RAQMS global chemical and aerosol assimilation and forecasting studies during the NOAA 2006 TEXAQS and 2008 ARCPAC field campaigns

R. Bradley Pierce (NOAA/NESDIS)
Todd Schaack (UW/SSEC)
Allen Lenzen (UW/SSEC)
Jassim Al-Saadi (NASA/LaRC)
Chieko Kittaka (NASA/LaRC)
Amber Soja (NASA/LaRC)
Murali Natarajan (NASA/LaRC)
Don Johnson (UW/AOS)

4th Workshop on the Use of Isentropic & other Quasi-Lagrangian Vertical Coordinates in Atmosphere & Ocean Modeling
October 7-9, 2008, Boulder, Colorado

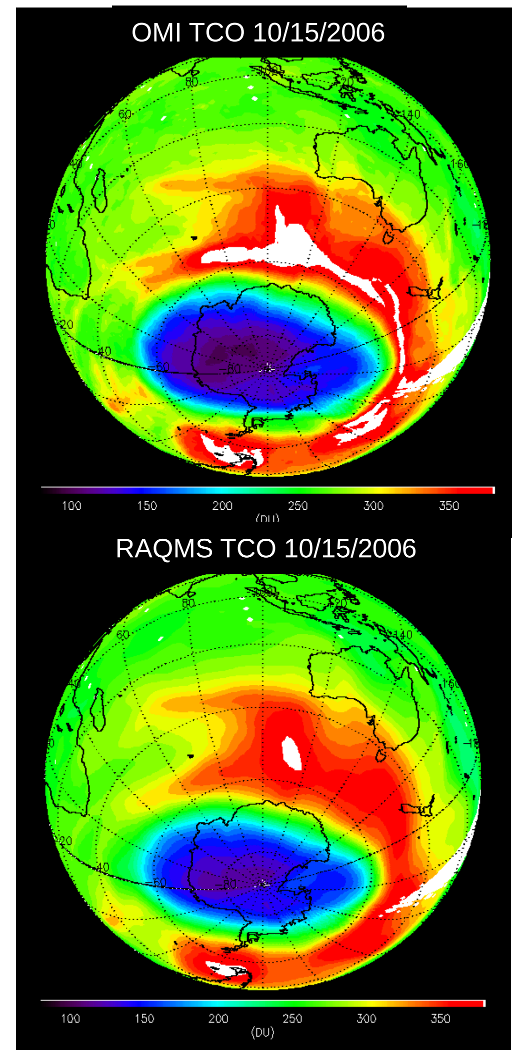
Satellite Retrievals → Global Assimilation → Regional Prediction → Validation

RAQMS Realtime Air Quality Modeling System

Real-time Air Quality Modeling System (RAQMS)

1) **Online global chemical and aerosol assimilation/forecasting system**
2) **University of Wisconsin sigma-theta hybrid coordinate model (UW-Hybrid) dynamical core**
3) **Unified stratosphere/troposphere chemical prediction scheme (LaRC-Combo) developed at NASA LaRC**
4) **Aerosol prediction scheme (GOCART) developed by Mian Chin (NASA GSFC).**
5) **Statistical Digital Filter assimilation system developed by James Stobie (NASA/GFSC)**
6) **36 levels (21 eta, 15 theta, 380K interface), 2x2 degrees**
7) **76 chemical/aerosol species**

RAQMS has been used to support airborne field missions [Pierce et al, 2003, 2007, 2008], develop capabilities for assimilating satellite trace gas and aerosol retrievals [Fishman et al., 2008, Sunita et al., 2008] and assess the impact of global chemical analyses on regional air quality predictions [Song et al., 2008, Tang et al., 2008]



2006 TexAQS / GoMACCS Texas Air Quality Study / Gulf of Mexico Atmospheric Composition and Climate Study

Where: East Texas and the Gulf of Mexico
When: August - September 2006

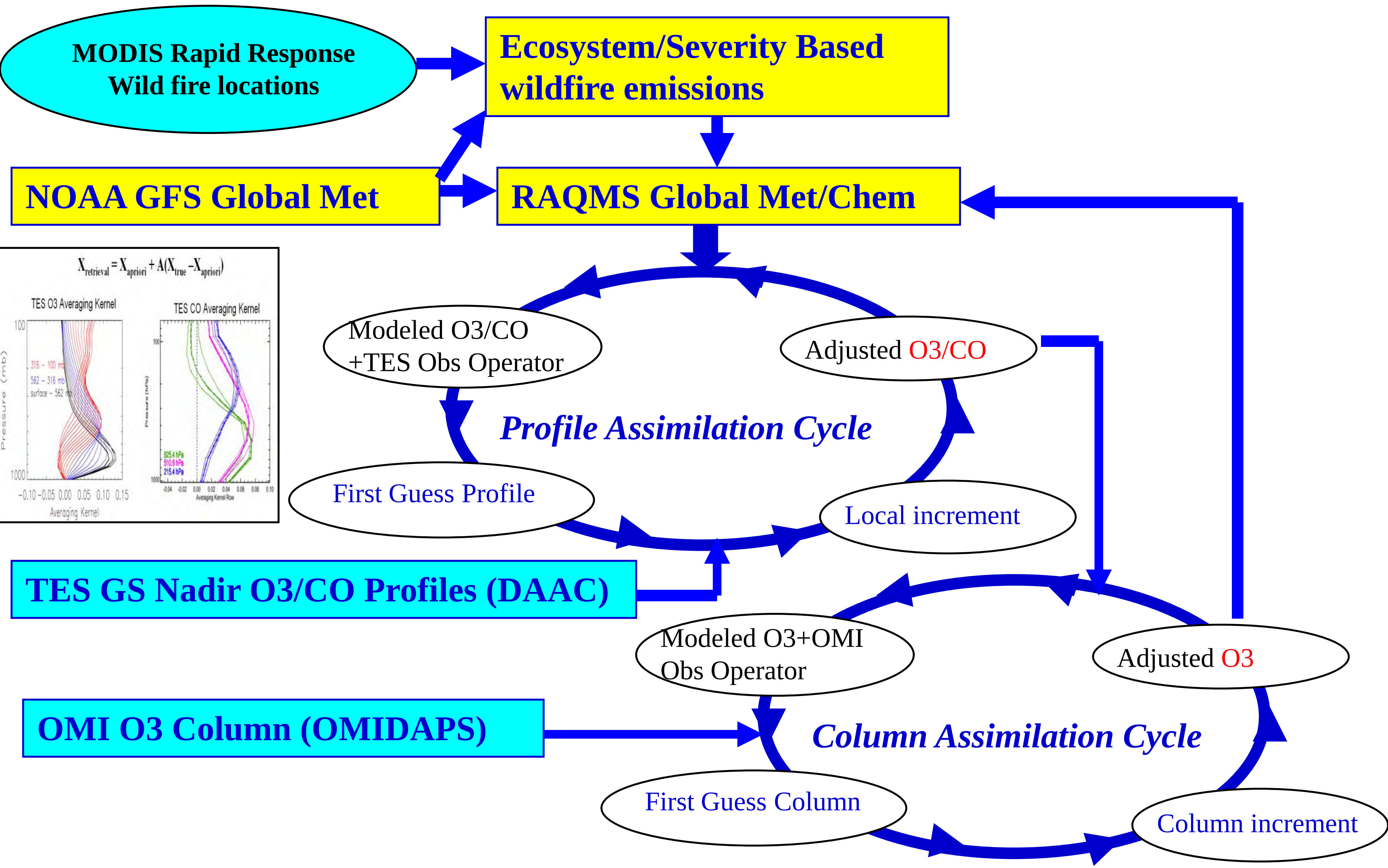
The TexAQS field studies supported the Texas Commission on Environmental Quality (TCEQ) in developing State Implementation Plans (SIPs) for attaining National Ambient Air Quality Standards (NAAQS) for ozone in the Houston and Dallas ozone non-attainment areas.

RAQMS was used to investigate the impact of continental scale ozone production on Houston and Dallas air quality during TEXAQS II.

How do emissions from local and distant sources interact to determine the air quality in Texas, and which areas outside of Texas adversely affect the air quality of non-attainment areas within Texas?

NOAA's Atmospheric Research Campaign
Combining Climate Change and Air Quality Research

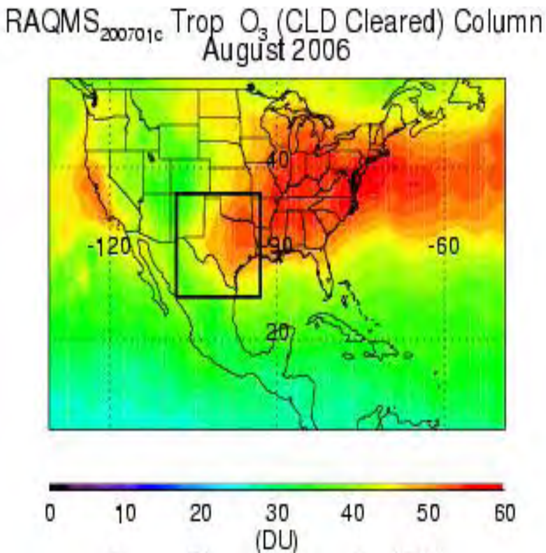
RAQMS$_{global}$ (2x2) 2006 OMI/TES Reanalysis O3/CO Assimilation Procedure

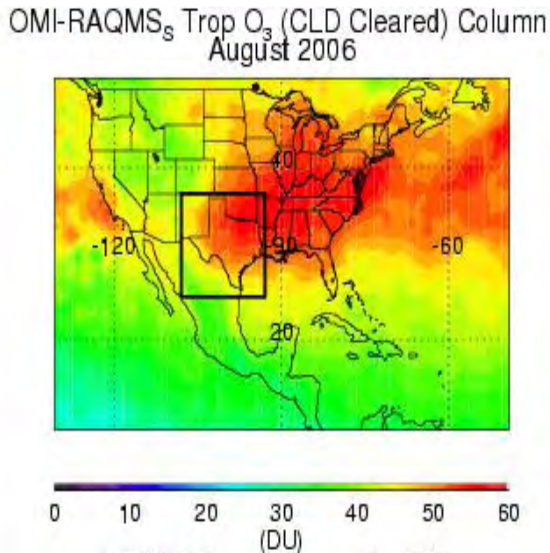


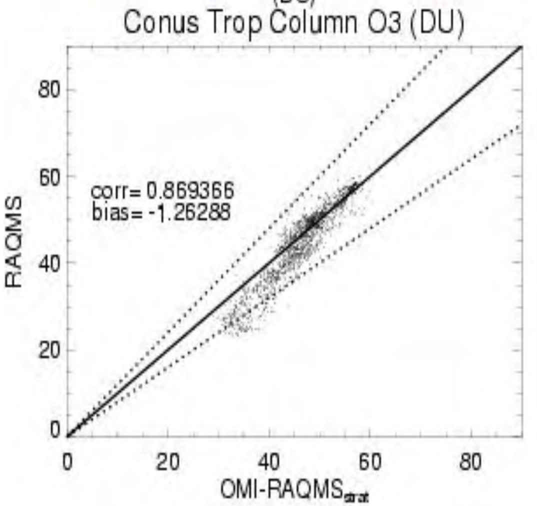
Fishman, J et al., "Remote Sensing of Tropospheric Pollution from Space", BAMS June 2008

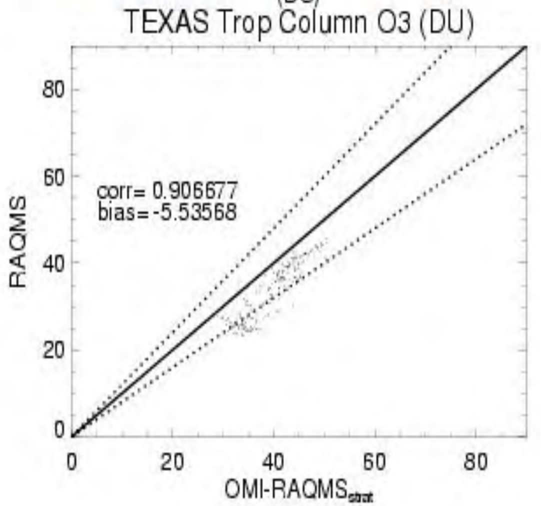
RAQMS Trop O3 vs OMI

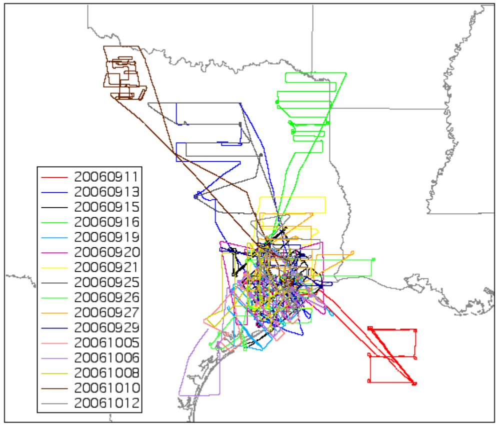
RAQMS O3 vs NOAA P3

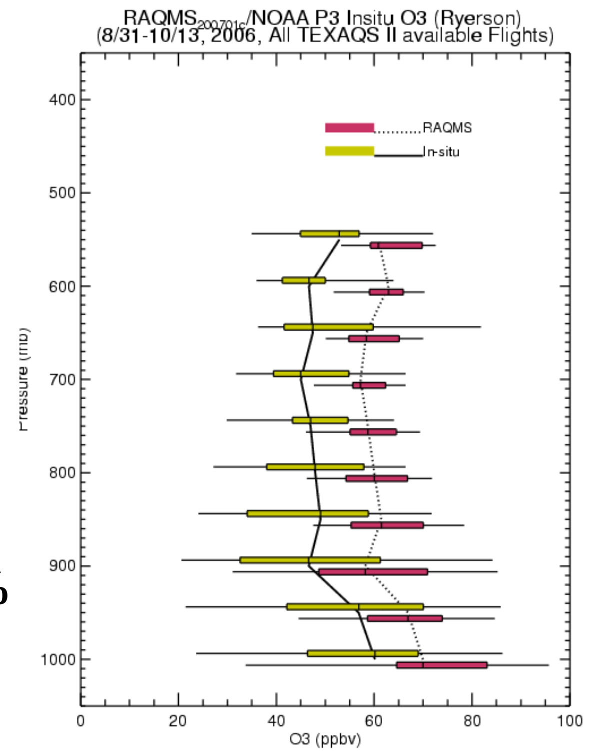








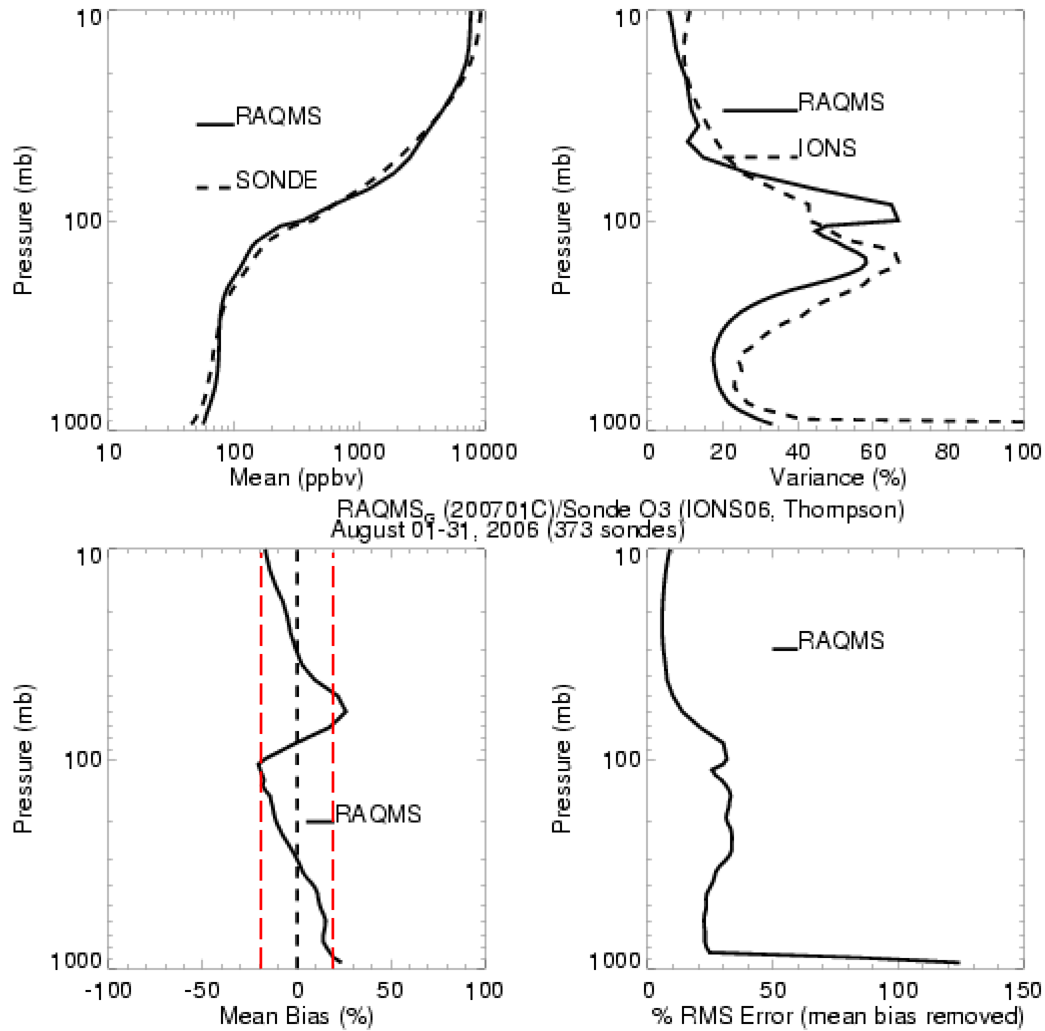




RAQMS <u>mean</u> trop O3 column is <u>low</u> by a factor of up to 20% relative to OMI-RAQMS$_{strat}$ over TX

