Air Quality Modeling of TexAQS-II Episodes

(1) Data Assimilation & reduce "input" uncertainties
(2) Secondary Organic Aerosol Modeling
(3) HONO Parameterization

"inputs" = meteorology, emissions, initial/boundary conditions

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Rob Griffin: *University of New Hampshire*

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(1) Data Assimilation & reduce “input” uncertainties

Task 1: improved model inputs with satellite and in-situ measurements

(a) Retrospective MM5 simulations with new LULC and MADIS/CAMS were mostly successful in improving wind fields → add TAMU met data

(b) Remaining meteorological modeling problems were associated with mostly either cloud/prcp or stable PBL height & nocturnal wind (TS/CLD)

(c) Incorporate diurnal SST variation to improve Galveston Bay simulation

(d) Assimilate GOES-R satellite cloud-data to improve cloud/prcp (UAH) (TS/CLD)

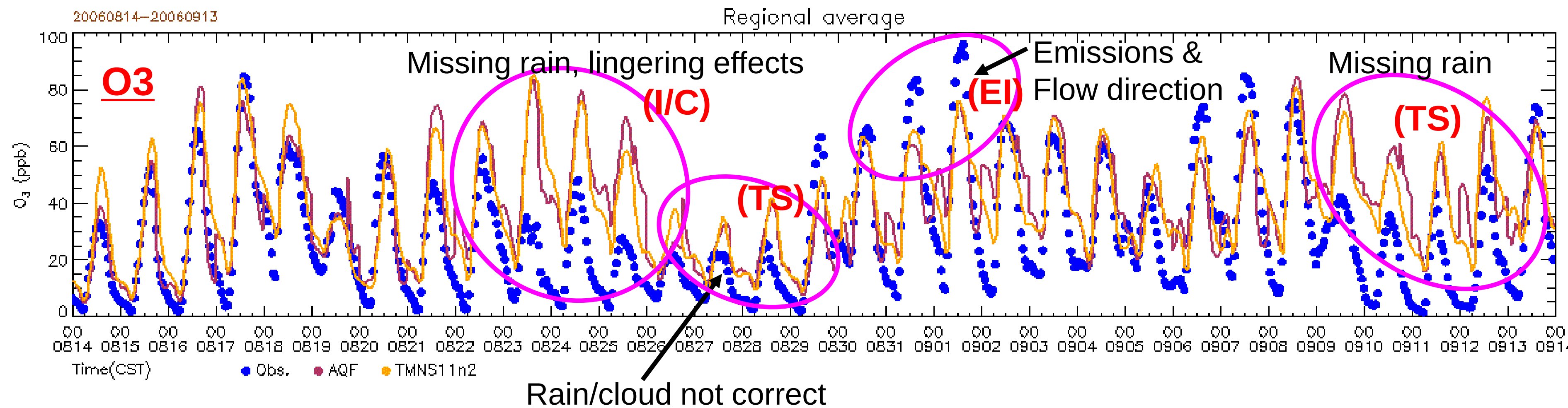
(e) Improve 2006 TPSI emissions using TCEQ’s EI “reconciliation” factors

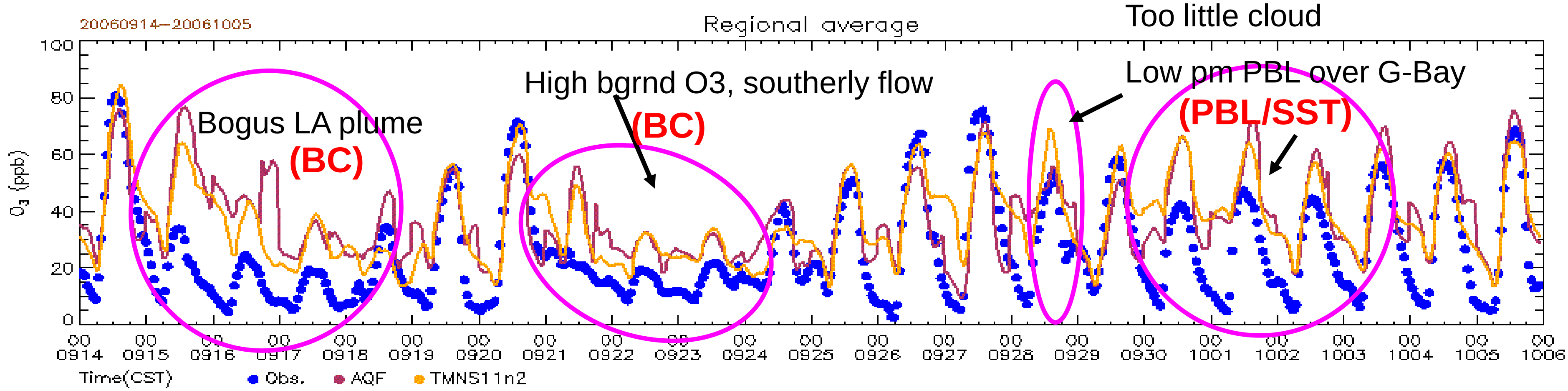
(f) Utilize trajectory, PCA, and HDDM to reduce EI uncertainties (Fire EI)

UH ($60K), Lamar University ($40K), Rice University ($40K)
*** Tech support from Univ. Alabama, Huntsville (McNider & Biazar) for GOES-R data for pilot)

Deliverables: Improved model inputs for TexAQS-II meteorology and air quality modeling

Reduce AQ modeling biases by improving meteorology through data assimilation





O3 averaged over the CAMS sites in the HGB domain
for Aug. 16-Sept. 14, 2006 (upper) and Sept. 15 – Oct. 6, 2006 period (lower).

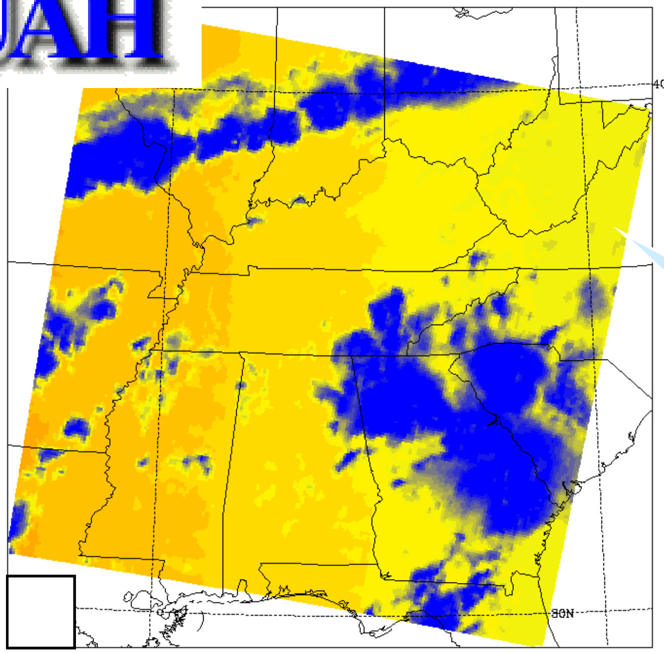
ASSIMILATION OF GOES-DERIVED CLOUD PRODUCTS IN MM5

From Dick McNider & Arastoo Biazar,
Univ. Alabama, Hunsville (UAH)

