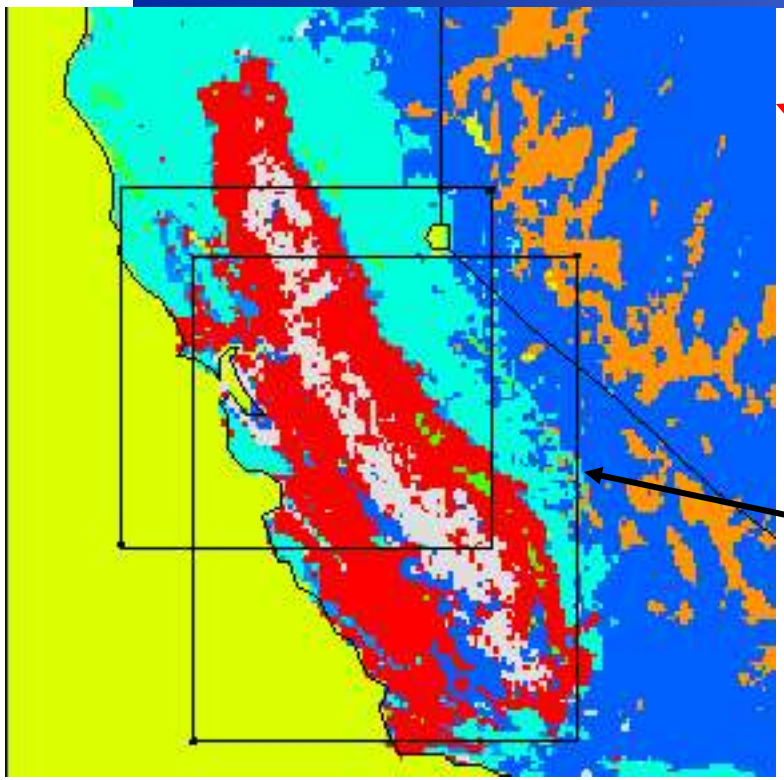
- **Simulation details**
  - Domain and resolution
  - Inputs (meteorology, emissions, boundary and initial conditions)

Computational details
  - LBNL Linux Cluster
  - CPU times and memory requirements
  - Estimates for 120 day run

CMAQ V4.5 (2005)

- Parallelized, F90, Linux, faster than CMAQ V4.3
- Chemistry:
  - SAPRC99 chemistry
  - Euler Backward Iterative (EBI) solver
  - Smvgear stiff solver
- Improved advection results in better mass conservation
- Improved vertical diffusivity algorithm

SARMAP domain within CCOS domain



CCOS
4km res.
190 x 190

SARMAP
4km res.
96 x 117

Vertical resolution: 27 layers.
Lowest layers: 20m thick
Uppermost layer at P=100 mbar, (16km) is 2km thick

Initial and Boundary Conditions

Initial condition files are created by 72 hour spinup runs using the appropriate boundary conditions and day-of-week specific emissions

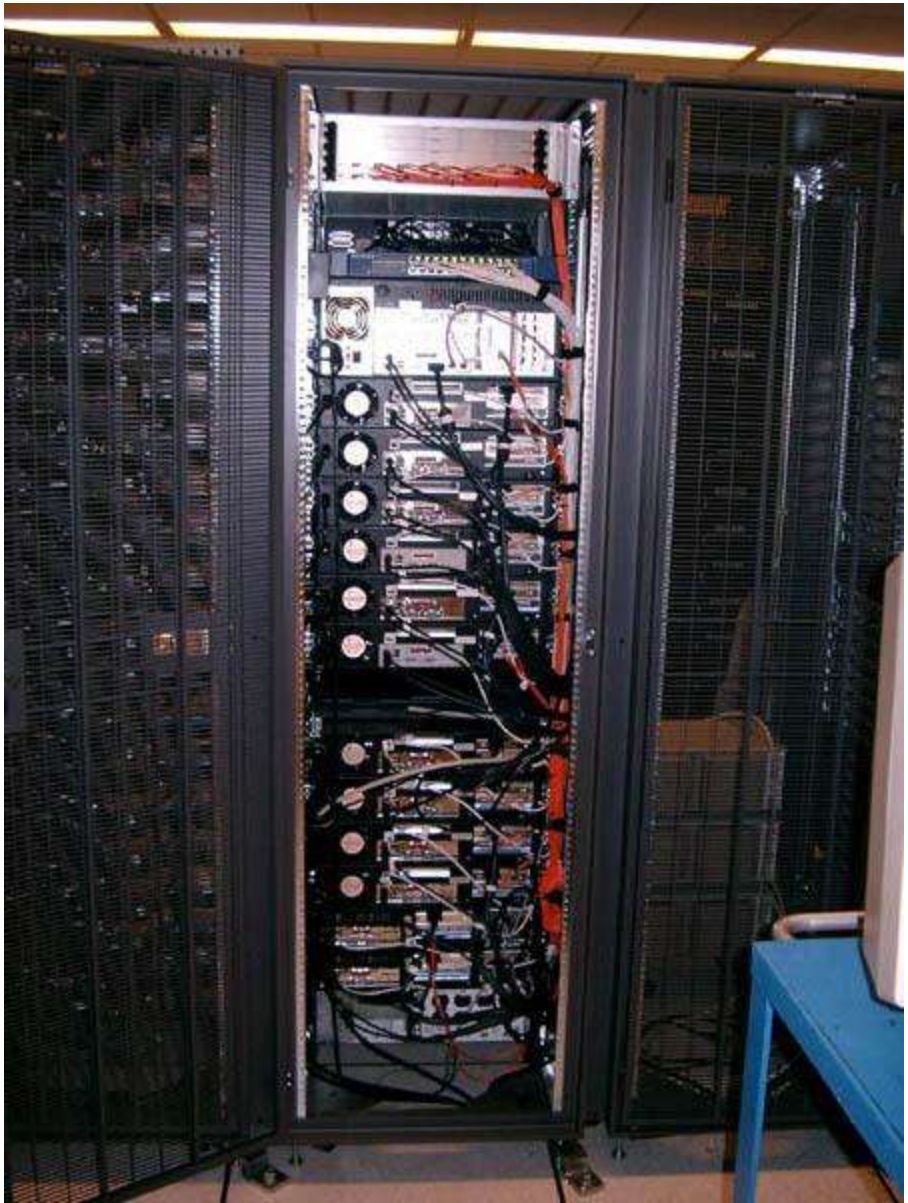
Selected boundary concentrations (in ppb)

Species	Western BC	Other BC
CO	200	200
NO	0.05	0.05
NO2	1	1
O3	22 - 70	40 - 70
ALK1+2	7	12.5
OLE1+2	0	0.7
Aldehydes	2.5	2.5

Computational Details

The "Mariah" Linux Cluster

- Provided by DOE
- Maintained by LBNL under the Scientific Cluster Support Program.
- 24 nodes, (2 processors and 2GB RAM per node)
- Centos Linux (similar to Red Hat Linux), run in a Beowulf-cluster configuration



