Evaluation of NASA Aura's Data Products for Use in Air Quality Studies Over the Gulf of Mexico

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Presented at

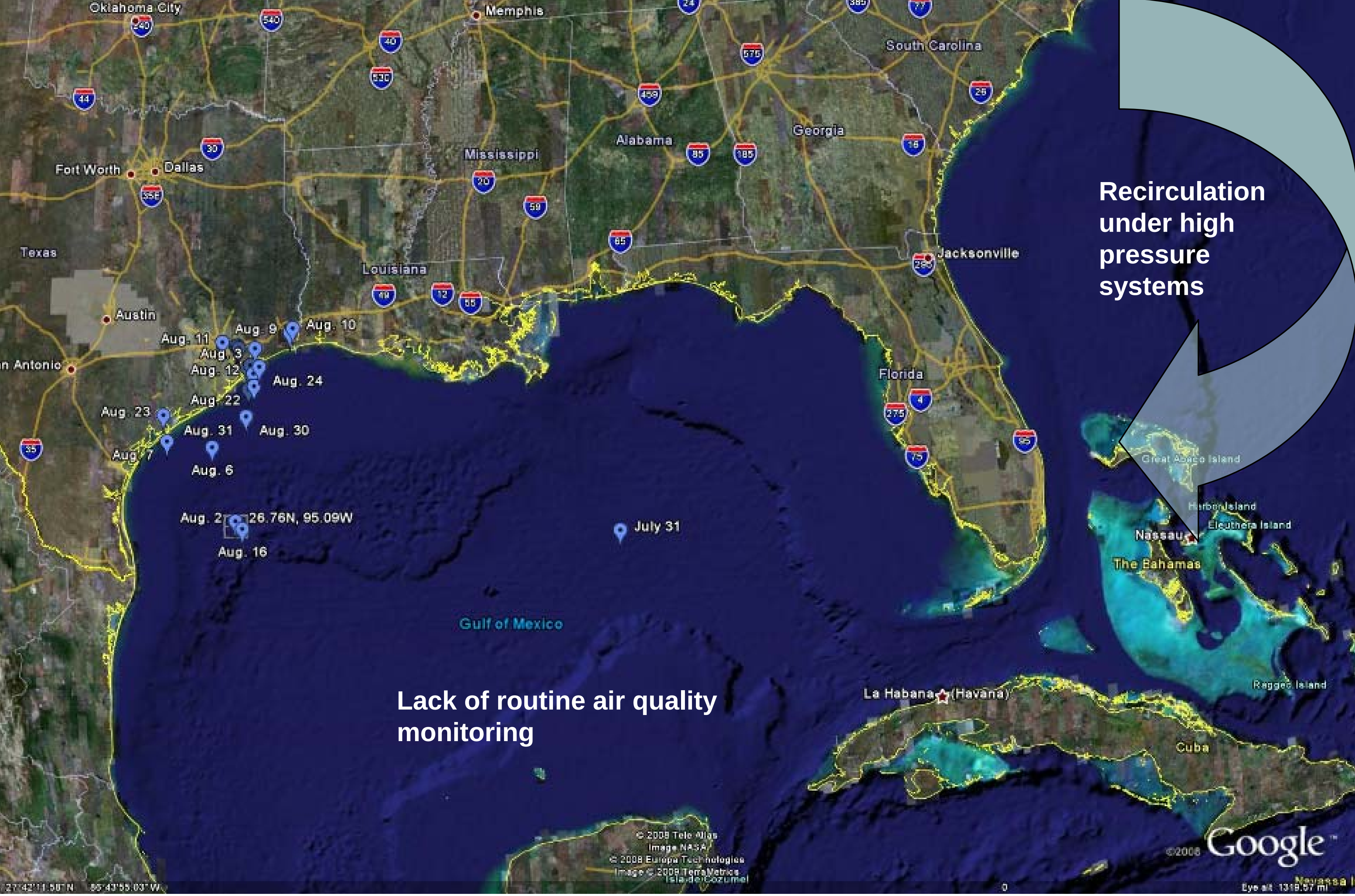
25th Minerals Management Service Information Transfer Meeting

6 – 8 January 2009

New Orleans, Louisiana

Motivation

- In assessing the potential onshore impact of outer continental shelf (OCS) sources on ozone, one of the sources of uncertainty in photochemical models is the characterization of the background air. Reducing such errors is of interest to MMS.
- Large scale atmospheric motions carry polluted air to a region far from the source
  - Natural background and setting of the federal standard
  - Effect of inter-continental transport on local pollution
  - Recirculation of pollution in southeastern United States under high pressure system
- Lack of routine air quality monitoring over open waters poses a challenge in specifying model IC/BC over regions such as GoM.
- Satellite observations of trace gases and aerosol can potentially address some of these issues.



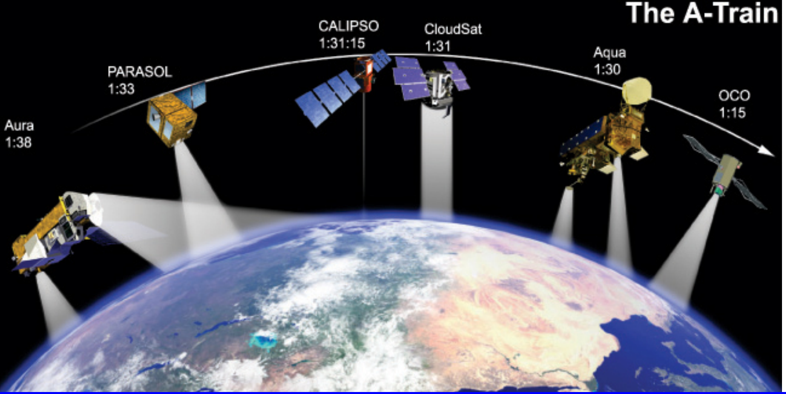
Recirculation under high pressure systems
Lack of routine air quality monitoring
Aug. 9
Aug. 10
Aug. 11
Aug. 3
Aug. 12
Aug. 24
Aug. 22
Aug. 23
Aug. 31
Aug. 30
Aug. 7
Aug. 6
Aug. 2
26.76N, 95.09W
Aug. 16
July 31
Gulf of Mexico
Oklahoma City
Memphis
South Carolina
Georgia
Alabama
Mississippi
Fort Worth
Dallas
Texas
Louisiana
Jacksonville
Austin
San Antonio
Florida
Great Abaco Island
Harbor Island
Eleuthera Island
Nassau
The Bahamas
La Habana (Havana)
Ragged Island
Cuba
Google

Utility of Satellite Data

1. Now the question is: Can satellite data improve air quality studies over GoM region?
2. We started to examine the viability of use of TES observations for improving air quality predictions, in particular to address the following questions:
    1. How reliable are TES observations in the boundary layer over GoM region?
    2. Given the sparseness of TES daily observations, does it still offer value for air quality simulations over GOM region?
    3. Can average ozone observations derived from TES observations on weekly and monthly timescales be useful in improving the air quality model performance?
    4. How useful are TES observations for air quality model evaluation?
3. With the availability of OMI/O3 profiles we started to utilize the new data product.
4. We also examined the utility of MODIS aerosol products.

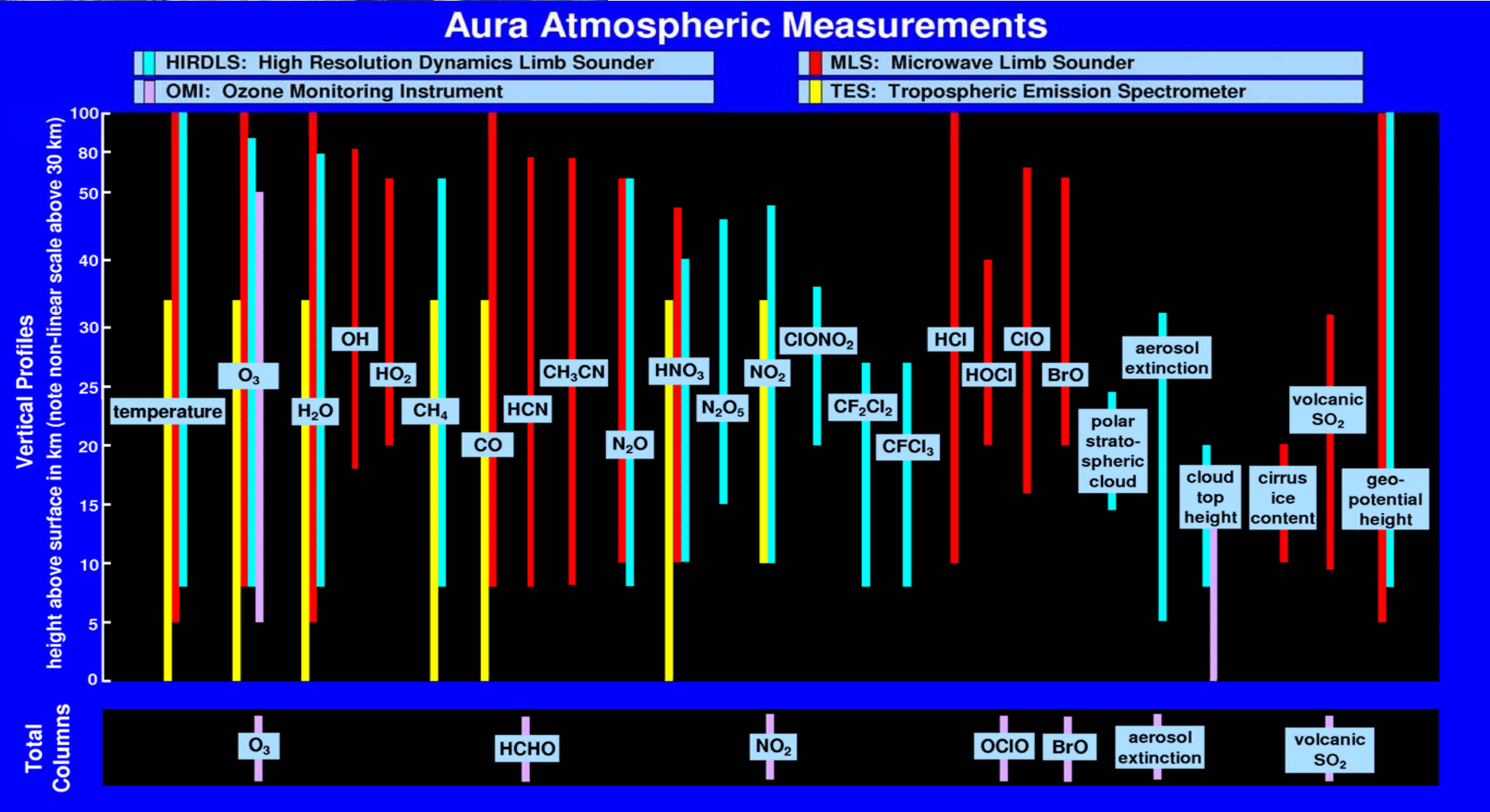
Satellite Data Used in This Study

- **Aura (NASA Earth Observing System)**
  - **Tropospheric Emission Spectrometer (TES)**
  - **Ozone Monitoring Instrument (OMI)**
- **Terra & Aqua (10:30 AM & 1:30 PM)**
  - **The Moderate Resolution Imaging Spectroradiometer (MODIS)**
- **GOES (Geostationary Operational Environmental Satellite)**
  - **Visible and IR sensors**