SATELLITE DATA IS UTILIZED TO CORRECT MODEL CLOUD FIELDS IN A DYNAMICALLY CONSISTENT MANNER

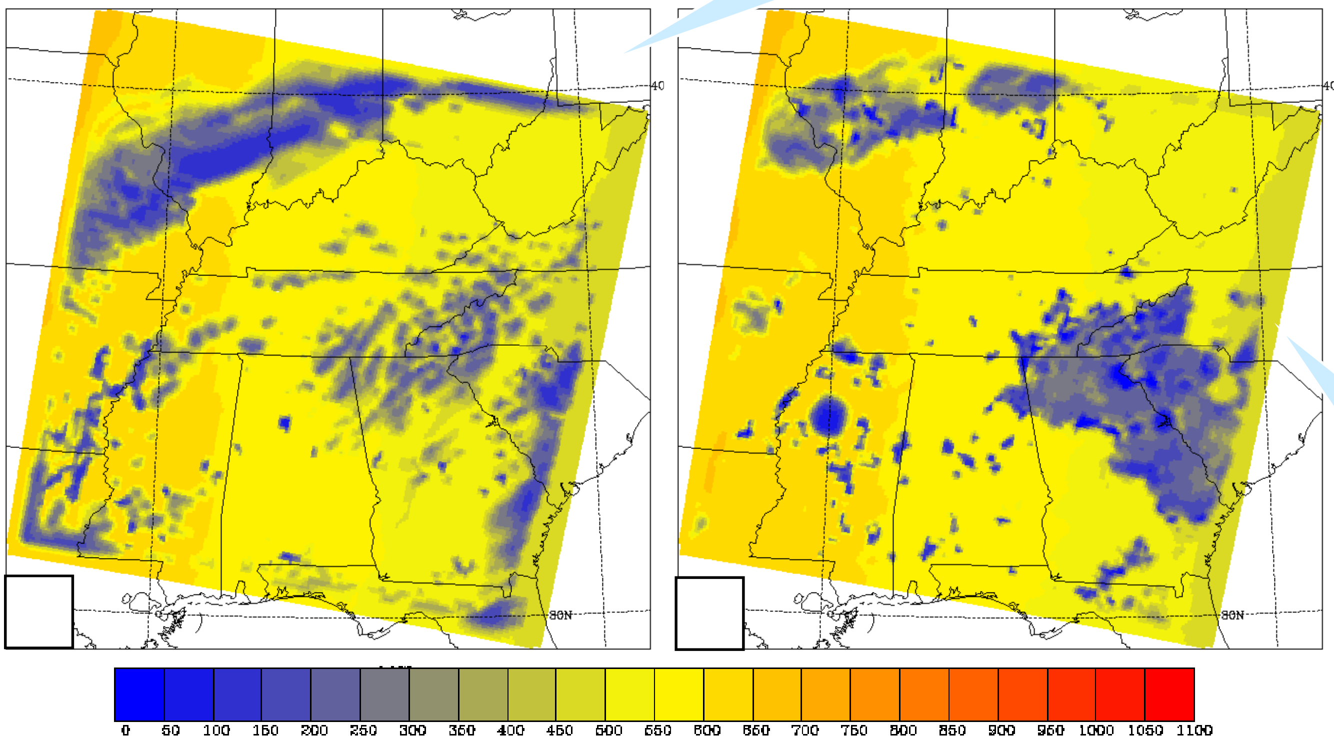
- Use GOES cloud top temperatures and/or cloud albedoes to determine a maximum vertical velocity (Wmax) in the cloud column.
- Adjust divergence to comply with Wmax in a way similar to O'Brien (1970).
- Calculate new horizontal divergent wind components.
- Nudge MM5 winds toward new horizontal wind field.
- Determine a way to remove erroneous model clouds.

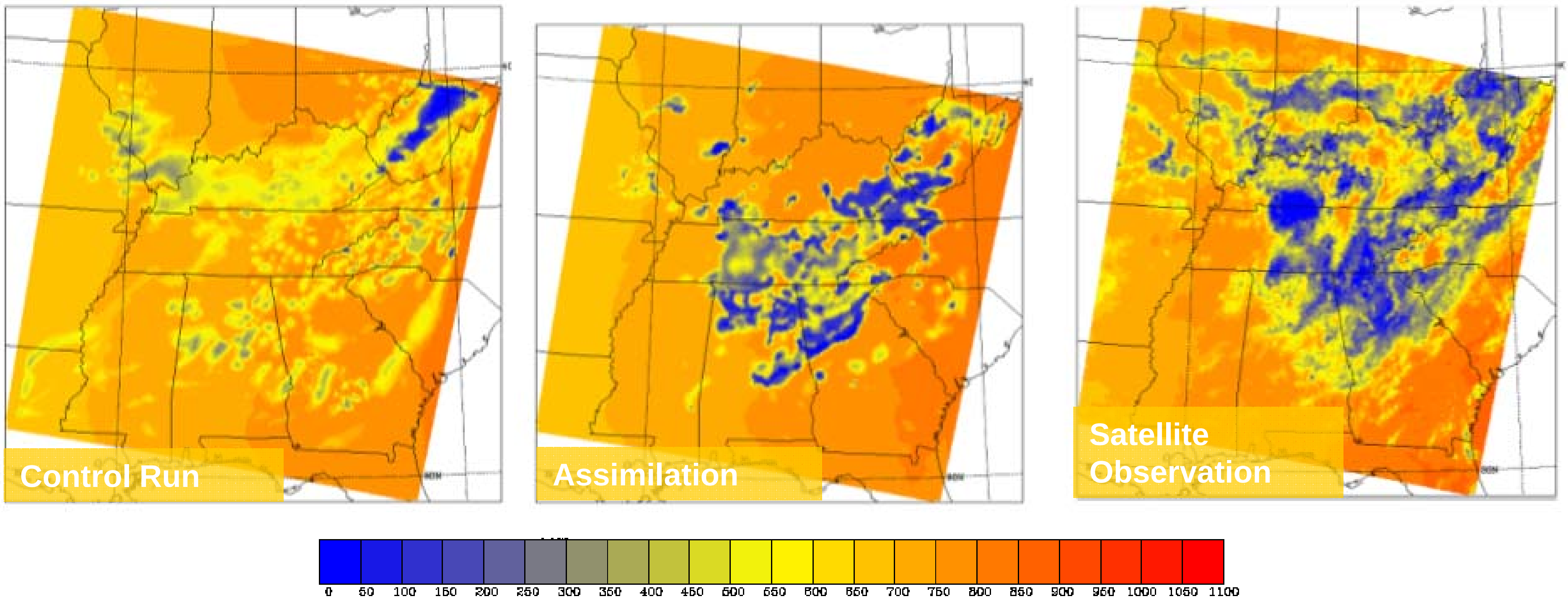
SATELLITE DATA IS UTILIZED TO CORRECT MODEL CLOUD FIELDS IN A DYNAMICALLY CONSISTENT MANNER



Downward shortwave radiation in W m^{-2} at 2200 UTC 6 July 1999.

