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Improving Air Quality Forecasting through Incremental Reduction of Input Uncertainties – focus on episodic fire emissions

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Governing Equation and Inputs Affecting AQF Results

$$\frac{\partial(\bar{\varphi}_i J_\xi)}{\partial t} + m^2 \nabla_\xi \bullet \left(\frac{\bar{\varphi}_i \hat{\mathbf{V}}_\xi J_\xi}{m^2} \right) + \frac{\partial(\bar{\varphi}_i \hat{v}^3 J_\xi)}{\partial \hat{x}^3}$$

$$+ m^2 \frac{\partial}{\partial \hat{x}^1}\left[\frac{\bar{\rho} J_\xi}{m^2} \hat{F}^1_{q_i} \right] + m^2 \frac{\partial}{\partial \hat{x}^2}\left[\frac{\bar{\rho} J_\xi}{m^2} \hat{F}^2_{q_i} \right] + \frac{\partial}{\partial \hat{x}^3}\left[\bar{\rho} J_\xi \hat{F}^3_{q_i} \right]$$

$$= J_\xi R_{\varphi_i}(\bar{\varphi}_1, \ldots, \bar{\varphi}_N) + J_\xi Q_{\varphi_i} + \left.\frac{\partial(\bar{\varphi}_i J_\xi)}{\partial t}\right|_{cld} + \left.\frac{\partial(\bar{\varphi}_i J_\xi)}{\partial t}\right|_{aero} + \left.\frac{\partial(\bar{\varphi}_i J_\xi)}{\partial t}\right|_{ping}$$

Quality of forecasting depends on both model formulations and inputs.

For AQF, daily meteorology is the main driver, but IC/BC & emissions can affect forecasting quality greatly.

Often current AQFs do not have event-based emission inputs.

Demonstrate how an AQF can be improved by re-initialization or further by improving episodic emission inputs

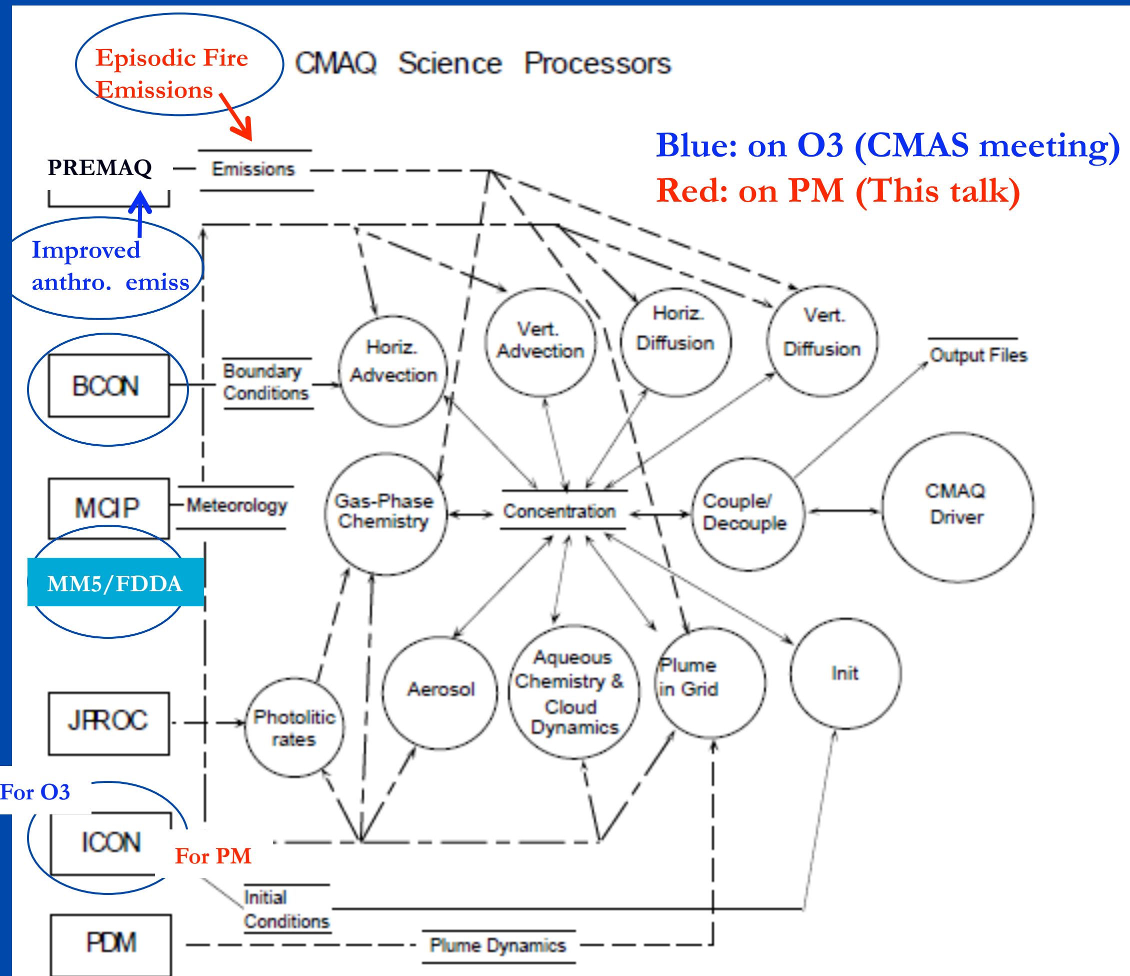

Figure 6-1. Science Process Modules in CMAQ. Interface processes are shown with rectangular boxes. Typical science process modules are updating the concentration field directly and the data-provider modules include routines to feed appropriate environmental input data to the science process modules. Driver module orchestrates the synchronization of numerical integration across the science processes. Concentrations are linked with solid lines and other environmental data with broken lines. (From Byun et al., 1998.)

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How to Improve AQF when Episodic Emissions Are Missing?

•Show problems with UH AQF
(36-km CONUS & 12-km Texas and Surrounding States)

•Example of improvement of CMAQ by means of adjusting aerosol ICs with MODIS-derived AOD (for UH CONUS)

•Example improvement of CMAQ by adding fire emissions from satellite obs. (with UH CONUS & 12-km domains)

Implementation of Episodic Emissions in NOAA NAQFS

•On-going implementation of HMS/Bluesky/HYSPLIT fire emissions for NAQFS

•On-going implementation of wind-driven dust in NAQFS

Improvement of UH-AQF without episodic fire emissions with improved IC

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•Errors in the IC can cause serious problems during the early part of the simulation.

•Hypothesis: Using IC based on satellite obs. can improve model predictions of PM2.5

•Many studies [Gupta et al. (2006), Engel-Cox et al. (2004), Kittaka et al. (2004)] revealed that the satellite-derived AOD and ground-based PM concentration are well correlated

•High possibility of improving AQF accuracy if AOD is used

•Retrospective test simulations with IC from MODIS-AOD and AQS PM2.5

Demonstrate if performance of CMAQ aerosol simulation can be improved by means of adjusting aerosol ICs with MODIS-derived AOD.

MODIS = Moderate Resolution Imaging Spectroradiometer
AOD = Aerosol Optical Depth, AQS = EPA Air Quality System

How IC was updated with AOD

- MODIS-derived AOD Product
  - Total AOD = 'Optical_Depth_Land_And_Ocean'
  - Fine mode fraction = 'Optical_Depth_Ratio_Small_Land_And_Ocean'

$$AOD_f = AOD_t \times FineModeFraction$$

- CMAQ-derived AOD estimation
  - 'Reconstructed mass-extinction' method.
    Malm et al. (1994), Binkowski and Roselle (2003), Roy et al. (2007)

$$AODmodel = \sum_{i=1}^{N} (\beta sp + \beta ap)_i \Delta Zi$$

Extinction coeff. for particle scattering & absorbtion

Model layer thickness

$$\beta sp = (0.003)\ f(RH)\ [Sulfate + Nitrate + Ammonium] + (0.004)\ [Organic\ Mass] + (0.001)\ [Fine\ Soil] + (0.0006)\ [Coarse\ Mass]$$

$$\beta ap = (0.01)\ [Light\ Absorbing\ Carbon]$$

Use Cressman Successive Correction method (Cressman, 1959)

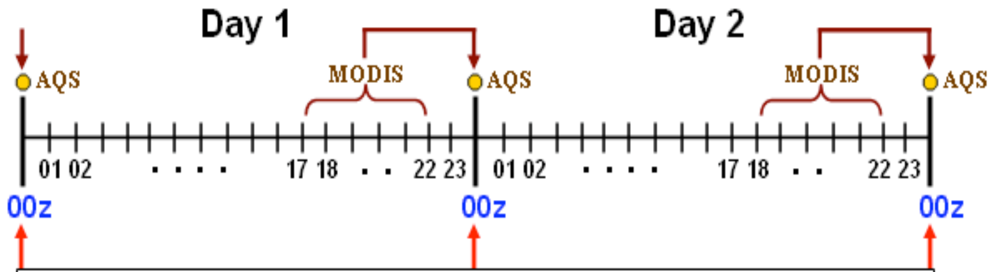
Two iterations with reducing radius of influence (R)

1st: R = 3 grid-length (108km)

2nd: R = 2 grid-length (72km)

Methodology

- <u>Two step adjustments of aerosol initial conditions</u>



Two Step adjustments of aerosol initial conditions

< **<u>Step 1: whole layer adjustment</u>** >

(1) First Guess: CMAQ_AOD (reconstructed mass extinction)
(2) Observation: MODIS_AOD (drop-in-grid)
(3) Analysis field: Objective analysis (Cressman scheme)
(4) Ratio = Analysis/First_Guess
(5) ***Adjusted ICs = CMAQ first guess conc. X Ratio***

< **<u>Step 2: surface layer adjustment</u>** >

(1) First Guess: Step 1 adjusted ICs
(2) Observation: AQS hourly PM2.5 data
(3) Analysis field: Objective analysis (Cressman scheme)
(4) Ratio = Analysis/First_Guess
(5) ***Adjusted ICs = CMAQ first guess conc. X Ratio***