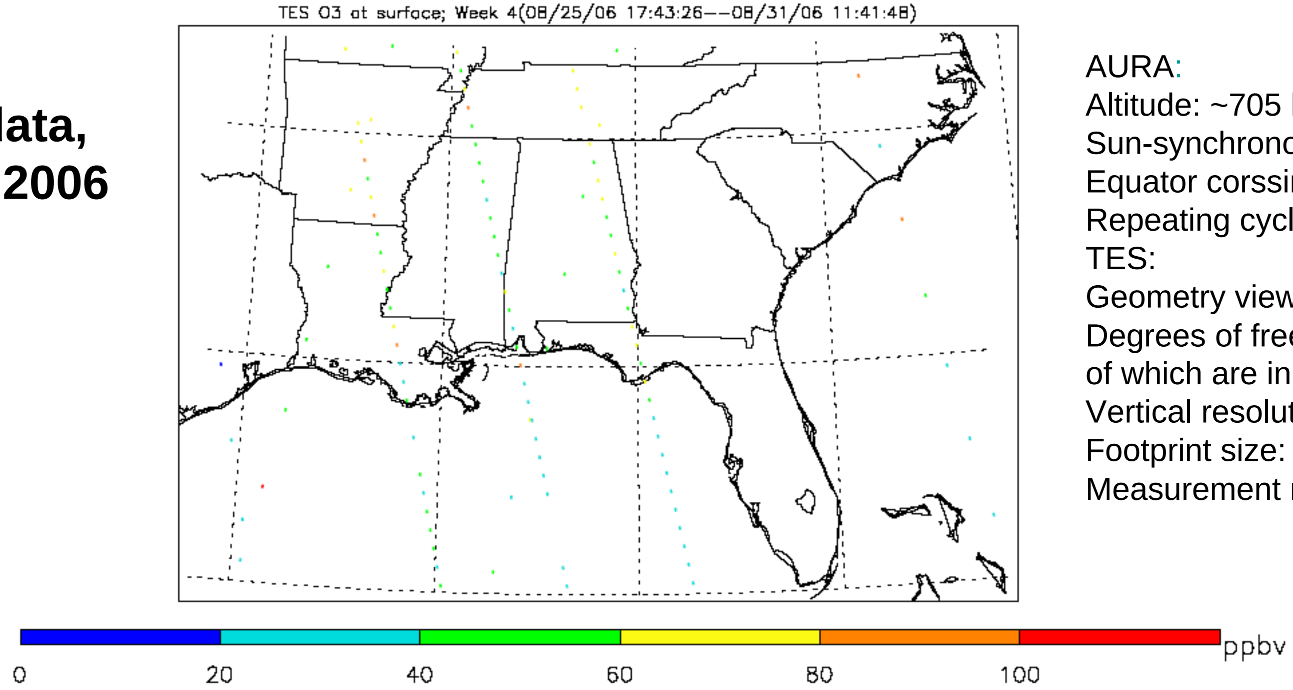


Available Data Products from Aura's Sensors

(adapted from Schoeberl et al. 2006)

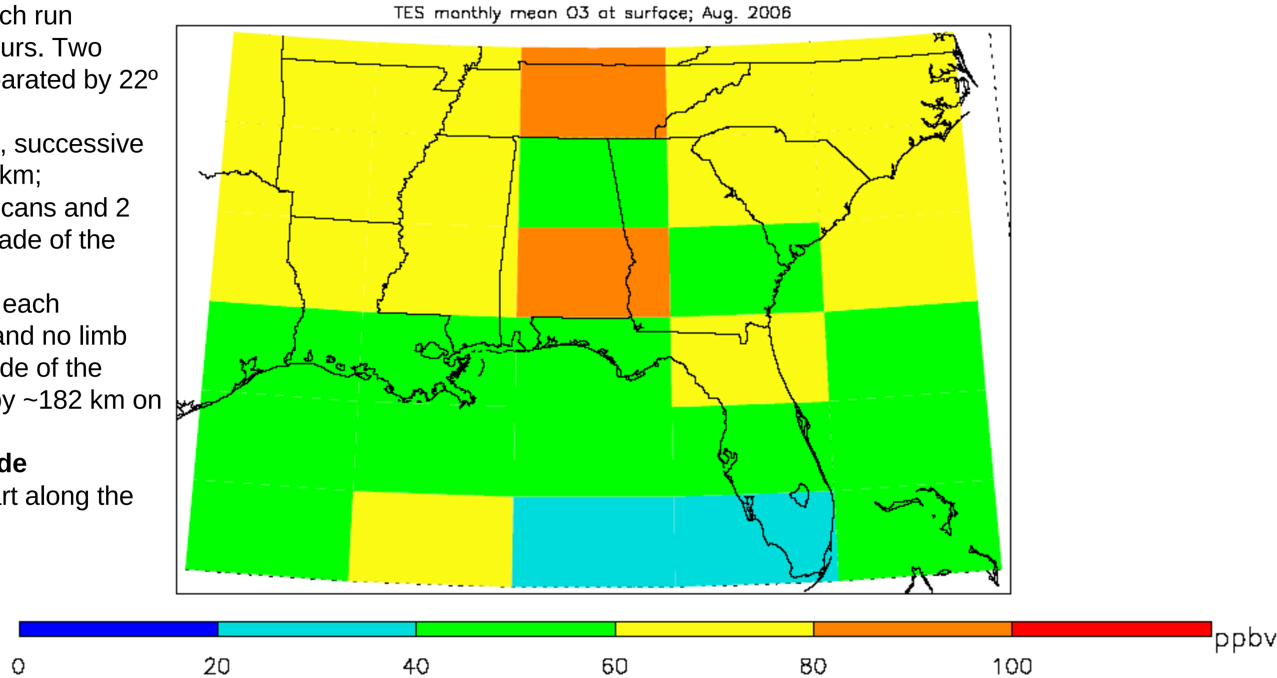


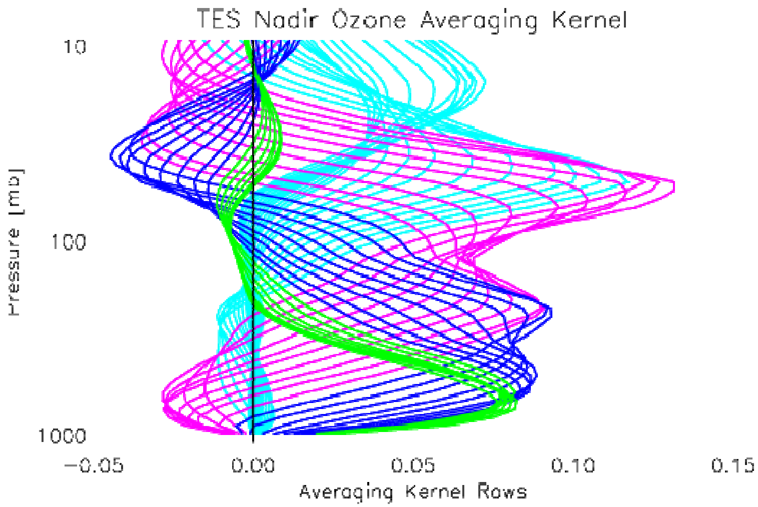
Actual TES data, 25 – 31 Aug. 2006



AURA:
Altitude: ~705 km
Sun-synchronous polor orbit
Equator corssing time: ~13:45
Repeating cycle: 16-day
TES:
Geometry views: nadir & limb
Degrees of freedom: 4, and two of which are in the troposphere
Vertical resolution: 6 km
Footprint size: 5.3 km by 8.3 km
Measurement mode: GS, SO

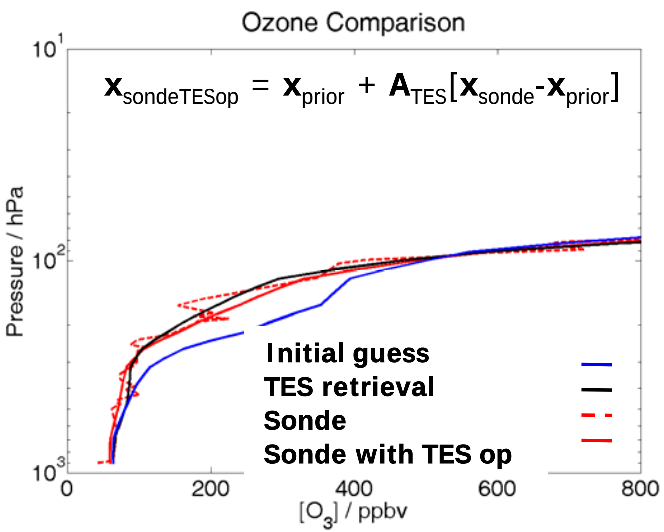
TES Global Survey (GS) mode: Each run contains 16 orbits within about 26 hours. Two neighboring TES orbit tracks are separated by 22º longitude (2118 km at 30N).
Old GS mode: Before May 21, 2005, successive sequences were separated by ~544 km;
Each sequence consisted of 3 limb scans and 2 nadir scans; the 2 nadir scans are made of the same spot.
New GS mode: After May 21, 2005, each sequence consists of 3 nadir scans and no limb scans. The 3 nadir scans are not made of the same spot; each scan is separated by ~182 km on the ground.
TES Special Observation (SO) mode
Step and Stare (SS): 40–45 km apart along the ground track
Transect mode: only ~12 km apart