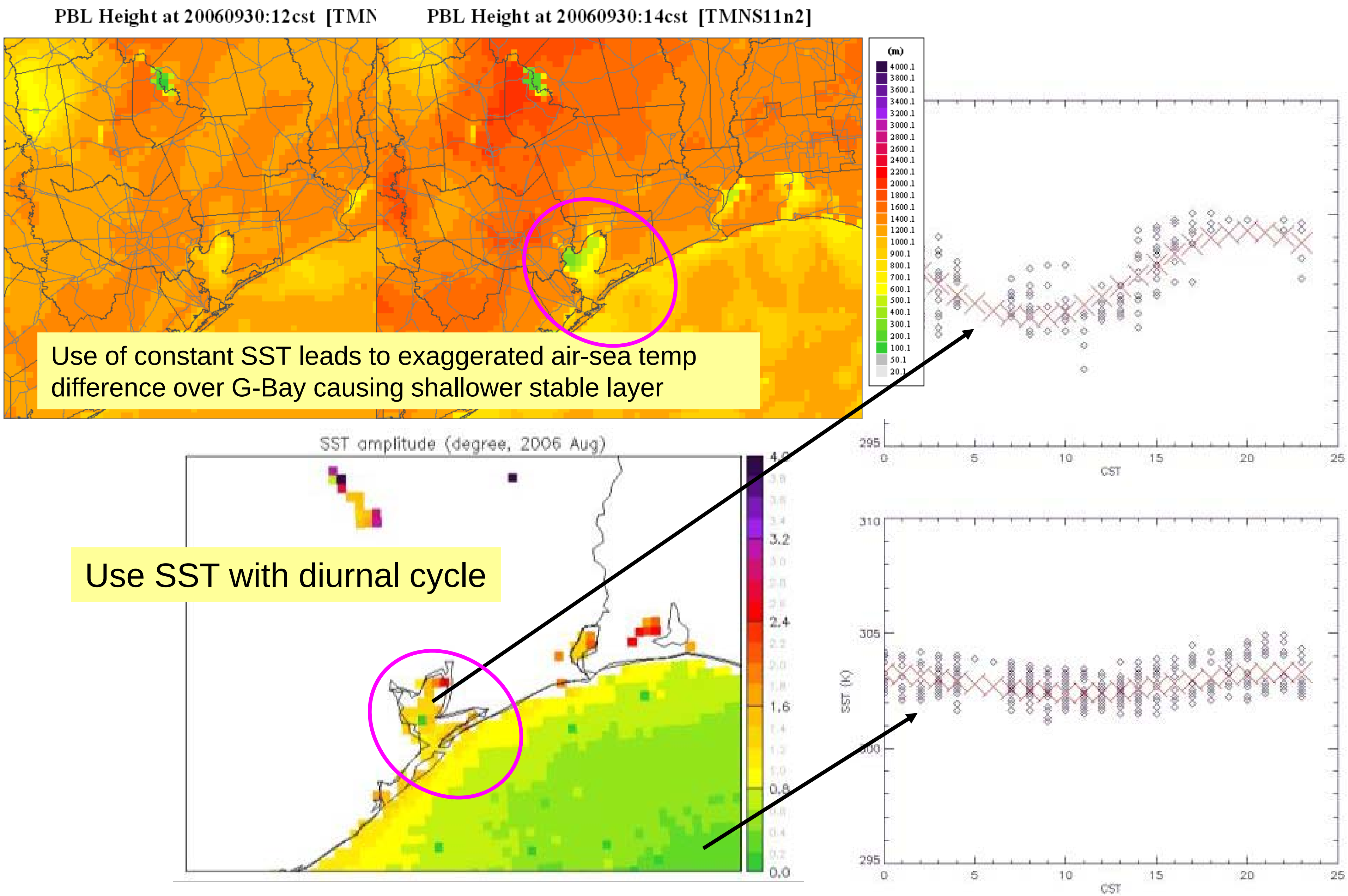
(A) Derived from GOES–8 satellite.
(B) Control run with no assimilation.
(C) Run with assimilation of satellite cloud information.





Surface incident shortwave radiation in W m^{-2} for July 2, 1999. Assimilation and satellite observation plots are @ 14:45 UTC, and the control run is @ 15:00 UTC. Control: Control run with no assimilation. Assimilation: Run with assimilation of satellite cloud information. Satellite Observation: Derived from GOES–8 satellite.