RAQMS <u>median</u> O3 profile is <u>high</u> by 20ppbv relative to P3 measurements

August 2006 OMI+TES ASSIM vs IONS

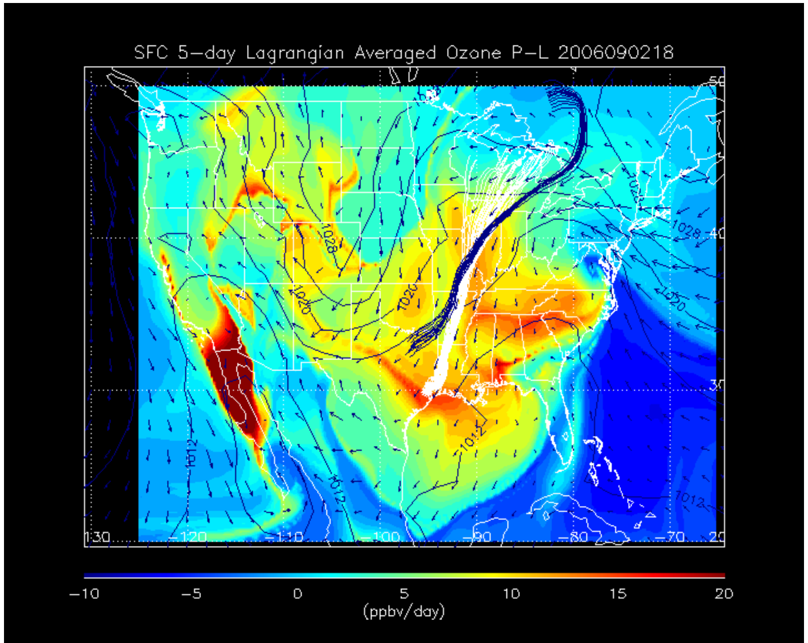


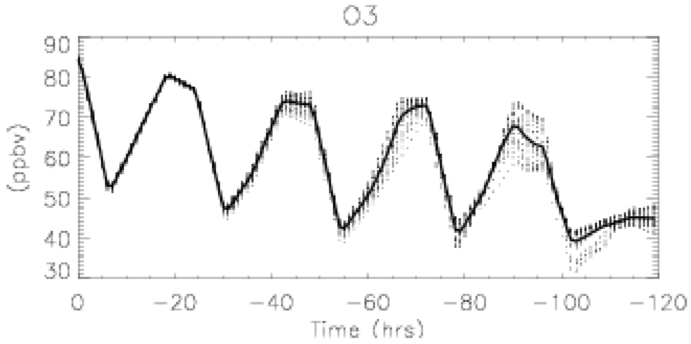
373 sondes

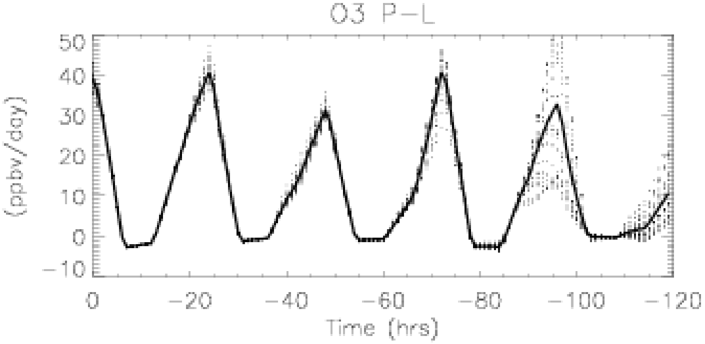
Tropospheric biases: +/- 20%

Approach:

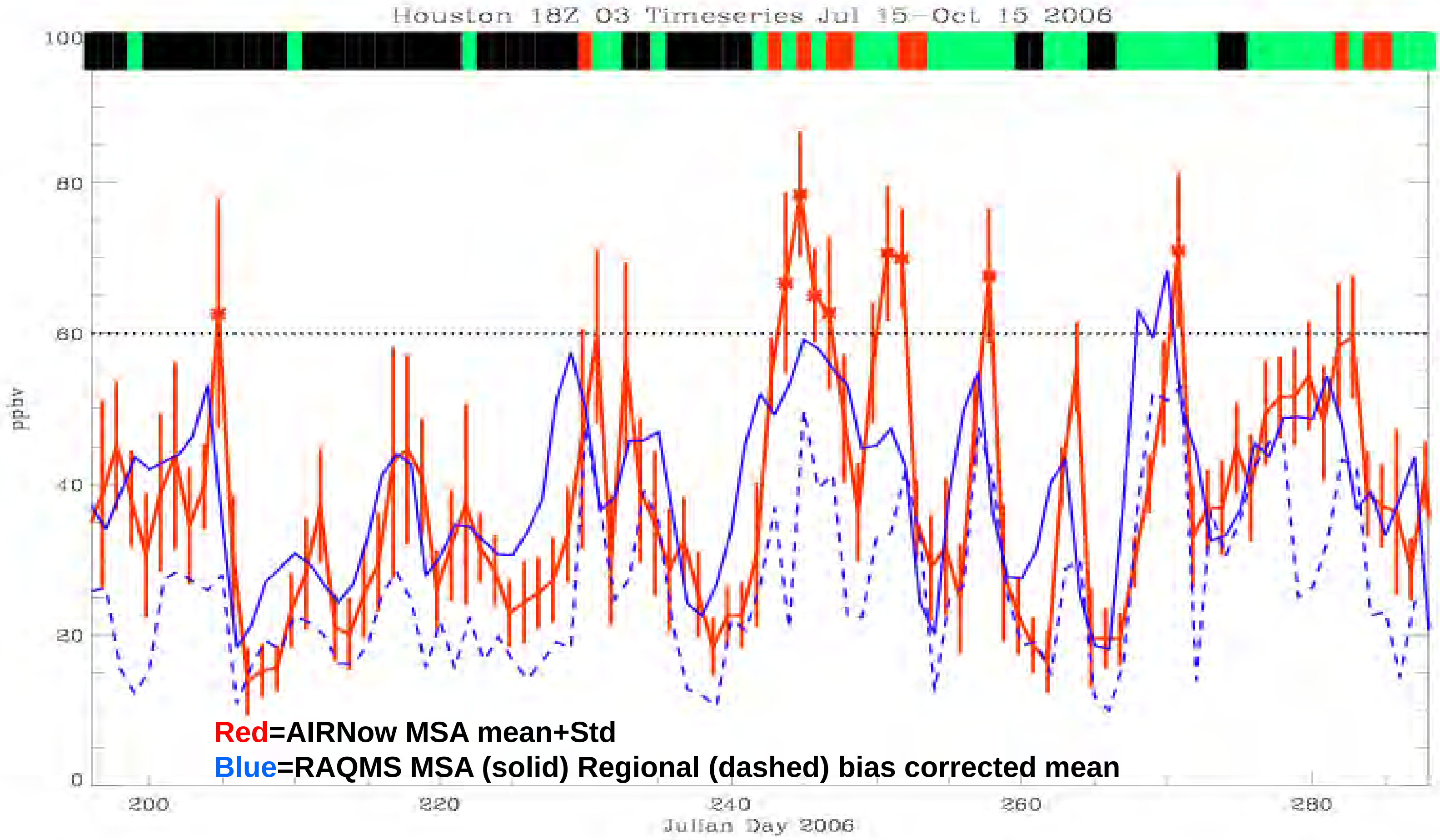
- Bias corrected RAQMS chemical analyses are used to provide estimates of background composition along ensemble back trajectories that are initialized at 18Z from surface EPA AIRNOW ozone monitoring stations within the Houston and Dallas metropolitan statistical area (MSA).
- Lagrangian averaged O3 Production-Loss (P-L) rates along the back trajectories are used as a metric to classify back trajectories.
-
- The Lagrangian averages are computed during time periods where the back trajectories are outside the respective MSA, defined as more than 2º in longitude or latitude away from central Houston or Dallas.







Impacts of background ozone production: Houston July 15-Oct 15, 2006



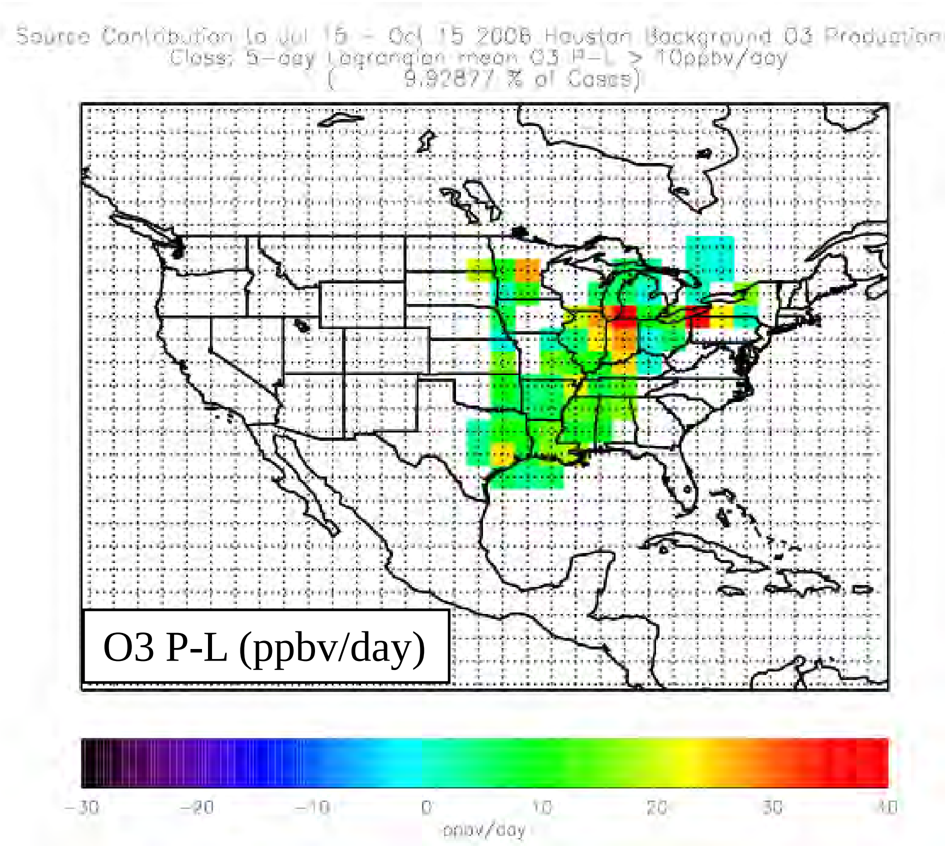
Classifications:

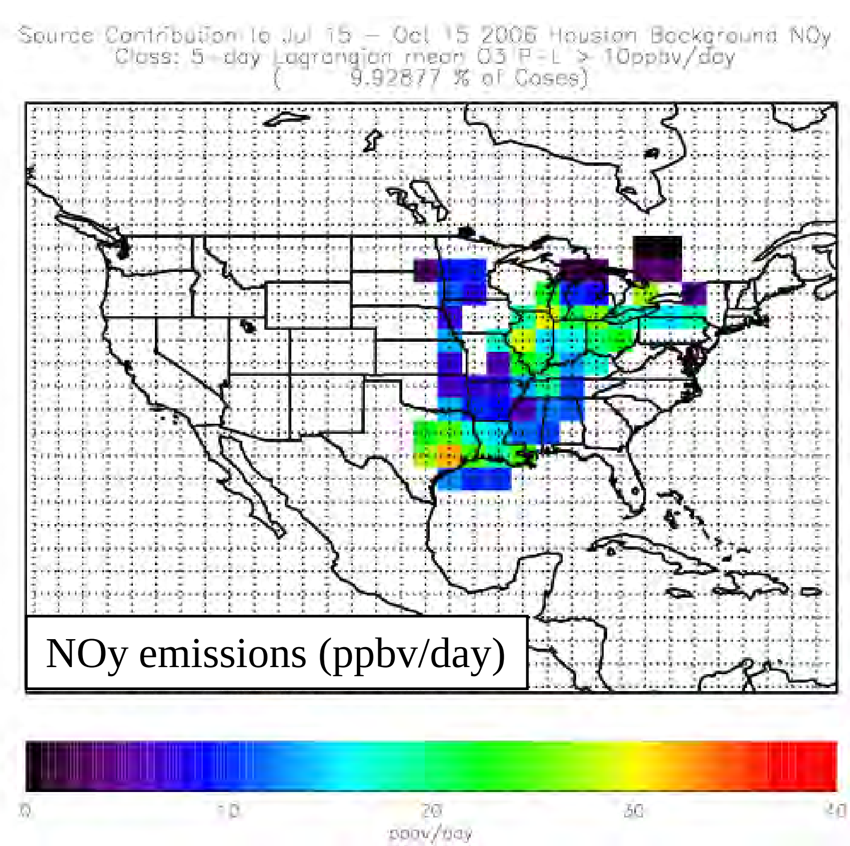
RED=<u>Class1</u>: Enhanced back ground ozone production (ensemble mean 5-day Lagrangian averaged O3 P-L > 10 ppbv/day)

GREEN=<u>Class 2</u>: Moderate back ground ozone production (ensemble mean 5-day Lagrangian averaged O3 P-L > 0 ppbv/day and < 10 ppbv/day).

BLACK=<u>Class 3</u>: Back ground ozone destruction (ensemble mean 5-day Lagrangian averaged O3 P-L < 0 ppbv/day).