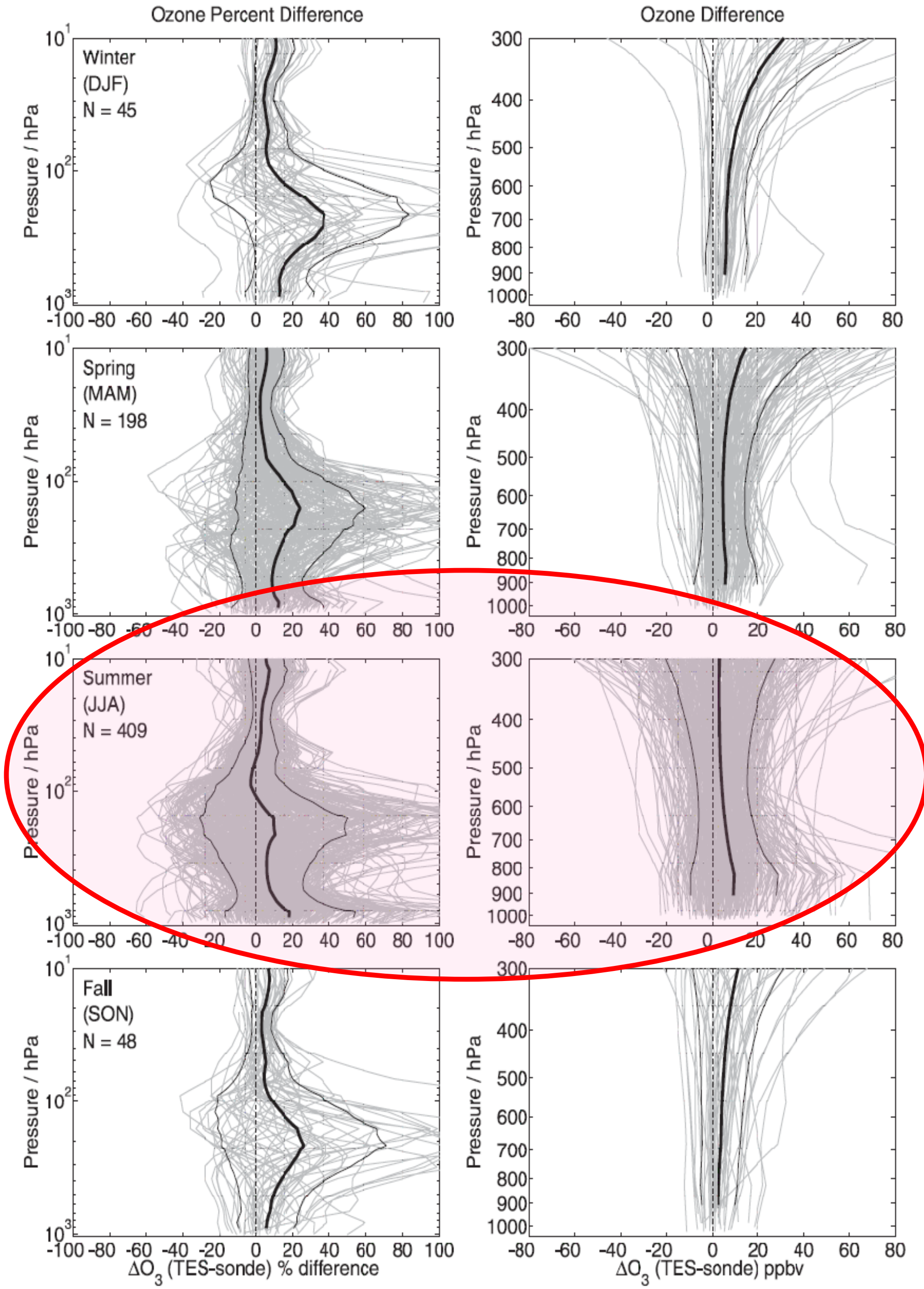




From Ray Nassar

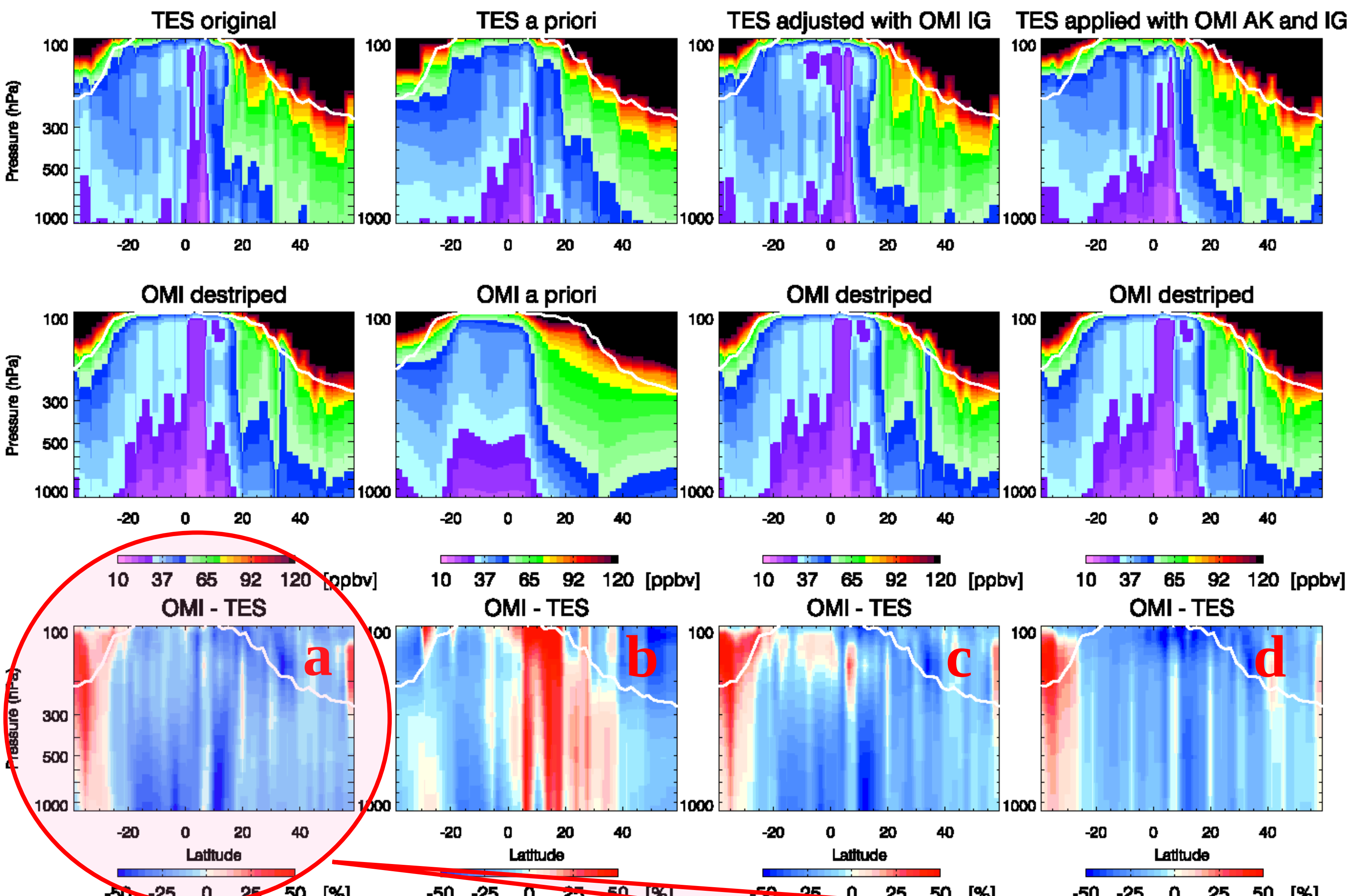
Nassar et al. 2008





Adapted from Xiong Liu, Harvard-Smithsonian Center for Astrophysics (personal communication)

OMI/TES Comparison



(b) Biases are not caused by a priori
(a, c, d) Mostly systematic differences

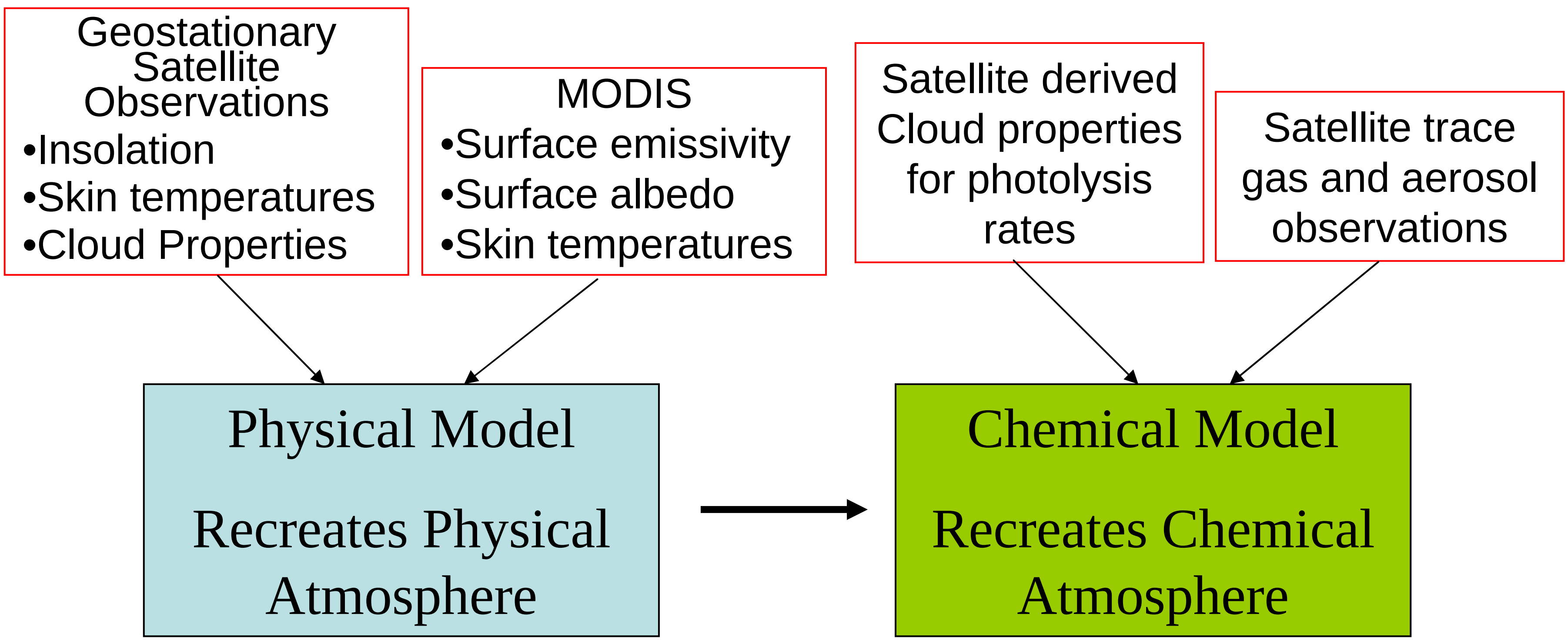
OMI is comparable to TES in mid-latitudes and provides a complete daily spatial coverage

August 2006 Case Study

- Study overview
- Methodology
- Utilization of satellite observations to provide boundary condition and initial condition for the AQ Model (CMAQ)
- Results and conclusions

Simulations – Satellite Inputs

Data available from:
http://sat_assim.nsstc.uah.edu/



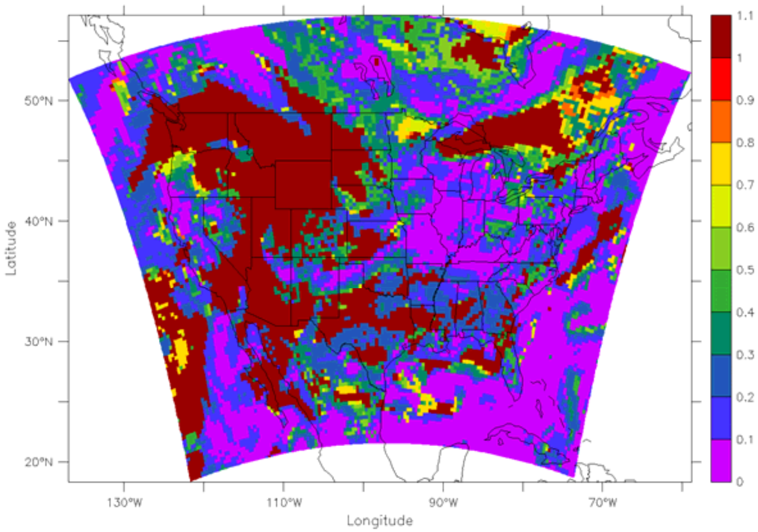
Overview of August 2006 Case Study

- MM5 and CMAQ simulations were performed for the summer of 2006 (15 July – 7 September). This period coincides with IONS06 and TexAQS06 field campaigns.
- MM5 simulation utilized ETA gridded analysis, surface and upper air observations. The results were evaluated and used in all subsequent CMAQ simulations.
- CMAQ simulations incrementally added the satellite observations.
- The results were evaluated against surface and ozonesonde observations.
- Results from the following simulations will be presented:

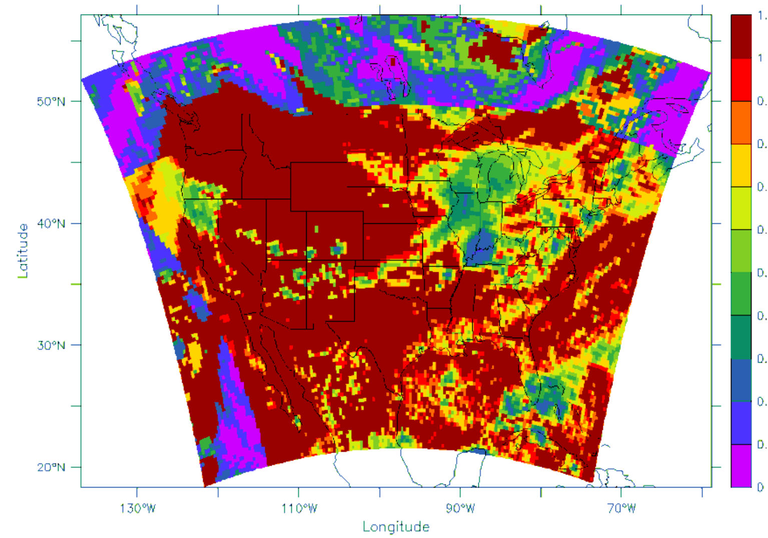
CNTRL	CMAQ simulation with U.S. EPA default boundary and initial conditions.
SATCLD	Similar to CNTRL except the use of GOES observed clouds to adjust photolysis rates.
SATCLD_ICBC	CMAQ simulations with GOES cloud adjustment + satellite O3 and PM2.5 BC + satellite O3 and PM2.5 every 24 hrs as initial condition.
SATBC	Similar to CNTRL except for BC. Satellite O3 and PM2.5 was used to provide BC.