Improve PBL simulations by applying SST diurnal variation obs. by satellite

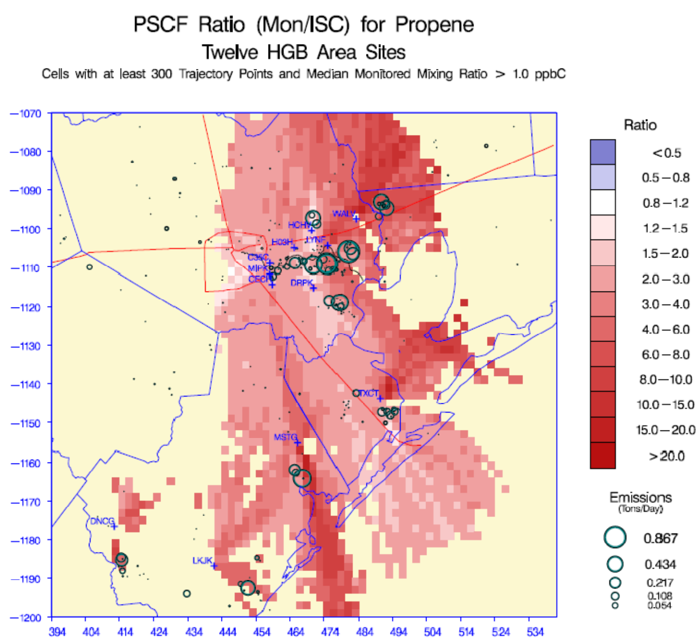


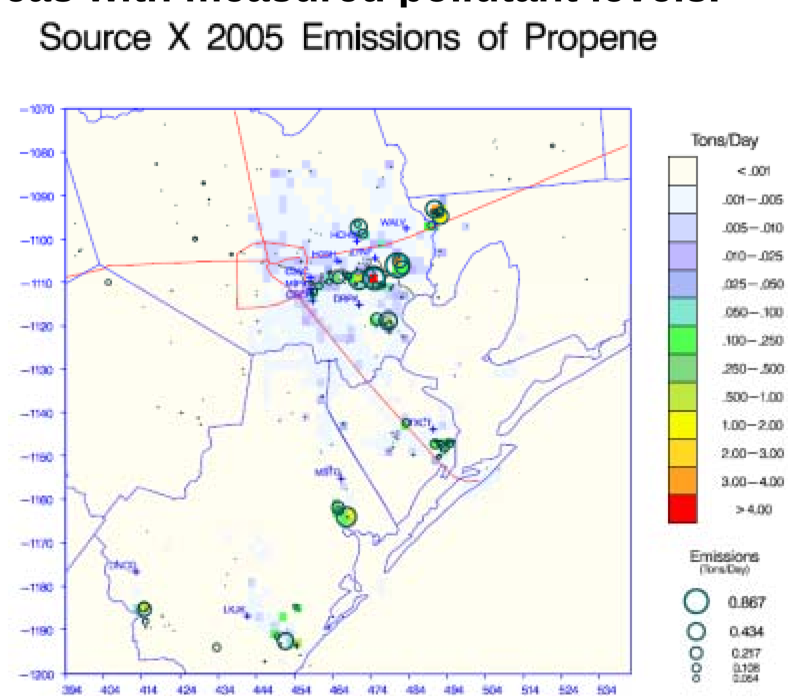
TCEQ HRVOC EI "Reconciliation"

Jim Smith & John Jarvie

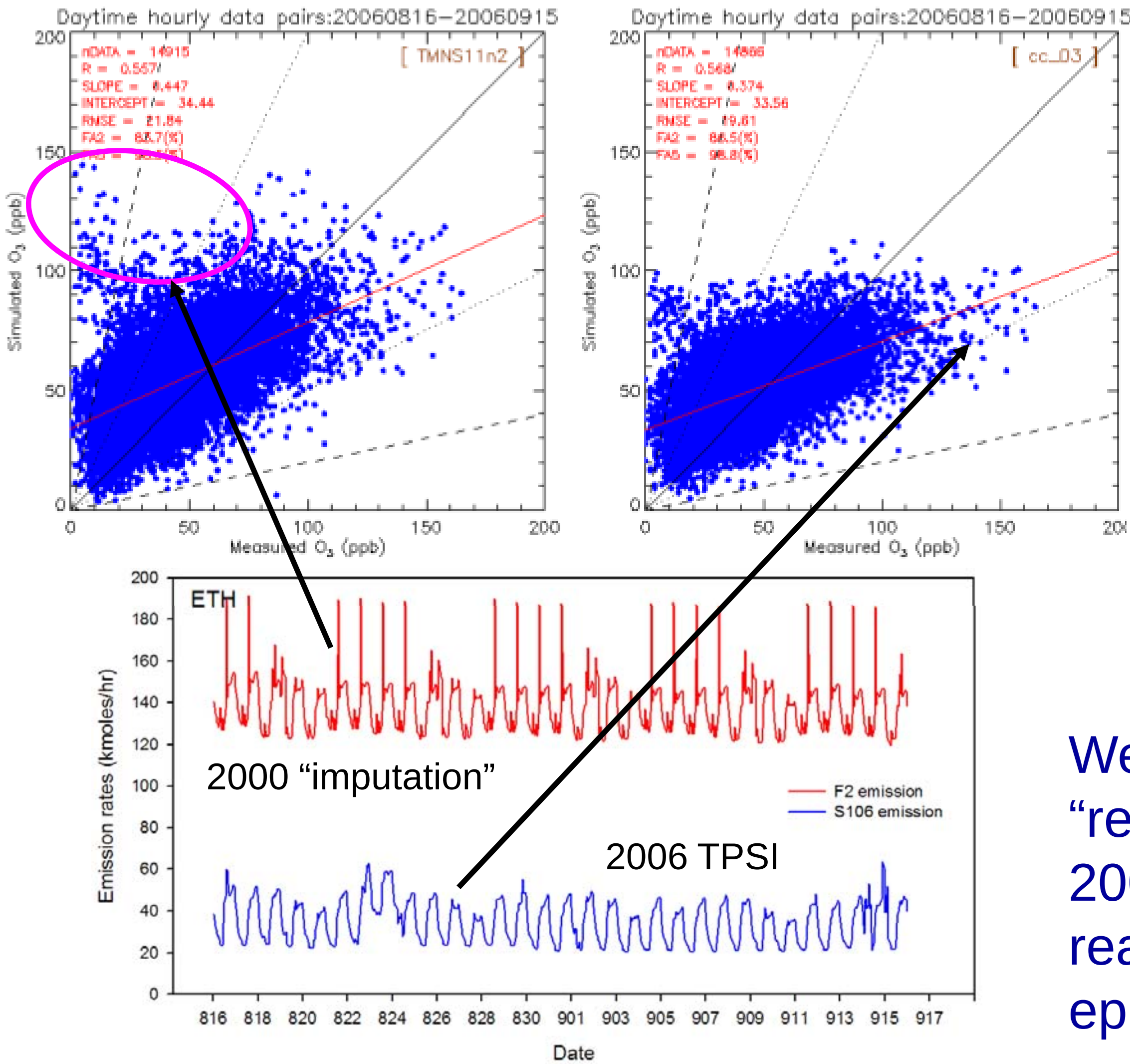
Southeast Texas Photochemical Modeling Technical Committee February 12, 2008

- **TCEQ modelers developed a methodology for reconciling reported emissions of HRVOCs (Ethene, Propene, Butenes, and 1,3-Butadiene) with measured ambient concentrations.**
- **Using hours with relatively "straight" winds, the Industrial Source Complex (ISC) model was used to predict concentrations at the monitors.**
- **Using the same hours as above, the Potential Source Contribution Function (PSCF) was used to associate source areas with measured pollutant levels.**





TCEQ HRVOC EI “Reconciliation”



TCEQ “reconciled”

Reconciled Emissions

- **Required additional emissions were calculated for each grid cell in the area (instead of only at point sources).**

Species	Reported Emissions	Reconciled Emissions	Est. Emiss. from unidentified sources
Ethene	16.813	32.241	15.428
Propene	12.078	40.628	28.55
1,3-Butadiene	2.673	3.841	1.168
1-Butene	3.322	6.787	3.465
c,2-Butene	0.904	1.68	0.776
t,2-Butene	1.146	3.553	2.407
isoButane	8.016	55.16	47.144
n-Butane	35.877	75.51	39.633

We expect application of TCEQ “reconciled emission factor” to 2006 TPSI will improve O3 reactivity without causing episodic biases

(1) Data Assimilation & reduce “input” uncertainties

Task 2: Synthesis datasets for chemical data assimilation

(a) Establish chemical datasets from various measurements

CAMS, UH/Moody, Aircrafts (Baylor, NOAA), DOAS, Lidar, Ozonesonde

Satellites (e.g., OMI O3, HCHO, NO2; AIRS CO; Aerosol, Fire emissions)

(b) Develop process analysis workbench for evaluation and assimilation utilizing GIS, IDL, Grads, and F90

(c) Sensitivity air quality simulations with different inputs to verify obs.

