Real-time Air Quality Modeling System

R. Bradley Pierce
NOAA/NESDIS

Team Members: Jassim Al-Saadi[1], Todd Schaack[2], Chieko Kittaka[1], Amber Soja[1],
T. Duncan Fairlie[1], Murali Natarajan[1], Allen Lenzen[2]

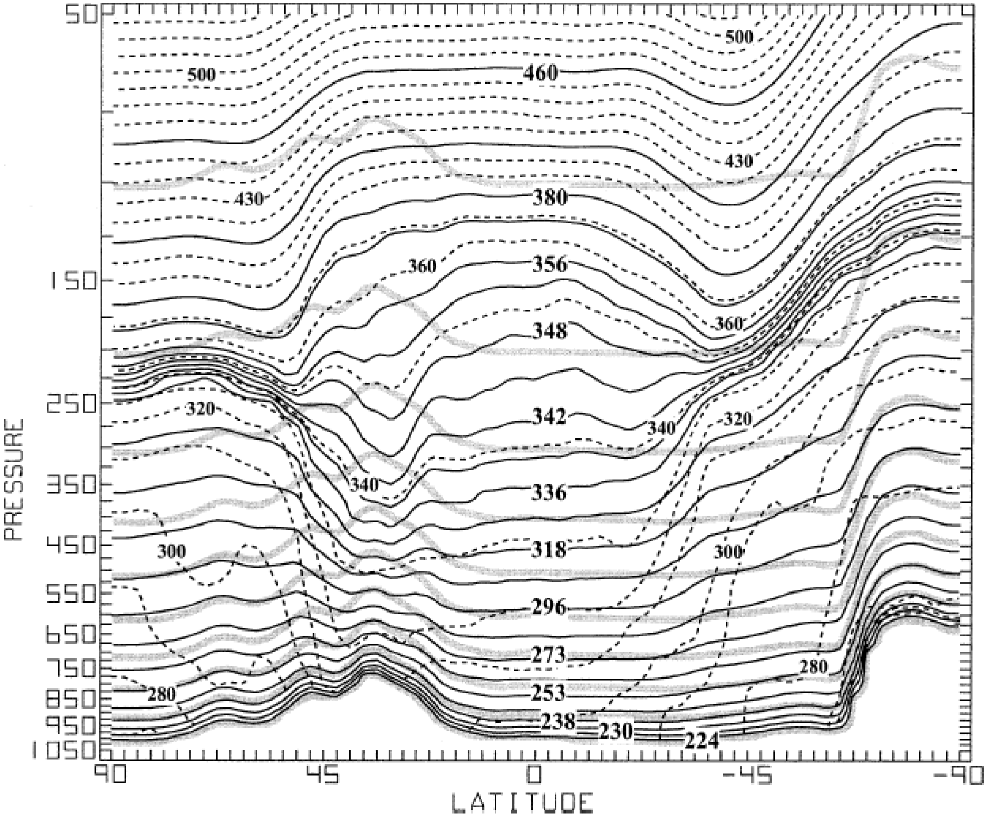
[1]NASA Langley Research Center, Hampton, VA
[2]Space Science and Engineering Center, Madison, WI

NOAA Atmospheric Chemical Modeling Workshop
10 - 11 October 2007 ~ Boulder, Colorado

Online unified tropospheric/stratospheric chemistry developed for global assimilation of satellite observations of atmospheric chemical composition and regional air quality prediction [Pierce et al., 2003, 2007].

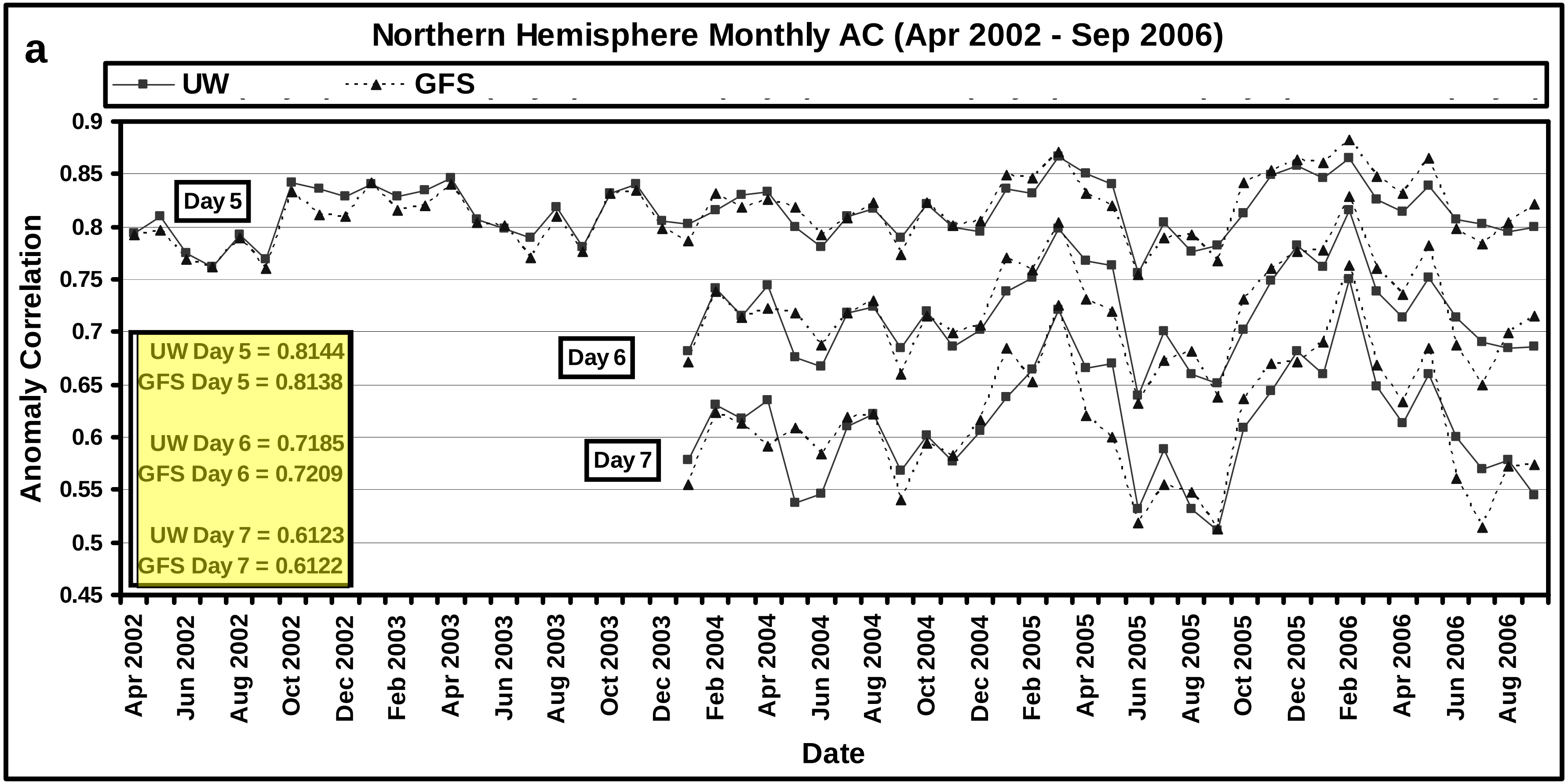
Dynamical core: UW hybrid isentropic coordinate model [Schaack et al., 2004]