CONTROL SIMULATION

SATCLD SIMULATION



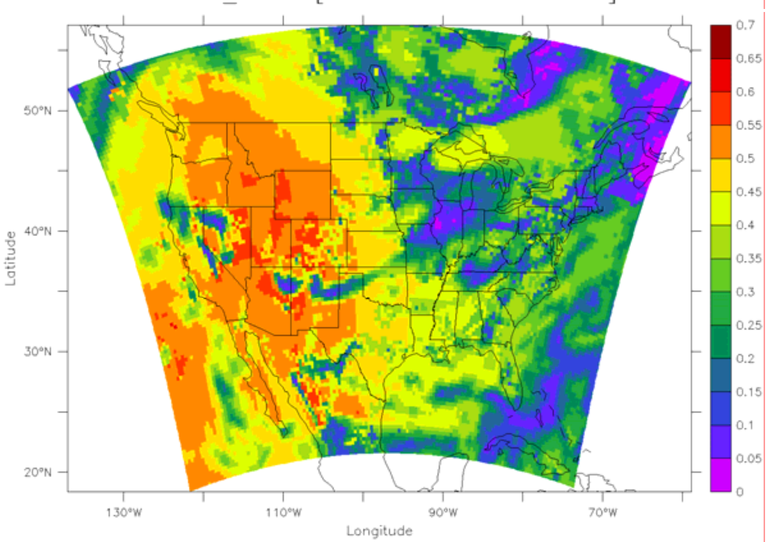
CLDTR_CNTRL[T=21–JUL–2006 20:00]



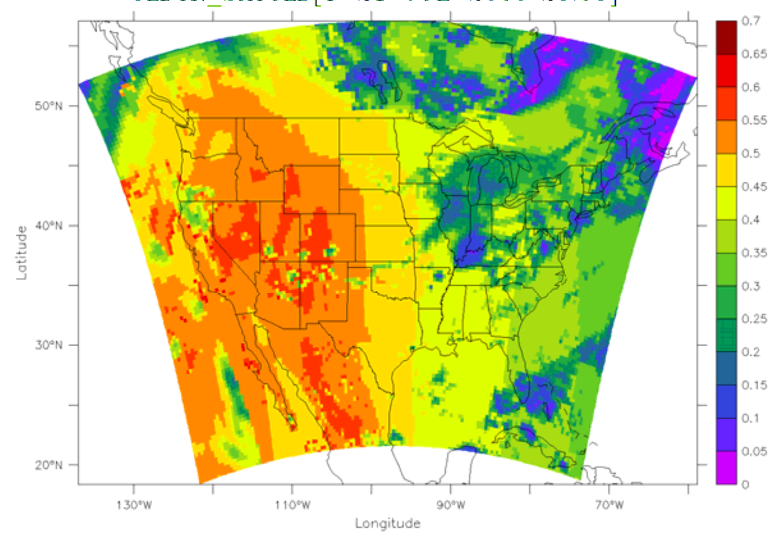
CLDTR_SATCLD[T=21–JUL–2006 20:00]

Transmissivity

CNTRL too opaque compared to satellite



JNO2_CNTRL[T=21–JUL–2006 20:00]

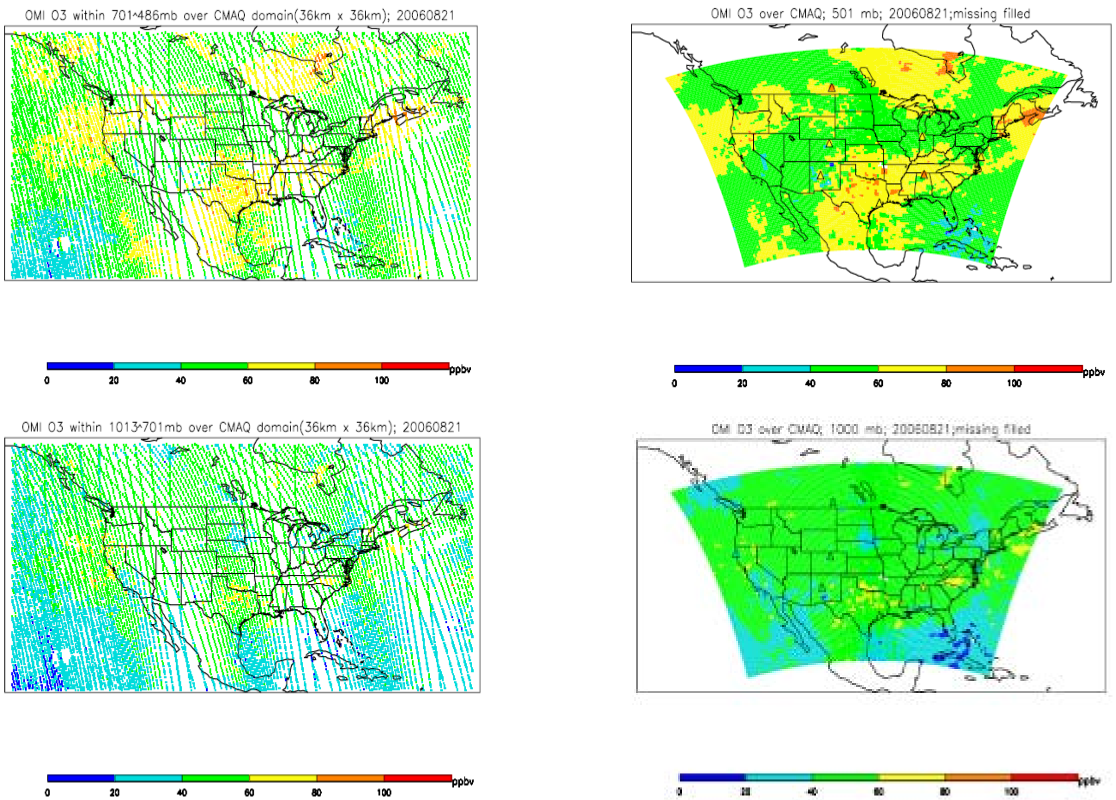


JNO2_SATCLD[T=21–JUL–2006 20:00]

NO2 photolysis rate

Generally CNTRL was close to observation

Aura/OMI O3 retrieval & IONS06 Network



424 ozonesondes were launched from 23 North American sites during August 2006.
(http://croc.gsfc.nasa.gov/intexb/ions06.html)

The ozonesonde data was used to evaluate both OMI profiles and model predictions.

OMI retrievals in the lateral boundaries of the domain were extracted and used as boundary condition (BC) and the full domain retrievals used as initial condition (0 GMT) for each daily run.

Aura/OMI Level 2 O3 profiles (24 layers; credit: Xiong Liu, GEST/UMBC/CFA) are mapped to CMAQ horizontal domain (36km x 36km) using a “drop-in-the-box” method; The daily-mean profiles are then interpolated to CMAQ 39 vertical layers.

Left: OMI O3 plotted with fixed pixel size (not real size, swath width ~ 2600 km)

Right: OMI O3 mapped to CMAQ 3-D domain (36kmx36km, 39 layers)

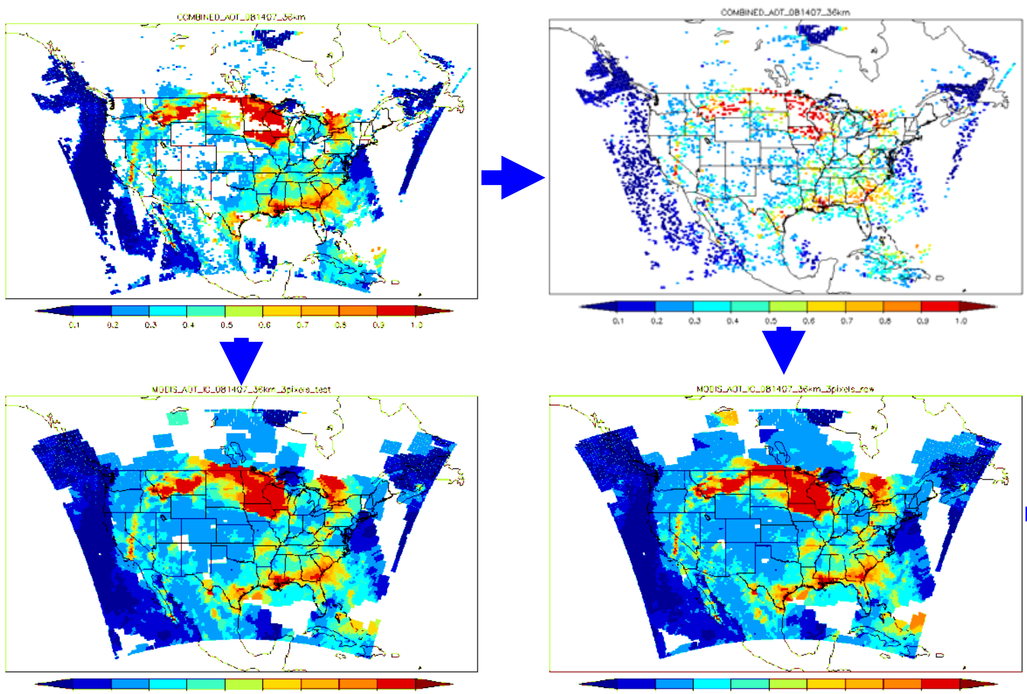
Assimilation of MODIS AOD

- MODIS L2 from Terra (10:30) and Aqua(13:30) are combined and mapped to CMAQ 36-km grid spacing
- Data coverage is increased by replacing missing pixels by the average of surrounding pixels
- MODIS fine fraction is used to partition fine & coarse mode aerosols
- CMAQ AOD is calculated based on IMPROVE equation
- For fine mode, CMAQ aerosol profiles are scaled as

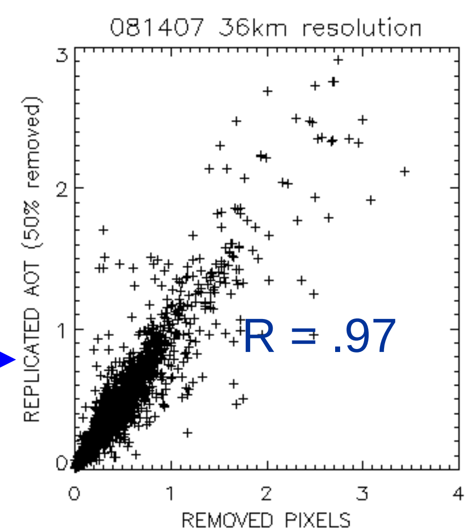
$$C(z) = C_{CMAQ}(z) \times \frac{\tau_{MODIS}}{\tau_{CMAQ}}$$

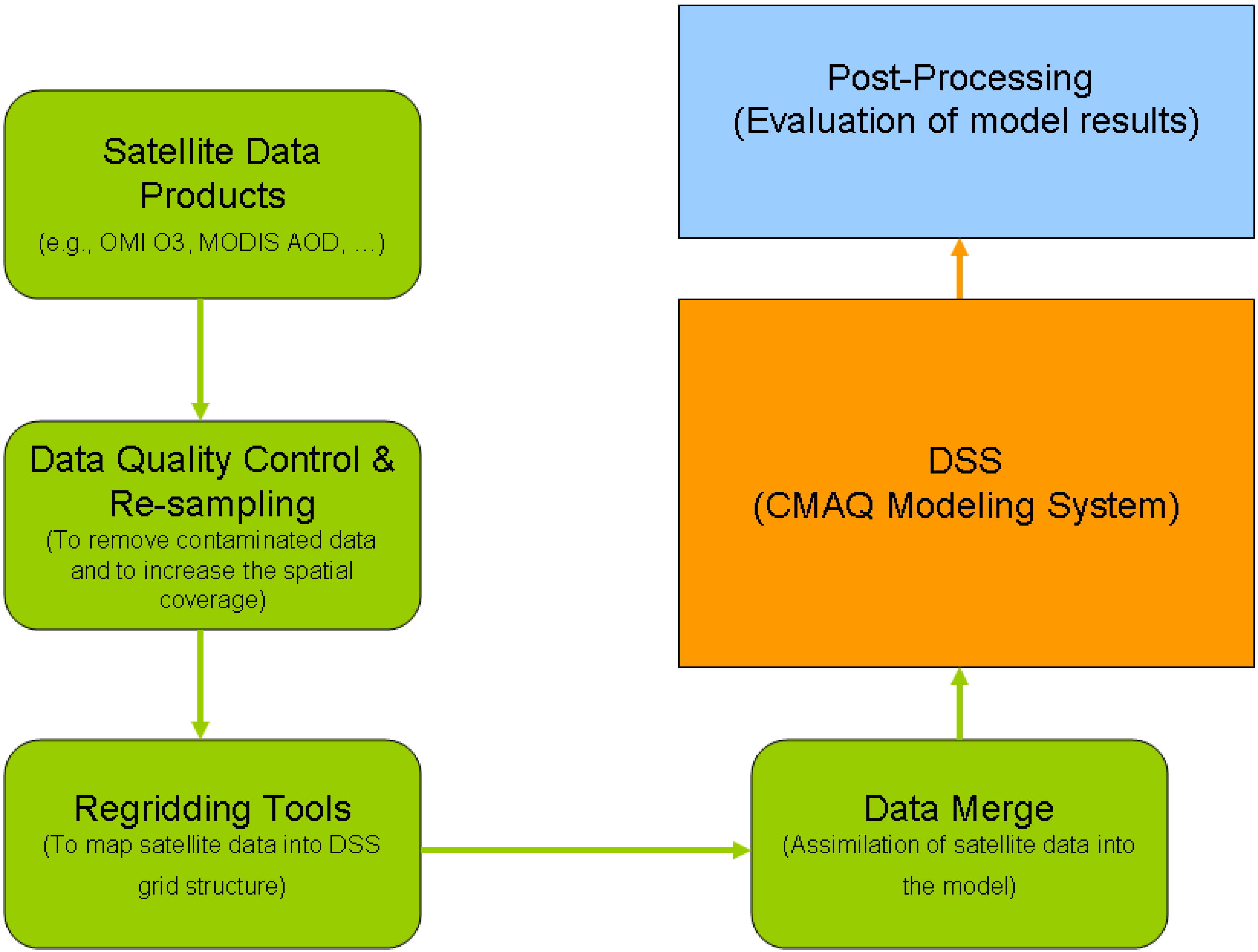
Original MODIS AOD Map for 14 August 2007 (AQUA & TERRA)