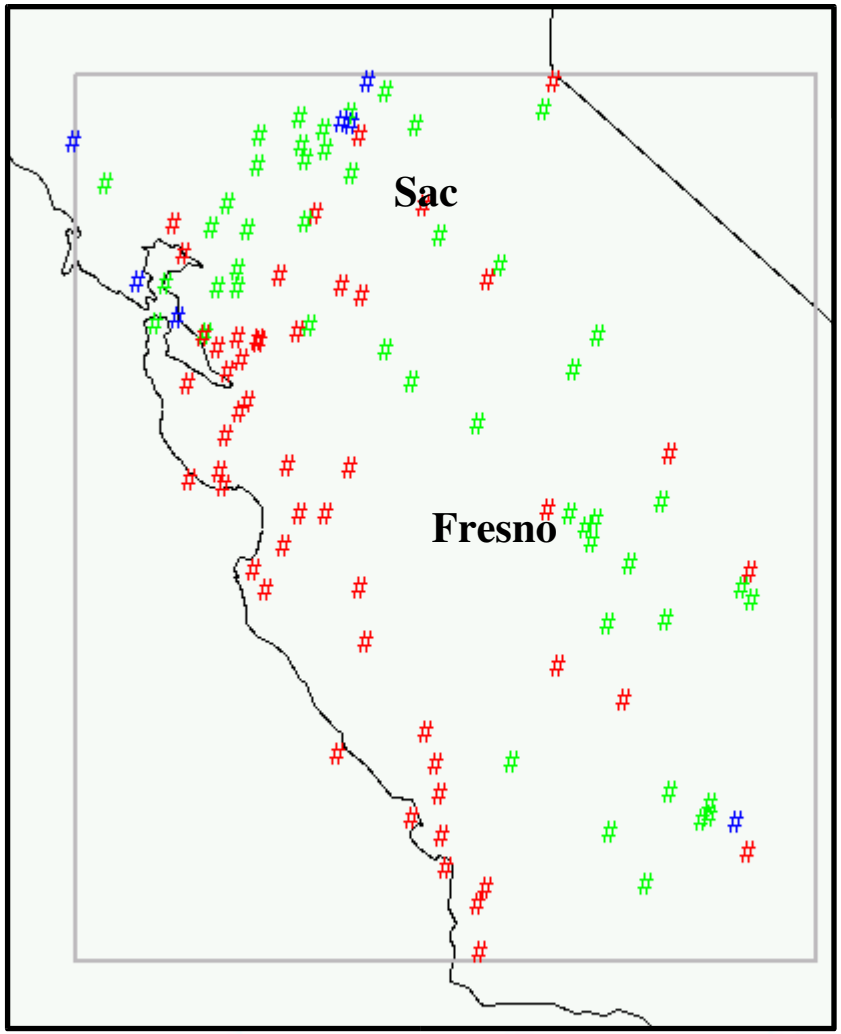
Computational Details

- Split the grid 3 ways in each direction and use 9 processor elements (PE's):
- Current run-times (96x117 domain):
  - 5-day run takes 48 hours with Gear solver
  - 5-day run takes 6 hours with EBI solver
- Projected seasonal run-times (190x190 domain):
  - 120 day run (EBI) will take 461 hours (19 days)
  - This can be accomplished in 70 hours by x8 splitting of the simulation period

Memory Requirements

File	Grid	days	Size	Comment
Meteorological	96x117	15	8GB	
Emissions	96x117	15	7GB	
Output Concentration	96x117	15	2GB	15 species
Meteorological	190x190	120	204GB	
Emissions	190x190	120	180GB	
Output Concentration	190x190	120	51GB	15 species