- •Terrain following (blended isentropic/sigma) coordinate in troposphere (below 380K)
- •Isentropic (potential temperature) coordinates in stratosphere (above 380K)
- •Arakawa A grid, flux form piecewise parabolic method (PPM) numerics
- •CCM3 physics (radiation, moist convection, vertical diffusion, gravity wave drag, PBL scheme, surface fluxes



Grey shading: Standard Sigma
Solid lines: Blended isentropic/sigma
Dashed lines: Isentrops

UW-Hybrid vs GFS Northern Hemisphere 500mb AC Scores



The UW model was run at 0.7 degree lat-lon, 28 layers throughout the record. Through May 2005 the GFS ran at T254L64 for the first 84 hours of the forecasts and finished the forecast with T170L42. After June 2005, the GFS ran at T382L64.
(Provided by Tom Zapotocny, SSEC/CIMSS)

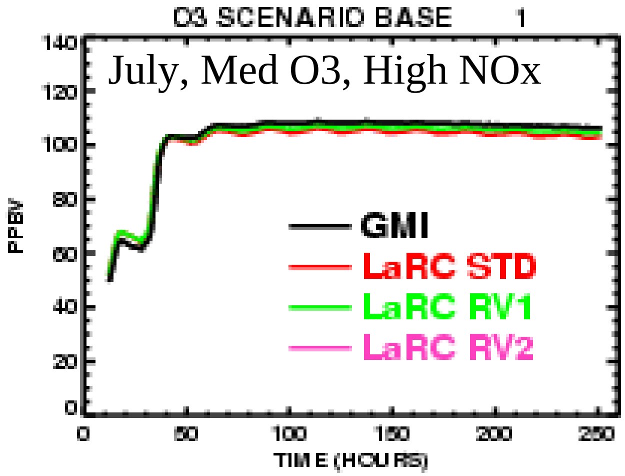
Chemical mechanism: Family approach for Ox-HOx-NOx-ClOx-BrOx cycles, extended carbon bond [Zaveri and Peters,1999] scheme for oxidation of non-methane hydrocarbons (NMHC) with semi-explicit treatment of propane and explicit treatment of isoprene oxidation [Carter, 1997]

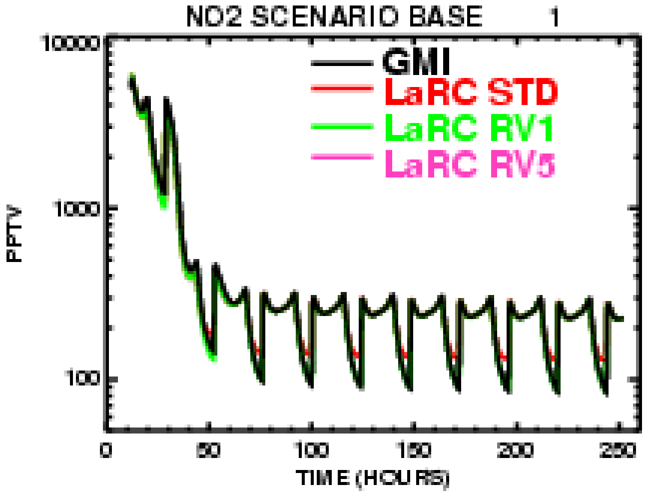
- 55 families and individual constituents transported, equilibrium concentrations of 86 separate species

- Photolytic rates are calculated using the Fastj2 method [Bian et al., 2002].

- Aromatic chemistry is not included. Concentrations of acetone and methanol are specified according to climatologies.

- Stratospheric heterogeneous reactions on liquid aerosol [Carslaw et al., 1995] and polar stratospheric cloud [Chipperfield, 1999] surfaces are considered.