50% of pixels were removed randomly



- 50% of data were removed randomly
- Data coverage were increased by replacing each missing pixel with the average of surrounding pixels
- Final product was well correlated with the original data



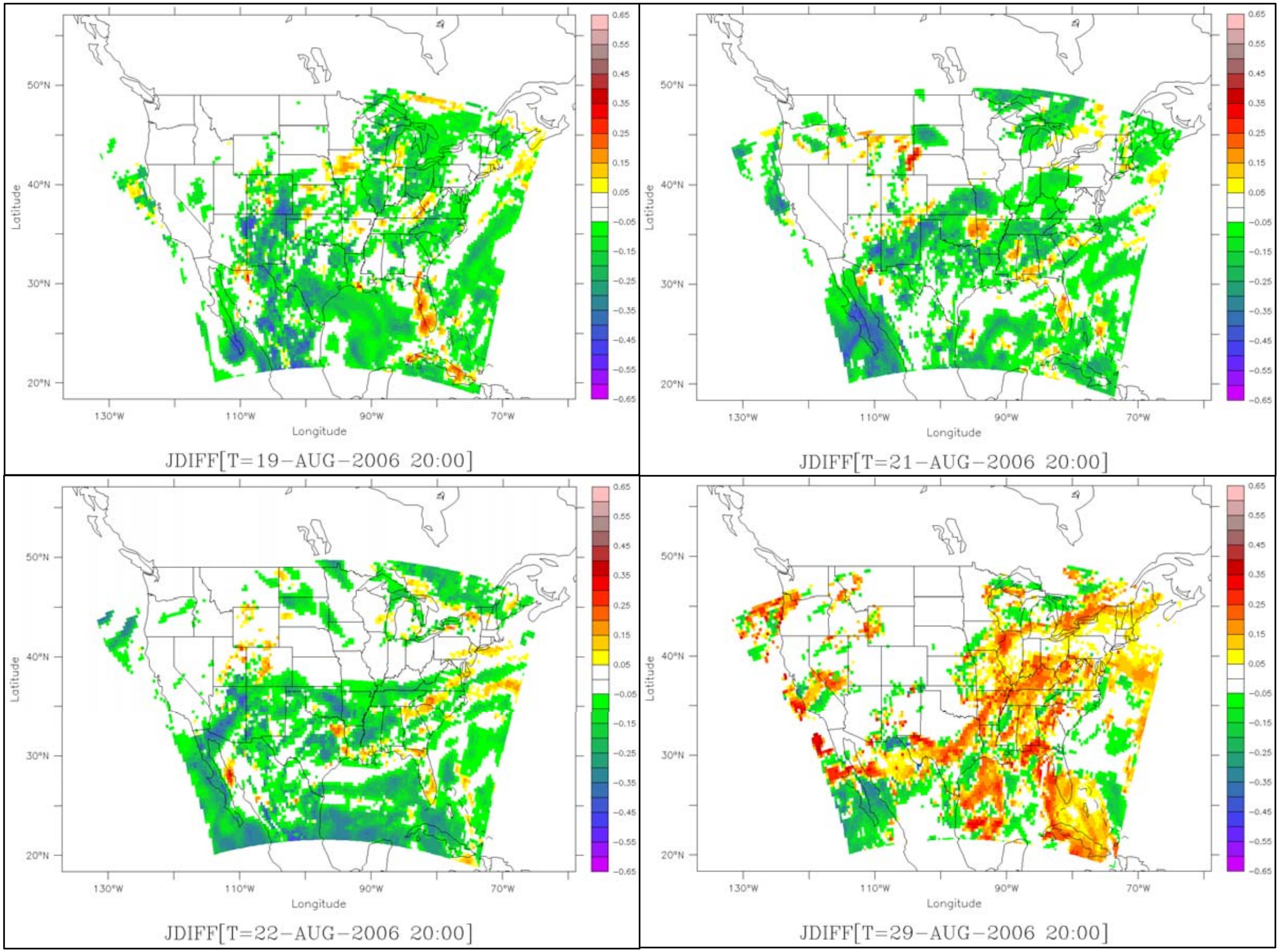


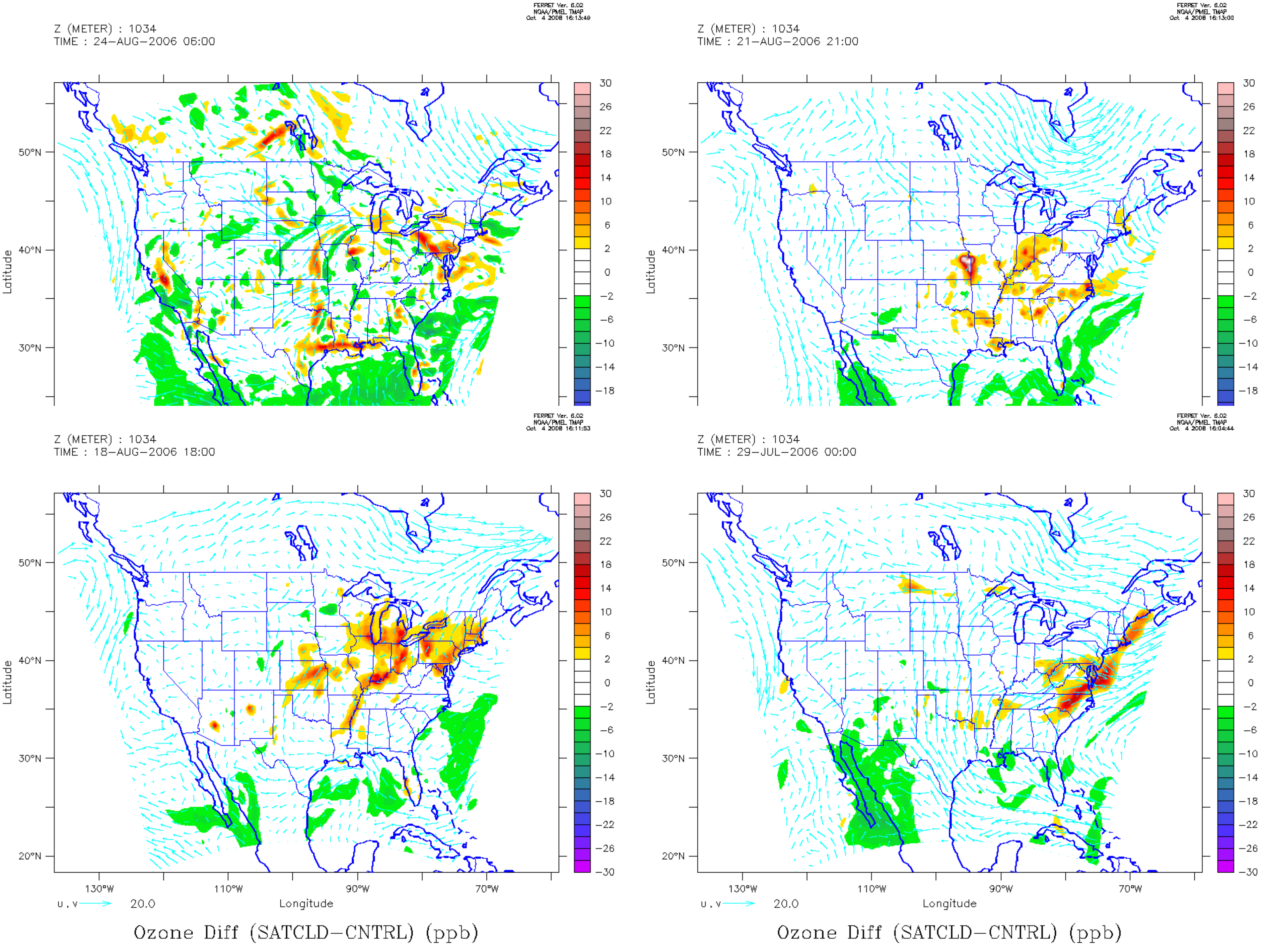
Post-Processing
(Evaluation of model results)
Satellite Data Products
(e.g., OMI O3, MODIS AOD, ...)
DSS
(CMAQ Modeling System)
Data Quality Control & Re-sampling
(To remove contaminated data and to increase the spatial coverage)
Regridding Tools
(To map satellite data into DSS grid structure)
Data Merge
(Assimilation of satellite data into the model)

RESULTS

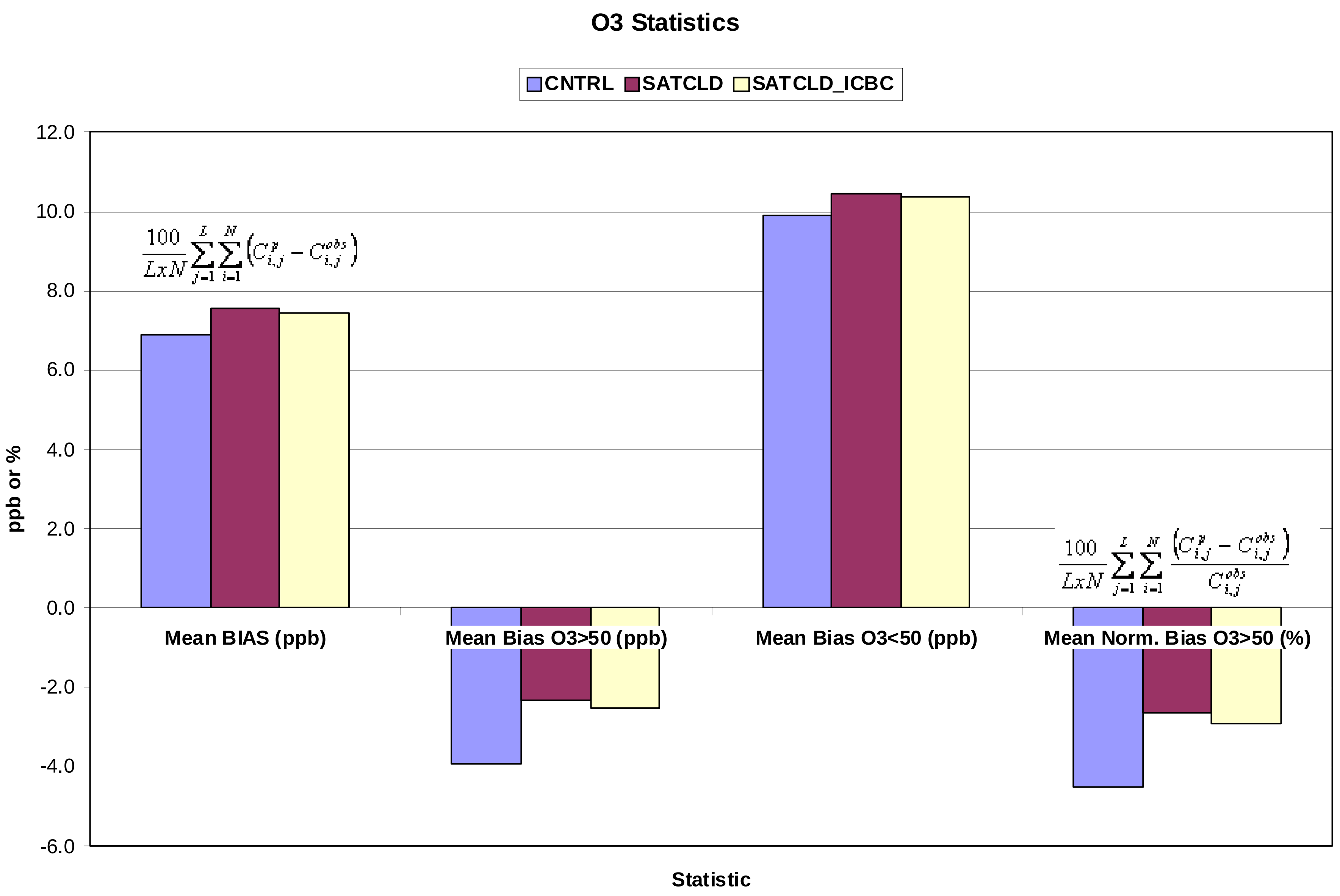
Difference in NO2 photolysis rates for selected days