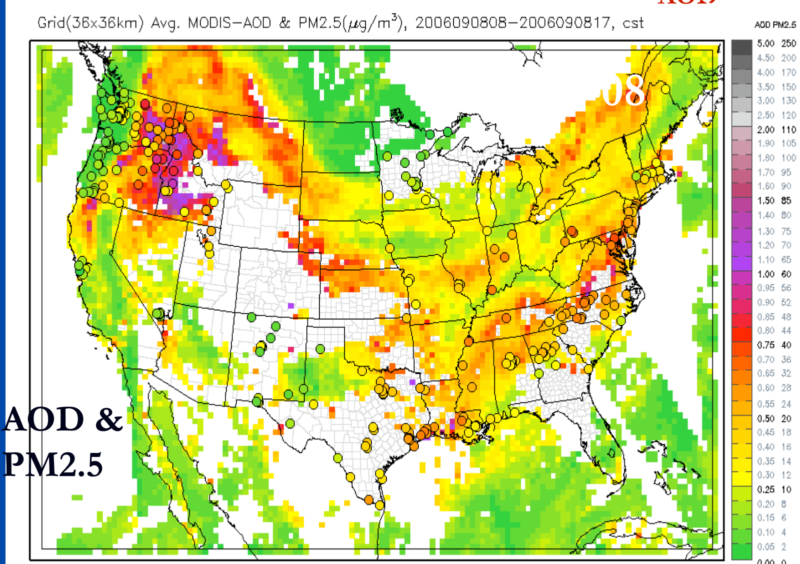
$$Adjusted\ CONC = CONC_{firstguess} \times \frac{AOD_{analysis}}{AOD_{firstguess}}$$

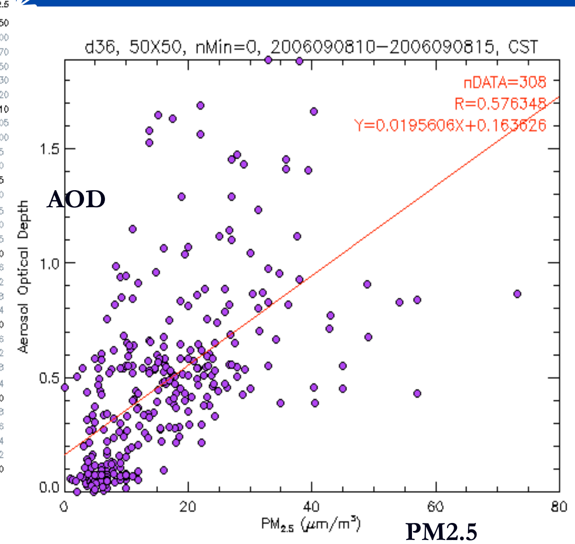
Species name	CMAQ variable names
Sulfate	ASO4J + ASO4I
Nitrate	ANO3J + ANO3I
Ammonium	ANH4J + ANH4I
Organic Mass	AORGAJ+AORGAI + AORGPAJ+AORGPAI + AORGBJ+AORGBI
Fine Soil	A25J
Coarse Mass	ACORS+ASOIL
Light Absorbing Carbon	AECJ+AECI

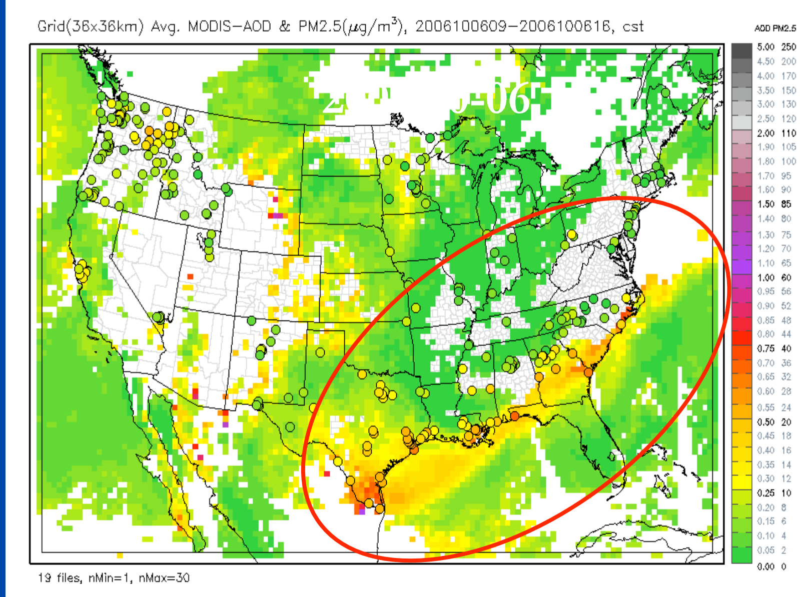
Total AOD: used all species IC adjustment
Fine AOD & PM2.5: exclude Coarse Mass

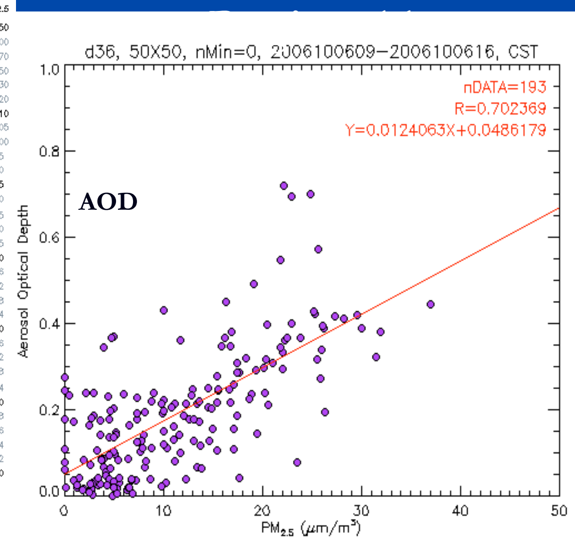
Correlation between MODIS AOD and AQS PM2.5

AOD-PM2.5 relationship provides the fundamental basis of this study.









9/8/2006 Wildfires

Fires in NW + local emission

continental haze day

High AOD, low PM2.5 due to smoke plume height

AOD: surface to TOA

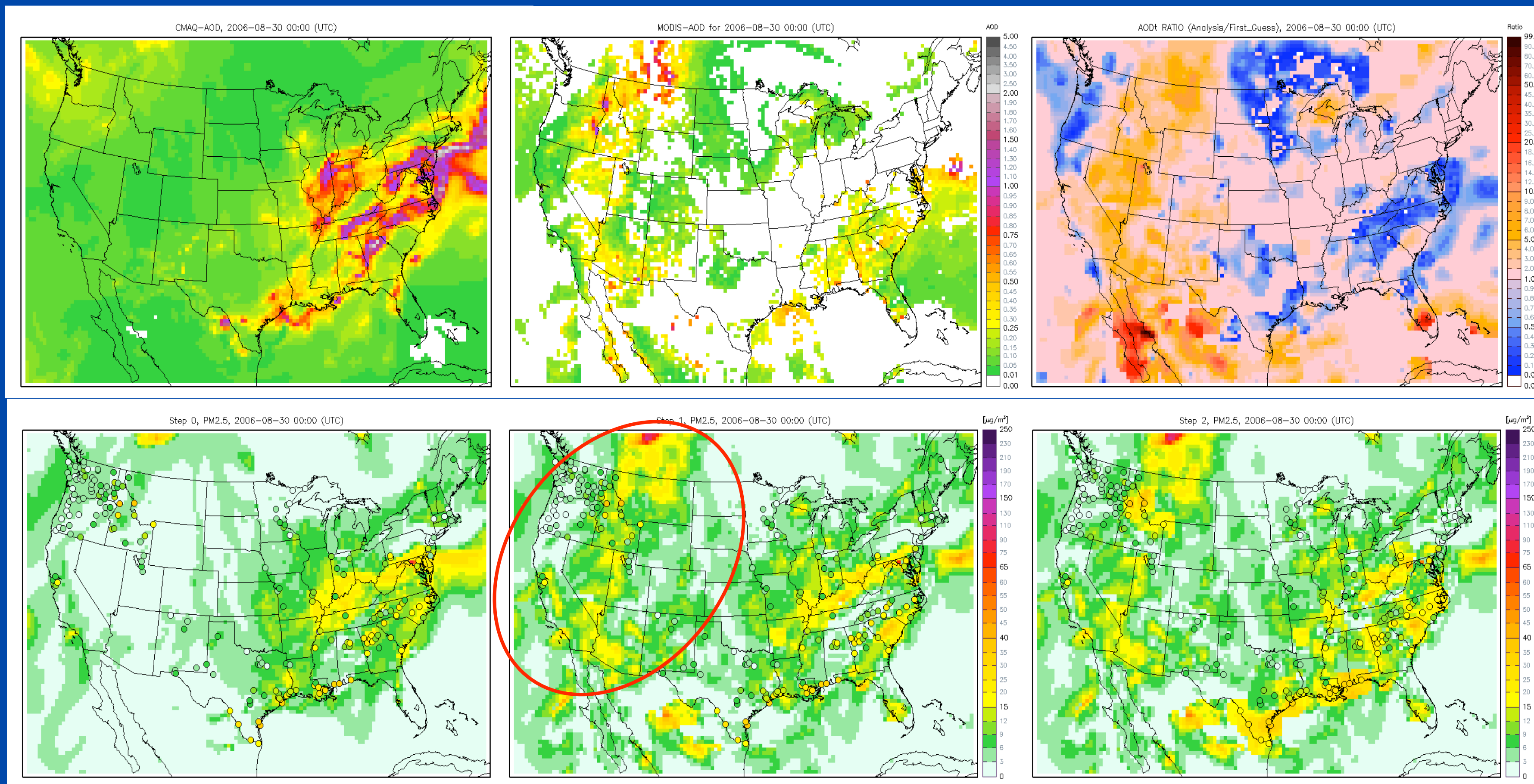
PM2.5: surface

10/6/2006 Regional haze

High AOD & PM2.5 in SE well correlated

Aerosol IC adjustments with Total AOD on 8/30/2006: first day example

< CMAQ AODt > < MODIS AODt > < AODt Ratio >



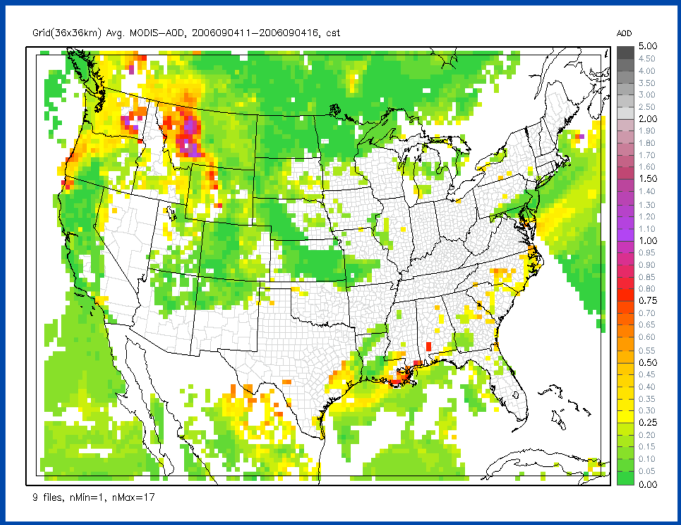
< PM2.5: Original IC > < PM2.5: After step 1 > < PM2.5: After step 2 >