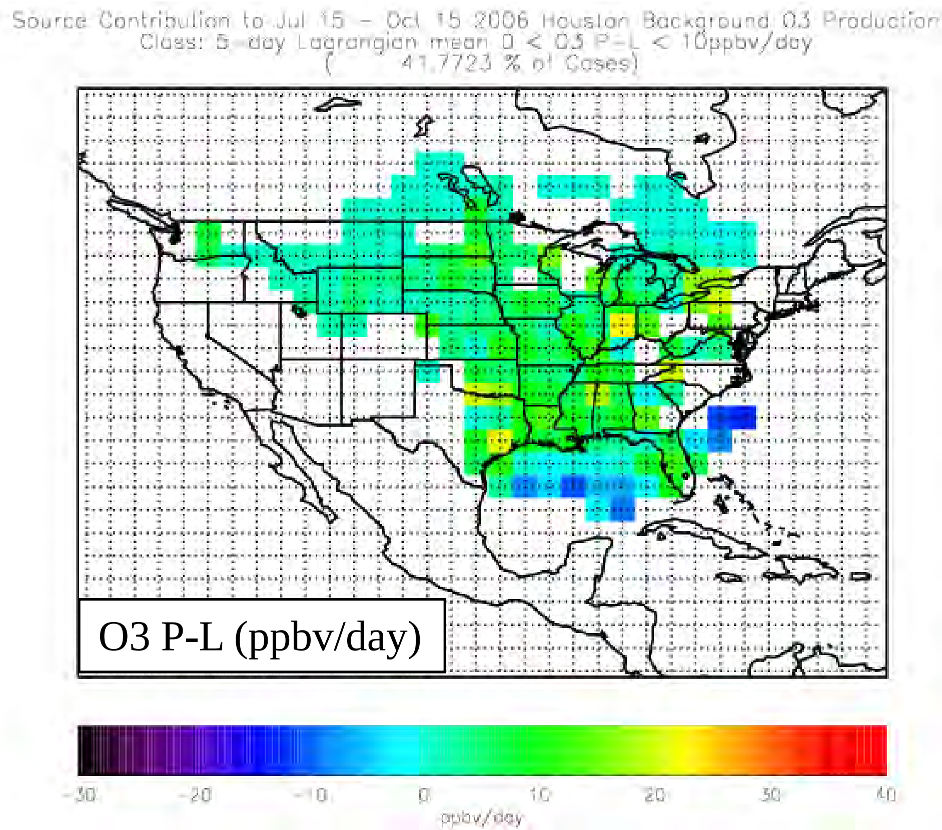
Houston Class 1 Source Contributions July 15-Oct 15, 2006

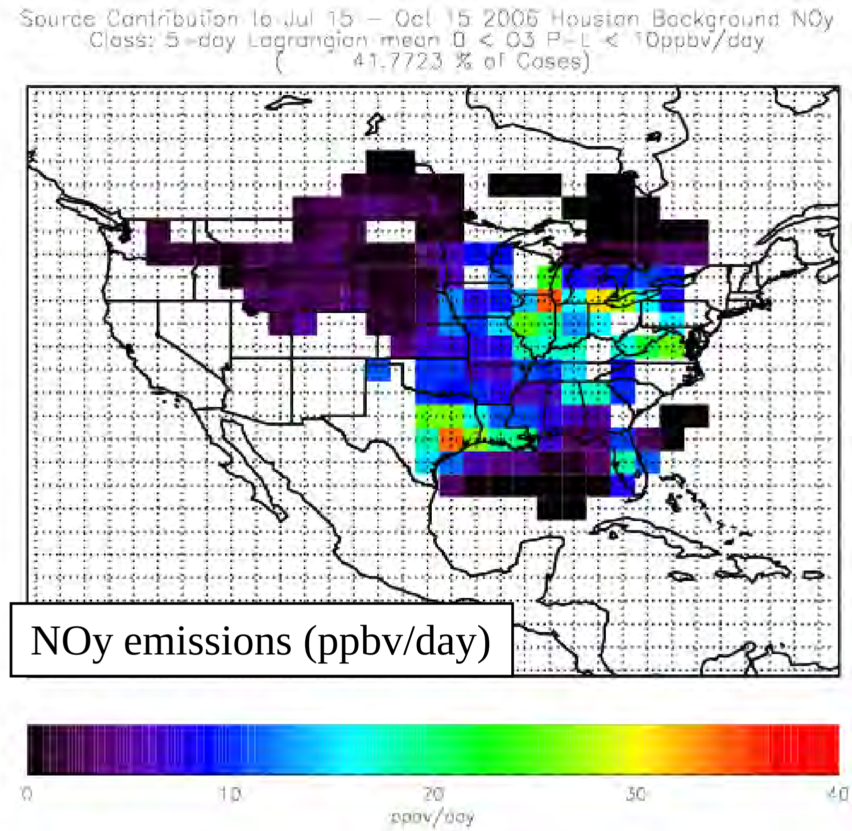




Class 1(10%) ➔Midwest/Ohio River Valley source with significant O3 P-L (40ppbv/ day) due to NOx sources along the southern Great Lakes.

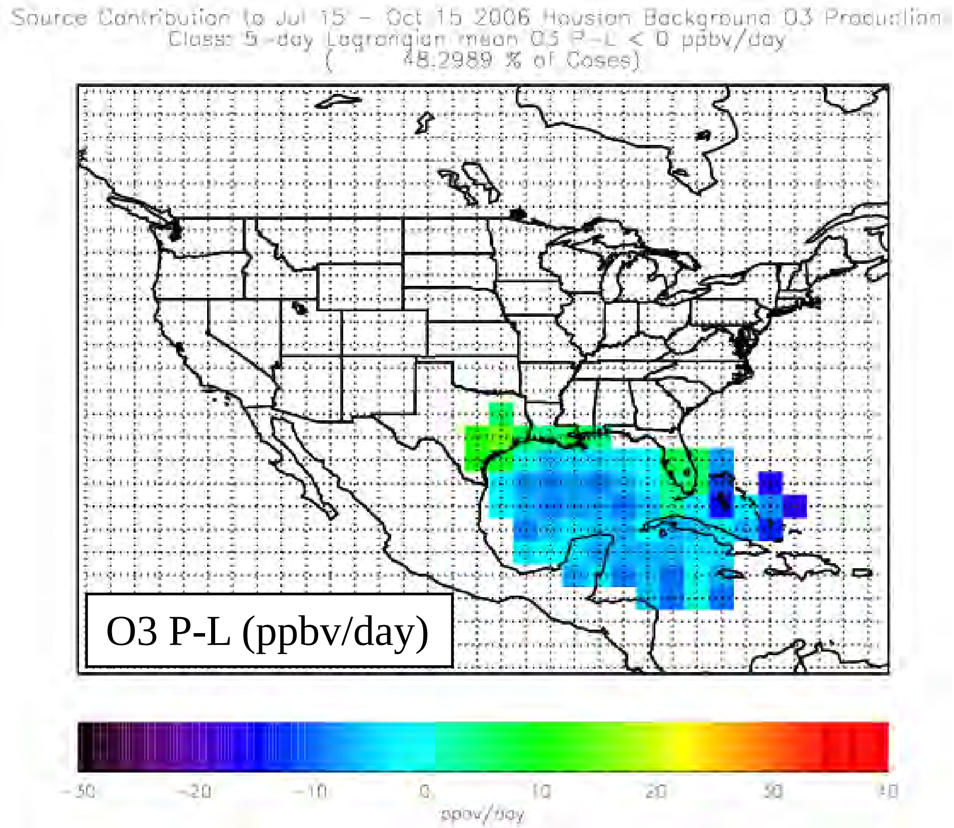
Houston Class 2 Source Contributions July 15-Oct 15, 2006

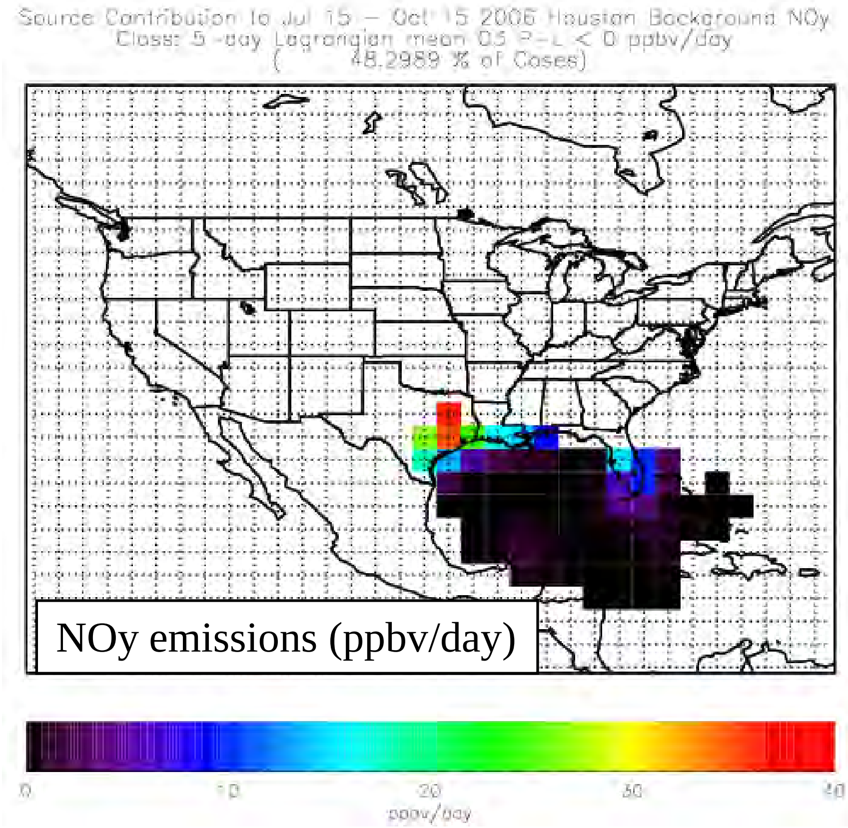




•**Class 2 (42%)** ➔Distributed Eastern US sources with moderate (10ppbv/day) O3 P-L due to biomass burning NOx sources in Pacific NW.

Houston Class 3 Source Contributions July 15-Oct 15, 2006





Class 3(48%)➔Net maritime O3 loss over Gulf of Mexico with moderate (10ppbv/day) O3 P-L due to NOx sources in Florida and Louisiana.

TEXAQS Summary

Continental US source contributions to daily 18Z mean Houston and Dallas ozone mixing ratios were estimated during July 15-Oct 15, 2006 using Lagrangian approaches to sample RAQMS chemical analyses

Three distinct regional influence classifications are developed based on the AIRNow ensemble mean 5-day Lagrangian averaged O3 P-L.

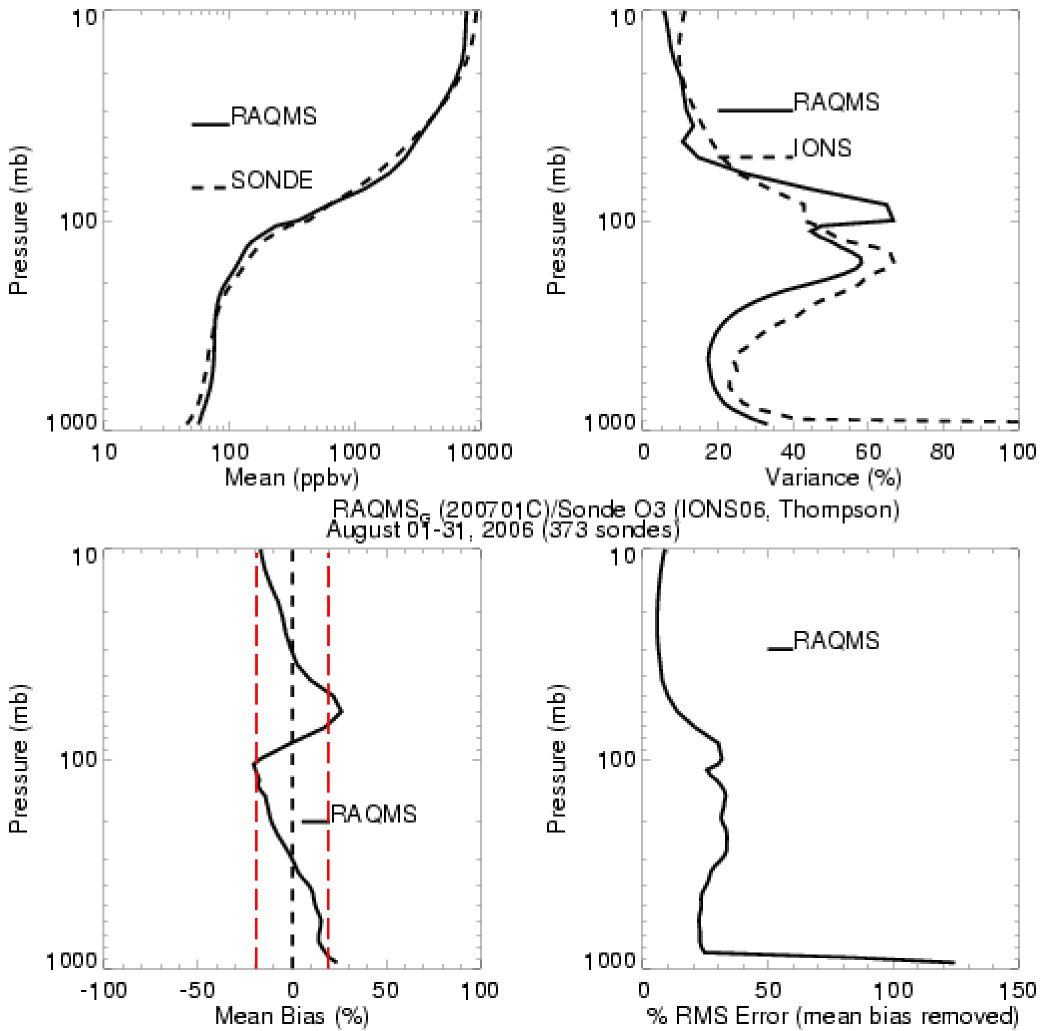
<u>Class 1</u> (Background O3 P-L > 10ppbv/day)
<u>Class 2</u> (Background 0<O3 P-L<10ppbv/day)
<u>Class 3</u> (Background O3 P-L<0ppbv/day)

Periods of enhanced regional ozone production (<u>Class 1</u>) preceed 66% (6 out of 9) and 46% (7 out of 15) of the periods with elevated (Mean >60ppbv) AIRNOW ozone within the Houston and Dallas MSAs respectively.