Spatial distribution of O3 normalized bias



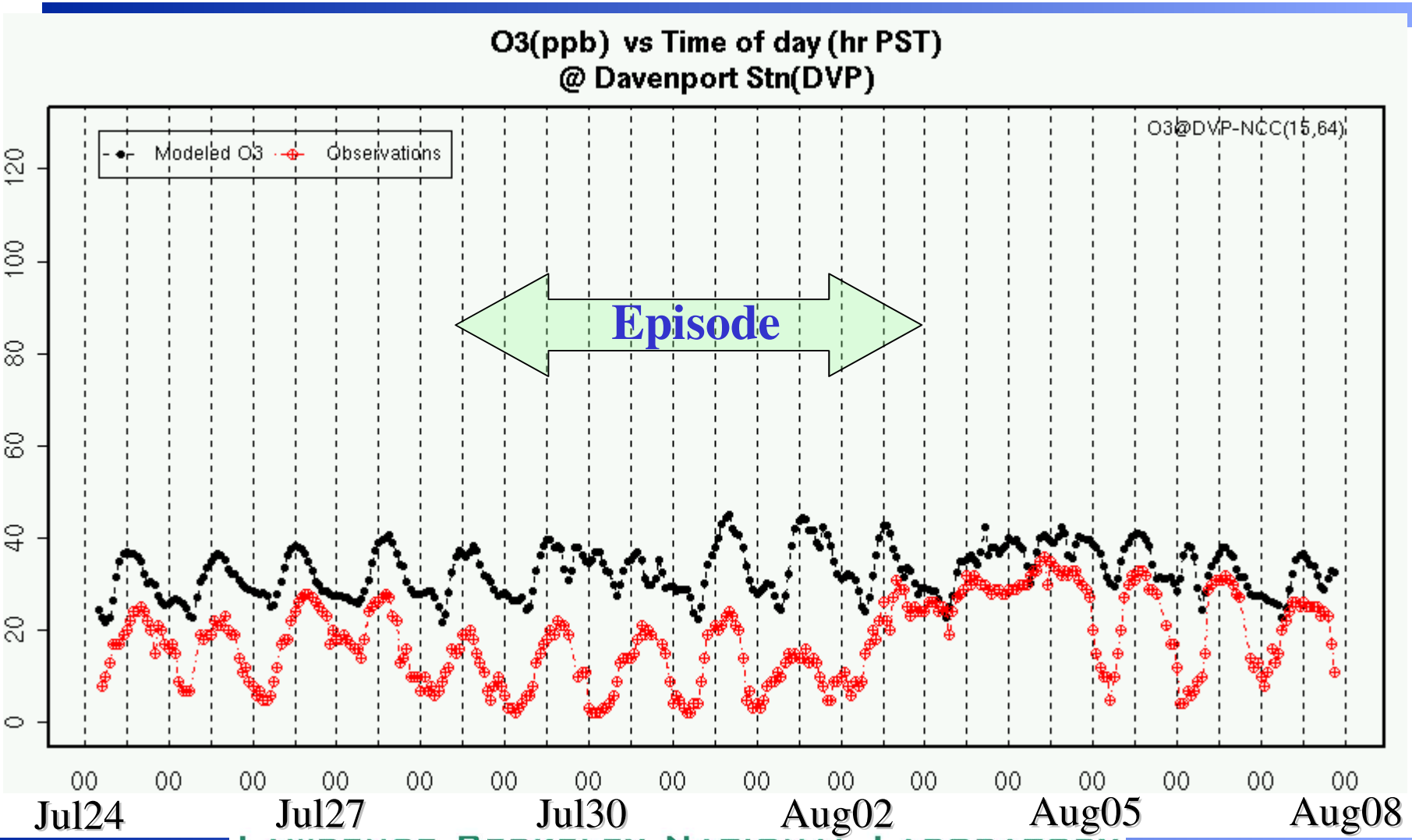
#: < -15%

#: -15 to 15%

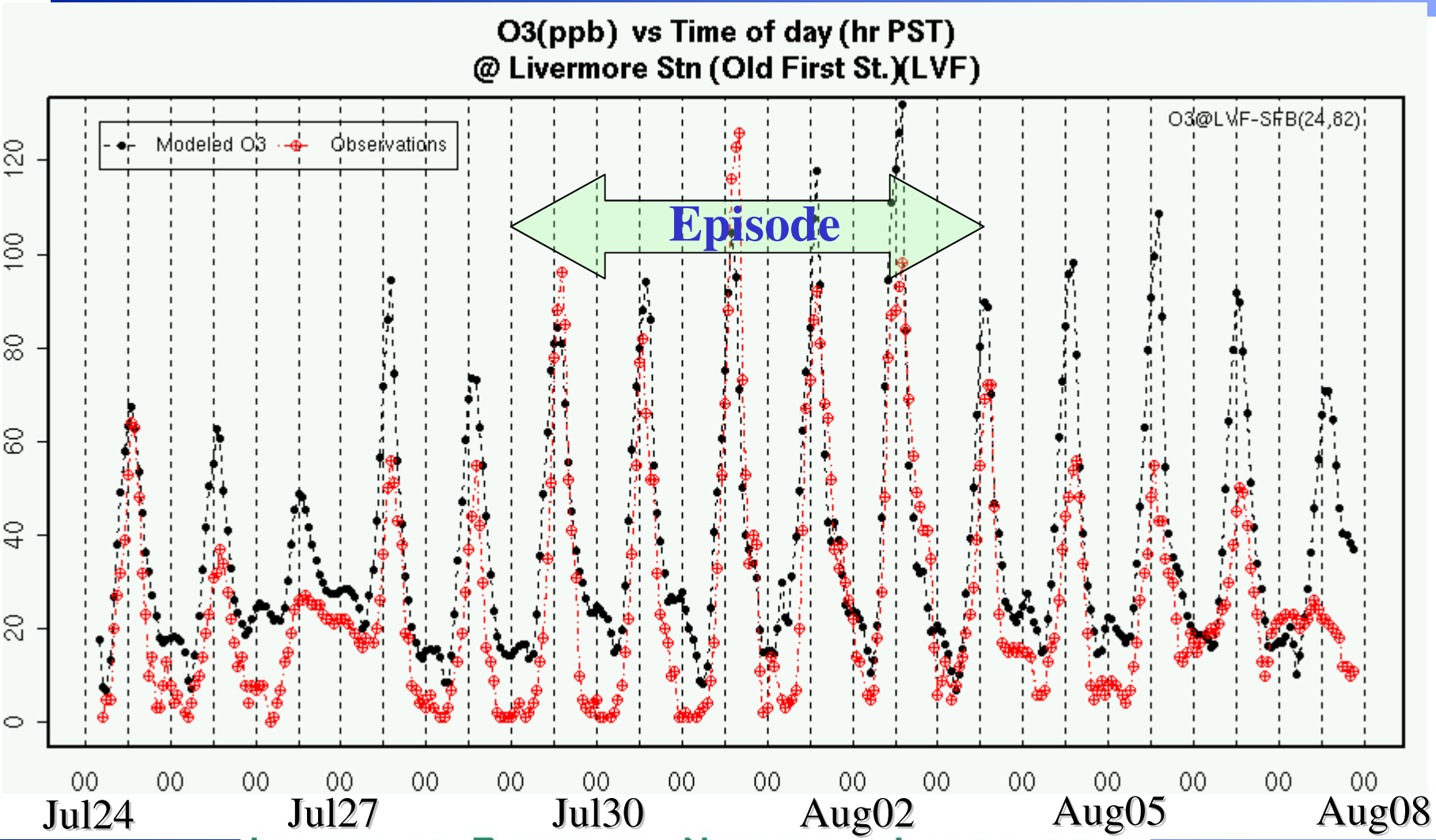
#: > 15%

cutoff at 25%

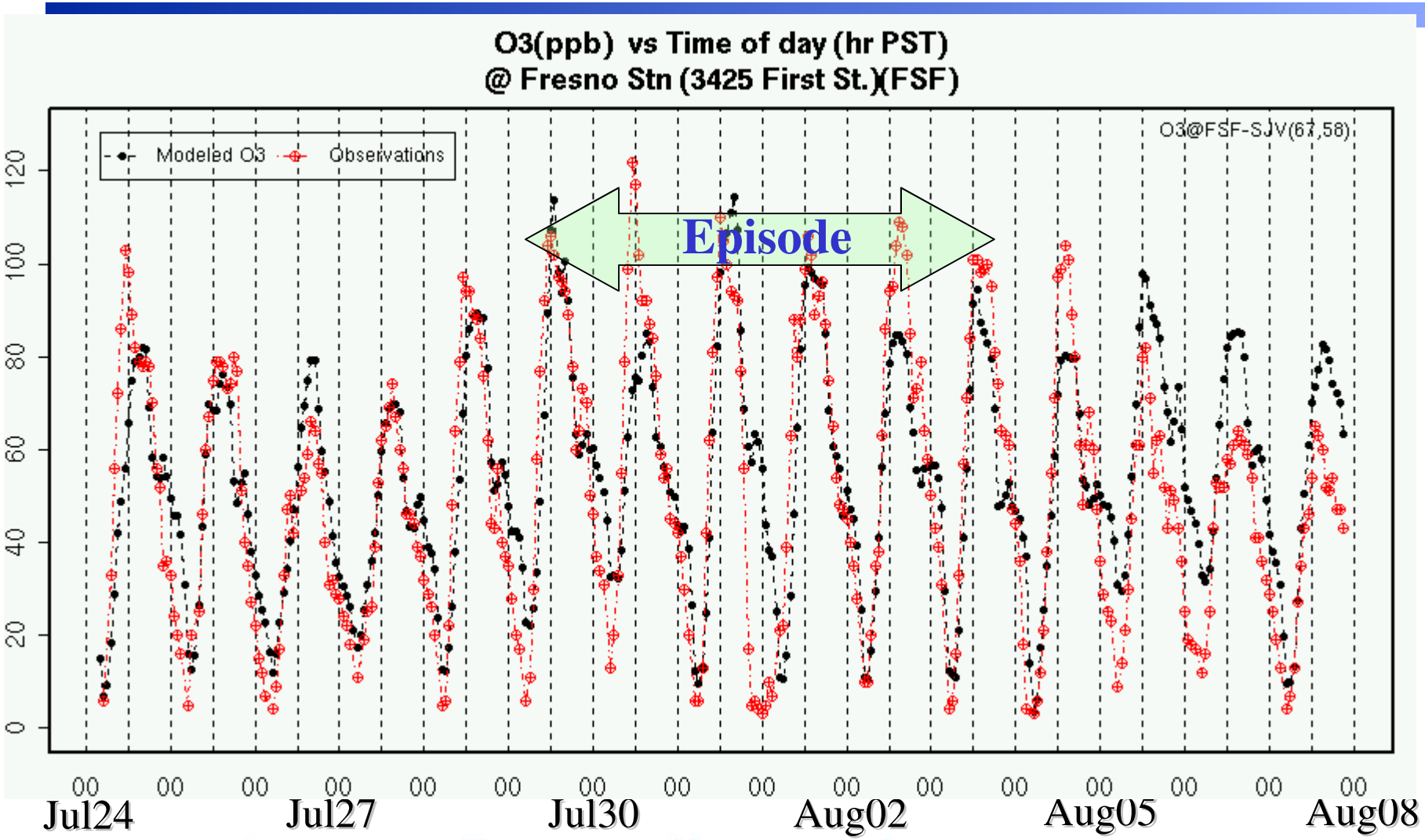
15-day ozone time series (north central coast)



15-day ozone time series (Livermore)



15-day ozone time series (SJV)