(CNTRL-SATCLD)



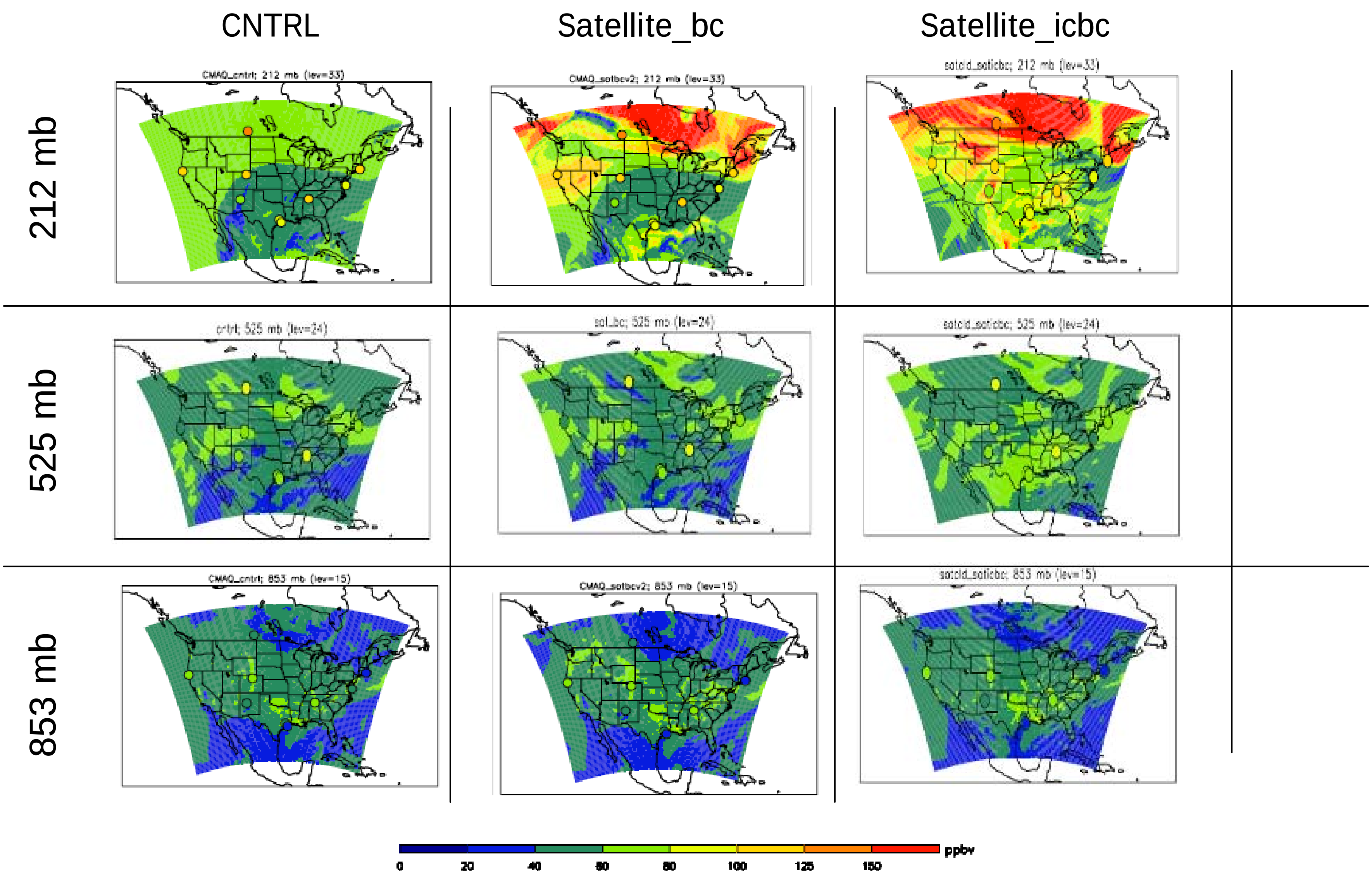


Z (METER) : 1034
TIME : 24-AUG-2006 06:00
Z (METER) : 1034
TIME : 21-AUG-2006 21:00
Z (METER) : 1034
TIME : 18-AUG-2006 18:00
Z (METER) : 1034
TIME : 29-JUL-2006 00:00
Latitude
Longitude
50°N
40°N
30°N
20°N
130°W
110°W
90°W
70°W
u,v 20.0
30
26
22
18
14
10
6
2
0
-2
-6
-10
-14
-18
-22
-26
-30
Ozone Diff (SATCLD-CNTRL) (ppb)
Ozone Diff (SATCLD-CNTRL) (ppb)



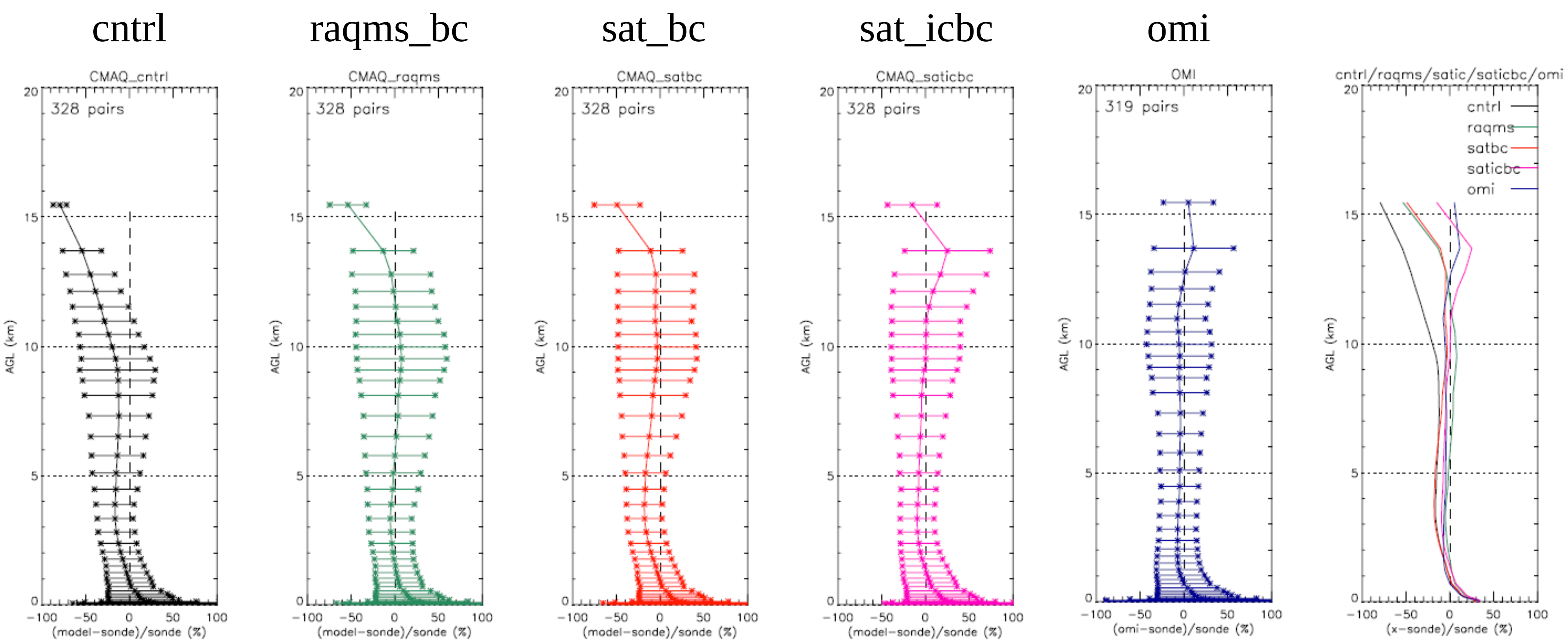
O3 Statistics
CNTRL
SATCLD
SATCLD_ICBC
12.0
10.0
8.0
6.0
4.0
2.0
0.0
-2.0
-4.0
-6.0
ppb or %
$\frac{100}{LxN}\sum_{j=1}^{L}\sum_{i=1}^{N}\left(C_{i,j}^{p}-C_{i,j}^{obs}\right)$
$\frac{100}{LxN}\sum_{j=1}^{L}\sum_{i=1}^{N}\frac{\left(C_{i,j}^{p}-C_{i,j}^{obs}\right)}{C_{i,j}^{obs}}$
Mean BIAS (ppb)
Mean Bias O3>50 (ppb)
Mean Bias O3<50 (ppb)
Mean Norm. Bias O3>50 (%)
Statistic

Preliminary Result (OMI/O3 & MODIS Aerosol Applied)