(1) Analysis field: CMAQ AODt=First guess, MODIS AODt=Obs. by Cressman scheme
(2) AODt ratio= Analysis/First guess

After Step 1 and Step 2 adjustments, Original PM2.5 IC are closer to obs
In W & NW region, PM2.5 IC are increased

CMAQ predicted PM2.5 on 9/3~9/5/2006 (wildfire) - Total AOD adjustment

< MODIS AOD >



MODIS

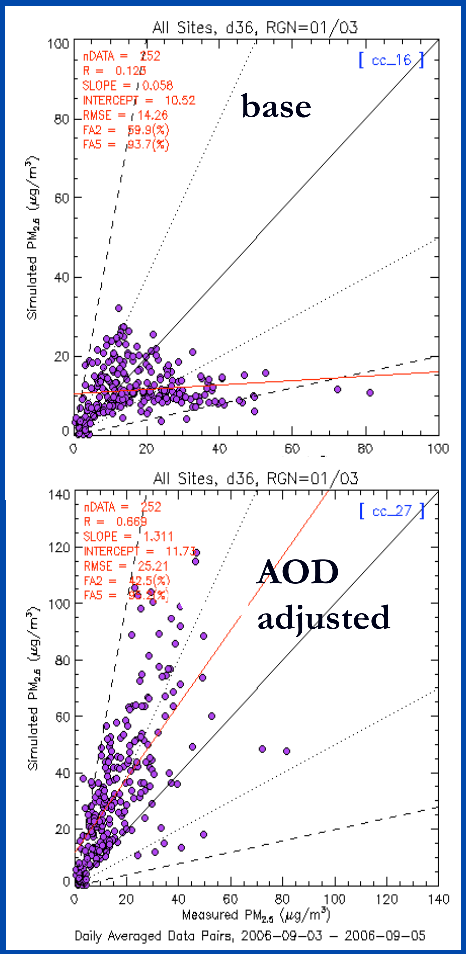
Wildfires in NW: high AOD
Regional haze in SE

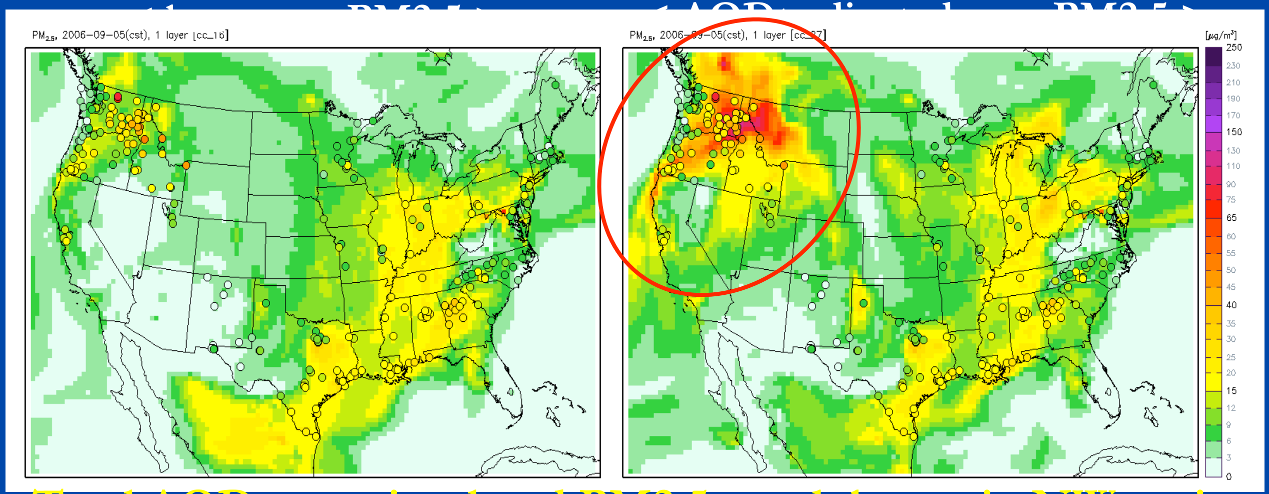
CMAQ

Central & E region=similar

Base case: low in NW
AODt case: high in NW

[Western region]





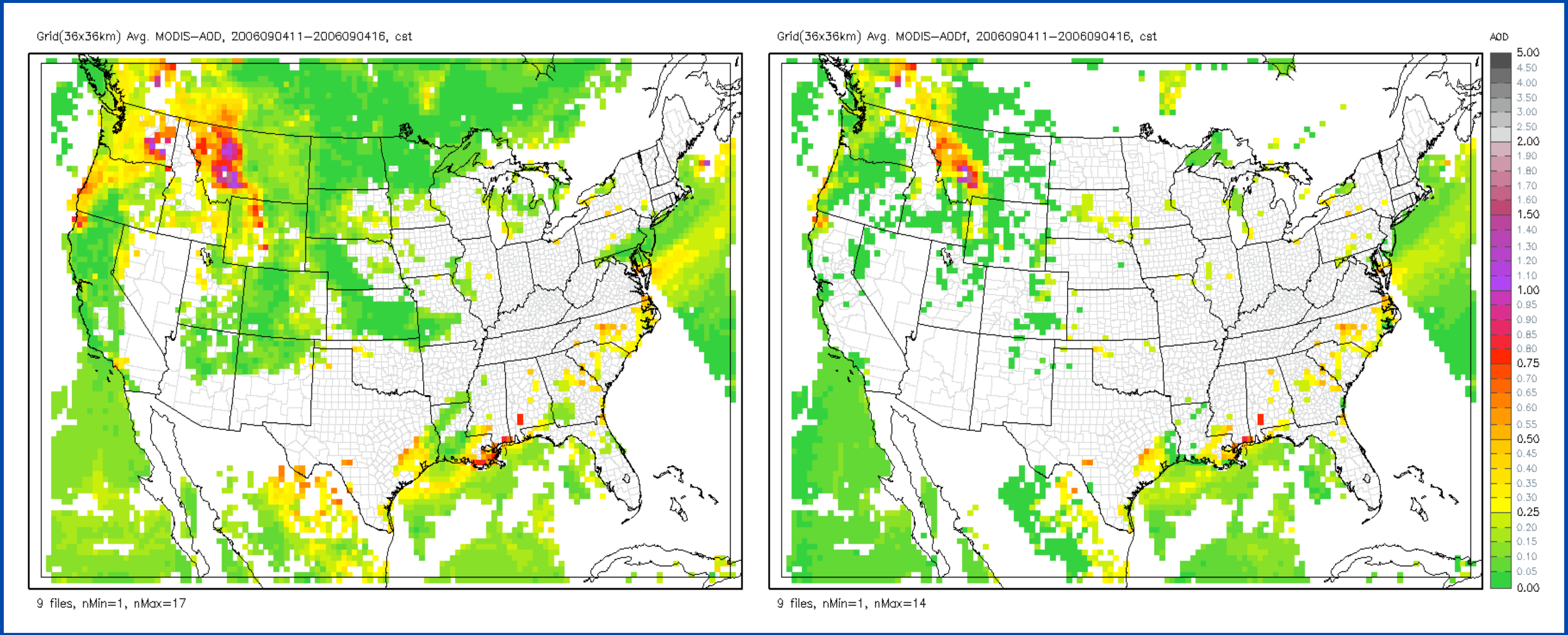
Total AOD case simulated PM2.5 much better in NW region

- but, unrealistic high peak PM2.5 appeared (obs=50, CMAQ=120ug/m^3)
- possibly due to elevated smoke plume (no consideration of vertical distribution) & large uncertainties in coarse mass emissions

CMAQ predicted PM2.5 on 9/3~9/5/2006 (wildfire) - Fine mode AOD adjustment

Due to unrealistic high peak PM2.5 with Total AOD case, in AODf adjustment, coarse masses are excluded in this adjustment

< MODIS AODt > < MODIS AODf >



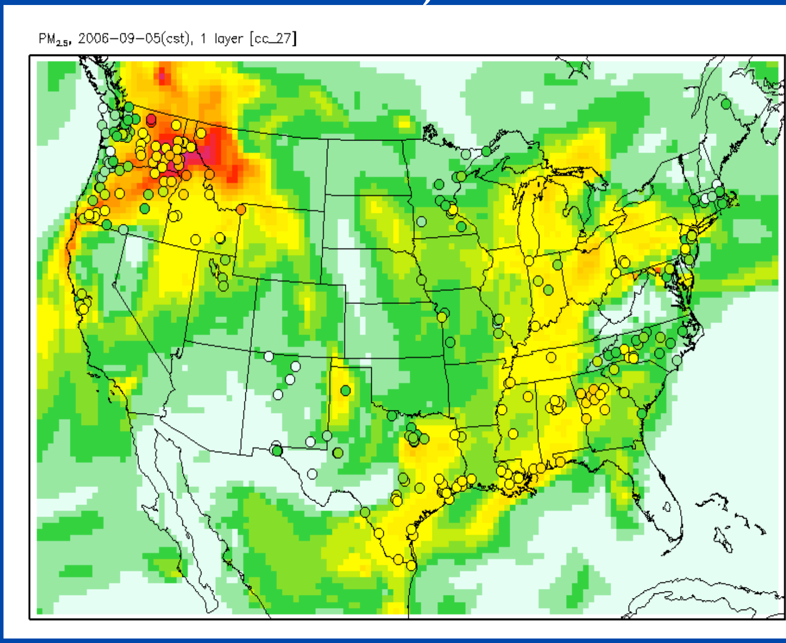
Total AOD vs Fine mode AOD

- NW: reduction of numerous number of pixels with decreased AOD values
- SE: AOD values remain almost the same