Task 4: Model Results Analysis

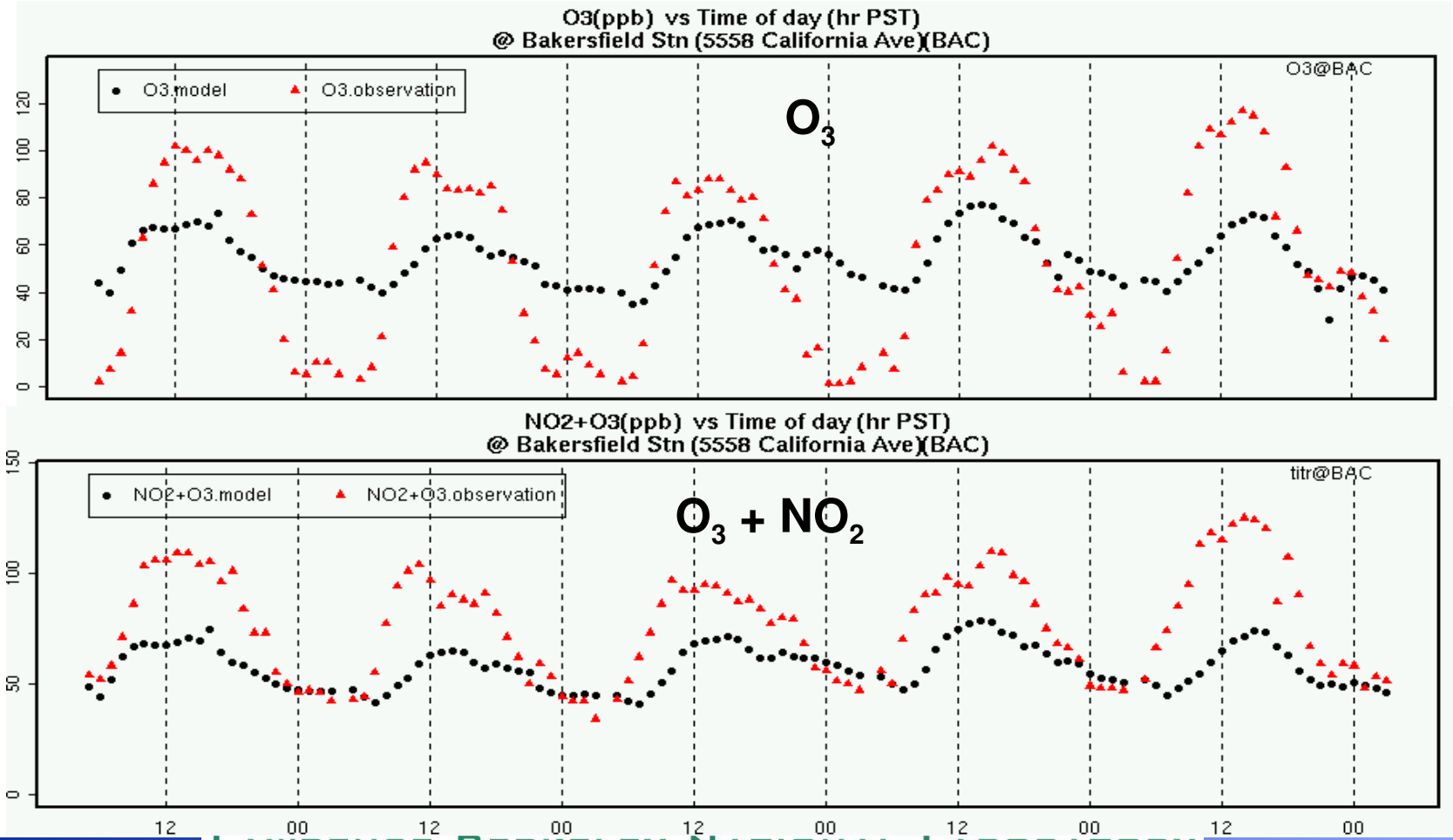
- Large emphasis on analysis tools used in concert
- Statistical tools
  - Physics analysis workstation (PAW), time series analysis, clustering of modeling results
- Sensitivity Analysis
  - DDM for emissions, boundary conditions, initial condition
- Process Analysis

5-day Diagnostic Simulations

- **Effect of different versions: CMAQ V4.3, V4.4, V4.5**
- **Met. diagnostics**
  - Nudged vs. un-nudged
  - Averaged met. wind fields vs. instantaneous
- **Other diagnostics**
  - Titration: compare to O_3+NO_2
  - Coastal overestimation of O_3:
    - O_3 deposition to ocean?
    - Effects of changing boundary conditions?
    - Light attenuation
  - Photochemistry albedo effects