Reported to the TEXAQS Rapid Science Synthesis Team for Incorporation into Texas Commission on Environmental Quality State Implementation Plan to US EPA

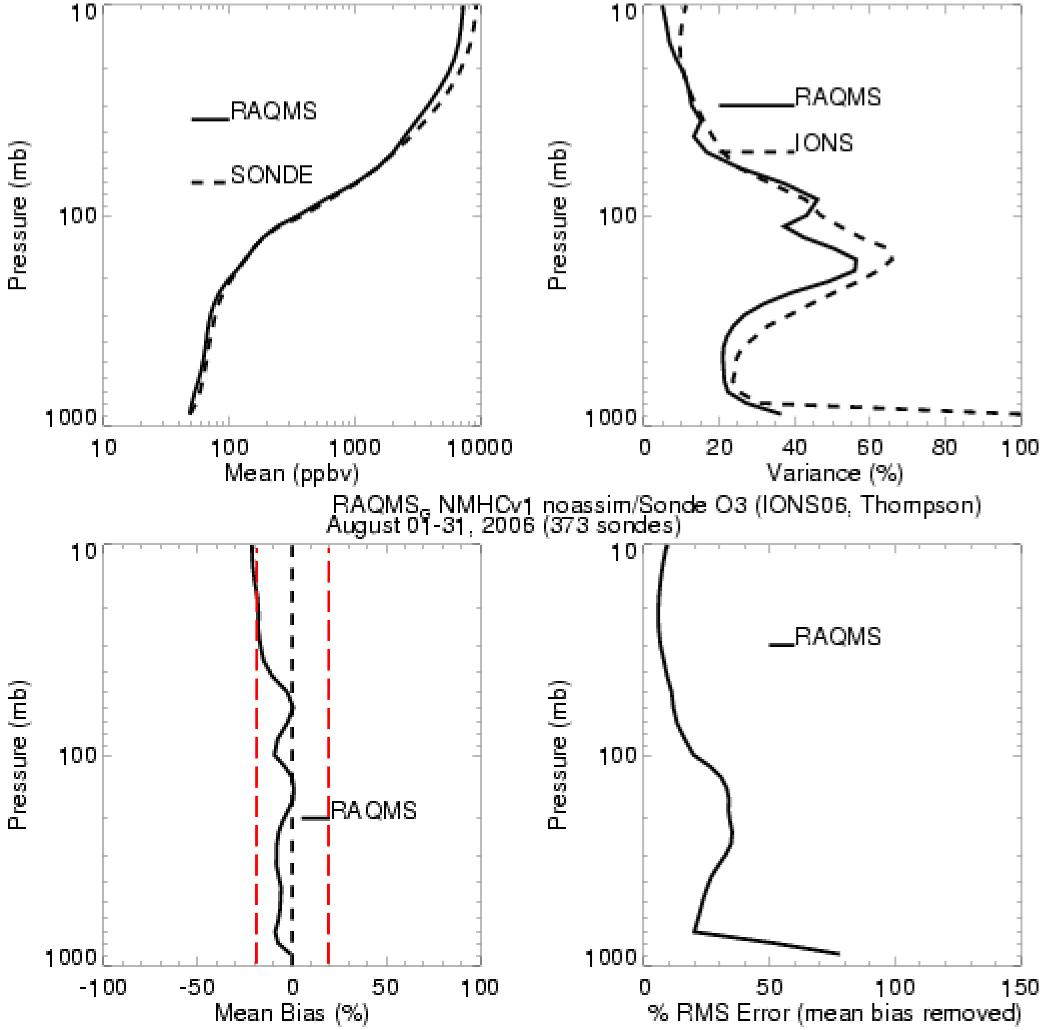
Pierce, et al. Impacts of background ozone production on Houston and Dallas, TX Air Quality during the TexAQS field mission, Submitted to J. Geophy. Res., Oct, 2008

August 2006 OMI+TES ASSIM vs IONS



Tropospheric biases: +/- 20%

August 2006 NO ASSIM vs IONS
(July 15, 2006 OMI+TES IC)



Tropospheric biases: -10%

RAQMS 2006 Data Denial Study

Time period: August 2006
Initial Conditions: July 15th, 2006
(Baseline RAQMS OMI+TES ozone analysis)
Validation: 2006 IONS ozonesonde network (373 sondes)

Ozone Analysis:
- Optimal Interpolation (IO) univariate (Pierce et al., 2007)
- OSIRIS assimilation restricted to tropopause and above
- MLS assimilation tests limited by tropopause (or 246mb) and 100mb
- unified online troposphere/stratospheric chemistry for first guess

Procedure:
Compare RAQMS analyses with ozonesonde
1) No Assimilation
2) OMI (Cloud Cleared) only
3) TES (O3&CO) only
4) MLS + TES CO
5) OSIRIS (Limb Scattering) + TES CO

Pierce et al., "RAQMS TES/OMI/MLS/OSIRIS data denial studies: Impacts of Satellite measurements on Tropospheric ozone" at the JCSDA workshop (June 9-10, 2008 Baltimore, MD)

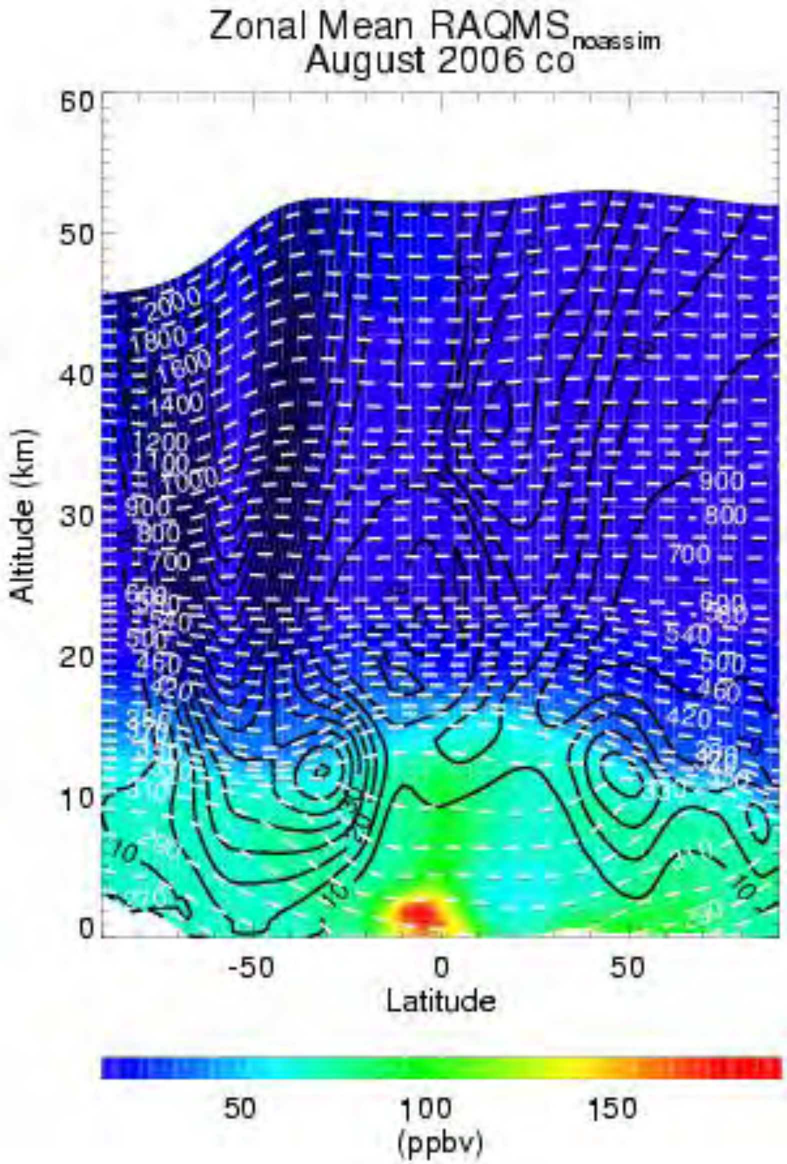
Optimal combination:

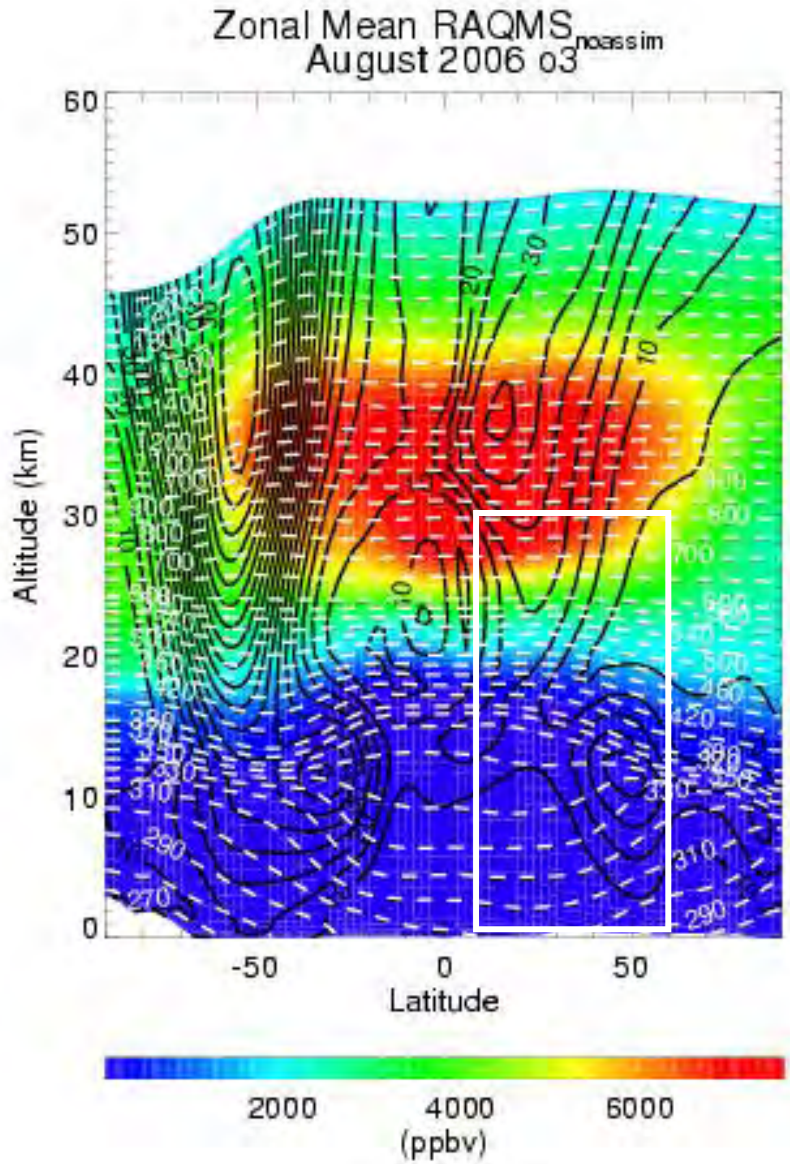
MLS (above 100mb)
TES CO (below 100mb)
MODIS AM/PM AOD ← Addition of Aerosol Assimilation

Improved Baseline:

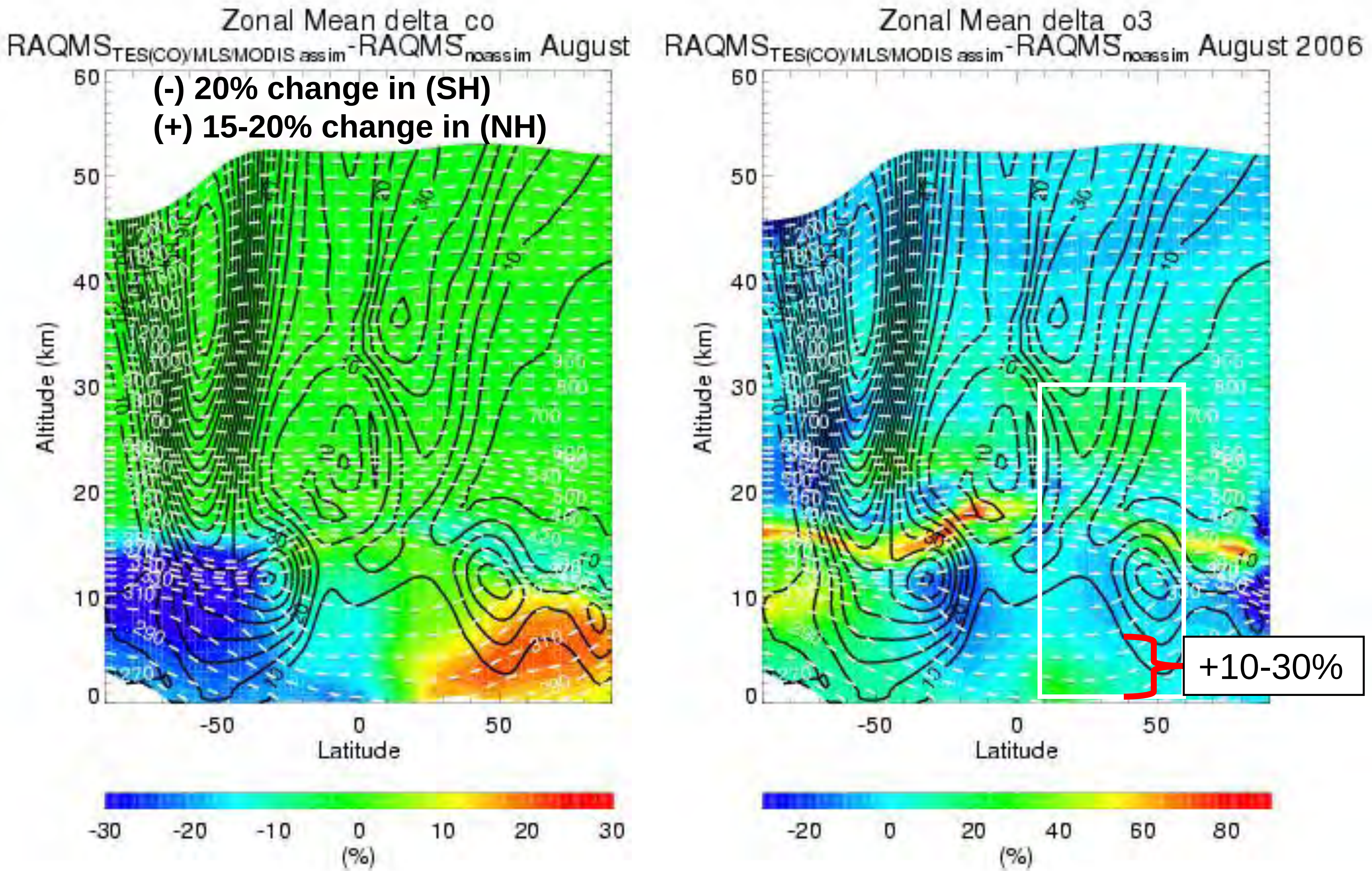
Corrected error in dz calculation (impacts emissions)
Improved tropical biomass burning estimates
Aerosol influence on photoysis calculations (GOCART aerosols)

August 2006 NO ASSIM Zonal mean CO/O3
(July 15, 2006 OMI+TES IC)

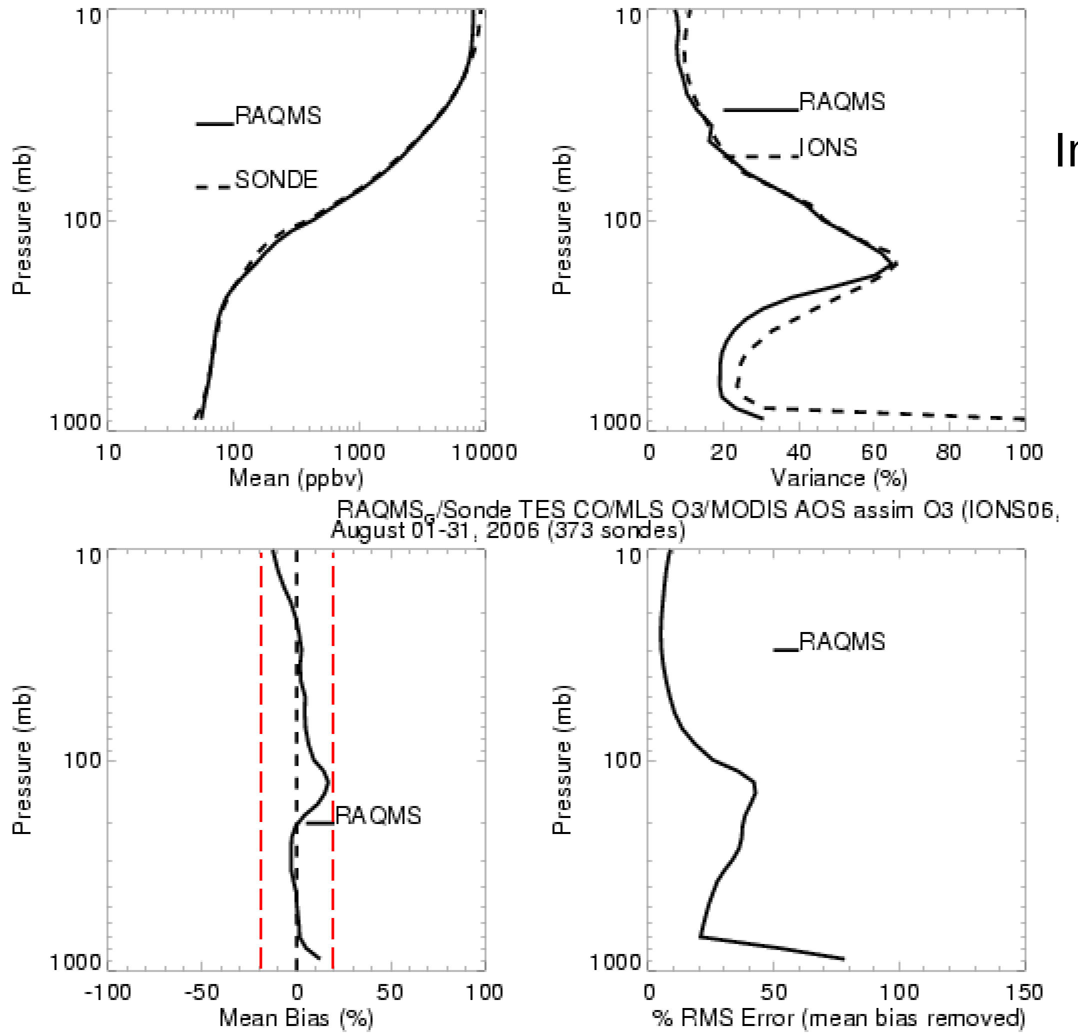




August 2006 TESCO/MLS/MODIS-NO ASSIM Zonal mean Delta CO/O3
(July 15, 2006 OMI+TES IC)