RAQMS unified (strat/trop) chemistry

(55 species/families explicitly transported, 86 calculated, PCE assumptions for “fast” species)

1) Ox
2) Noy
3) Cly
4) Bry
5) HNO3
6) N2O5
7) H2O2
8) HCl
9) ClONO2
10) OClO
11) N2O
12) CFCl3 (F11)
13) CF2Cl2 (F12)
14) CCl4
15) CH3Cl
16) CH3CCl3 (MTCFM)
17) CH3Br
18) CF3Br (H1301)

19) CF2ClBr (H1211)
20) HF
21) CFClO
22) CF2O
23) CH4
24) HNO4
25) HOCl
26) H2O
27) NO3
28) NO2
29) CH2O
30) CH3OOH
31) CO
32) HBr
33) BrONO2
34) HOBr
35) BrCl
36) Cl2

Stratosphere+CH4&CO oxidation

37) C2H6 (ethane, 2C)
38) ALD2 (acetaldehyde+higher group, 2C)
39) ETHOOH (ethyl hydrogen peroxide, 2C)
40) PAN (2C)
41) PAR (paraffin carbon bond group, 1C)
42) ONIT (organic nitrate group, 1C)
43) AONE (acetone, 3C)
44) ROOH (C3+hydrogen peroxides group, 1C)
45) MGLY (methylglyoxal, 3C)
46) ETH (ethene, 2C)
47) XOLET (terminal olefin carbon group, 2C)
48) XOLEI (internal olefin carbon group, 2C)
49) XISOP (isoprene, 5C)
50) XISOPRD (isoprene oxidation product-long lived, 5C)
51) PROP_PAR (propane paraffin, 1C)
52) CH3OH (methanol)
53) XMVK (methyl vinyl ketone, 4C)
54) XMACR (methacrolein, 4C)
55) XMPAN (peroxymethacryloyl nitrate, 4C)