Night time Ozone Titration: $O_3 + NO \rightarrow NO_2$

Red: Observations **Black: Model predictions**

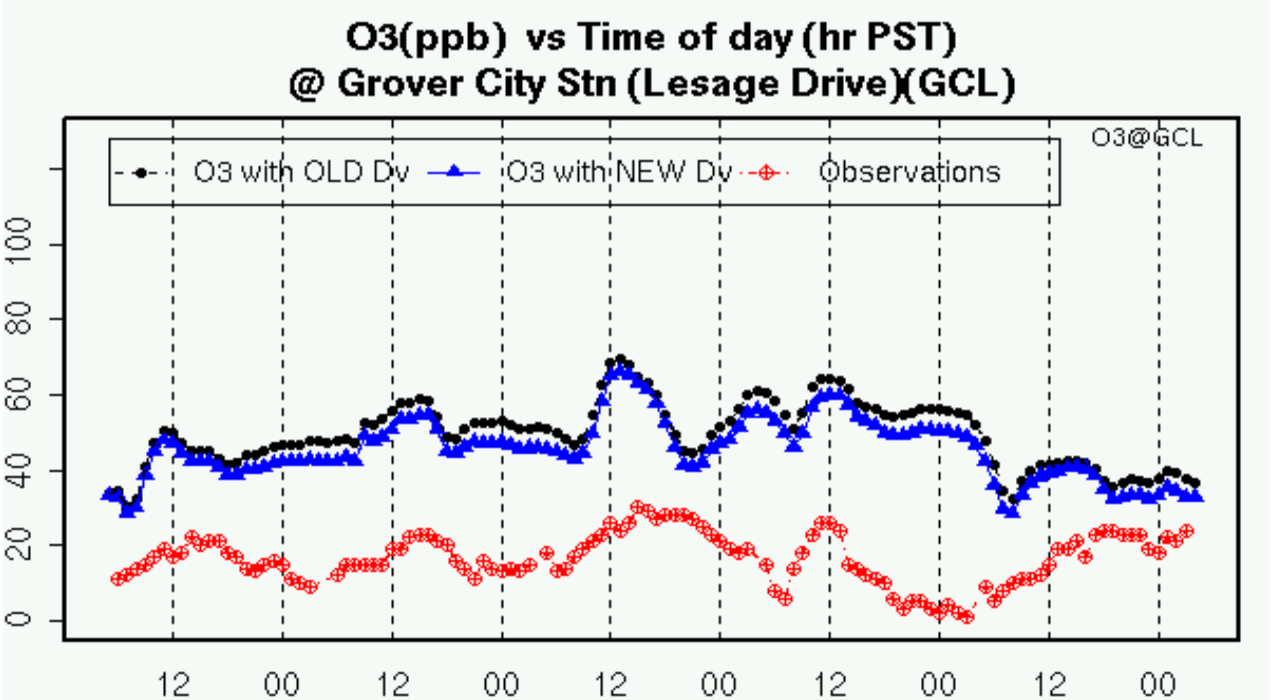


Ocean deposition

Coastal sites overestimate O_3 in CMAQ

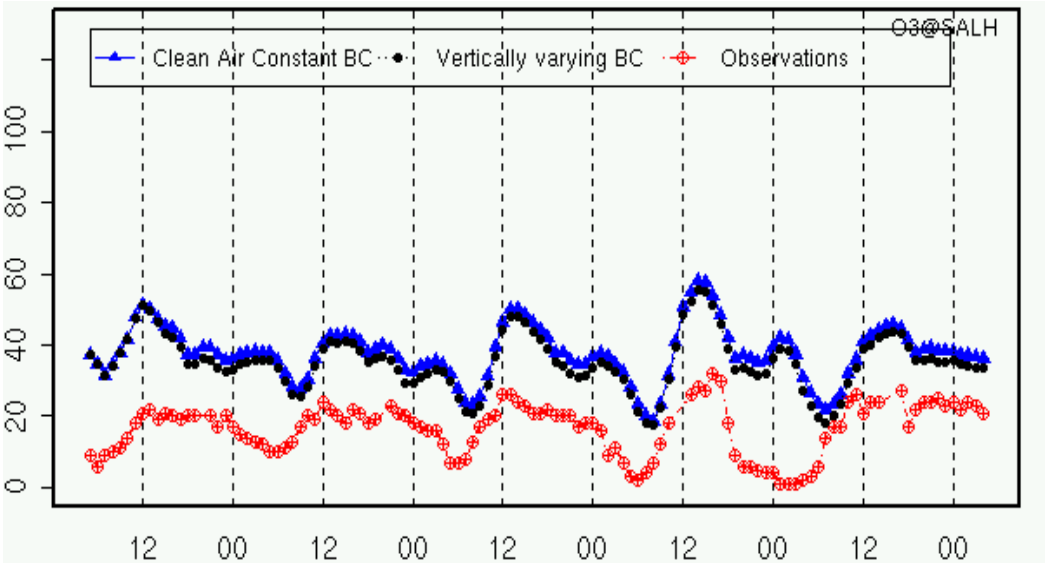
Dry deposition to ocean too low in CMAQ

Reasonable deposition velocity of O_3 to ocean: 0.05 cm/sec



Vertically varying O3 BC

•Observations
•BC clean air-constant
•BC vertical varying



Coastal Sites

•~2-5ppb lower
•Correct direction but problem not fixed

Photochemistry: Albedo Effects

(Change seen in SF Bay Area)

***O3a*: Zeroed albedo**

***O3b*: Original albedo**

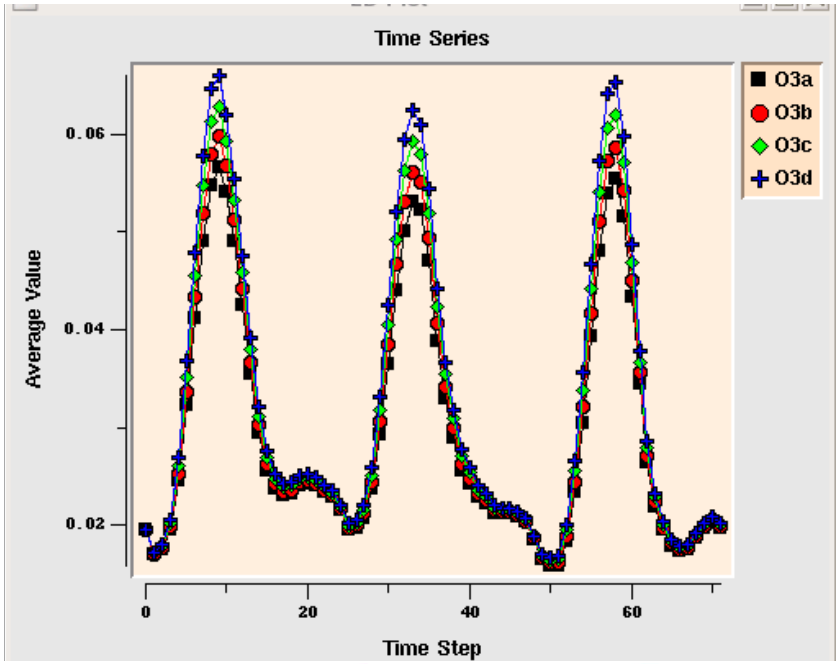
***O3c*: Doubled albedo**

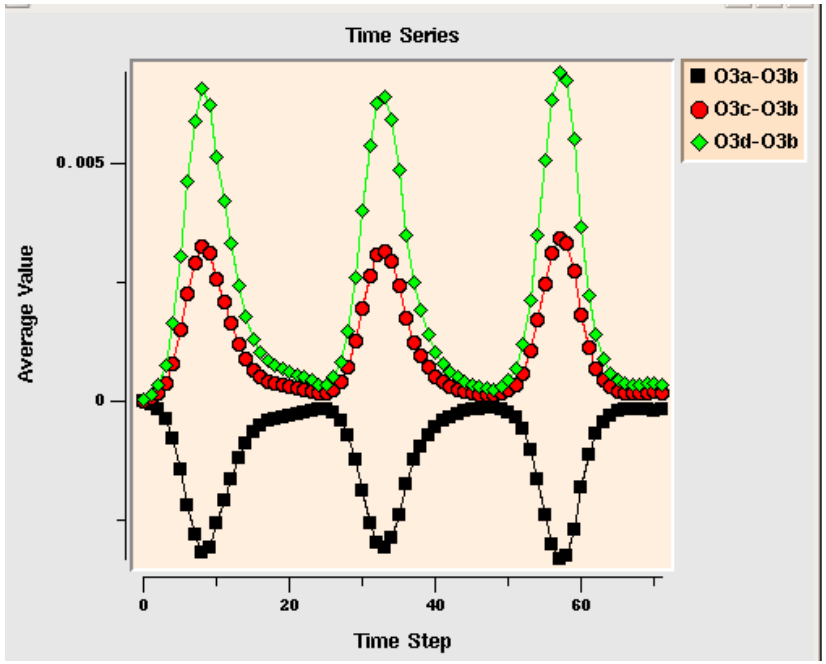
***O3d*: Tripled albedo**

Zeroed minus orig.

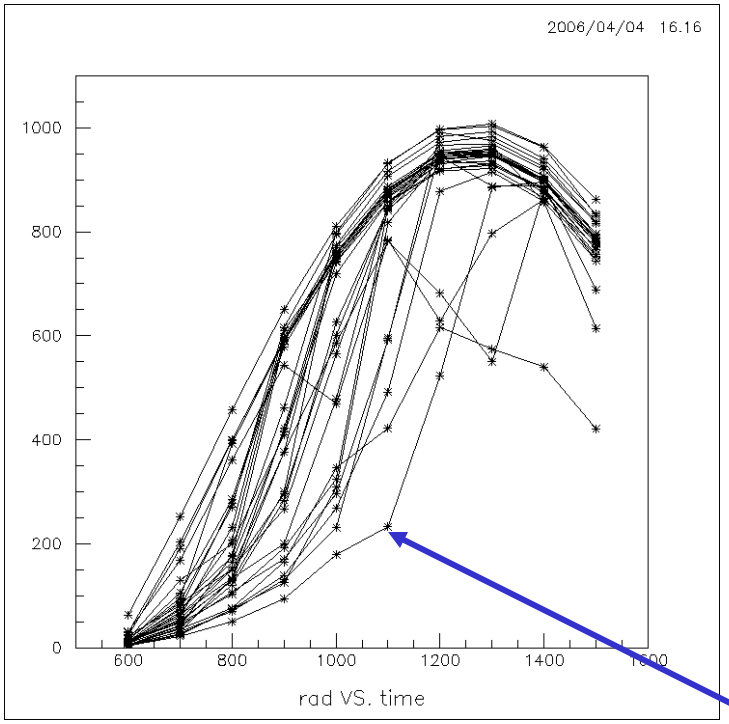
Doubled minus orig.

Tripled minus orig.