(d) Assembly of inputs for chemical data assimilation and development of cost functions and covariance matices.

UH ($60K)

*** Satellite data support from NASA (Langley) and NOAA (Brad Pierce & Shobha Kondragunta)

Deliverables: Synthesized dataset for chemical data assimilation, CMAQ process analysis output

(1) Data Assimilation & reduce "input" uncertainties

Task 3: 4-DVar chemical data assimilations to improve IC, BC, and EI

(a) CMAQ/4Dvar code development for improving IC, BC, and EI through assimilation of chemistry data (from Task 2)

(b) Assimilate satellite data with RAQMS to improve BC conditions

(c) Study model & input uncertainties with and without chemical 4Dvar

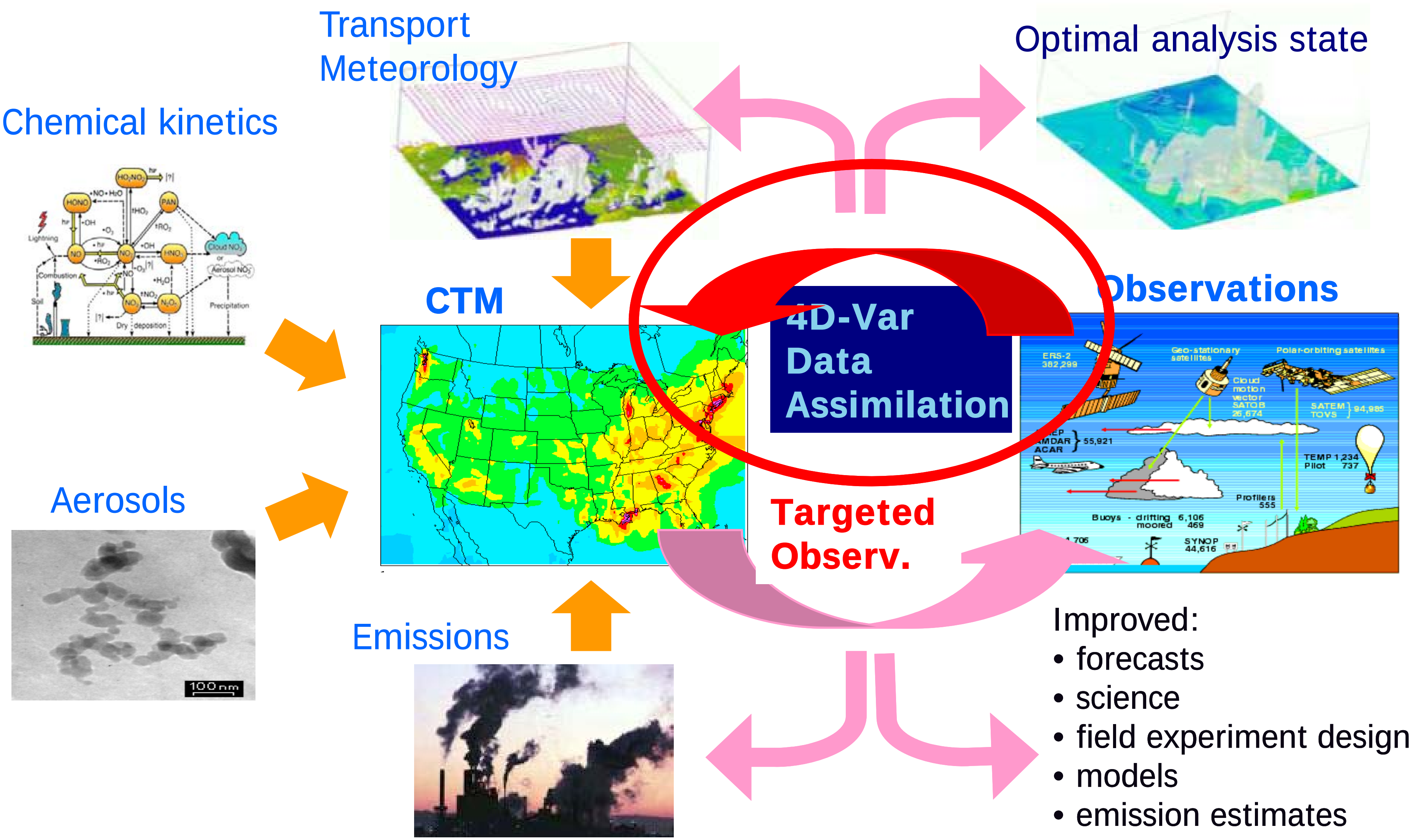
(d) Assembly of inputs for chemical data assimilation and development of cost functions and covariance matrices.

UH ($70K), Virginia Tech ($60K), NOAA & NASA (in-kind--RAQMS output)

*** Satellite data support from NASA (Langley) and NOAA (Brad Pierce & Shobha Kondragunta)

Deliverables: CMAQ/4DVar code and assessment of uncertainties in emissions & model boundary conditions

Information feedback loops between CTMs and observations: data assimilation and targeted meas.



Goal is to improve I/C, B/C, EI through assimilation

Adrian Sandu, Virginia Tech

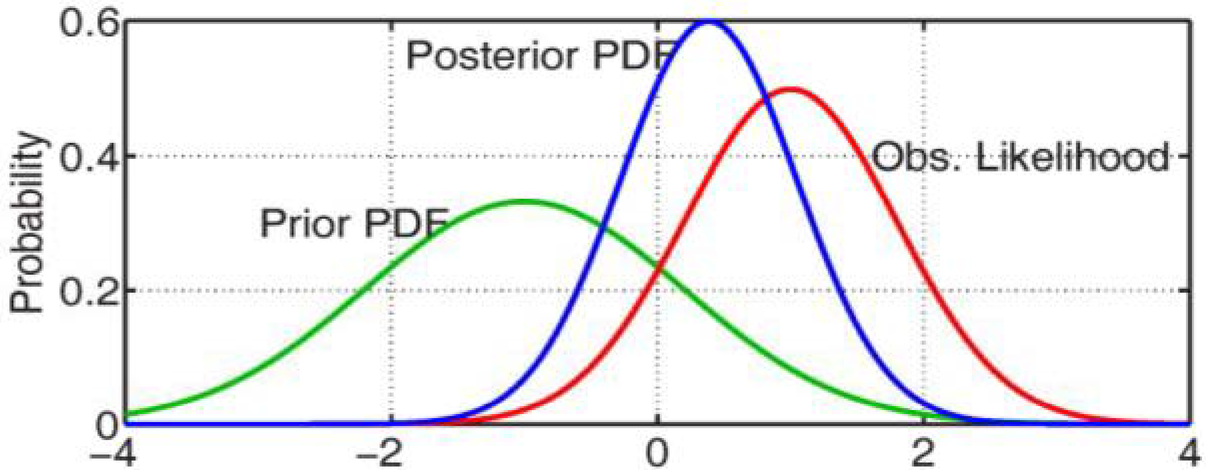
Best estimate of the state is obtained by combining multiple sources of information