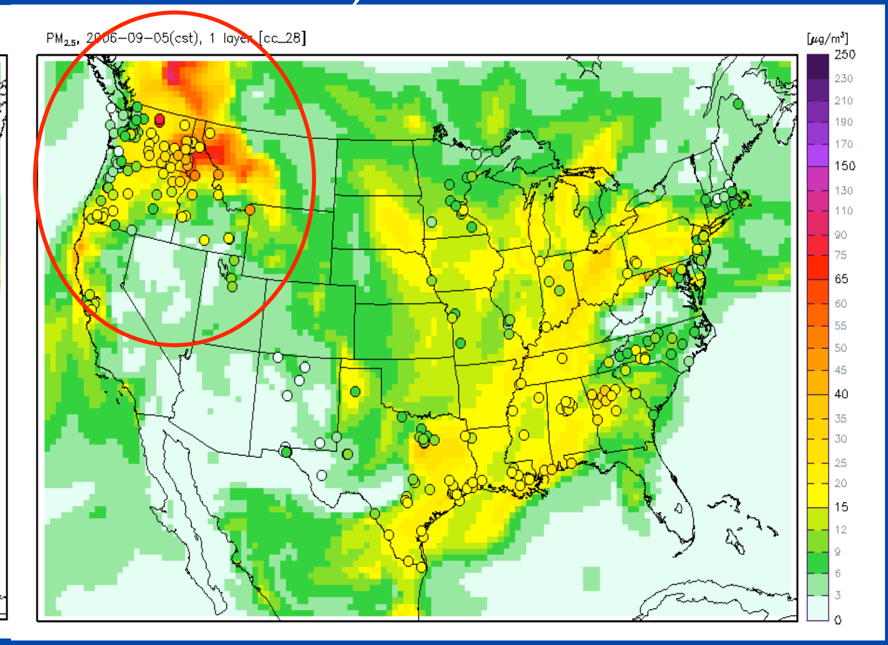
- NW: coarse aerosols from fires are dominant
- SE: fine aerosols produced by local pollution are dominant

CMAQ predicted PM2.5 on 9/3~9/5/2006 (wildfire) - Fine mode AOD adjustment

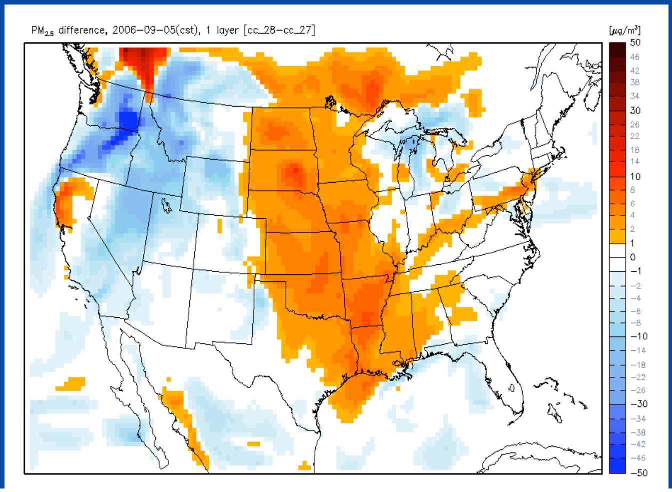
< AODt adjusted case PM2.5 >



< AODf adjusted case PM2.5 >



< difference: AODf-AODft >



SE in Fine mode AOD case

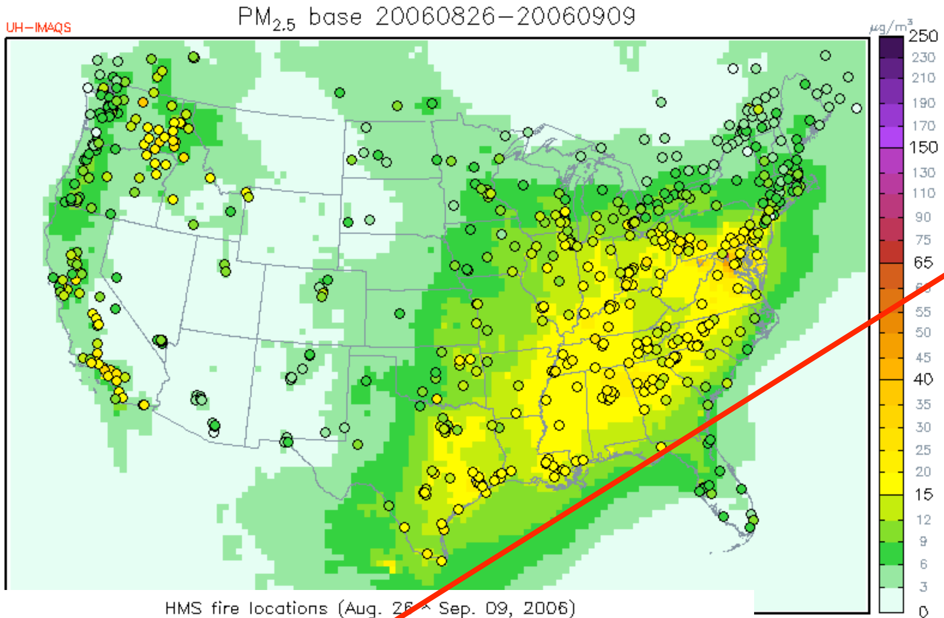
decrease/increase by 1~10ug/m^3
similar to Total AOD case
well simulated

NW in Fine mode AOD case

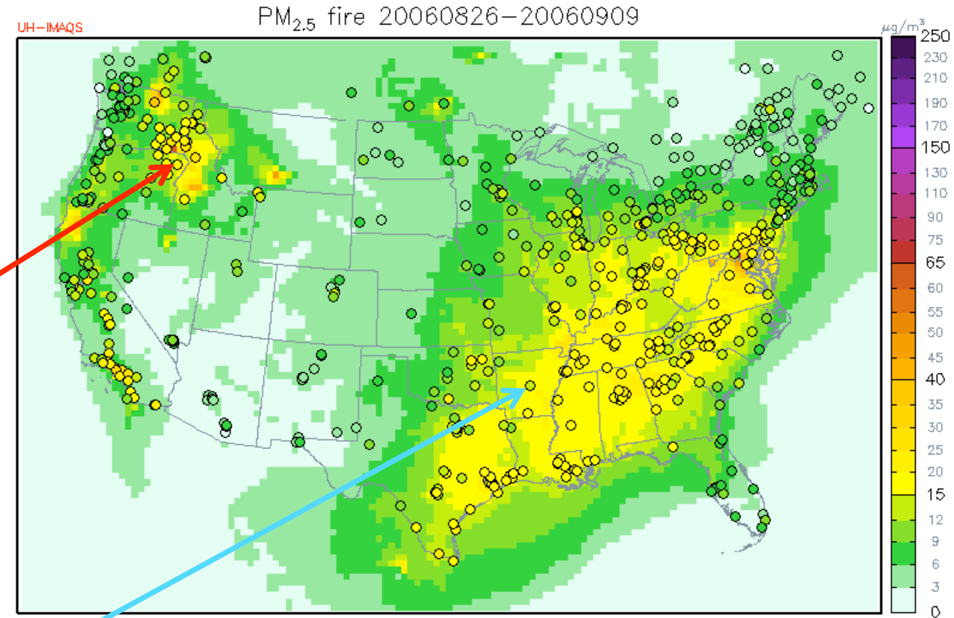
decreased PM2.5 by -10 ~ -50ug/m^3
reduced unusual high peak cells
more realistic spatial distribution of PM2.5

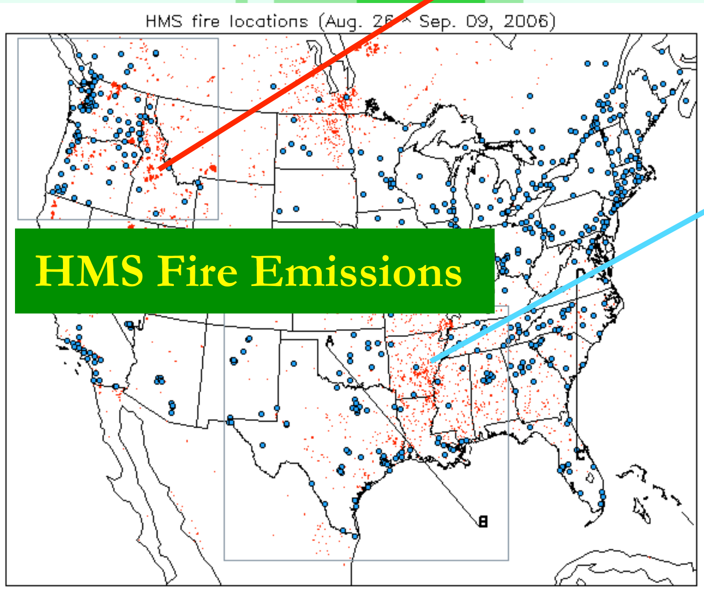
Now with HMS Fire Emissions Included (no IC Correction)

< Base Case>



< With HMS fire emissions>





HMS Fire Emissions

CMAQ-ready emissions (g s^{-1})

	CONUS			NW_US			TX		
	base	fire	change	base	fire	change	base	fire	change
PEC [2]	7847.82	15750.4	100.70%	595.818	4711.93	690.83%	1361.39	2675.18	96.50%
PMFINE [2]	125693	149752	19.14%	7313.65	19844.9	171.34%	30867.5	34867.3	12.96%
POA [2]	30170.7	86015.6	185.10%	2766.64	31853.8	1051.35%	5749.22	15033.3	161.48%