August 2006 TES (CO)/MLS/MODIS ASSIM vs IONS
(July 15, 2006 OMI+TES IC)

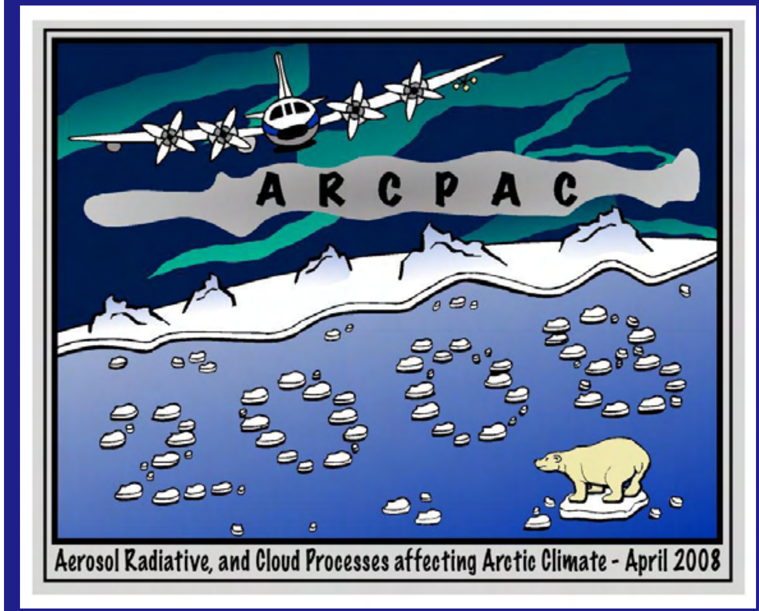


Improved Variance

Tropospheric biases: <10%
Stratospheric biases: <10%
Tropopause biases: +20%

Thanks to:

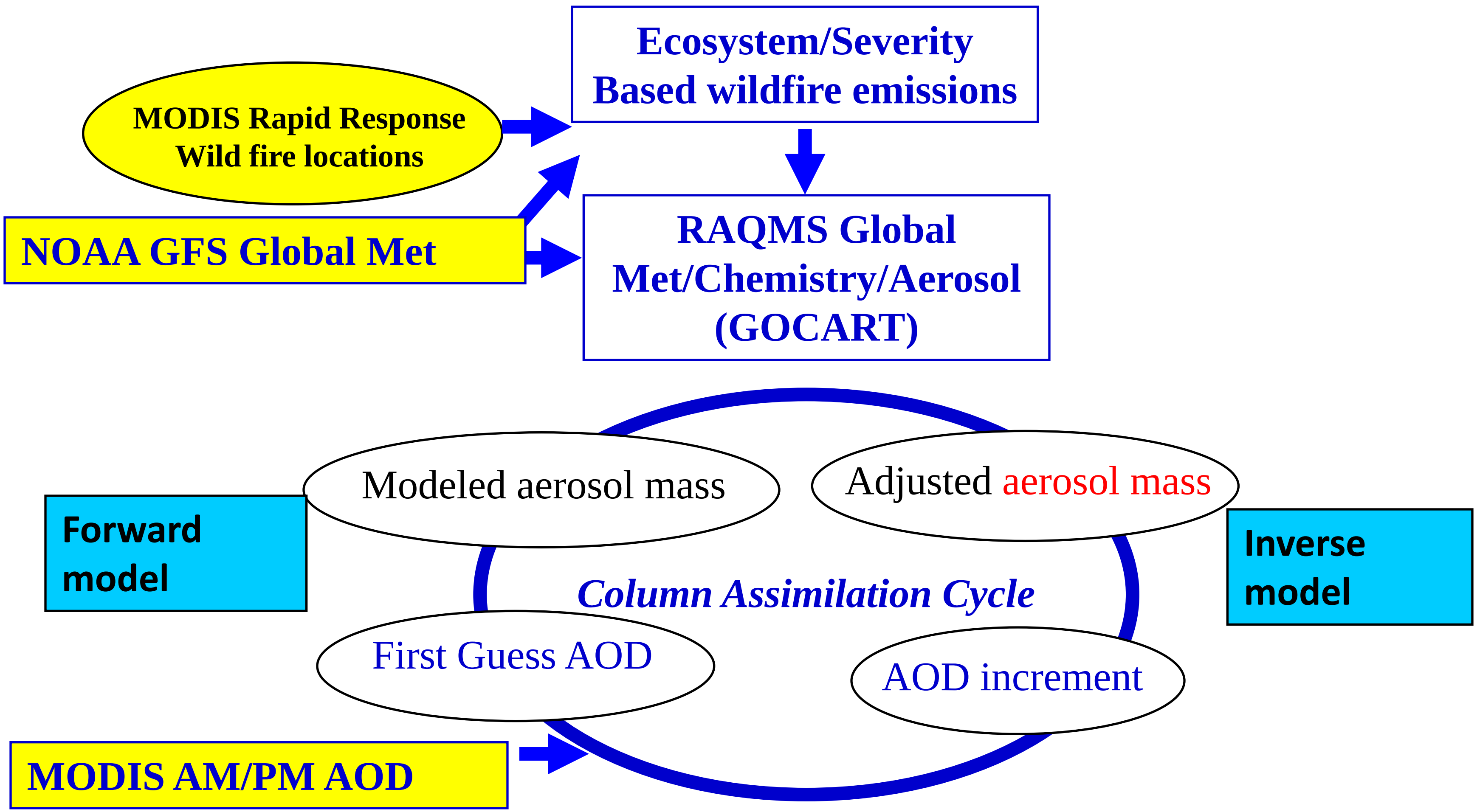
Fred Fehsenfeld, Bruce Doddridge & James Meagher
for coordinating the NASA/NOAA, Satellite/Airborne
collaboration during TEXAQS2006



During April 2008, as part of the International Polar Year (IPY), NOAA's Climate Forcing and Air Quality Programs engaged in an airborne field measurement campaign in the Alaskan Arctic. The Aerosol, Radiation, and Cloud Processes affecting Arctic Climate (ARCPAC) field mission (Fairbanks AK) focused on direct measurements of properties and processes associated with non-greenhouse-gas atmospheric climate forcing.

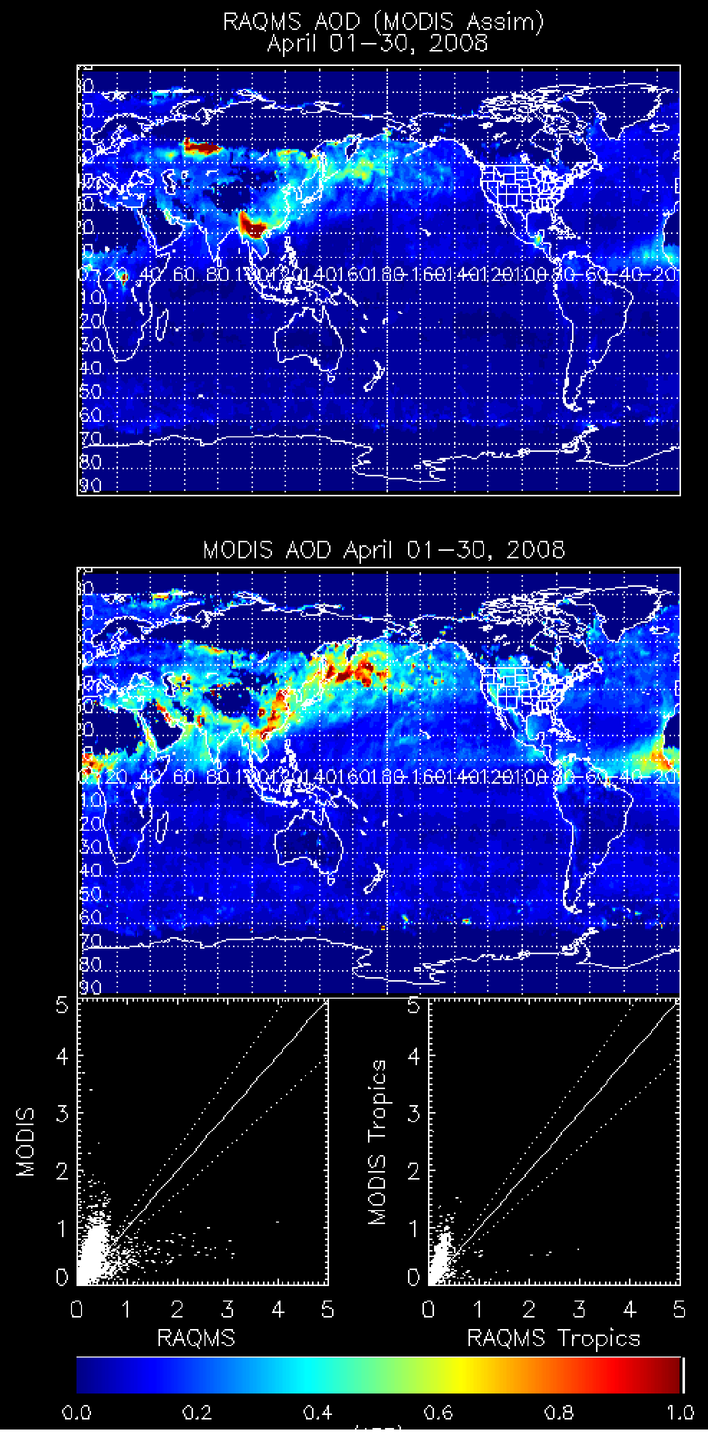
The Real-time Air Quality Modeling System (RAQMS) chemical and aerosol forecasts, initialized with real-time satellite measurements (e.g. Aura OMI column ozone and MLS ozone profiles, Terra and Aqua MODIS AOD) were used for daily flight planning activities during ARCPAC.

$RAQMS_{global}$ (2x2) ARCPAC AOD Assimilation Procedure



<u>Forward model:</u>
Compute layer/species extinction based on tabulated extinction efficiency and hydroscopic growth factors

<u>Inverse model:</u>
Distribute total AOD increment across aerosol dry mass based on layer/species extinction accounting for extinction due to hydroscopic growth

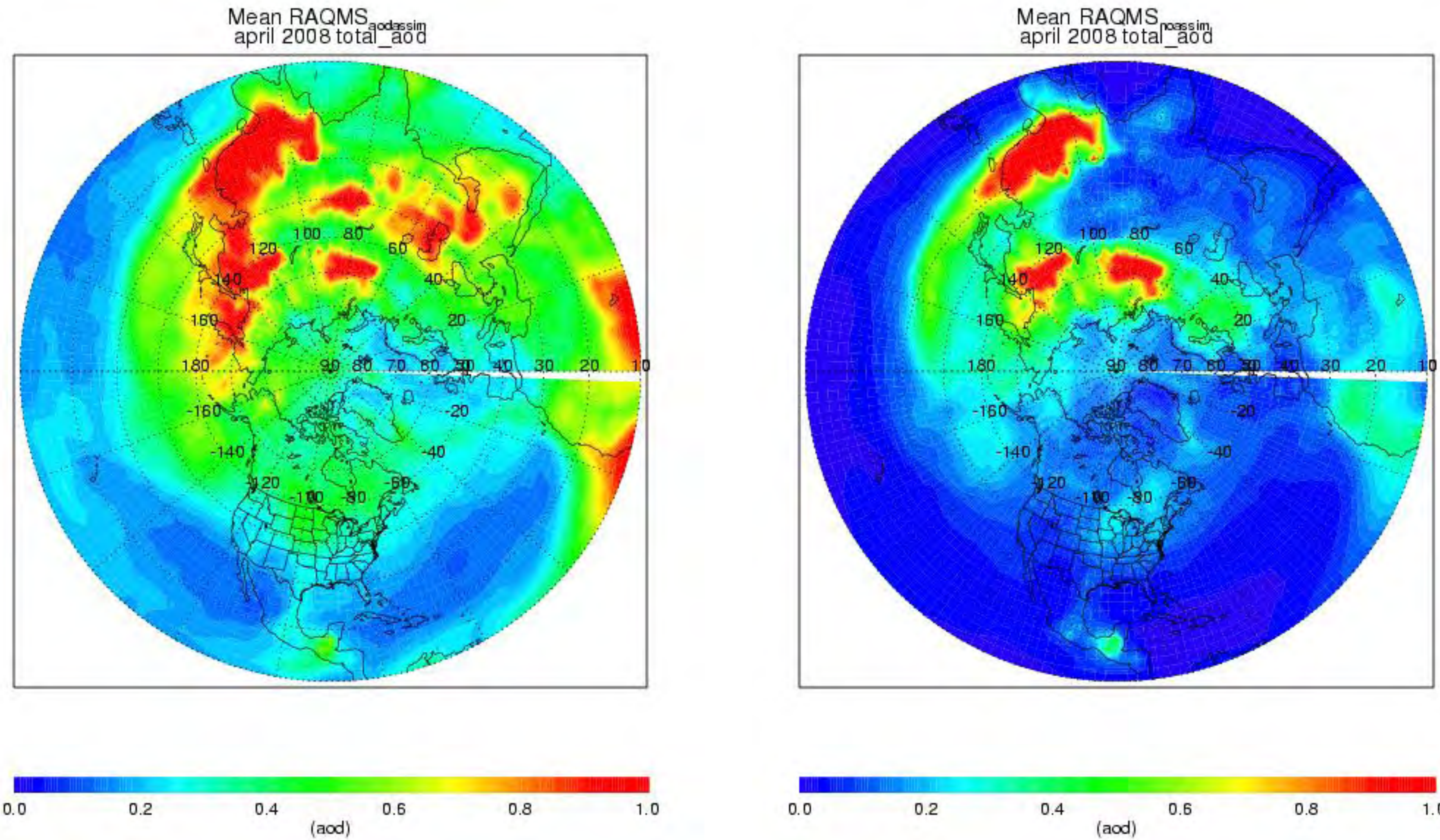


Monthly mean comparisons between the RAQMS AOD analysis and MODIS Aqua L2 retrievals for April, 2008.

RAQMS assimilates 1^{o} averaged MODIS AOD at hourly increments.

<u>The RAQMS analysis generally underestimates AOD relative to the L2 MODIS AOD retrieval.</u>

RAQMS April 2008 AOD with/without MODIS assimilation.