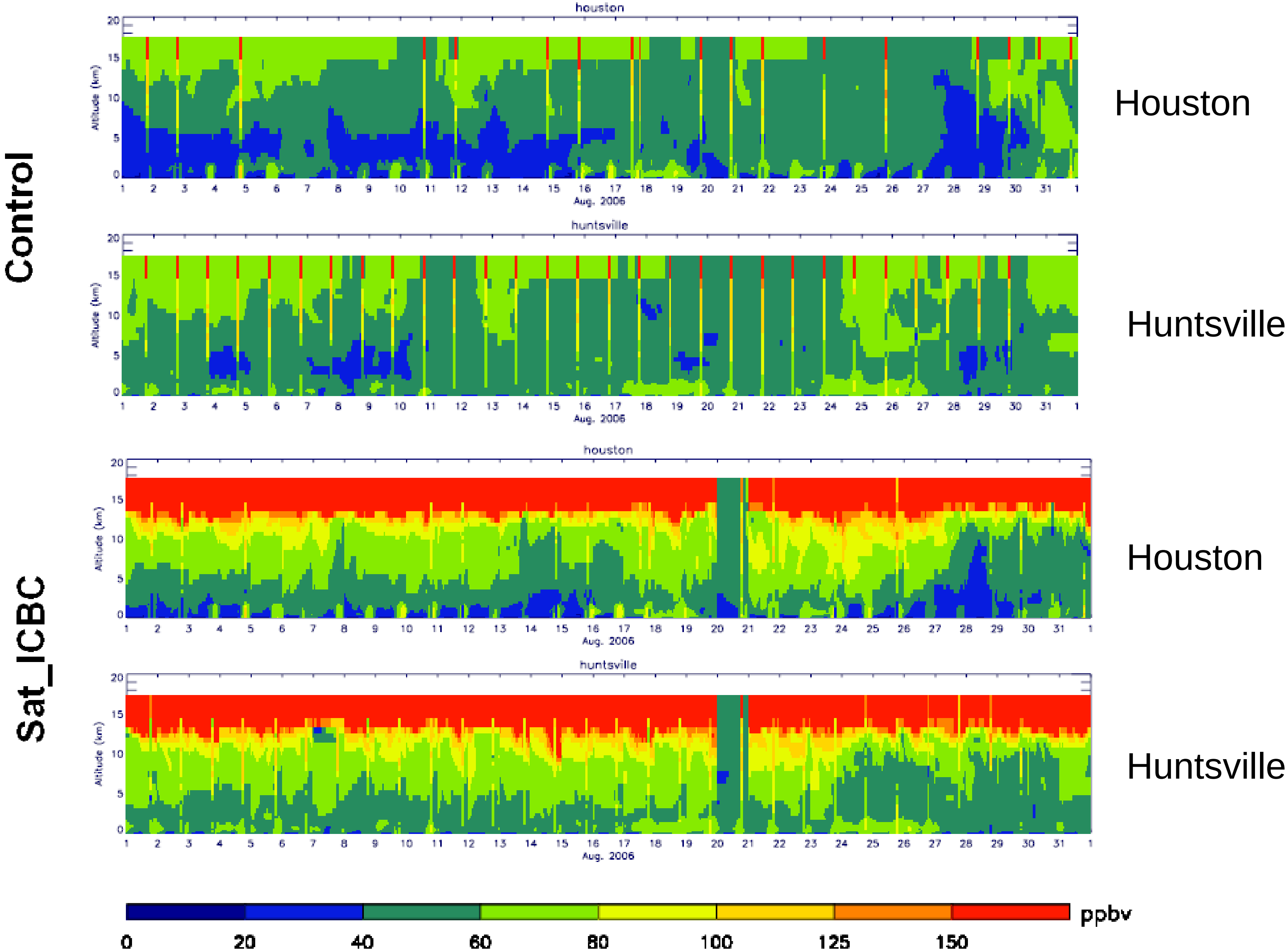
Ozone concentrations at 1900 UTC from 4 CMAQ simulations. Top pannel: 212 mb; Bottom: 853 mb. Ozonesondes within 1500 UTC ~ 2300 UTC are overplotted with same color scale.

Evaluation OMI O3 and CMAQ results with ozonesondes August 2006; 17 stations together (total 328 ozonesondes)

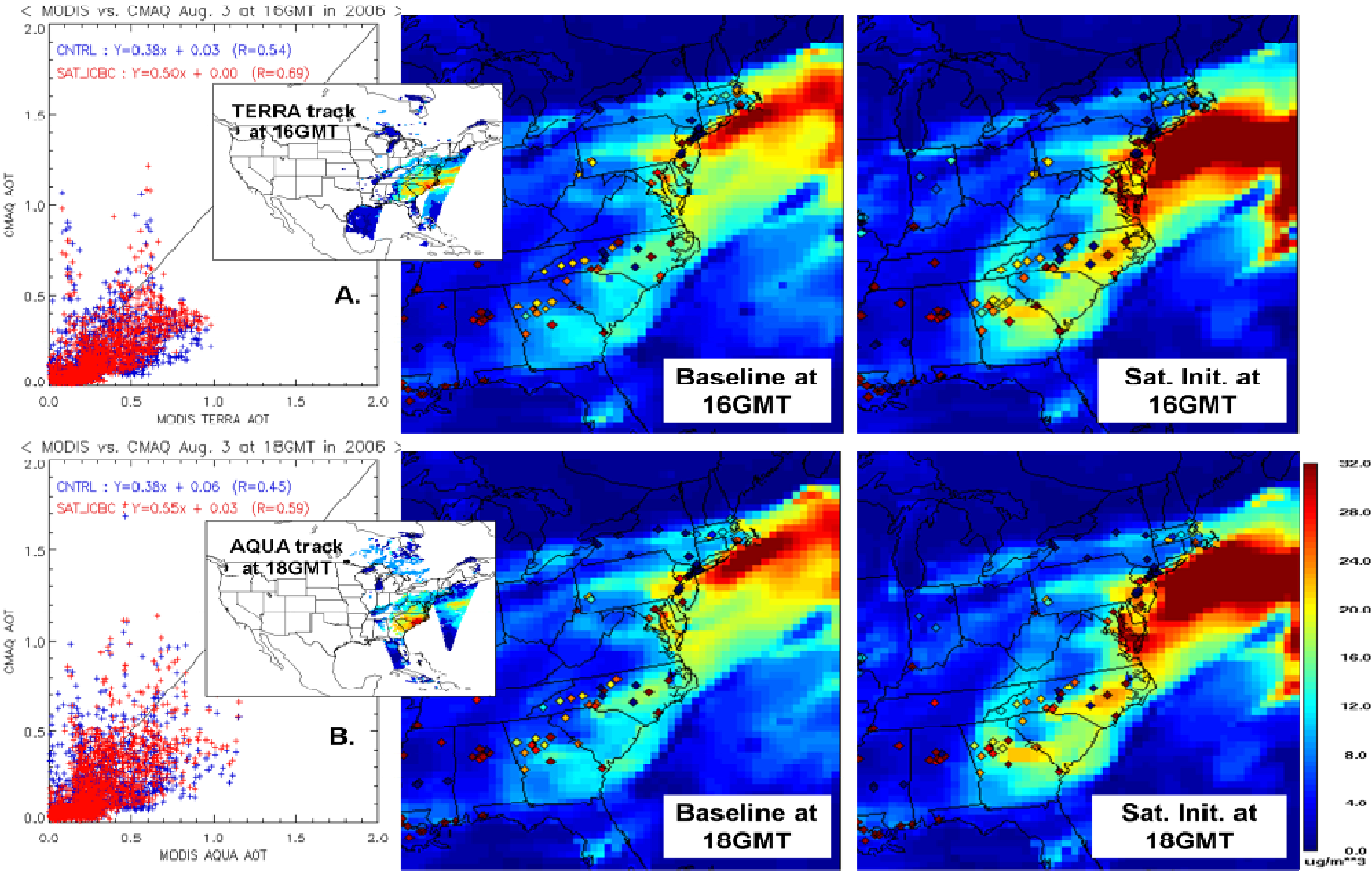


Mean and standard deviation of percent differences (x-sonde)/sonde (%) are plotted above, where x represents O3 simulated from 4 CMAQ runs or OMI/O3, respectively.

USE OF OMI O3 FOR IC/BC IMPROVES MODEL PREDICTIONS IN FT

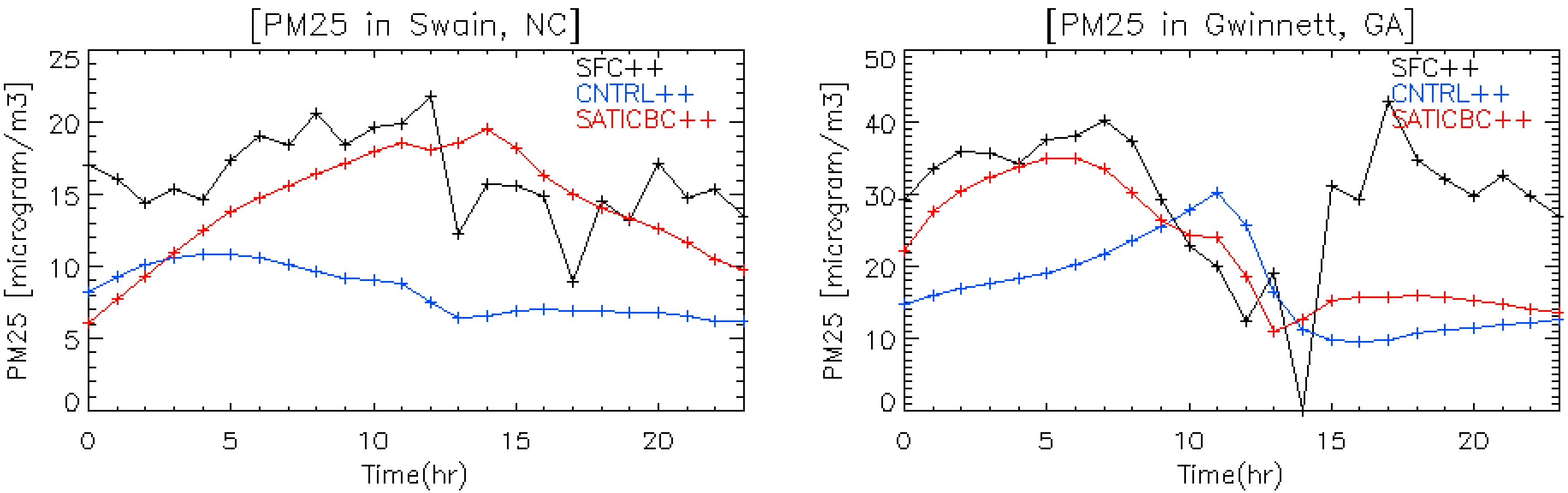


Utilization of MODIS AOD improves model predictions of PM2.5 mass concentration, speciation remains a concern.

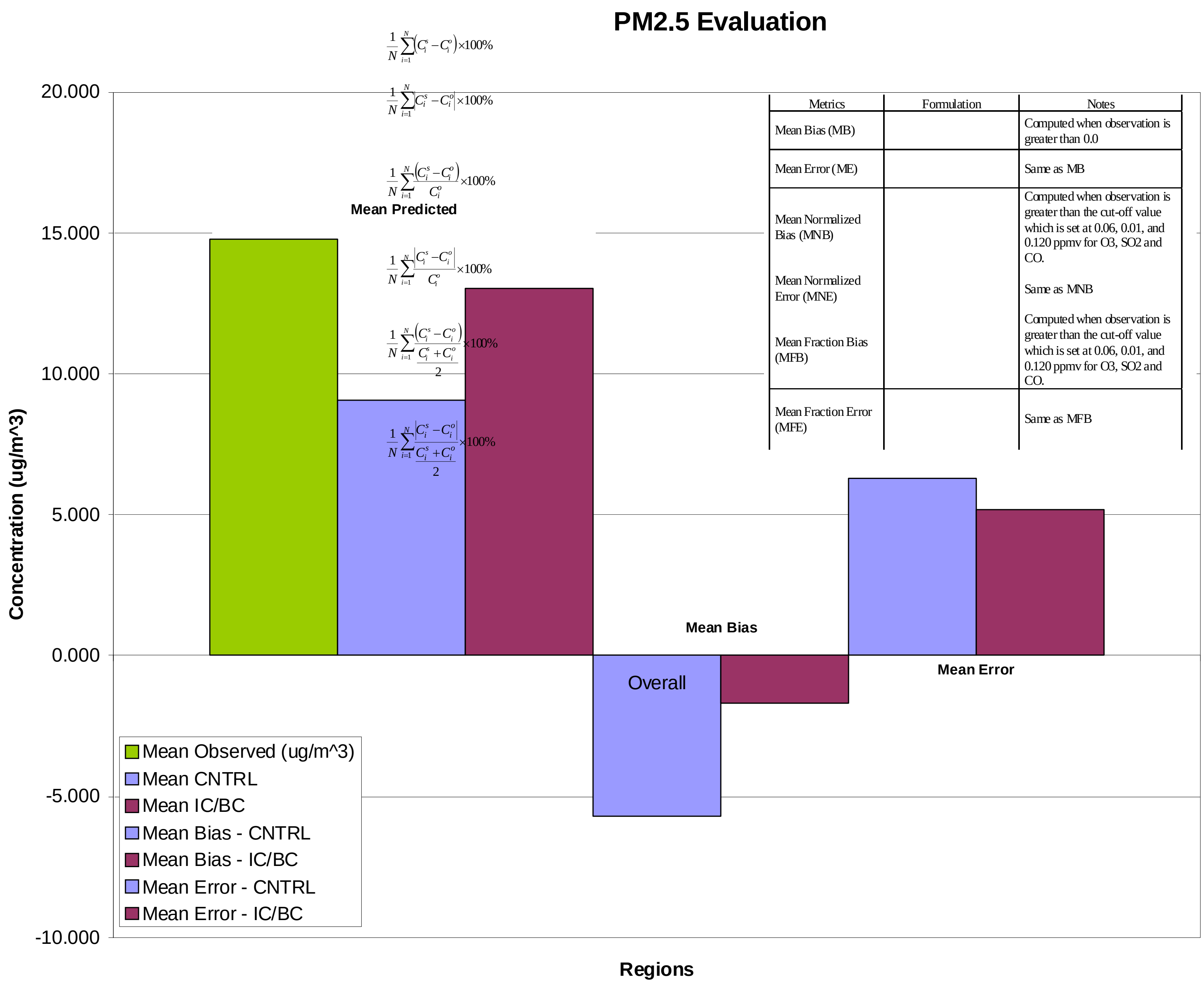


Baseline CMAQ output PM2.5 mass concentration

Applied satellite IC/BC CMAQ output PM2.5 mass concentration



Figures present time series of PM2.5 mass concentration from surface observation (black), baseline CMAQ (blue), and CMAQ simulation utilizing MODIS data (RED) for Swain in North Carolina and Gwinnett in Georgia.