Model (encapsulating knowledge on the physics, chemistry, thermodynamics, etc)

Background (encapsulating best a-priori knowledge of the state)

Observations (encapsulating new information about reality)

Bayes:
$$P\left[y^k \,\middle|\, z_{\rm obs}^k \ldots z_{\rm obs}^0\right] = \frac{P[z_{\rm obs}^k | y^k] \cdot P[y^k \,|\, z_{\rm obs}^{k-1} \ldots z_{\rm obs}^0]}{\int P[z_{\rm obs}^k | y] \cdot P[y | z_{\rm obs}^{k-1} \ldots z_{\rm obs}^0]\, dy} = \frac{P_R[\varepsilon_{\rm obs}^k] \cdot P_B[y^k]}{\cdots}$$

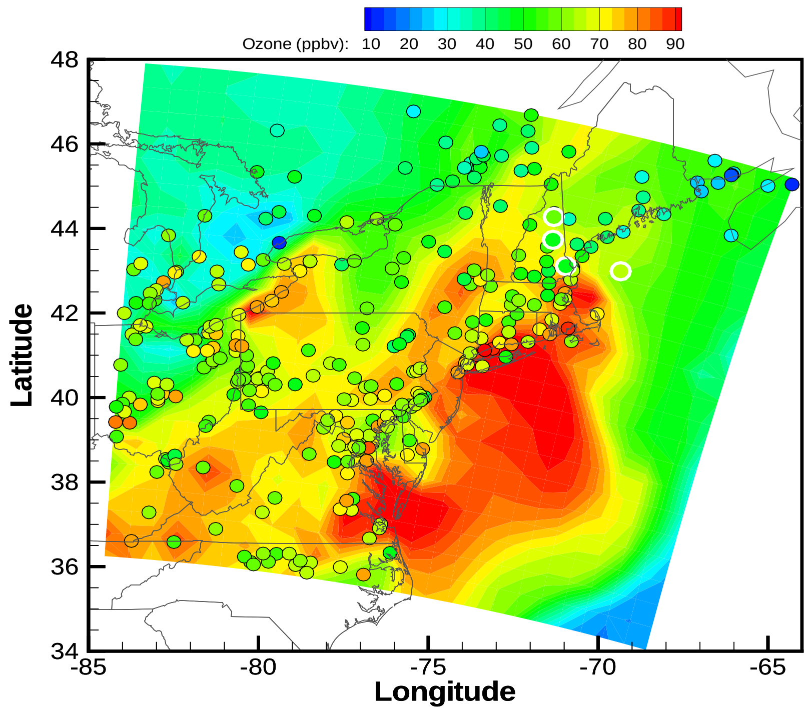


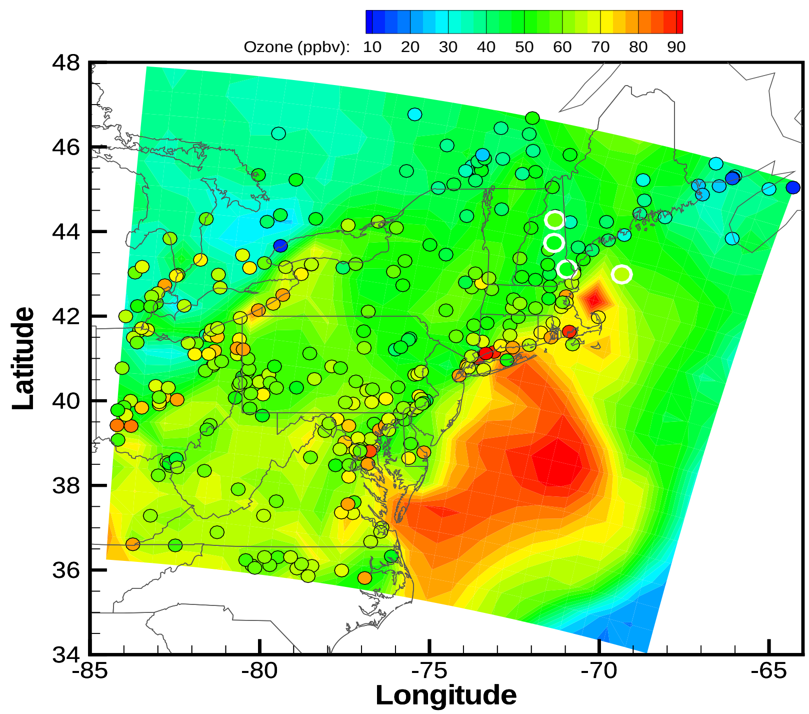
Methods:
4D-Var, EnKF

[Picture from J.L. Anderson]

Example: data assimilation adjusts O_3 predictions c onsiderably at 4pm EDT on July 20, 2004

Observations: circles, color coded by O_3 mixing ratio





[Chai et al., 2006]

Adrian Sandu, Virginia Tech

(1) Data Assimilation & reduce "input" uncertainties

Task 4: Air quality forecasting of Houston and Dallas Metropolitan areas

(a) Establish 2008/2009 Eastern Texas Air Quality (ETAQ) forecasting for Houston and Dallas-Fort Worth areas at 36- (CONUS), 12- and 4- km domains.

(b) Provide daily air quality forecasting continuously for 16 months with two different emission inputs (NEI2002+TSPI2006+Reconciliation vs. 2005 Projected with 2000 imputed).

(c) Include the near real-time satellite-observed fire emissions and SST

(d) Apply screening trajectory ozone prediction system (STOPS) for fast model re-simulation of emissions upset events.

(e) Provide modeling data for other TERC/TCEQ measurement projects.