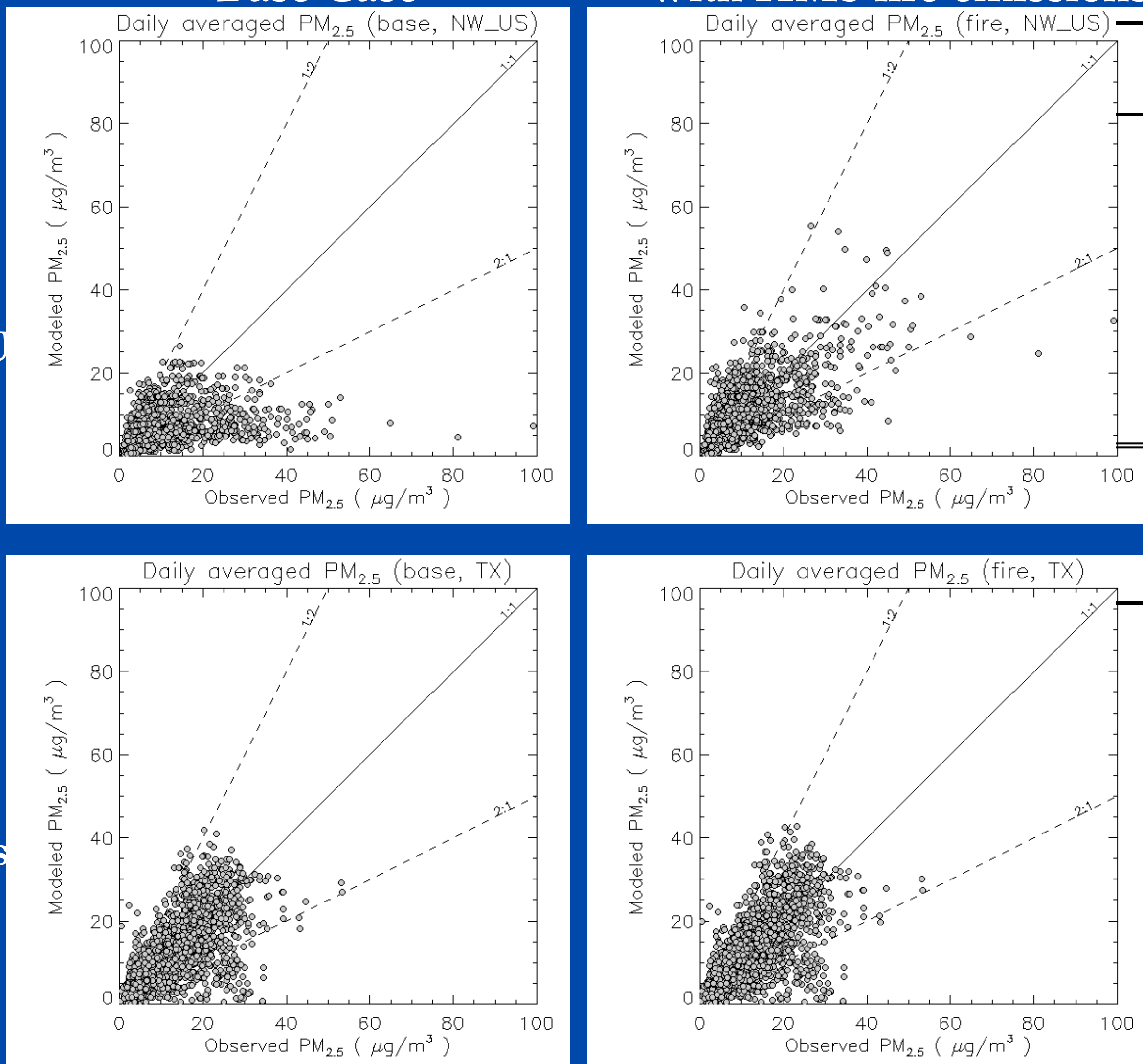
Inclusion of HMS fire emissions improved model

Now with HMS Fire Emissions Included (no IC Correction)

< Base Case> < With HMS fire emissions>

NW U

Texas



	E12			TX		
	base	fire	AQS	base	fire	AQS
ASO4	5.44	5.48	4.82	4.95	5.01	4.45
OC	1.45	1.89	3.79	1.65	2.41	3.43
EC	0.22	0.27	0.6	0.26	0.35	0.6
ANO3	0.77	0.79	0.47	2.43	2.5	0.52
PM2.5	15.2	16.3	15.39	15.2	16.3	15.39
C/PM2.5	0.095	0.12	0.25	0.11	0.15	0.22
C/PM2.5	0.014	0.02	0.04	0.017	0.02	0.039

$\mu g / m^3$

With fire E, slight Overprediction of PM2.5

Not much Change in ASO4
But it was overpredicted even for Base case

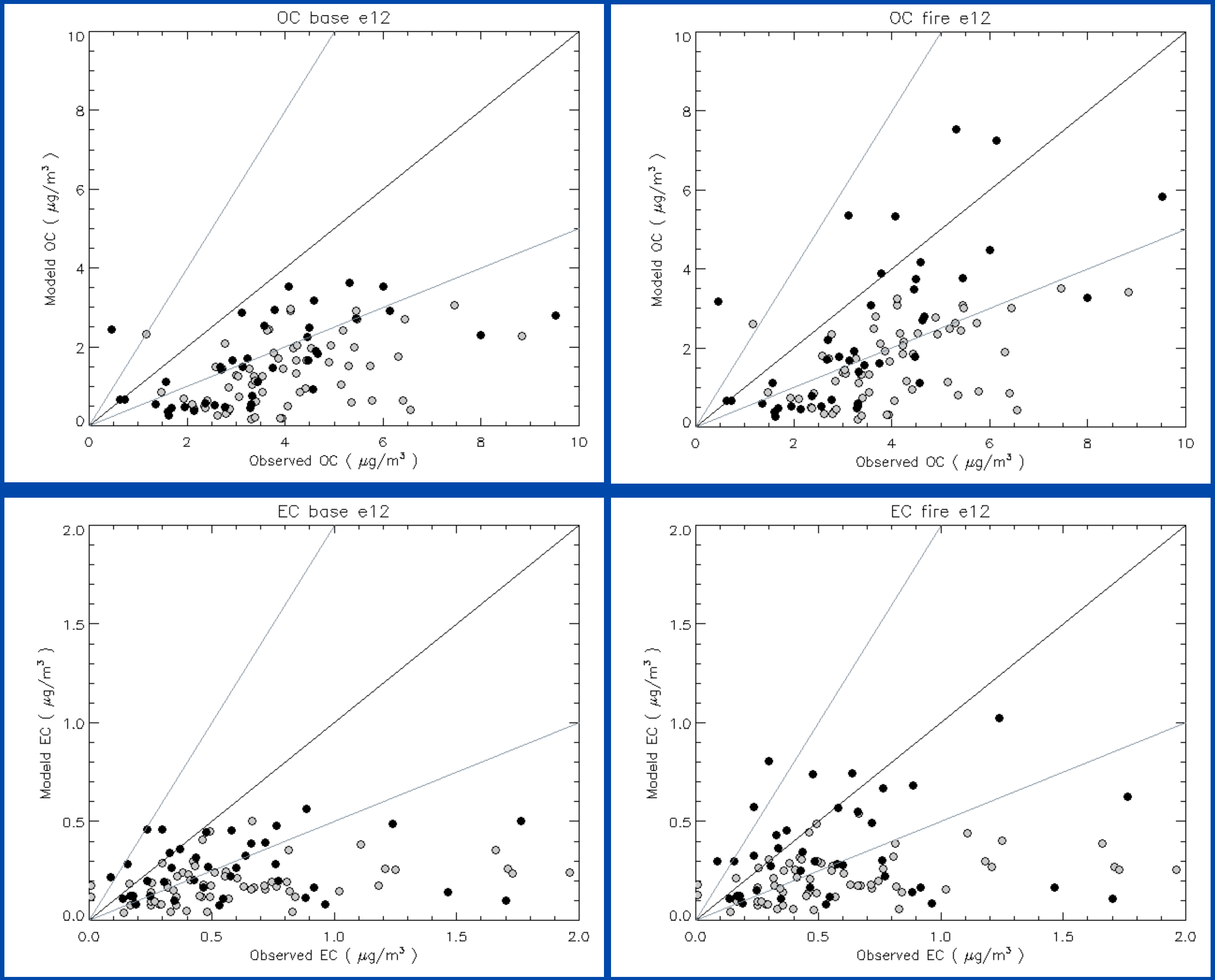
Now with HMS Fire Emissions Included (but no IC Correction)

< Base Case>   < With HMS fire emissions>

Texas

OC

EC



Interim Summary for Improving AQF

In order to improve CMAQ aerosol predictions,
the aerosol IC are adjusted at the simulation start time-step
utilizing the MODIS-derived AOD and AQS PM2.5 observations.

In case of aerosol events such as wildfires
- impacts of IC adjustments could be significantly big
- due to lack of episodic fire emission inputs, CMAQ could not simulate the event
- such deficiencies can be mitigated by improved IC with MODIS-AOD & AQS

Wildfire case with total AOD adjustment,
- CMAQ could simulate high PM2.5, but unrealistic high peak values appeared,
due to uncertainties in coarse mass emissions and elevated smoke plume

Wildfire case with fine mode AOD adjustment,
-Helped reducing unrealistic high peak PM2.5 concentrations

Wildfire case with HMS fire emissions,
-Improves simulation of PM2.5 (in particular for EC and OC)