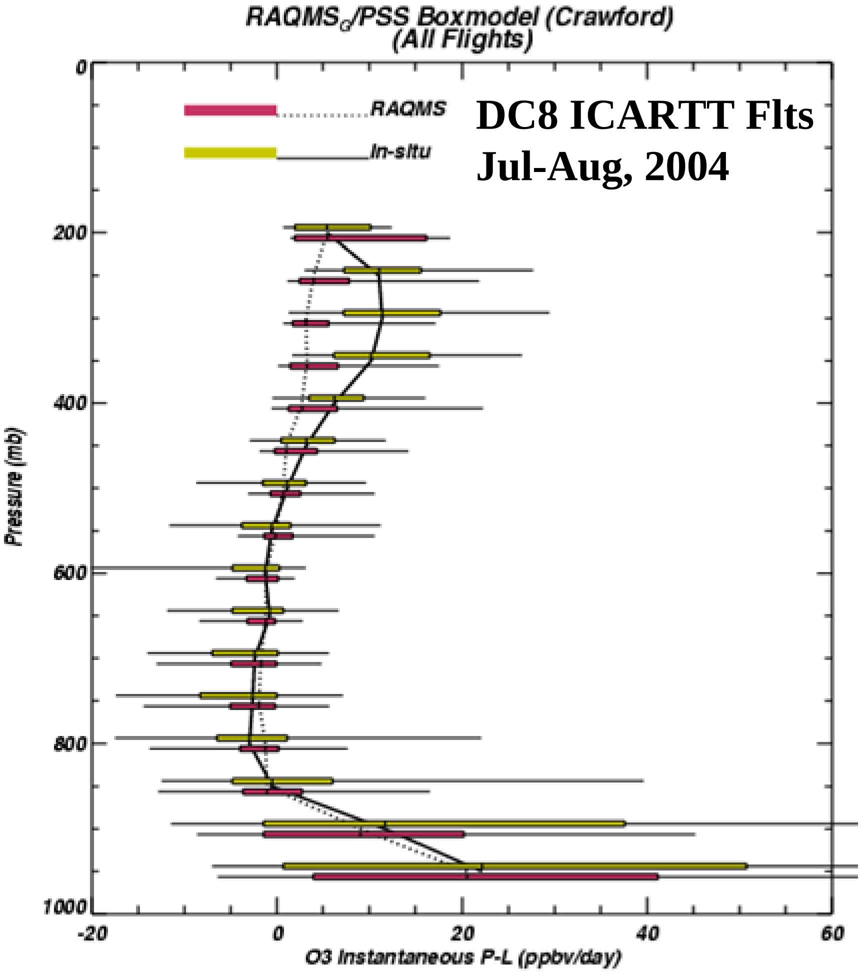
NMHC Chemistry

Chemical families

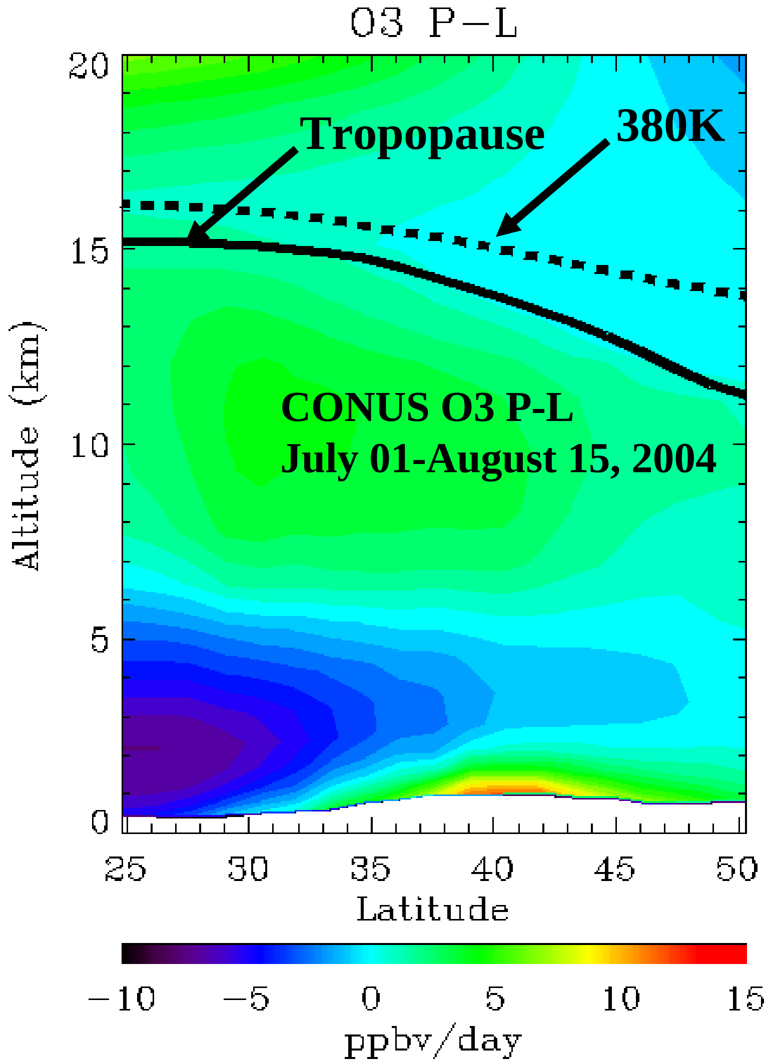
Ox=O(1D)+O(3P)+O3+NO2+HNO3+2(NO3)+3(N2O5)+HNO4+PAN+MPAN
NOy=N+NO+NO2+NO3+2(N2O5)+HNO3+HNO4+BrNO3+ClNO3+PAN+ONIT+MPAN
Cly=HCl+ClONO2+ClO+2(Cl2O2)+OClO+ClO2+2(Cl2)+BrCl+HOCl+Cl
Bry=HBr+BrONO2+BrO+BrCl+HOBr+Br

Comparison between RAQMS O3 P-L and Box Model ICARTT 2004

(Box model is observationally constrained with DC8 measurements)



DC8 ICARTT Flts
Jul-Aug, 2004



Tropopause

380K

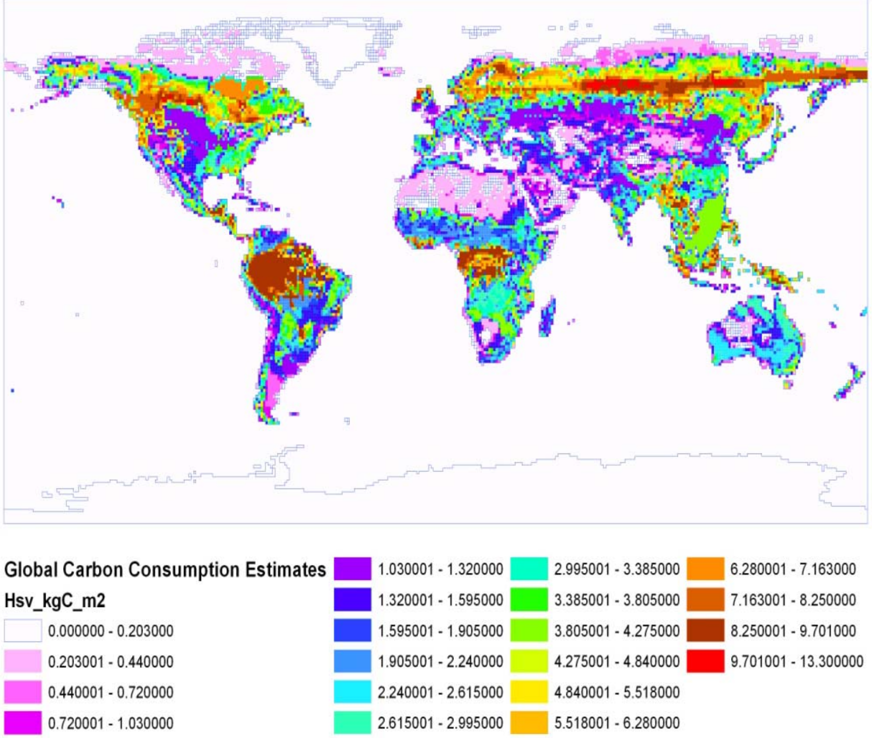
CONUS O3 P-L
July 01-August 15, 2004

Underestimate in ozone P-L at 300mb is consistent with factor of 2 underestimate of NO2 (likely due to underestimate in lighting NOx)

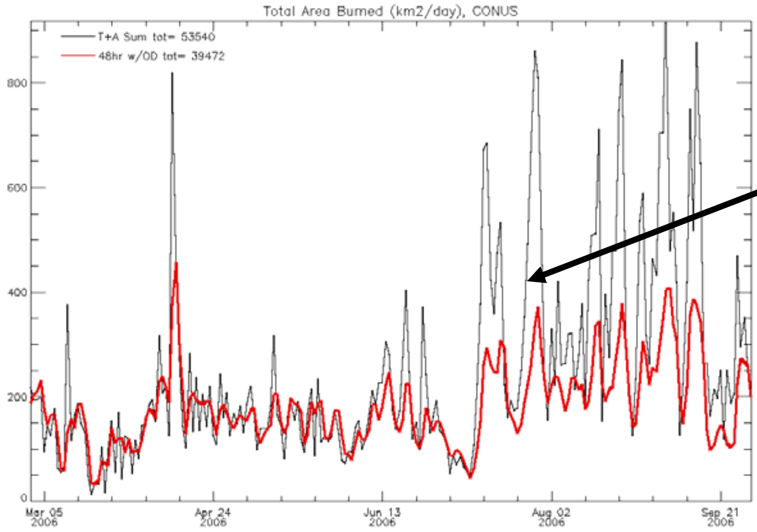
Emissions: Climatological anthropogenic and natural sources based on 1x1 degree GEIA/EDGAR data base with updates for Asian emissions from Streets et al. [2003] and additional biogenic CO sources as described by Duncan et al. [2004]