$$\frac{1}{N}\sum_{i=1}^{N}\left(C_i^s - C_i^o\right)\times 100\%$$

$$\frac{1}{N}\sum_{i=1}^{N}\left|C_i^s - C_i^o\right|\times 100\%$$

$$\frac{1}{N}\sum_{i=1}^{N}\frac{\left(C_i^s - C_i^o\right)}{C_i^o}\times 100\%$$

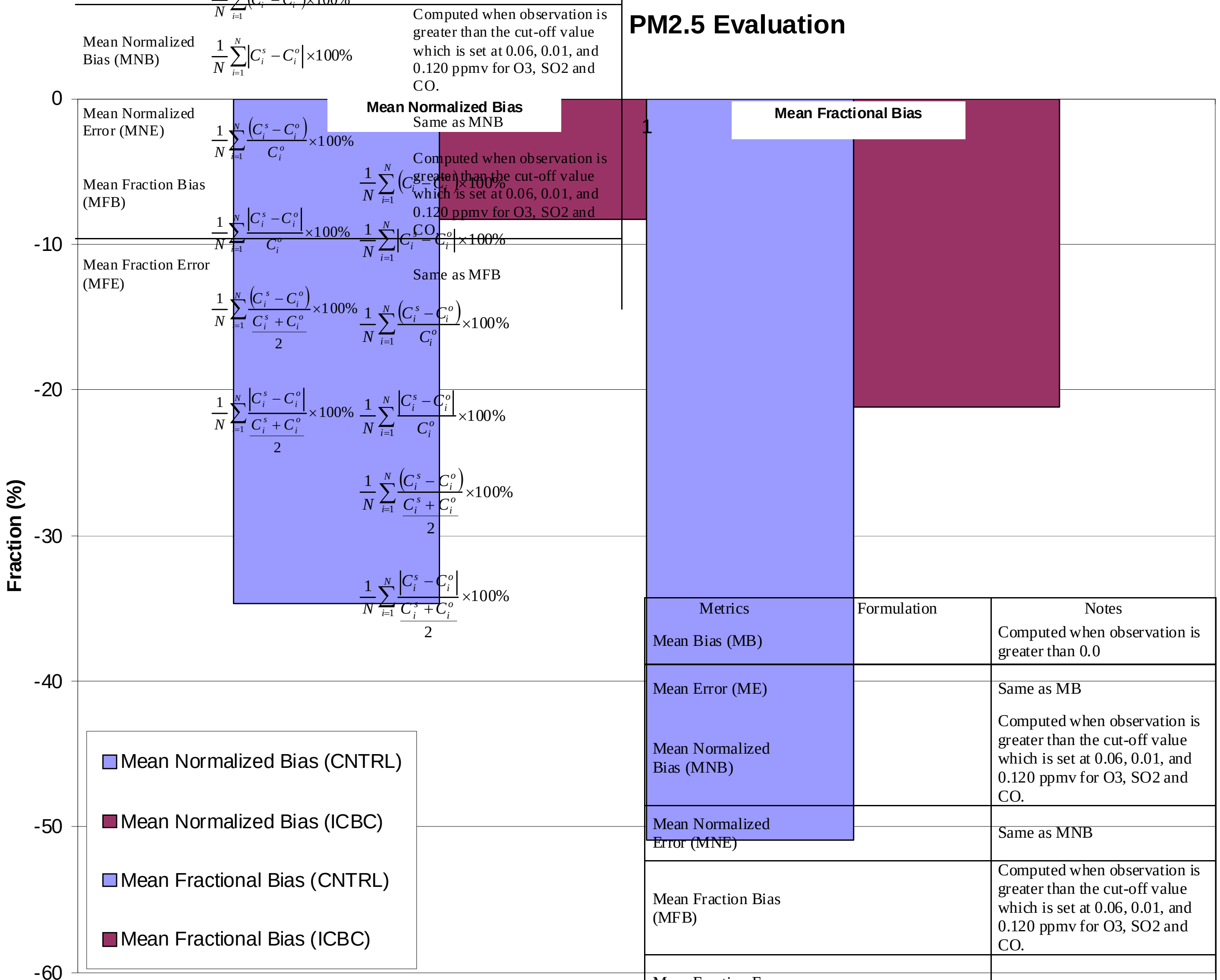
$$\frac{1}{N}\sum_{i=1}^{N}\frac{\left|C_i^s - C_i^o\right|}{C_i^o}\times 100\%$$

$$\frac{1}{N}\sum_{i=1}^{N}\frac{\left(C_i^s - C_i^o\right)}{\frac{C_i^s + C_i^o}{2}}\times 100\%$$

$$\frac{1}{N}\sum_{i=1}^{N}\frac{\left|C_i^s - C_i^o\right|}{\frac{C_i^s + C_i^o}{2}}\times 100\%$$

Metrics	Formulation	Notes
Mean Bias (MB)		Computed when observation is greater than 0.0
Mean Error (ME)		Same as MB
Mean Normalized Bias (MNB)		Computed when observation is greater than the cut-off value which is set at 0.06, 0.01, and 0.120 ppmv for O3, SO2 and CO.
Mean Normalized Error (MNE)		Same as MNB
Mean Fraction Bias (MFB)		Computed when observation is greater than the cut-off value which is set at 0.06, 0.01, and 0.120 ppmv for O3, SO2 and CO.
Mean Fraction Error (MFE)		Same as MFB

PM2.5 Mean Fractional Bias was reduced by about 30%



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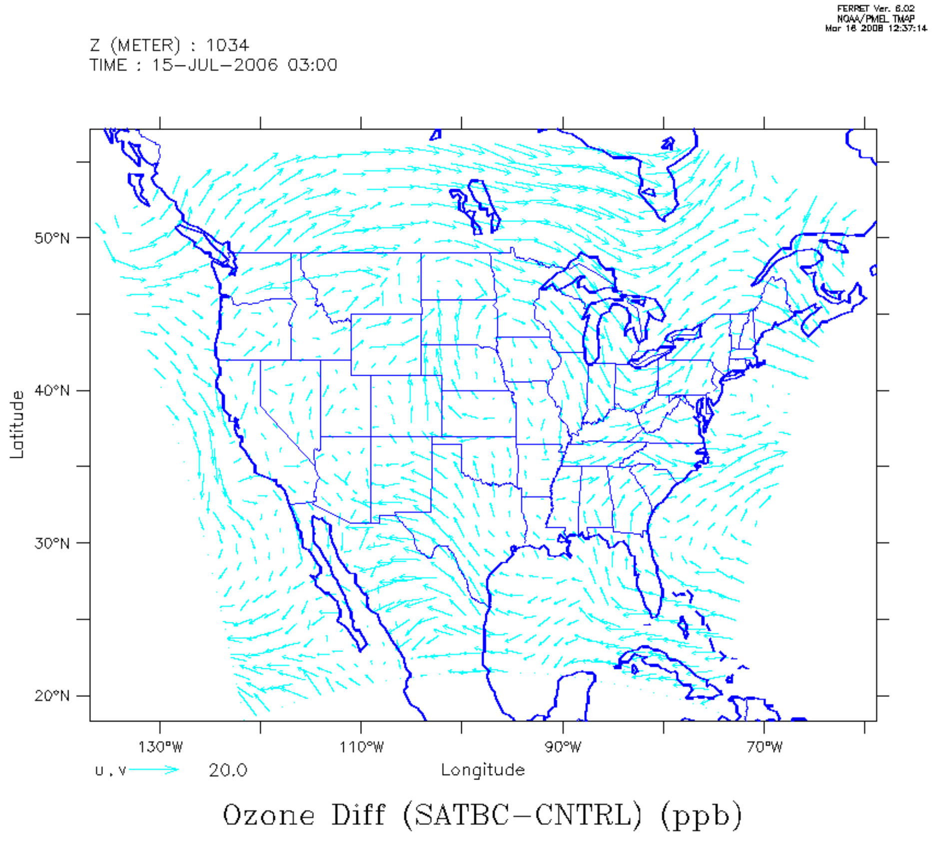
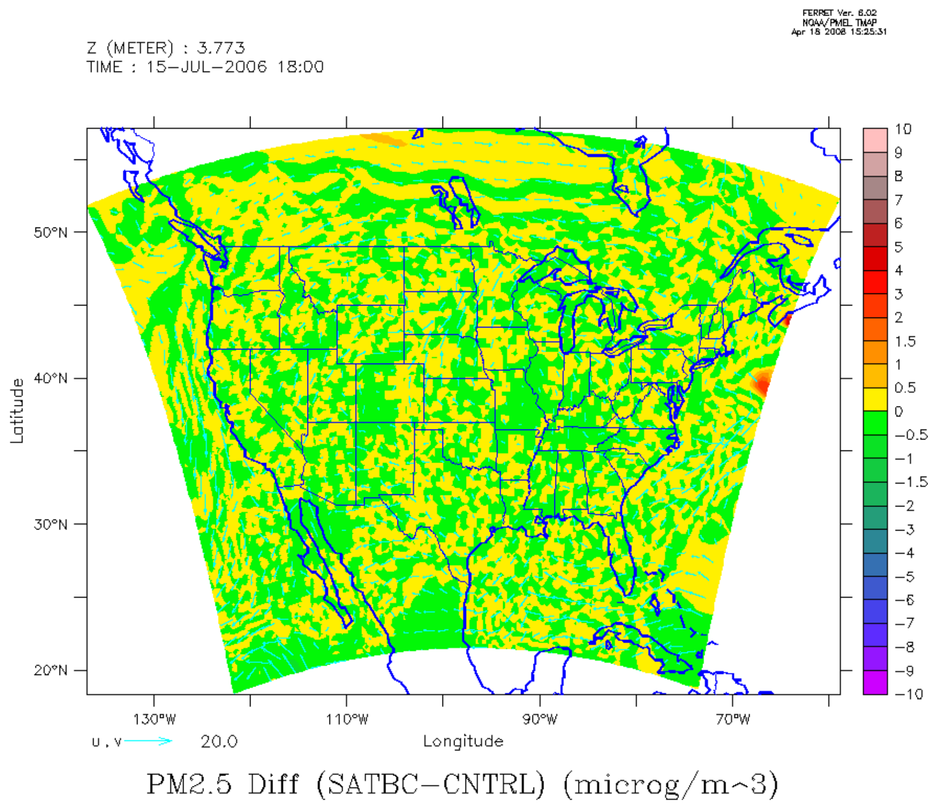


Difference in O3 concentration

(BC from OMI profiles)

Animations of PM2.5 difference

(sat_bc – control)



CONCLUSION & FUTURE WORK

- OMI O3 profiles can potentially be used to provide lateral BC. This is important to the GoM region.
- USE of OMI O3 for lateral BC will correct the model top boundary.
- Use of OMI O3 profiles for IC/BC greatly improved model performance in middle/upper troposphere.
- Assimilation of MODIS AOD greatly improved PM2.5 mass concentration predictions.
- Utilization of GOES observed clouds slightly improved model performance. Model performance at reduced grid spacing is required.

- The work presented here needs further refinements for satellite data ingestion.
- Additional simulations at higher resolution are needed to realize the impact of satellite data products on GoM region.
- Additional satellite observations of trace gases such as HCHO and NO2 can be utilized to better quantify the BL chemical composition.

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