2009 NOAA NAQF Performance –Developmental PM2.5, US (CB05/Aero4, Daily Max)

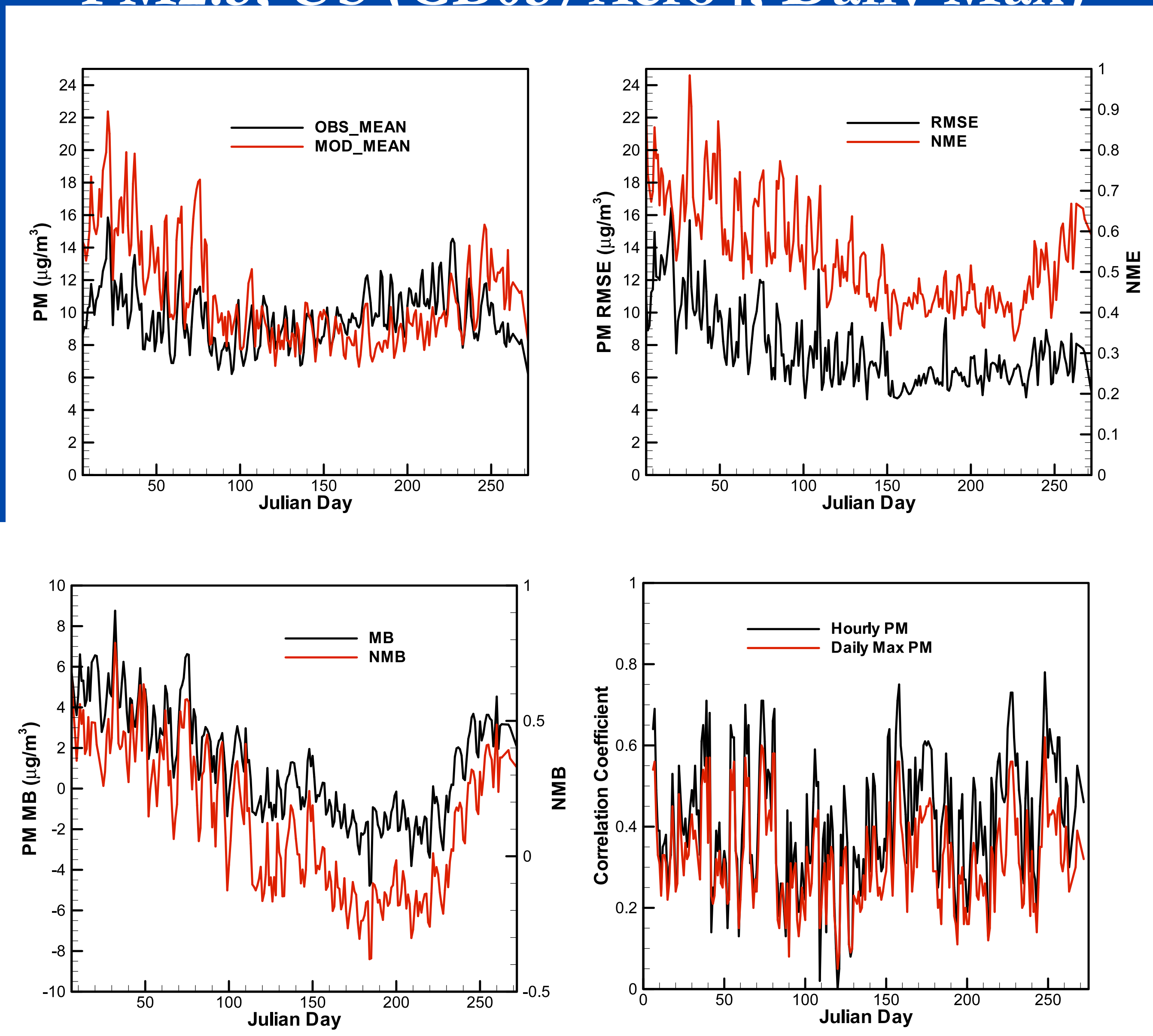
OBS mean
CMAQ mean

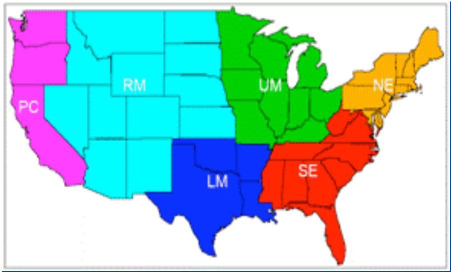
RMSE
Normalized
Mean Error

Mean Bias
Normalized
Mean Bias

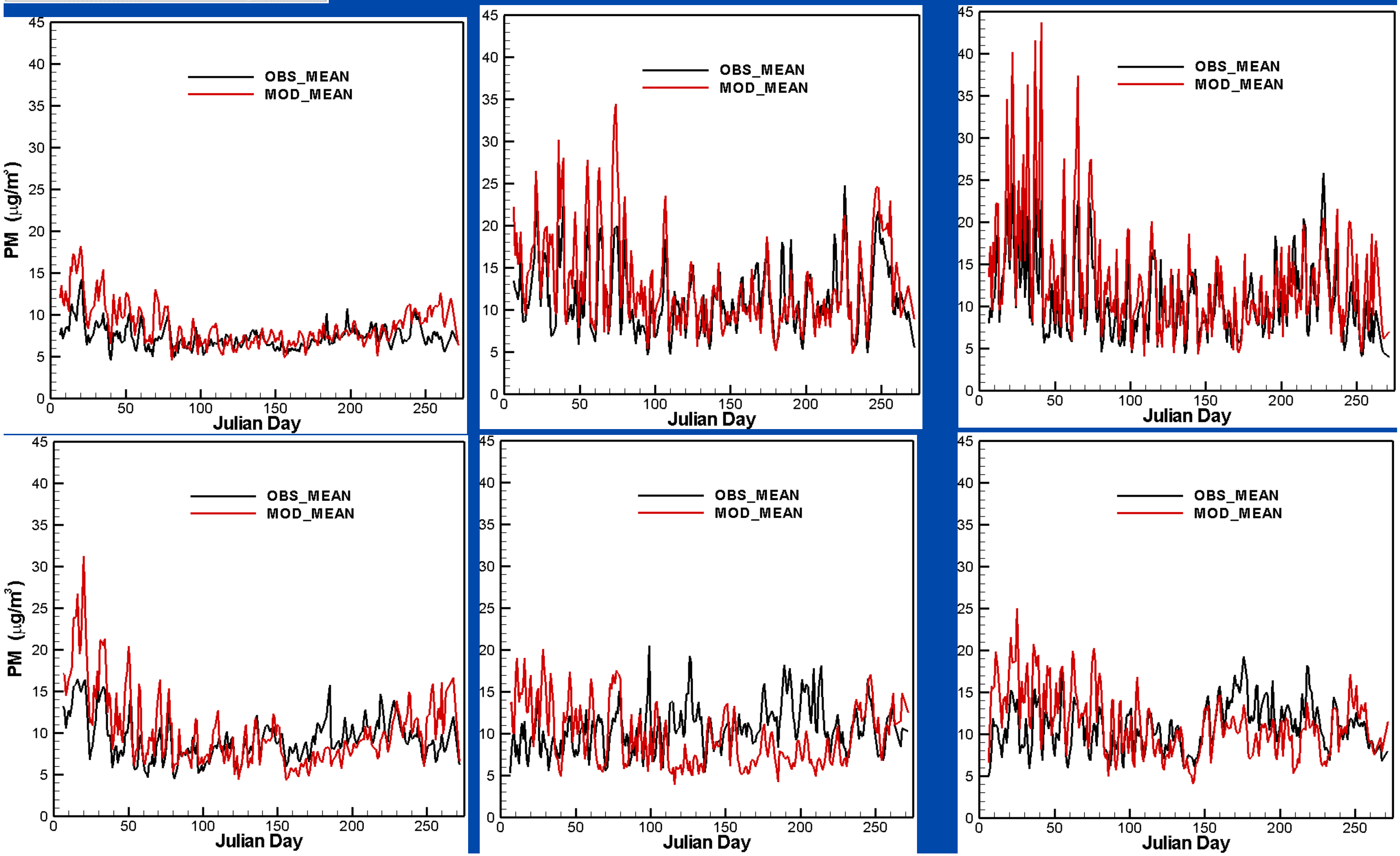
Correlation
(hourly)

Correlation
(daily max)

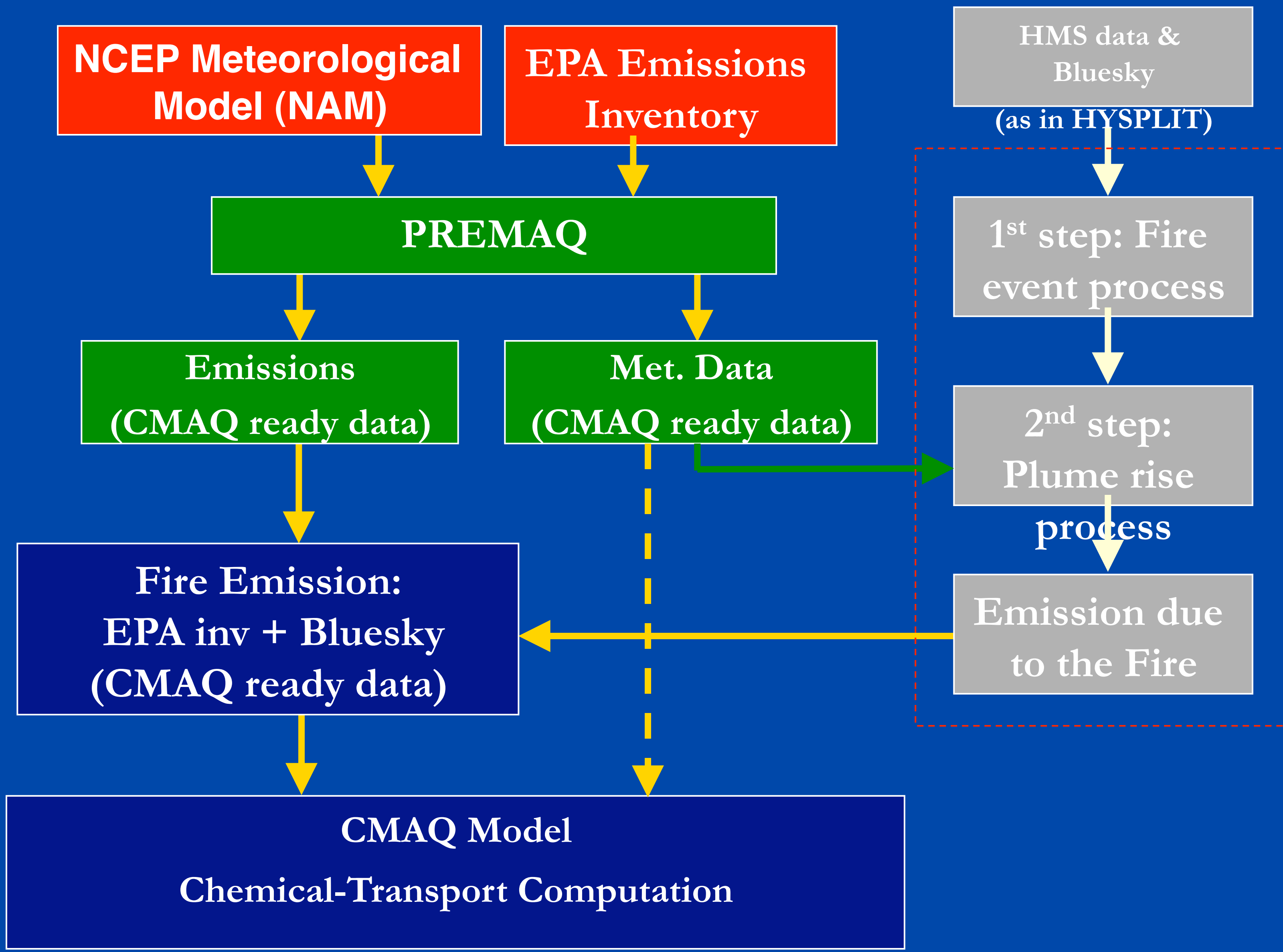




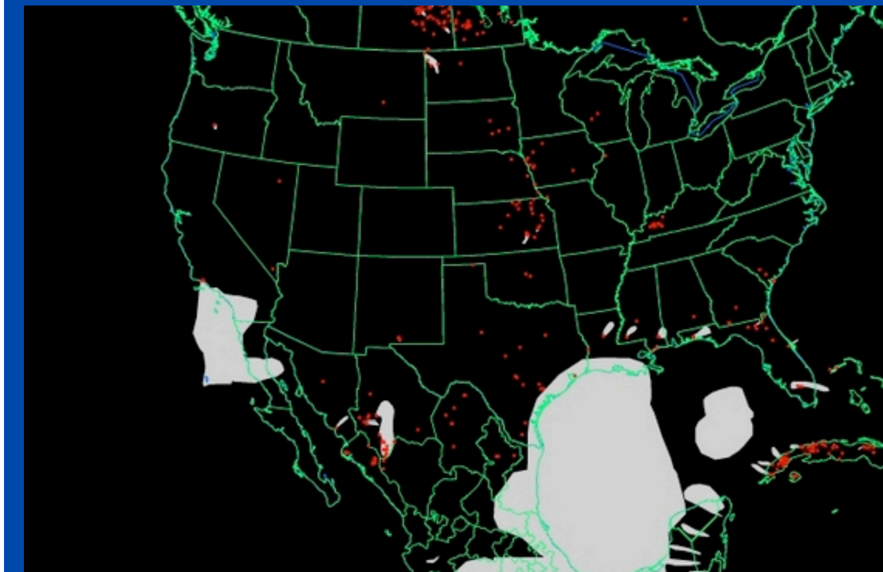
Rock Mountain Region	Upper Midwest	Northeast US
Pacific Coast Region	Lower Midwest	Southeast US