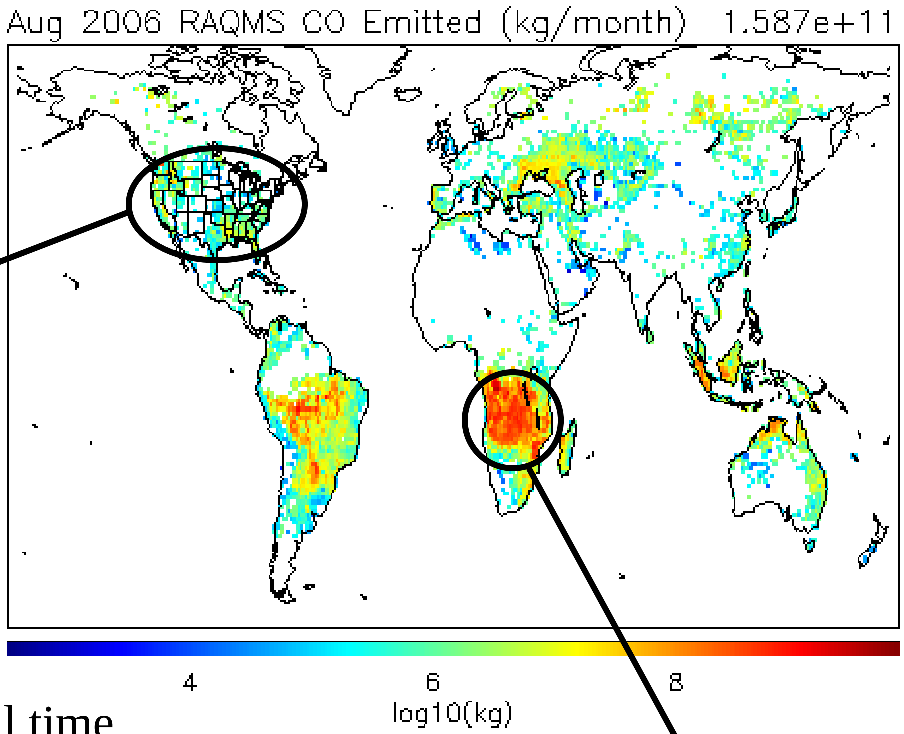
- Aircraft NOx emissions are obtained from the HSRP database [Stolarski et al., 1995]
- Lightning NOx emissions [Price et al., 1997, Pickering et al., 1998] use instantaneous convective cloud heights
- Twice daily updates in biomass burning emissions based on MODIS fire detection, Haines fire severity, and static ecosystem/severity based fuel loading.

Global carbon consumption estimates for *high-severity* fires

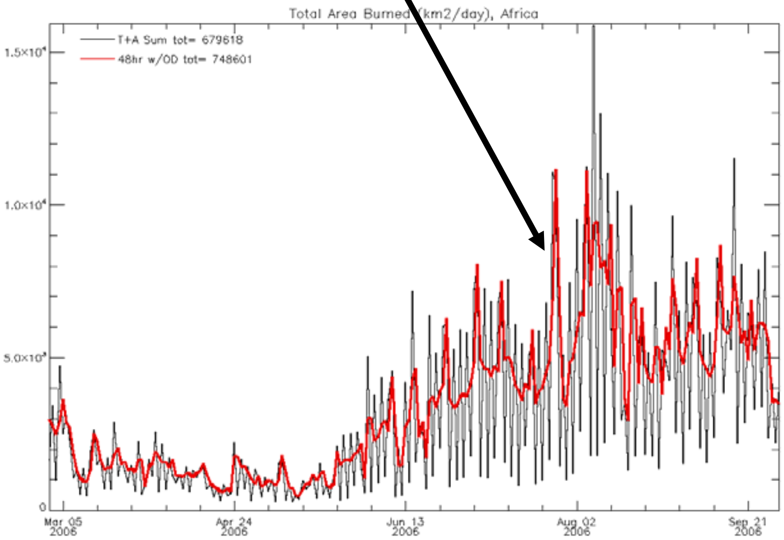


RAQMS Global BB CO Emissions: August 2006





- Need for global emissions in near real time dictates the use of MODIS Rapid Response fire detections for estimating area burned
- Terra/Aqua orbit parameters yield latitude-dependent sampling biases in daily estimates
- Current approach combines 48hrs of detections from Terra and Aqua and eliminates multiple detections