UH ($70K), NOAA & NASA (in-kind--satellite data products)

Deliverables: F1 & F2 daily Air Quality Forecasting for Houston-Galveston-Brazoria & Dallas-Fprt Worth areas

Satellite detected Fire emissions

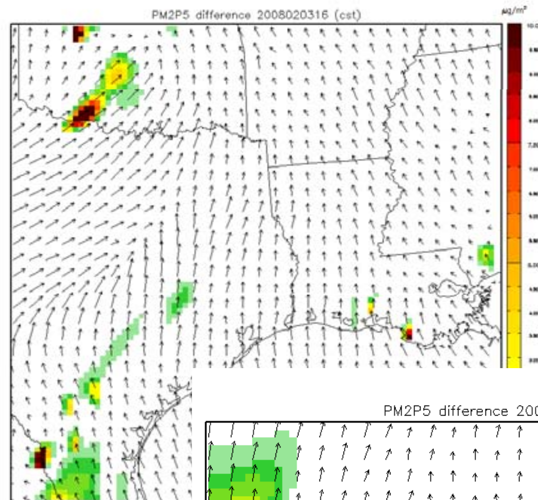
- Implemented forest fire emissions detected from satellites into the UH-IMAQS daily Air Quality Forecast (AQF) system
- We retrieved near-real time forest fire emission from the Hazard Mapping System (HMS) using the method of Wiedienmyer et al. (2006)
- Fire information is retrieved from HMS data of NESDIS.
- We assume 50%/day decaying of fire intensity from the detection time of forest fire. Previous 3 days of fires are considered
- Plume rises are estimated based on the PBL heights that MCIP forecasts, with 300 m minimum plume height.
- Assumed 80% of total emission is well distributed within the PBL height, and 20% of emission can rise over the PBL height and reaches up to 5km.

Satellite detected Fire emissions

Emission processing time depends on the number of forest fire pixels detected.

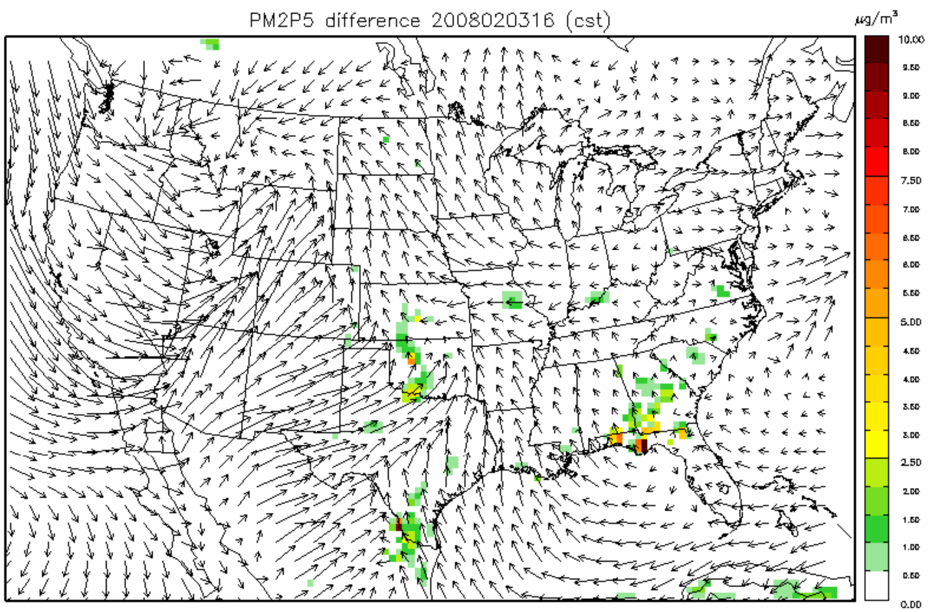
For the case of Feb. 2, 2008 run, 2555 fires pixels are detected during the previous 3 days in the CONUS domain.

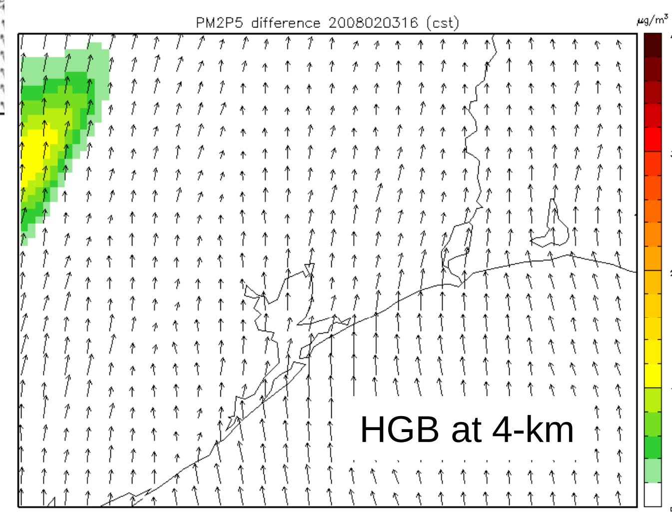
Total time for forest fire emission processing for Feb. 2 is 28 min, 5 min, and 2 min, for 36km CONUS domain (2555 fire pixels), 12km Eastern Texas domain (250 fire pixels), and 4km Houston-Galveston domain (12 pixels), respecti