On-going work → Include Fire Emissions: Link NESDIS HMS/USDA BlueSky/ARL HYSPLIT input

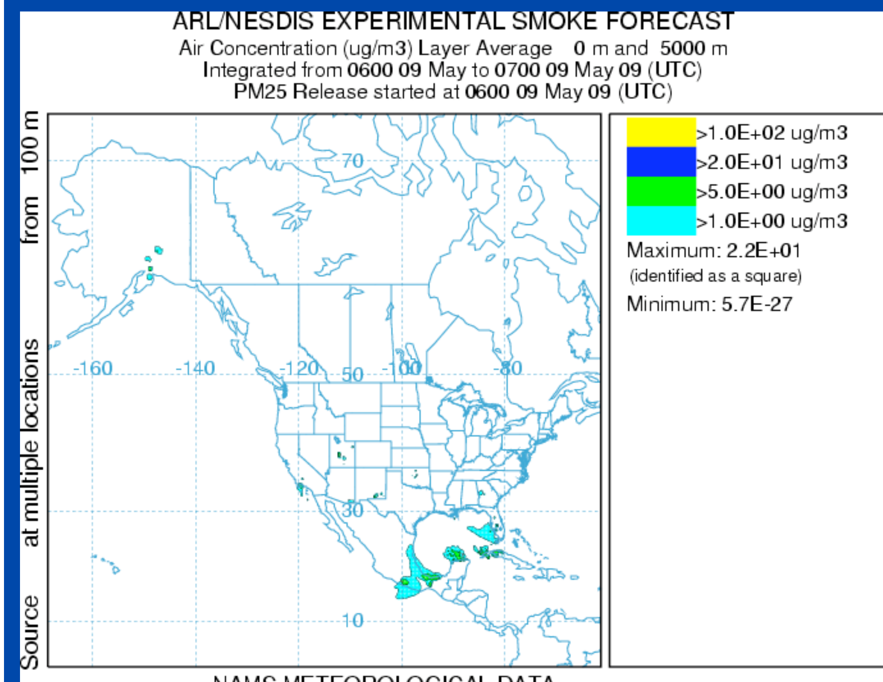


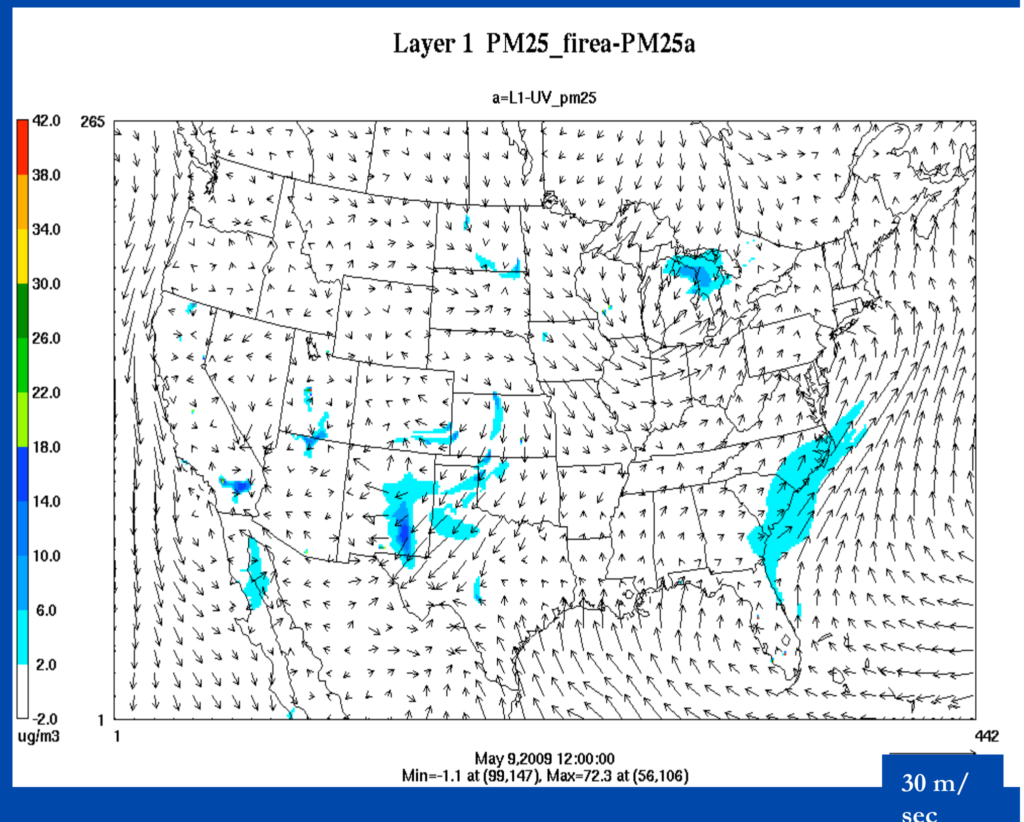
HMS



Case for 2009-05-09 1200Z run

This plot show difference of PM2.5 between the CMAQ with and without Smoke Emissions Comparison with the satellite fire detection and HYSPLIT PM product are also provided



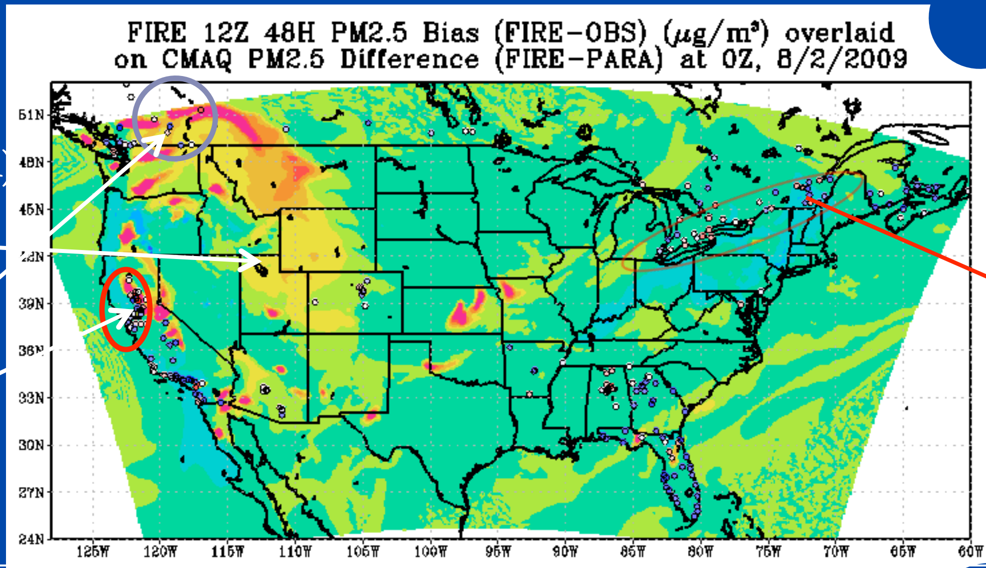


PM2.5 bias to observation (small circles) with & without fire emissions

(* climatological fire emission was removed from the HMS/BlueSky/HYSPLIT emissions)

CMAQ PM2.5 Difference (HMS – PARA) in mg/m^3

Improved with fire emissions



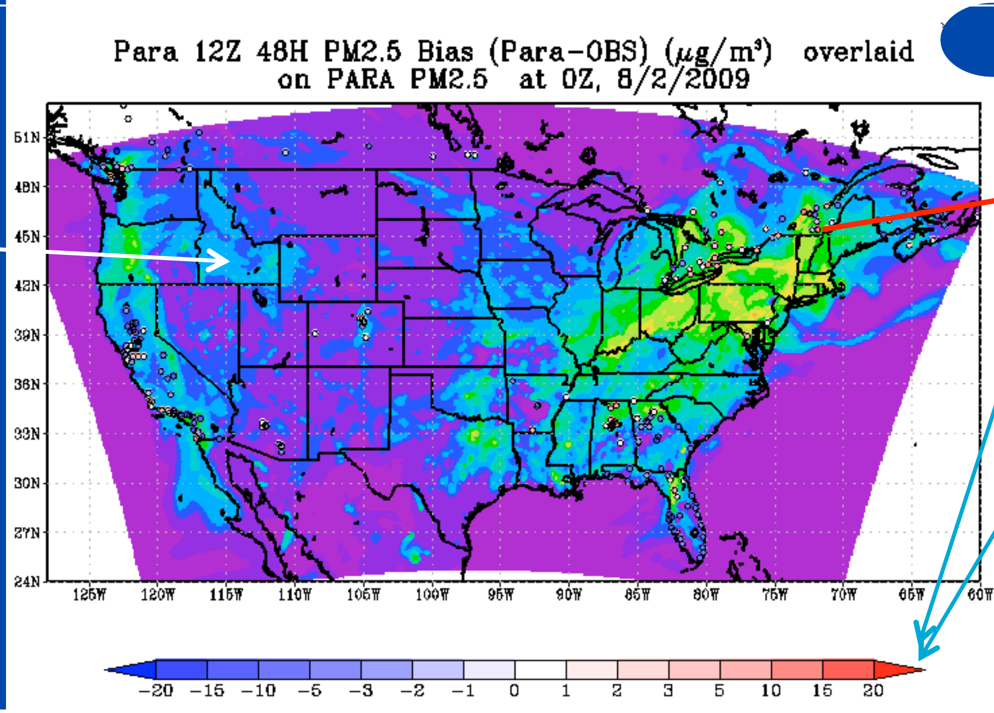
Case for 2009-08-02

Circles:
Bias with episodic fire
(but no climatological) emissions
CMAQ (with fire E) - OBS