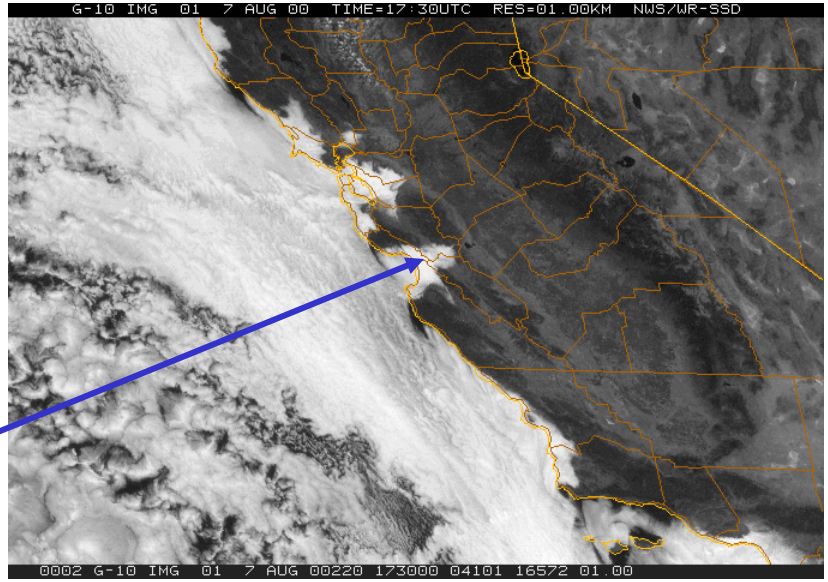




Attenuation of light in coastal stratus



Hourly CIMIS solar radiation (W/m^2) measurements near Monterey Bay, 7/20 - 8/20/2000. (1 curve per day)



11am 7th Aug 2000

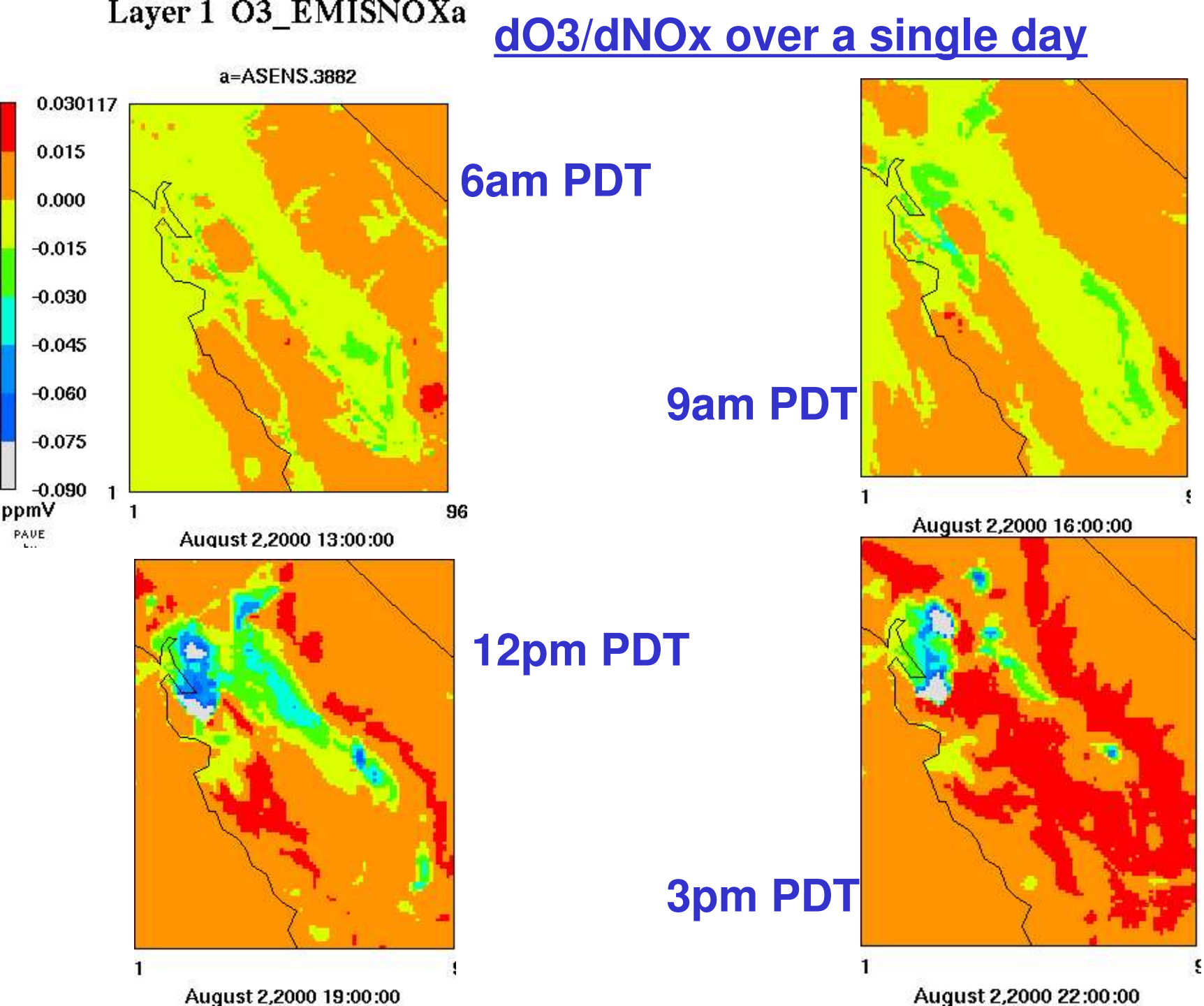
Sensitivity Analysis
CMAQ DDM V4.3

5-day and 15-day runs of :dO3/d(NOx), dO3/d(AVOC), dO3/d(BVOC)

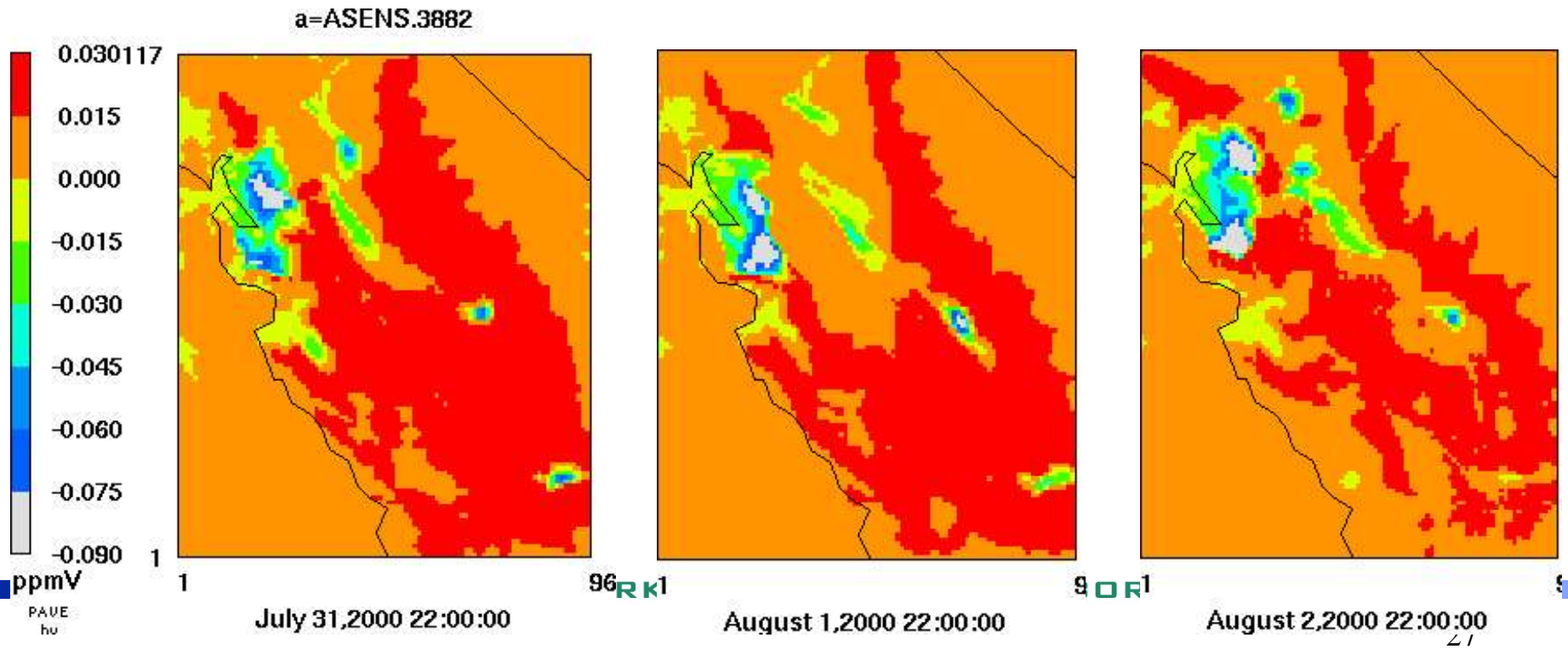
- **w.r.t boundary, initial conditions**
- **w.r.t. emissions from selected regions or full domain**
- **w.r.t. time-of-day of emissions from selected region**