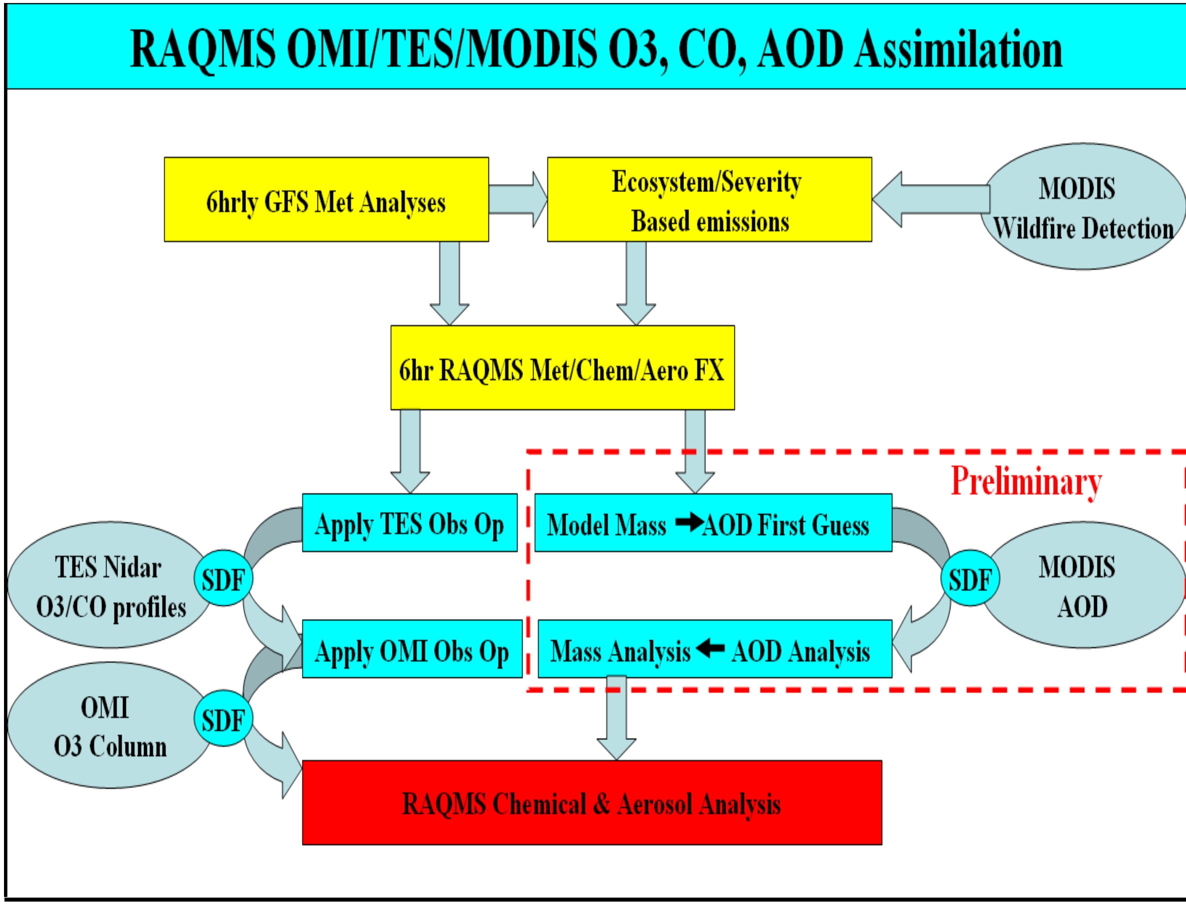


Assimilation: Statistical digital filter (SDF) analysis system [Stobie 1985, 2000] to perform a univariate Optimal Interpolation assimilation of satellite profile and total column retrievals of O3, CO, AOD.

- Retrieval apriori and averaging kernels accounted for in observation operator.

- Forecast error variances are calculated by inflating the analysis errors [Savijarvi, 1995]

- Quality control employed during the analysis includes a gross check, suspect identification and a buddy check for suspect observations.