E-Texas at 12-km

CONUS at 36-km

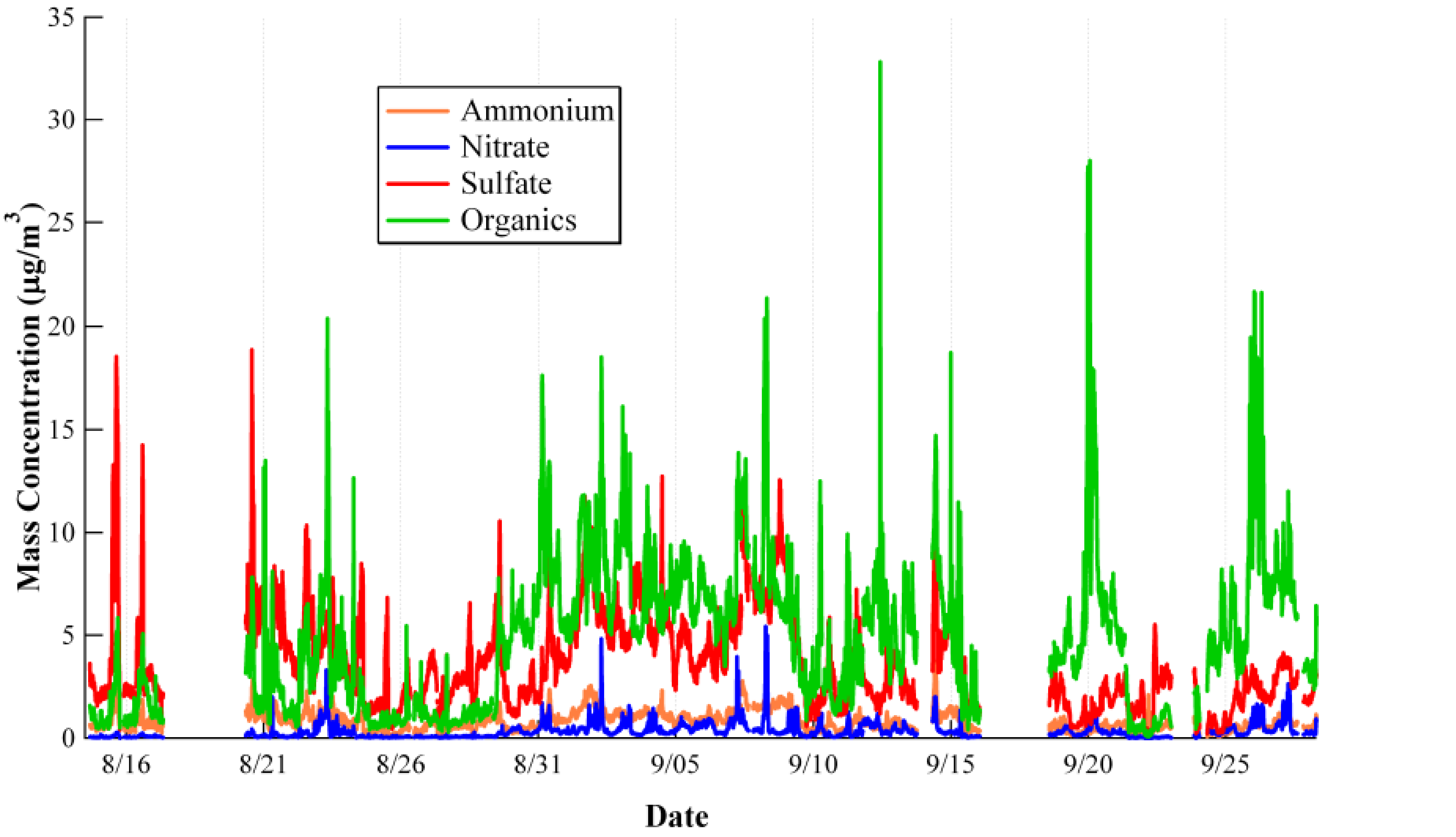




HGB at 4-km

Rob Griffin, UNH: Modeling of SOA in Houston in Summer

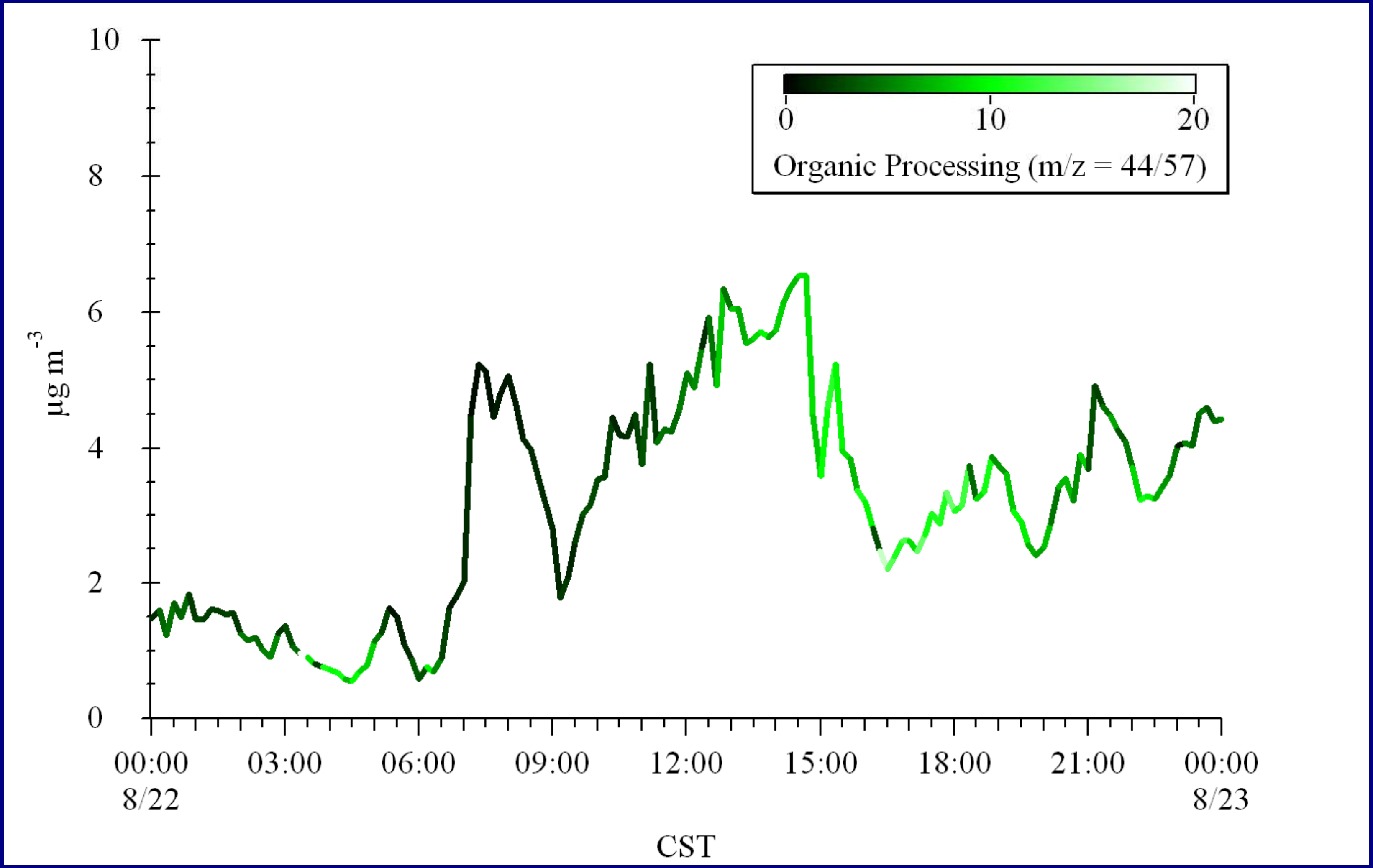
Dominance of Organics



Measured during TRAMP using AMS

Rob Griffin, UNH: SOA Modeling

Varying Contributions of POA/SOA



Processing defined by level of oxidation (43 to 57 ratio) of the primary and secondary organic aerosol

Model Questions To Address

1. On average, what are the relative contributions to OA loadings of POA and SOA?
2. What are the relative contributions to SOA of biogenic and anthropogenic precursors?
3. How much does the presence of elevated levels of smaller VOCs affect SOA formation?
4. How does SOA in Houston respond to changes in emissions profiles (speciation and amount) and is this sensitivity similar to that in other regions (eastern United States, Los Angeles, etc.)
5. How do the results from our mechanistic model compare to default CMAQ empirical SOA modules?
6. Can these exercises be used to refine emissions inventories?

(Rob Griffin, UNH: SOA Modeling)