Following slides show semi-normalized sensitivities: first derivative extrapolated to predict ozone as if 100% change in denominator value

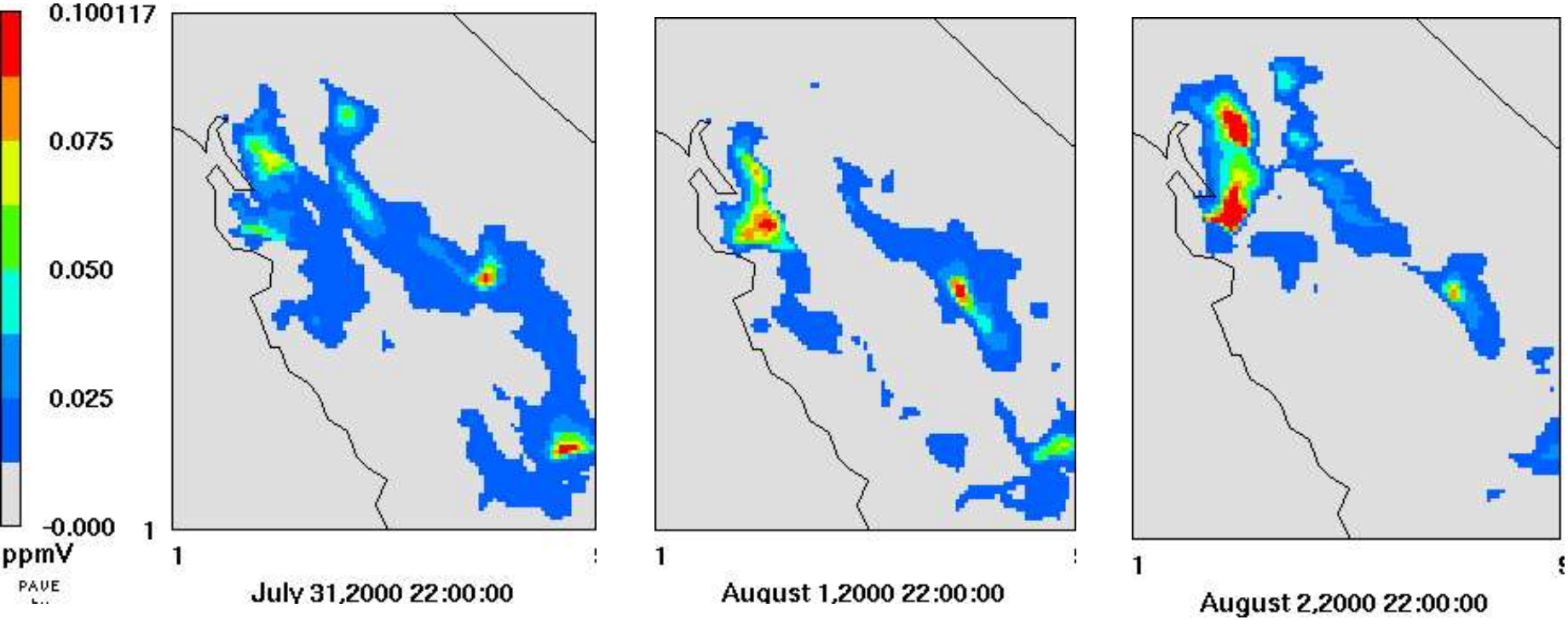
dO3/dNOx over a single day



dO3/dNOx at 3pm PDT on 3 successive days



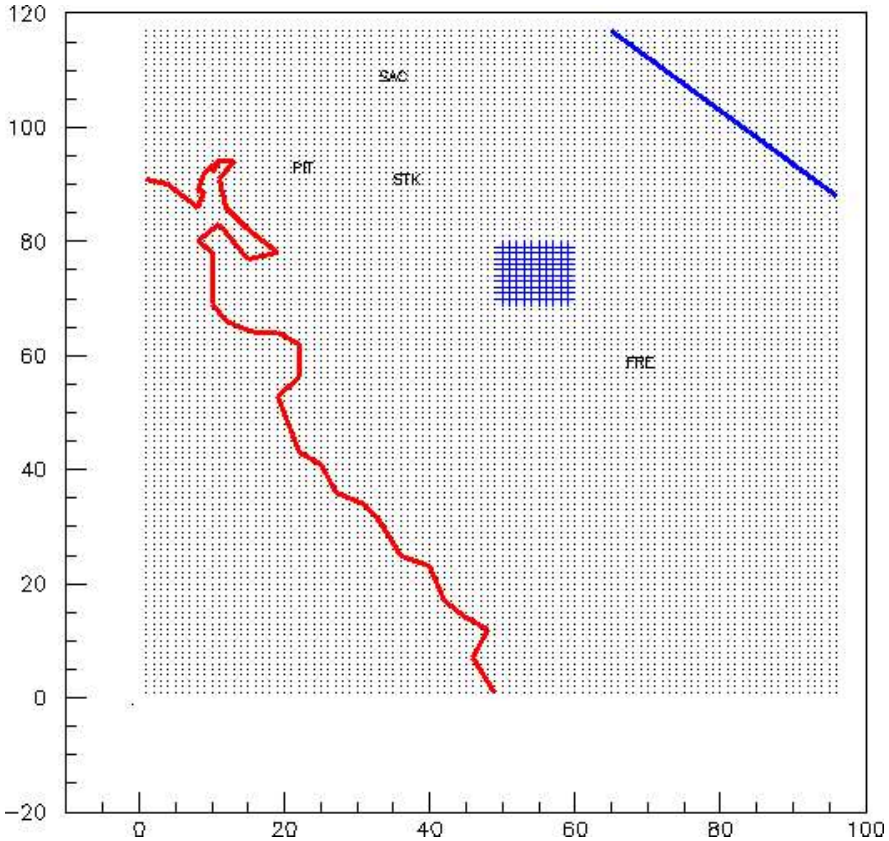
dO3/d(AVOC) at 3pm PDT on 3 successive days