Bias here did not improve with the addition of fire emissions

(good model prediction if color between circles and background cells are close)

Without fire emissions:
CMAQ PM2.5 in mg/m^3



Circles:
Bias without episodic
(but with climatological) fire emissions
CMAQ - OBS

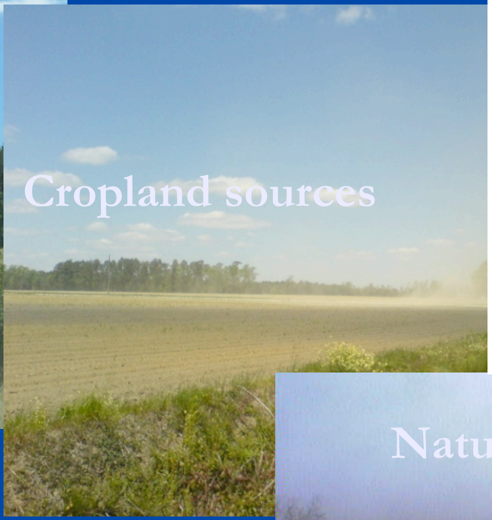
in mg/m^3

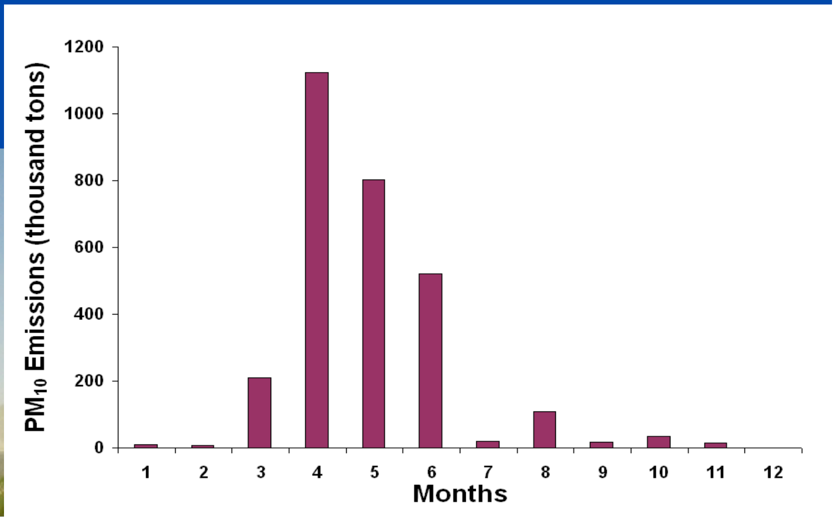
(Colors for circles and background Have no relations)

On-going work to include Wind-Blown Dust Emissions

Natural dust not accounted for yet in NAQFS

Major Dust Emission Sources





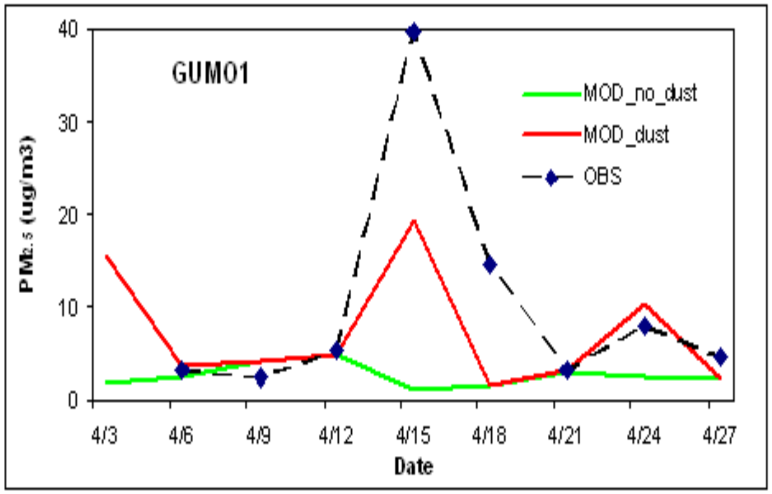
EPA's NEI includes anthropogenic dust sources

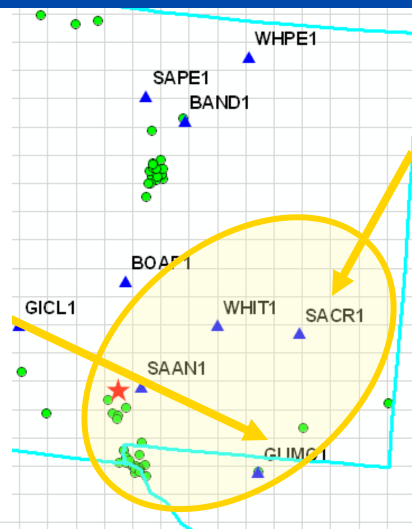
Modeling Natural Dust requires

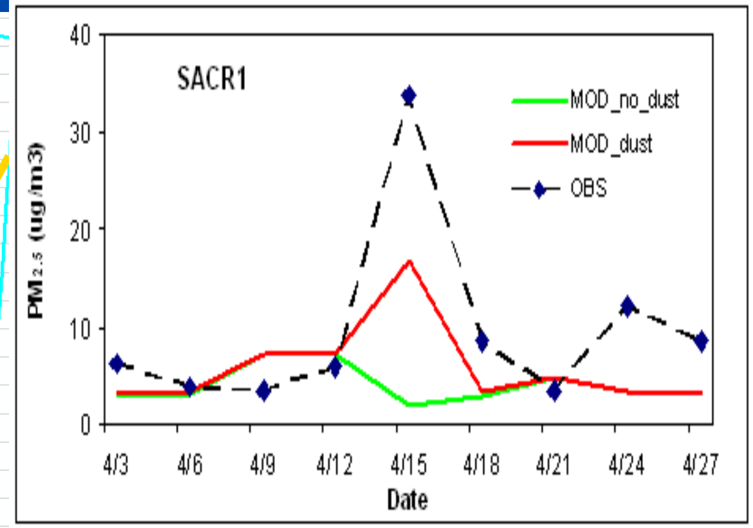
- **Owen's flux equation**
- **Threshold friction velocities from field and wind tunnel measurements;**
- **USGS land use and soil data;**
- **Vegetation growth and near source enhanced deposition;**

Testing algorithms -- Comparison with IMPROVE & MODIS

(April 2003 Case Study)

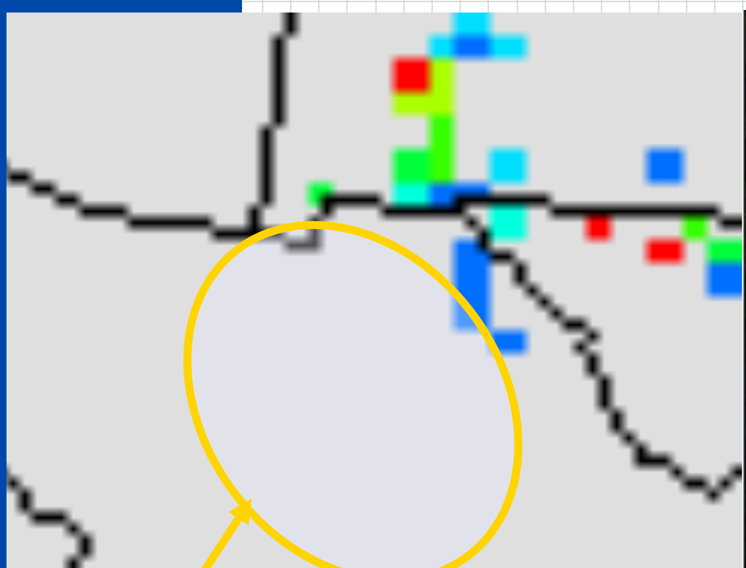


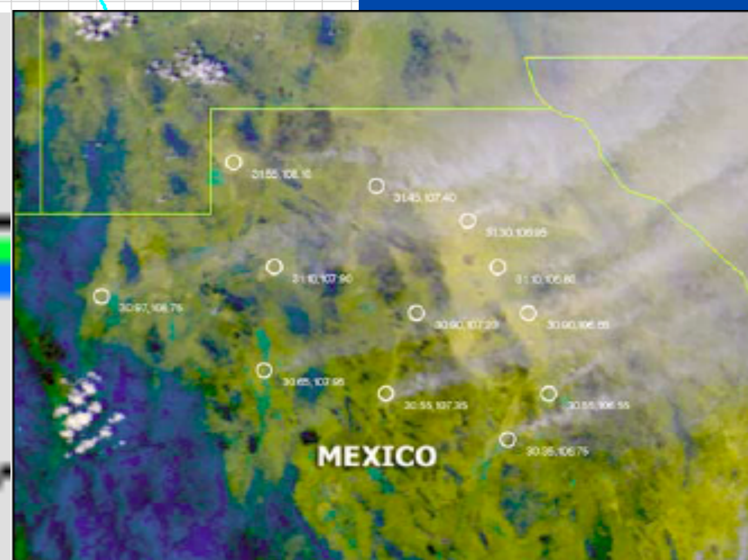




Improved, but not enough.

MODEL





MODIS

Missing Sources in Mexico

(Source: Rivera et al., 2006)

Conclusive Remarks

Investigating causes of bad forecasting may lead to future improvements

Previous talk …. For O3 at CMAS meeting

- First, look at the impact of meteorological forecasting (winds, clouds, precipitation, temperature, humidity …)
- If met forecasting was quite wrong previous day, consider "reinitializing" before next forecasting (not easy!) by assimilating met. Inputs & rerun AQ modeling
- Improve BCs into the system using global scale models
- Reduce anthropogenic emission uncertainties

This talk …. For PM2.5

If no episodic emissions and/or long-range transport BCs in the system

-Could use satellite and surface obs to re-initialize ICs

Better to develop methods (data/algorithms) for including intermittent emissions from **forest fires**, **wind-driven dust events**, (**volcanic ashes, etc & BCs)**