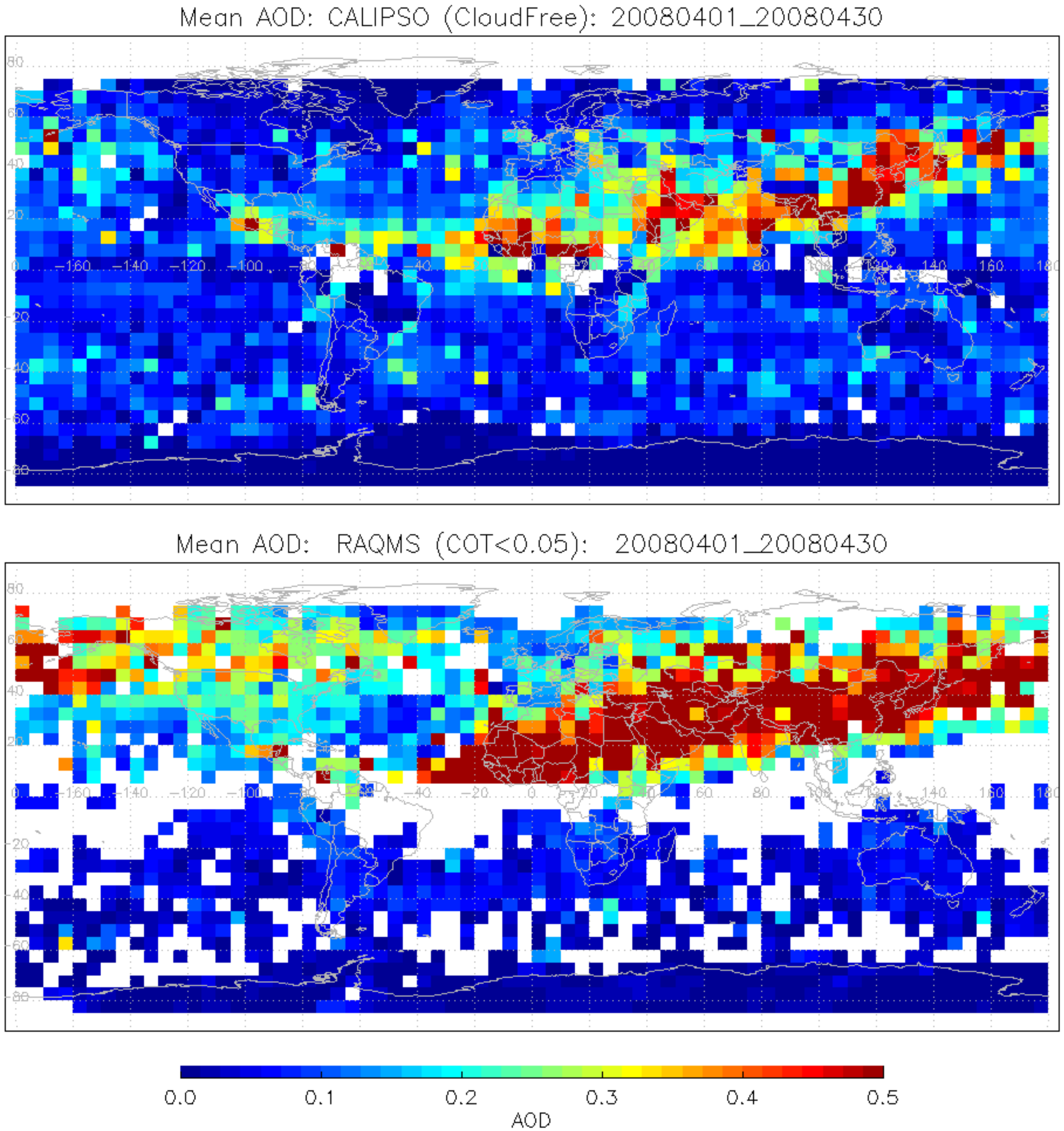


With AOD Assim

Without AOD Assim

<u>Assimilation increases RAQMS AOD, particularly over Central Asia and Africa.</u>

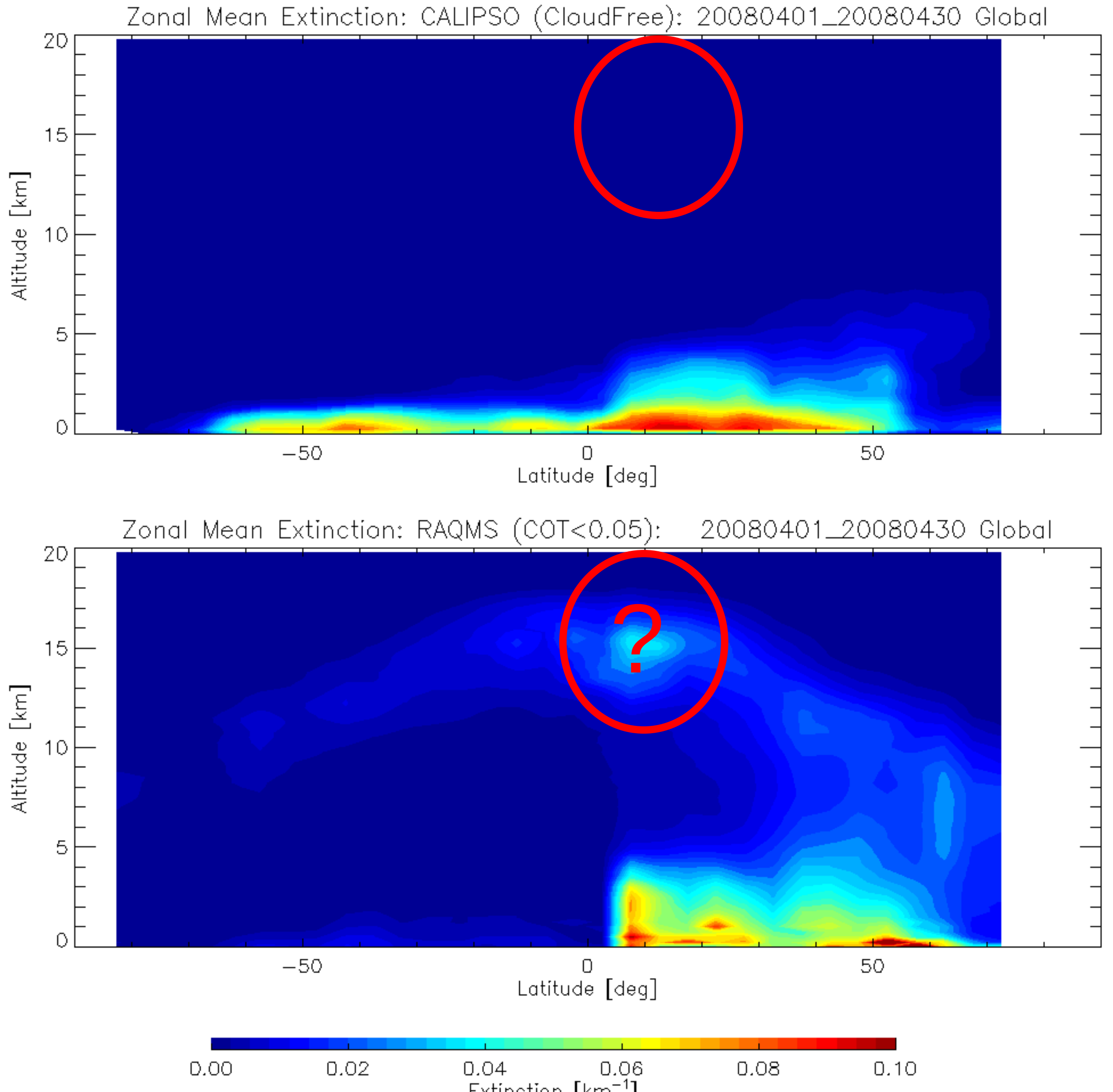
Cloud-free April 2008 comparisons between CALIPSO and RAQMS column AOD



<u>RAQMS overestimates AOD relative to CALIPSO</u>

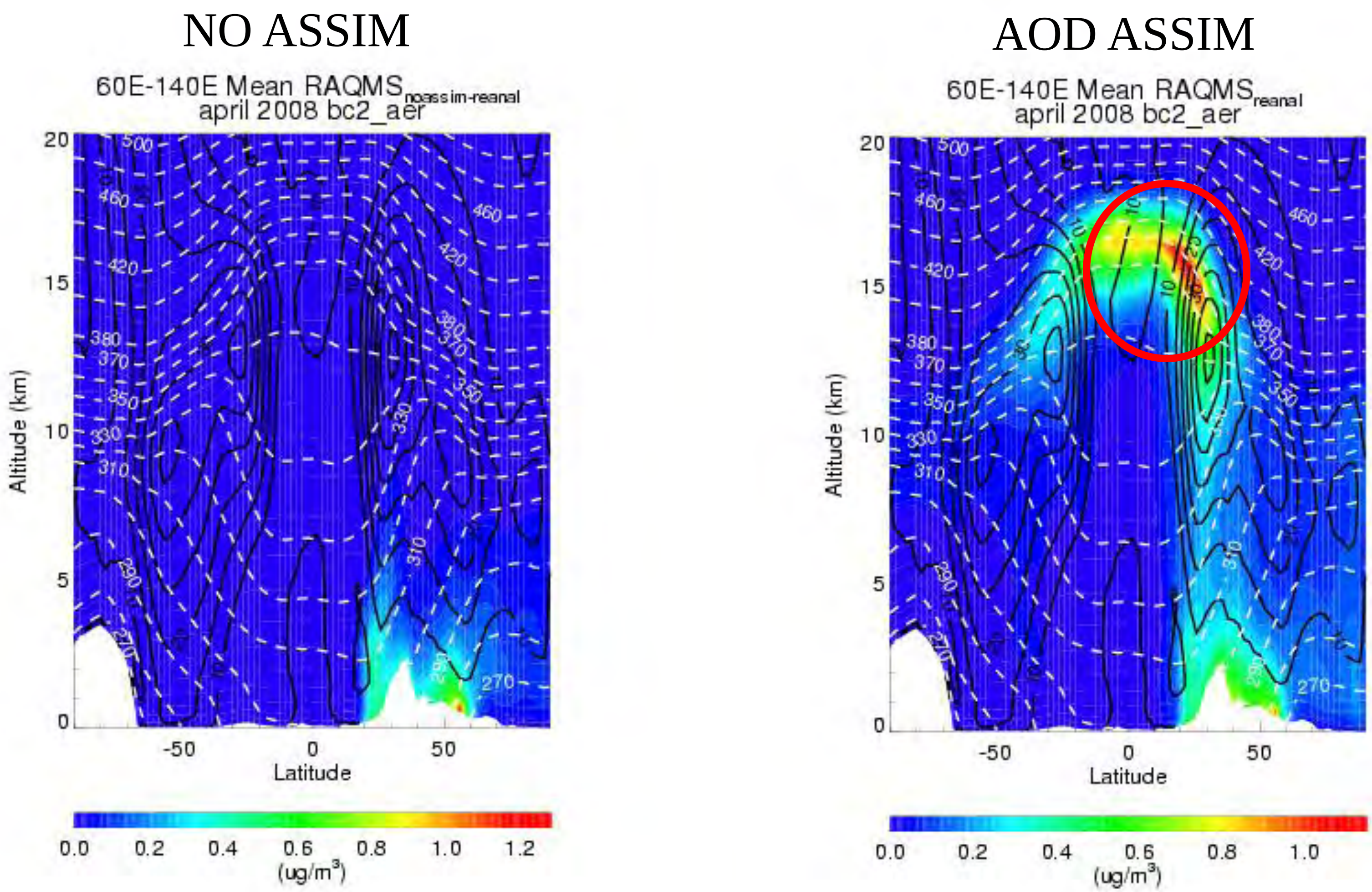
RAQMS/CALIPSO comparison provided by Chieko Kittaka, (NASA LaRC)

CALIPSO and RAQMS zonal mean extinction for April 2008



<u>RAQMS overestimates extinction in the upper troposphere relative to CALIPSO.</u>

Comparisons of hydrophilic black carbon (BC2) at 60E-140E with/without AOD assimilation



<u>Assimilation introduces hydrophilic BC mass near tropopause over SE Asian biomass burning region</u>

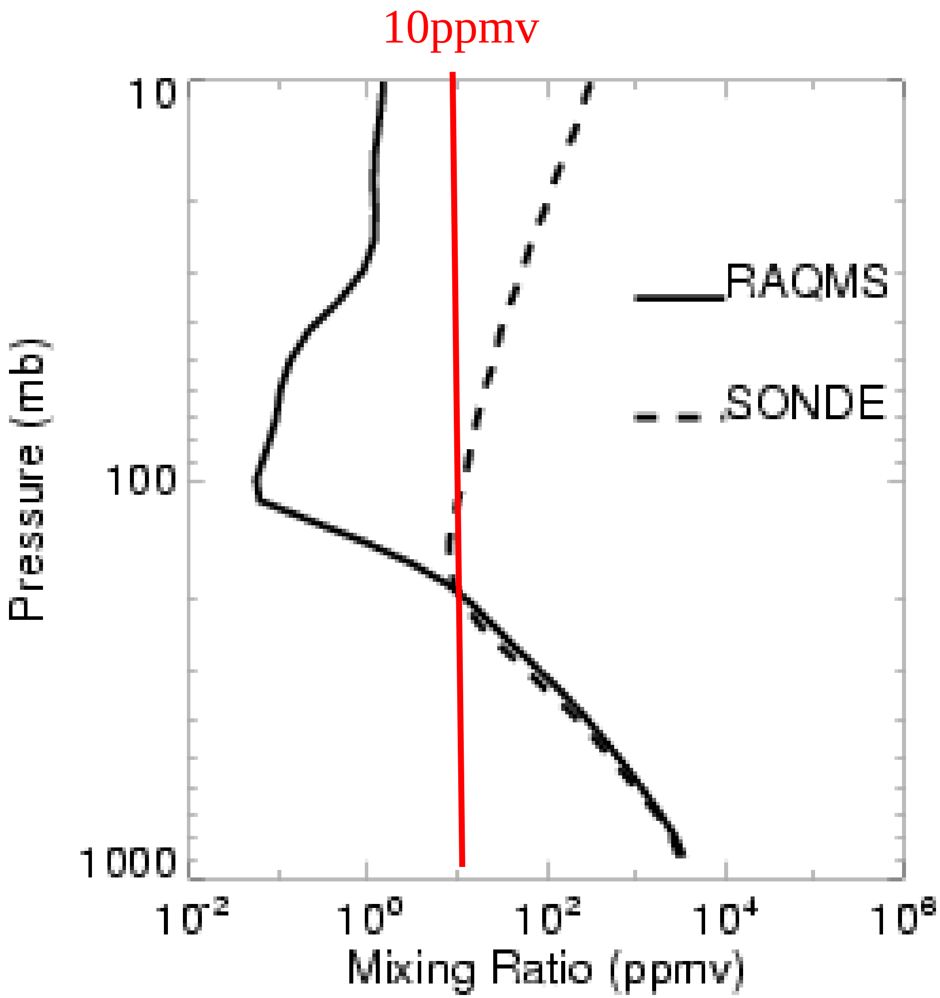
Hypothesis:

- **GFS water vapor is too low at tropopause.**

- **Correction for water vapor contribution to AOD during assimilation is significantly underestimated, resulting in over estimate of hydrophilic aerosol mass near tropical tropopause.**

- **Quasi-isentropic meridional transport results in elevated hydrophilic aerosols within the mid-latitude UT/LS.**