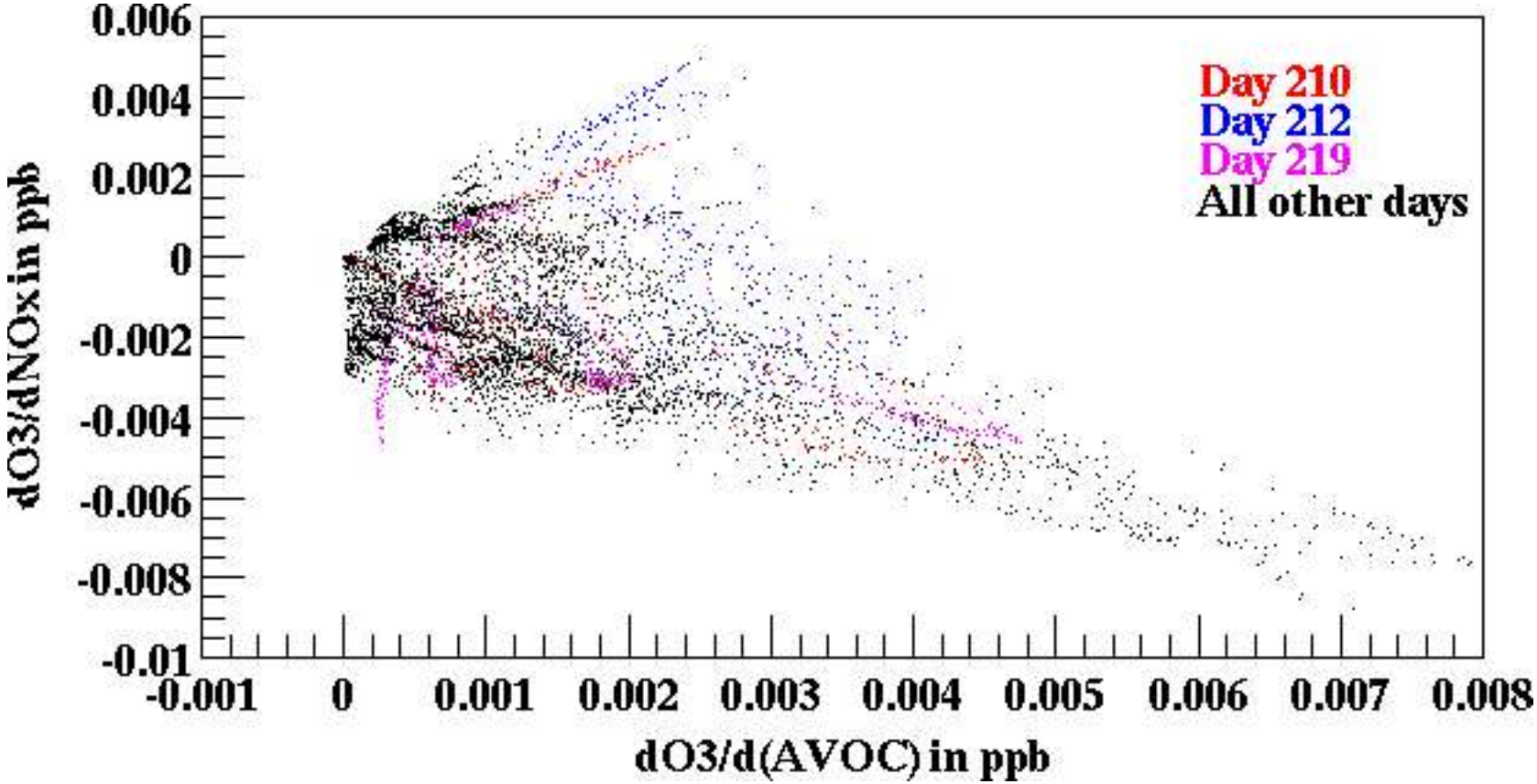
Combine analysis methods: DDM and PAW

For shaded region, compare O_3 sensitivities to emissions from specific regions: SF Bay Area and Sacramento for a prolonged period.

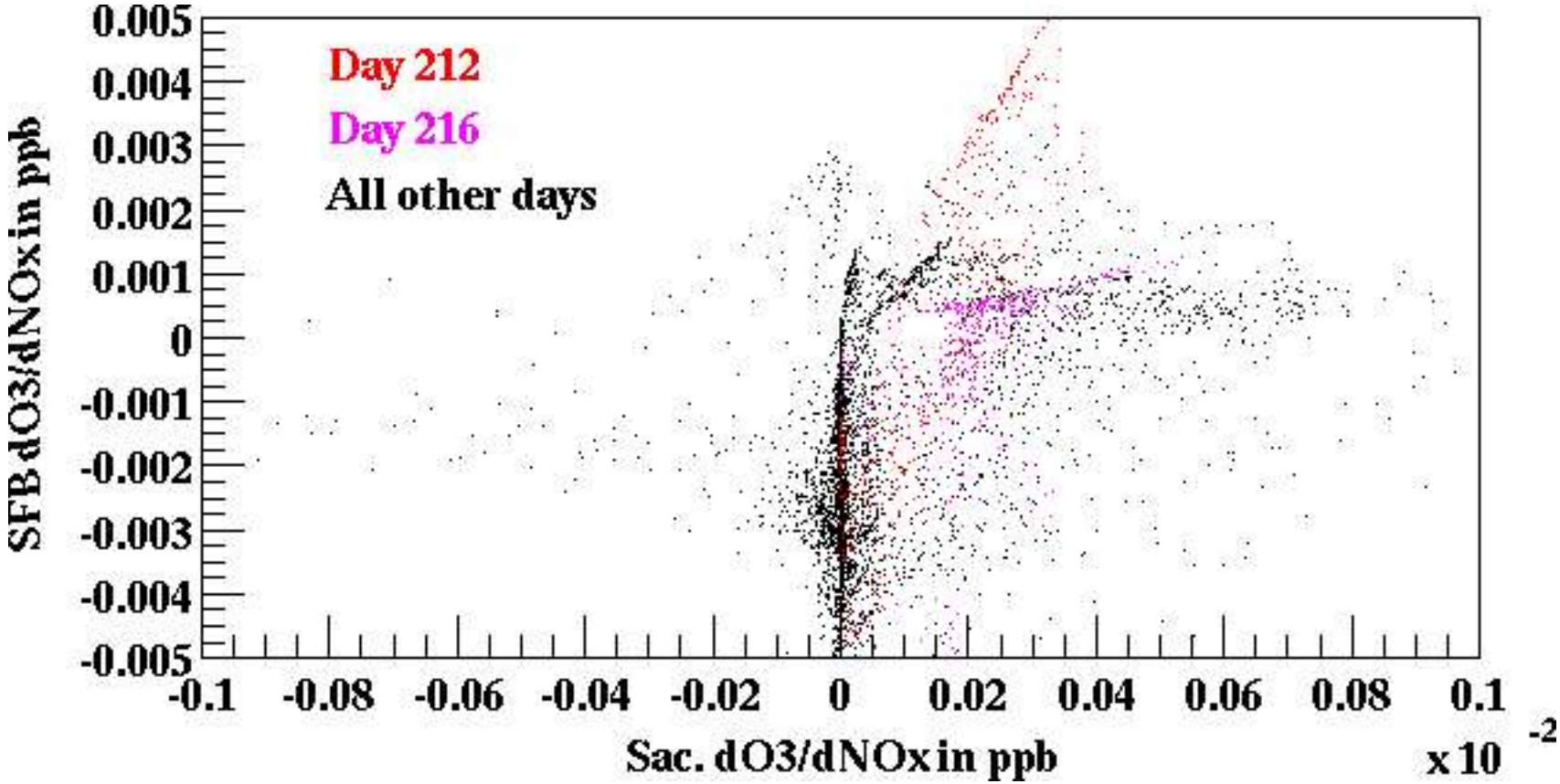
Following plots present O_3 sensitivities for the 12 noon – 4pm period for all 15 days



Comparison of O_3 sensitivities to SFB NOx and SFB VOC emissions



Comparison of O_3 sensitivities to SFB NOx and Sac. NOx emissions



Summary

Conducted and evaluated CMAQ 15 day simulations

Diagnosing model performance

- Photochemistry: Albedo, cloud attenuation
- Model performance on coast

Sensitivity and other analysis tools used in concert can help classifying day's meteorology when large data set available