RAQMS OMI/TES/MODIS O3, CO, AOD Assimilation

6hrly GFS Met Analyses

Ecosystem/Severity Based emissions

MODIS Wildfire Detection

6hr RAQMS Met/Chem/Aero FX

Preliminary

TES Nidar O3/CO profiles

SDF

Apply TES Obs Op

Model Mass → AOD First Guess

SDF

MODIS AOD

OMI O3 Column

SDF

Apply OMI Obs Op

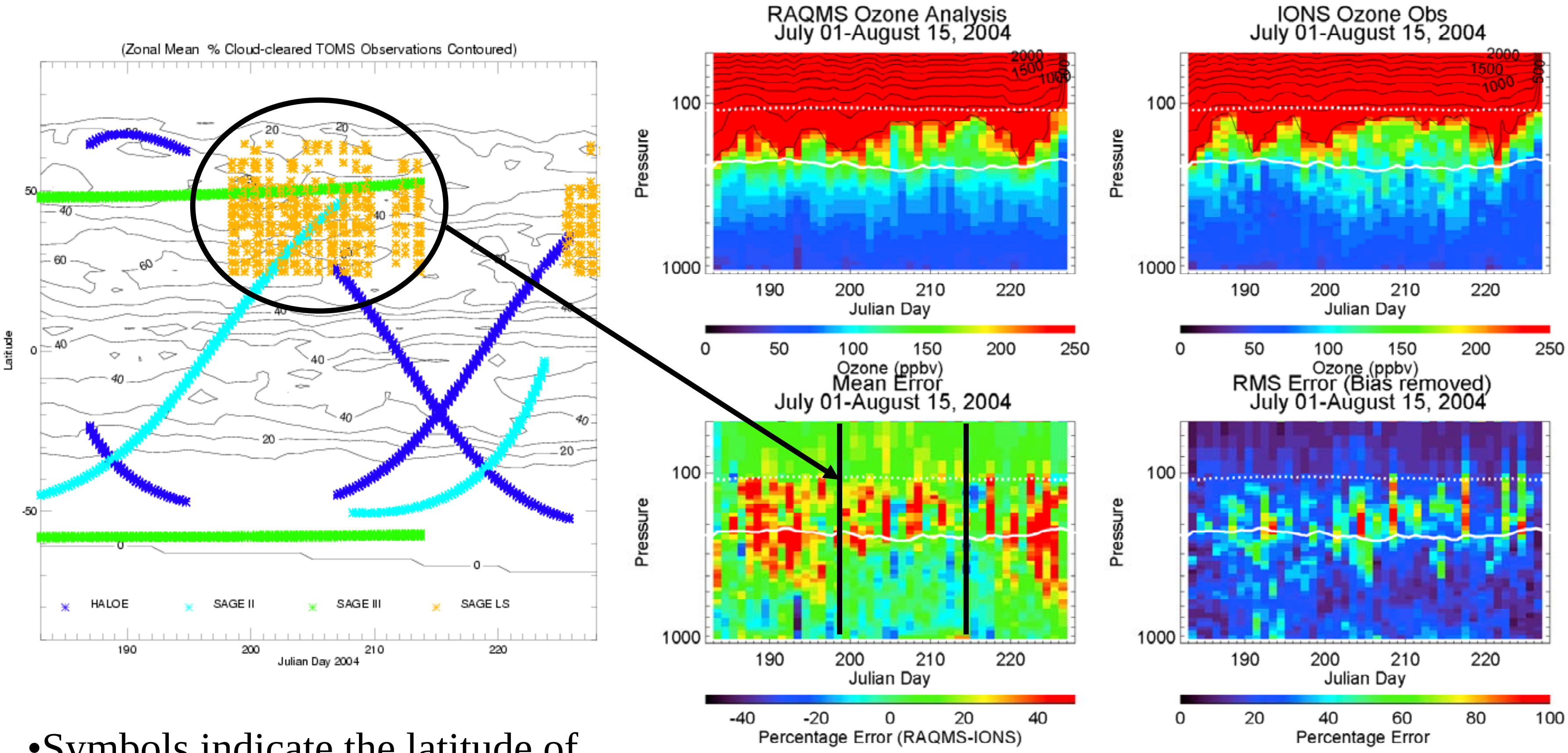
Mass Analysis ← AOD Analysis

RAQMS Chemical & Aerosol Analysis

Currently porting GSI to SGI Itanium at CIMSS (Linux Intel compiler)

RAQMS 1.4x1.4 2004 ICARTT Assimilation

(HALOE, SAGE II+III, SAGE LS, TOMS)

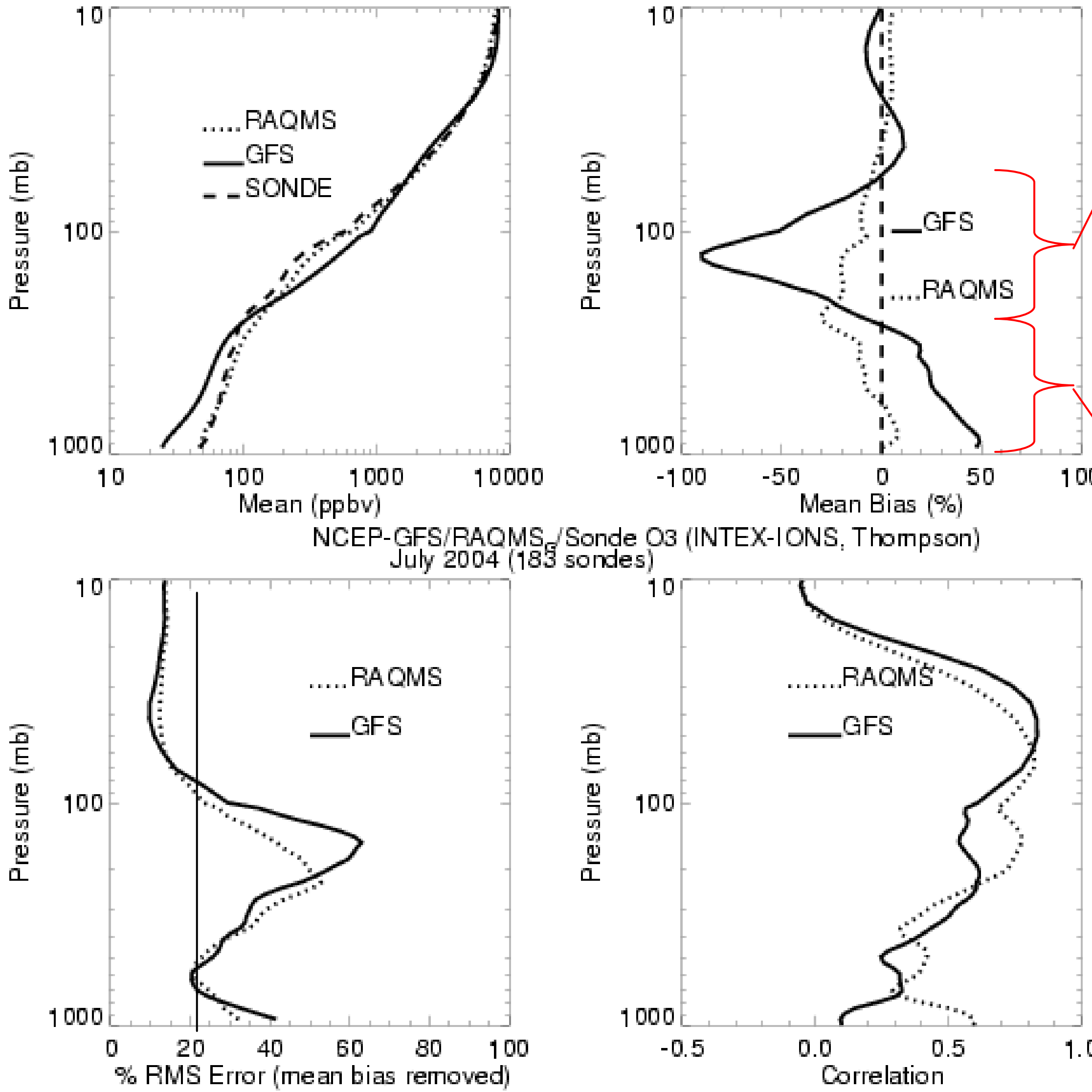


- Symbols indicate the latitude of solar occultation and limb scattering observations.