RAQMS (GFS) vs ARCIONS water vapor April 2008



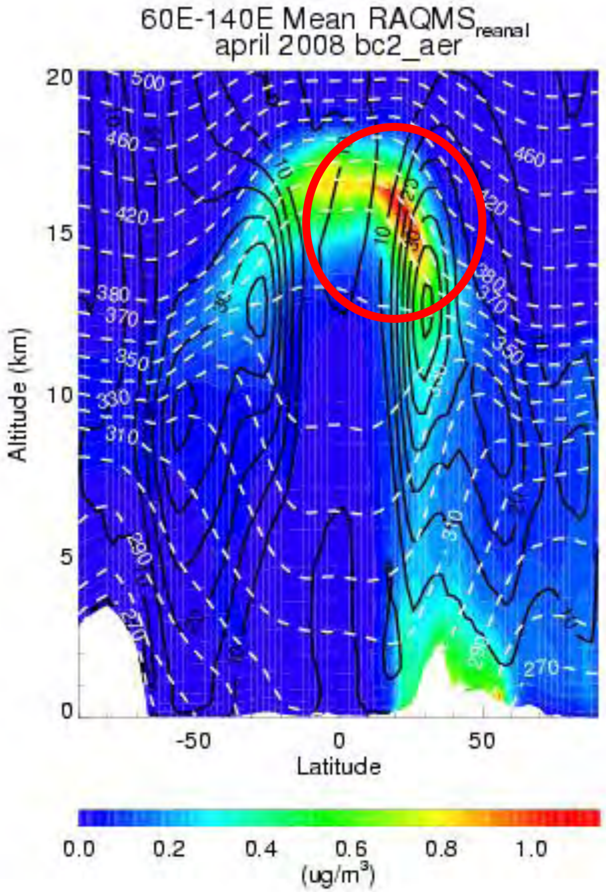
182 Sondes

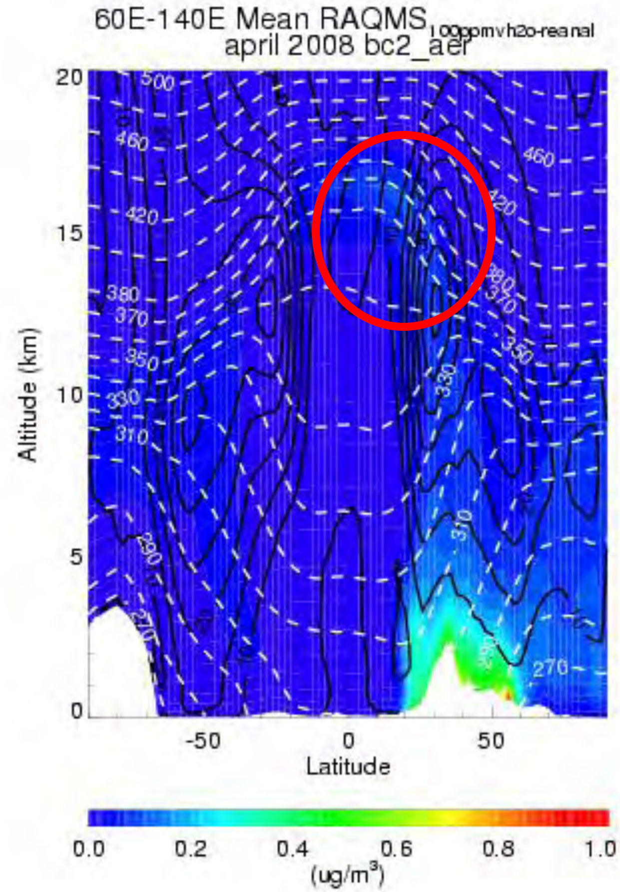
<u>RAQMS (GFS) is dry by over 2 orders of magnitude at 100mb.</u>

ARCIONS ozonesondes provided by Ann Thompson, (Penn State)

AOD ASSIM (baseline)

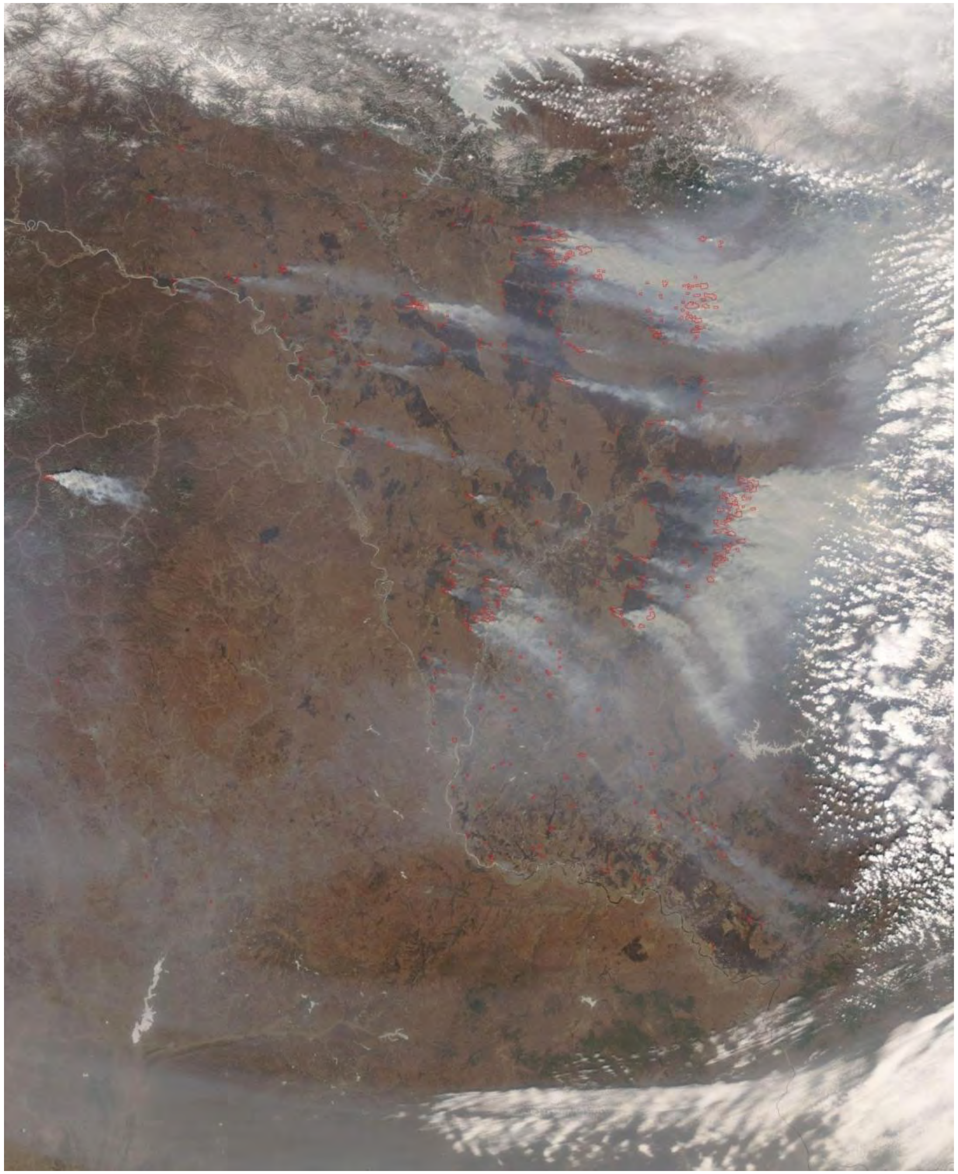
AOD ASSIM (H2O>100ppmv)





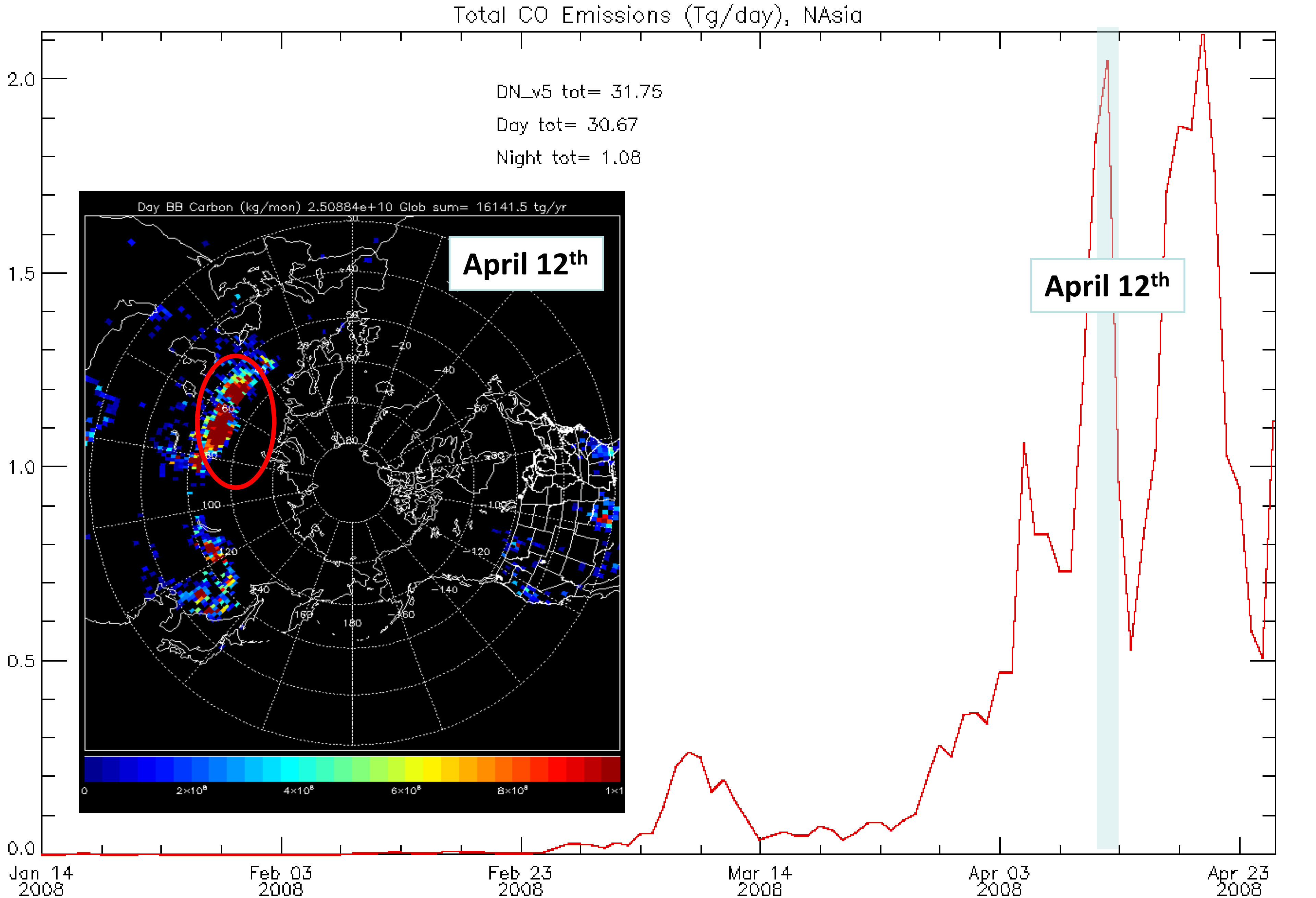
BC2 results of a preliminary sensitivity study where the minimum H2O used in the aerosol forward/inverse modeling was set to 100ppmv. ***The dry mass analysis increment for hydrophilic aerosols obtained from AOD assimilation is very sensitive to biases in the GFS analyzed water vapor in the upper troposphere due to the need to determine hydrophilic growth*.**

Case study of ARCPAC biomass burning influences (April 18th, 2008 NOAA P3 flight)



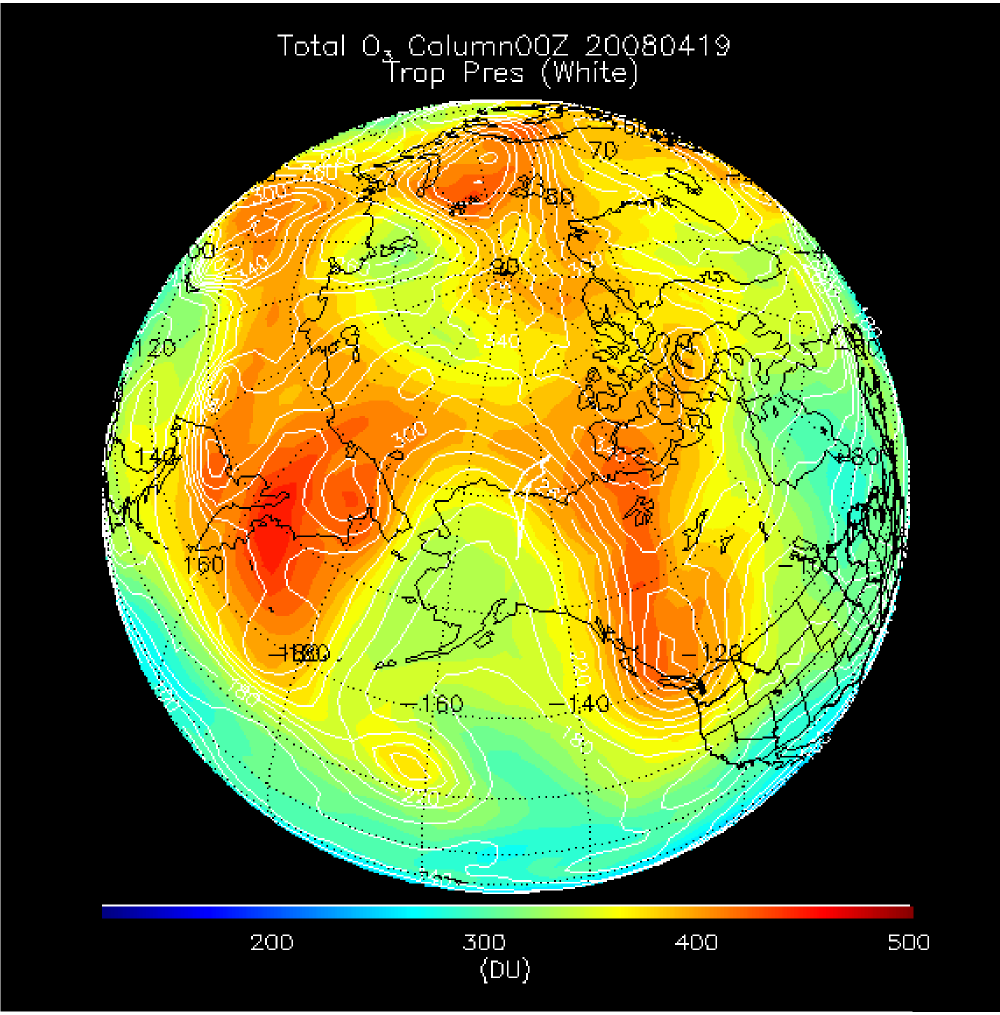
Fires in Southern Siberia attributed to unusually dry ground due to early loss of snow cover and agricultural burning activities

RAQMS N Asia Biomass Burning Emissions

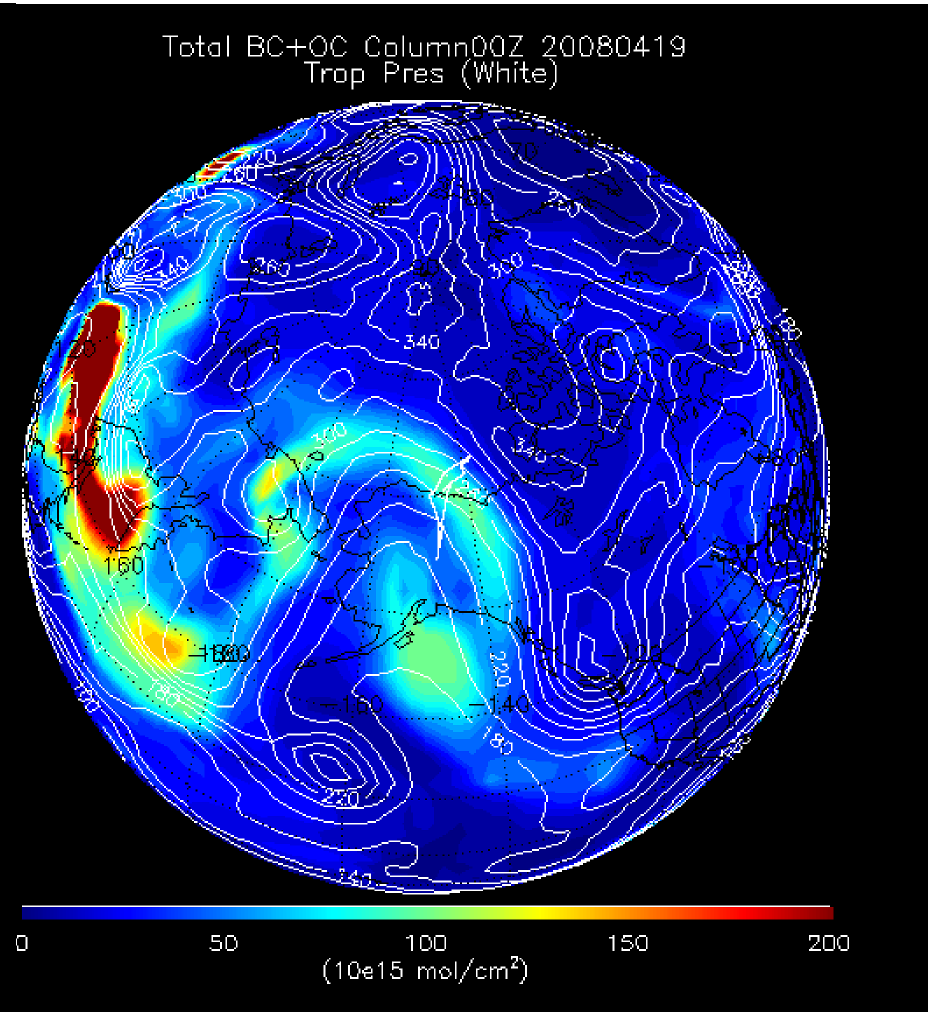


RAQMS 00Z April 19th, 2008 Analysis

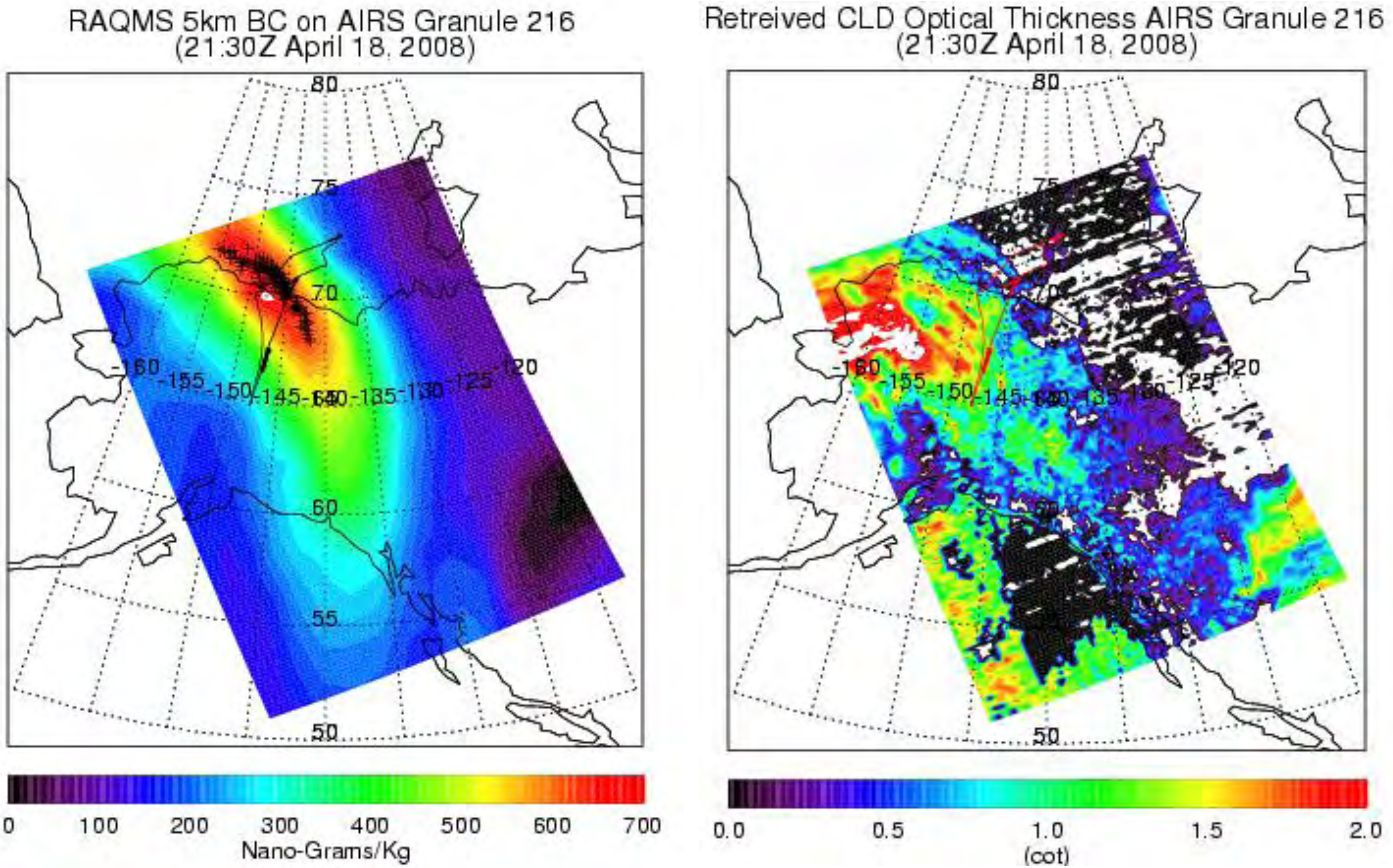
Total Colum Ozone



Carbonaceous (Black + Organic) aerosol



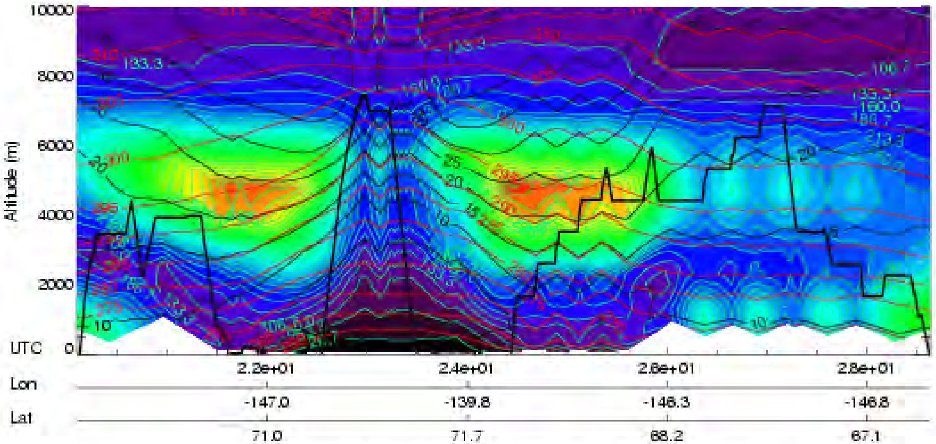
RAQMS total column O3 (DU, left) and BC+OC (x1015 mol/cm2, right) analyses at 00Z on April 19th, 2008. The tropopause pressure is contoured. The flight track of the NOAA P3, which sampled the predicted biomass burning plume is also shown.



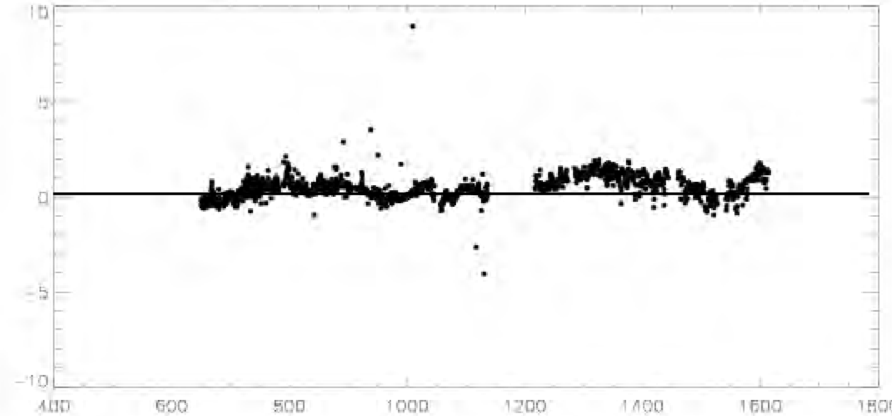
5km RAQMS Black Carbon (BC) aerosol analysis mapped onto AIRS Granule 216 (21:30Z) on April 18th, 2008 (left) and AIRS SFOV [Li et al, 2000, 2007] retrieval of cloud cloud optical thickness (right). The flight track of the NOAA P3 is also shown. Clear sky AIRS pixels with heavy aerosol loading are indicated by (+).

Black Carbon (BC) and Clear Sky AIRS Brightness Temperatures (T_b) April 18th, 2008

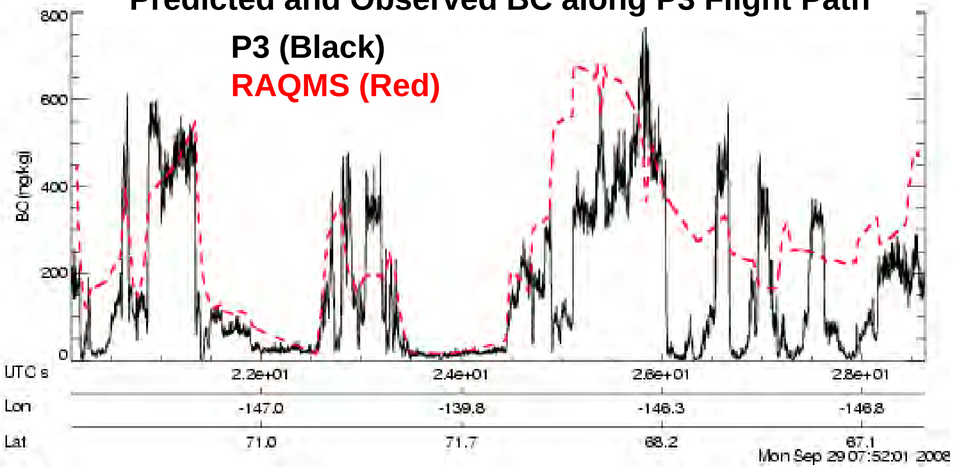
RAQMS BC Curtain along P3 Flight Path



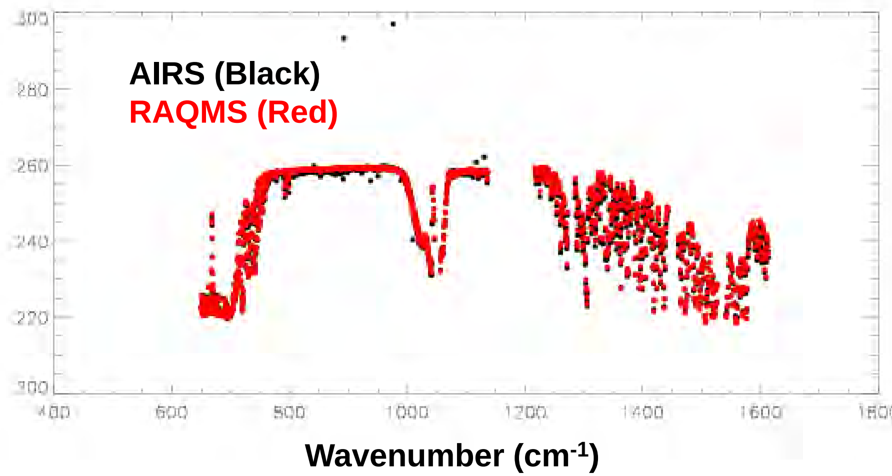
Delta T_b (RAQMS/CRTM-AIRS)



Predicted and Observed BC along P3 Flight Path



Clear Sky Tb for Granule 216



P3 SP-2 BC data provided by Ryan Spackman (NOAA/ESRL)

Predicted Black Carbon (BC) curtain and predicted (red) and observed (black) BC along April 18th, 2008 P3 flight track. Predicted (red) and observed (black) AIRS clear sky radiances in the vicinity of the P3 flight track and RAQMS/CRTM-AIRS brightness temperature differences for AIRS granule 216 on April 18th, 2008.

Future Directions:

- ***Alignment with NCEP operational system***

  •Update UW-Hybrid Physics (CCM3) to GFS (explicit clouds/improved convective exchange)

  •Update RAQMS SDF assimilation to GSI (3D-Var, testing underway)

- ***Develop capabilities to utilize future NPOESS (CrIS, VIIRS, OMPS) and GOES-R (ABI) aerosol and ozone***

  •Contribute to development of GFS global chemistry/aerosol assimilation/forecasting system (with Steve Lord, Sarah Lu NCEP)

  •Contribute to development of FIM global chemistry/aerosol assimilation forecasting system (with Stan Benjamin, Georg Grell ESRL)

  •Test CRTM aerosol forward modeling (with Fuzhong Weng, Quanhua "Mark" Liu, NESDIS)

- ***Participation on NOAA airborne field campaigns***

  •Post mission ARCPAC analysis (nested RAQMS/WRF-CHEM, with Lun Li, CIMSS and Georg Grell, ESRL, NOAA Climate Research Program)

  •CalNex (2010 California Air Resources Board)

References:

Fishman, J., K. W. Bowman, J. P. Burrows, A. Richter, K. V. Chance, D. P. Edwards, R, V. Martin, G. A. Morris, R. B. Pierce, J. R. Ziemke, J. A. Al-Saadi, T. K. Schaack, A. M. Thompson, Remote Sensing of Chemically Reactive Tropospheric Trace Gases from Space, BAMS, Vol 89, no 6, pages 805-821, June 2008.

Li, J., Jinlong Li, Elisabeth Weize, and D. K. Zhou, 2007: Physical retrieval of surface emissivity spectrum from hyperspectral infrared radiances, Geophysical Research Letters, 34, L16812, doi:10.1029/2007GL030543.

Li, J., W. Wolf, W. P. Menzel, W. Zhang, H.-L. Huang, and T. H. Achtor, 2000: Global soundings of the atmosphere from ATOVS measurements: The algorithm and validation, *J. Appl. Meteorol.*, 39: 1248 – 1268.

Pierce, R. B., et al. (2003), Regional Air Quality Modeling System (RAQMS) predictions of the tropospheric ozone budget over east Asia, J. Geophys. Res., 108(D21), 8825, doi:10.1029/2002JD003176.

Pierce, R. B., et al. (2007), Chemical data assimilation estimates of continental U.S. ozone and nitrogen budgets during the Intercontinental Chemical Transport Experiment–North America, J. Geophys. Res., 112, D12S21, doi:10.1029/2006JD007722.

Pierce, R. B., J. A. Al-Saadi, C. Kittaka, T. Schaack, A. Lenzen, K. Bowman, J. Szykman, A. Soja, T. Ryerson, A. Thompson, P. Bhartia, Impacts of background ozone production on Houston and Dallas, TX Air Quality during the TexAQS field mission, Submitted to J. Geophy. Res., Sept, 2008

Song, C.-K., D. W. Byun, R. B. Pierce, J. A. Alsaadi, T. K. Schaack, and F. Vukovich (2008), Downscale linkage of global model output for regional chemical transport modeling: Method and general performance, J. Geophys. Res., 113, D08308, doi:10.1029/ 2007JD008951.

Sunita V, J. Worden, R. B. Pierce, D. Jones, J. A. Al-Saadi, K. Bowman, F. Boersma, Ozone Production in Boreal Fire Smoke Plume as observed by the Tropospheric Emission Spectrometer and the Ozone Monitoring Instrument, Accepted to J. Geophys. Res. August, 2008

Tang, Y., P. Lee, M, Tsidulko, H. C. Huang , J. T. McQueen, G. DiMego , L. K. Emmons, R. B. Pierce, A. M. Thompson, H-M. Lin, D. Kang, D. Tong, S. Yu, R. Mathur, J. E. Pleim, T. L. Otte, G. Pouliot, J.O. Young, K. L. Schere, P.M. Davidson, I. Stajner, "The impact of chemical lateral boundary conditions on CMAQ predictions of tropospheric ozone over the continental United States", Accepted to Environ Fluid Mech, August 2008