- Contours indicate the density (% of total at each latitude) of cloud-cleared total column measurements

Reduction in mean biases during period of SAGE III Limb Scattering measurements

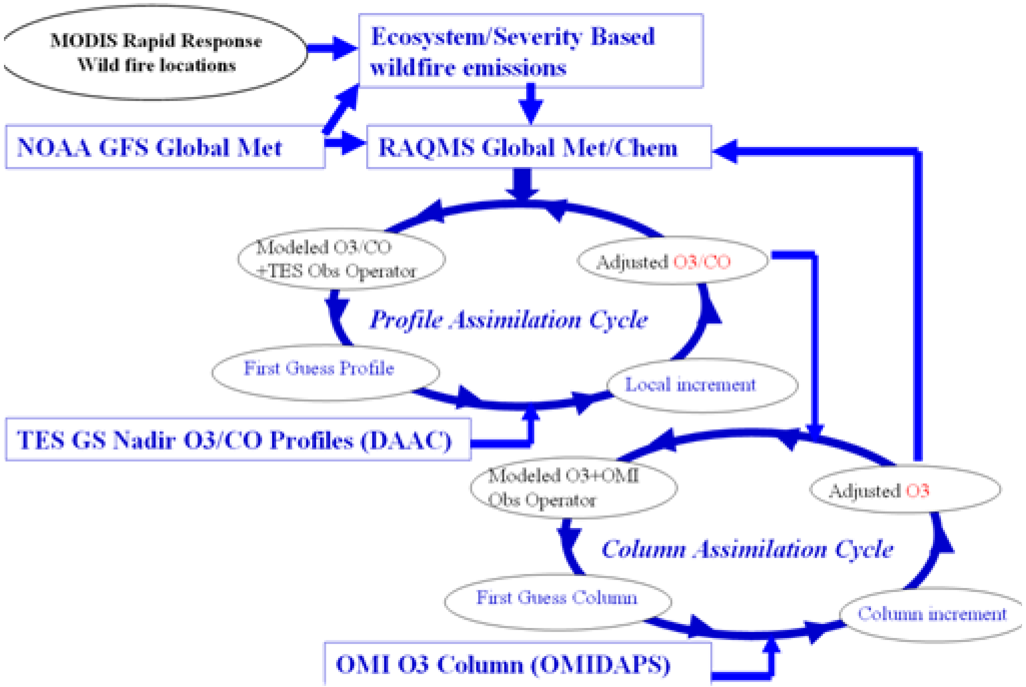
RAQMS (1.4x1.4) and Operational (T256) GDAS vs IONS July 2004



Reductions in the high biases due to assimilation of high vertical resolution solar occultation and limb scattering measurements.

Reductions in mean low biases due to the inclusion of realistic tropospheric ozone photochemistry.

RAQMS$_{global}$ (2x2) 2006 INTEX-B/TEXAQS Assimilation



MODIS Rapid Response Wild fire locations

Ecosystem/Severity Based wildfire emissions

NOAA GFS Global Met

RAQMS Global Met/Chem

Modeled O3/CO +TES Obs Operator

Adjusted O3/CO

Profile Assimilation Cycle

First Guess Profile

Local increment

TES GS Nadir O3/CO Profiles (DAAC)

Modeled O3+OMI Obs Operator

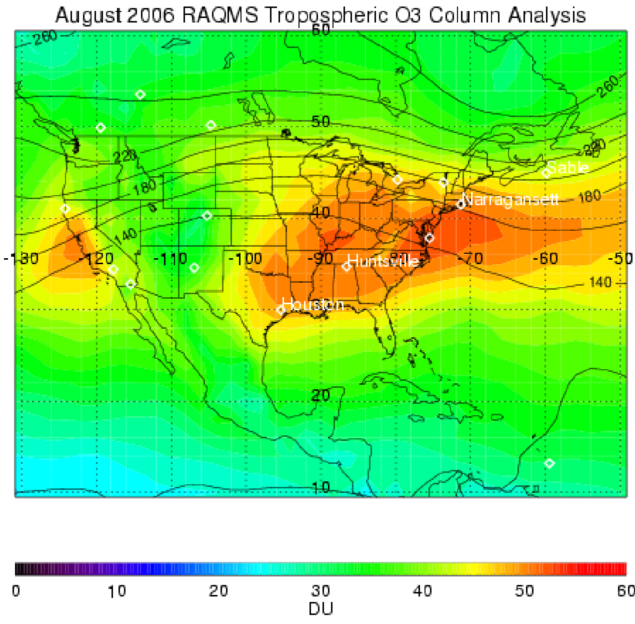
Adjusted O3

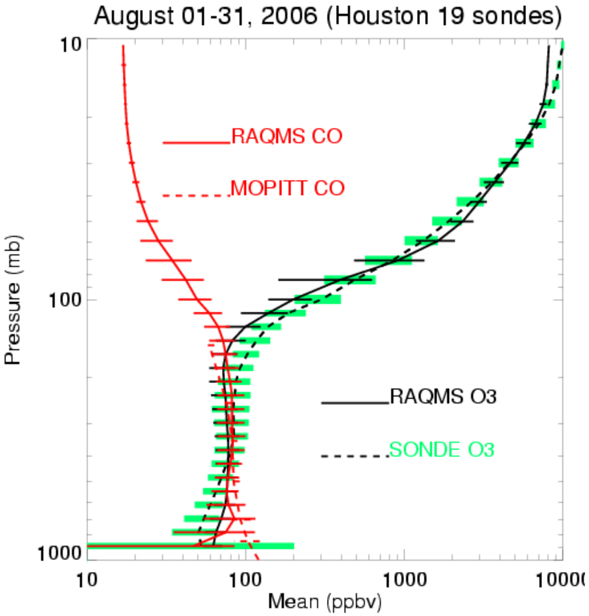
Column Assimilation Cycle

First Guess Column

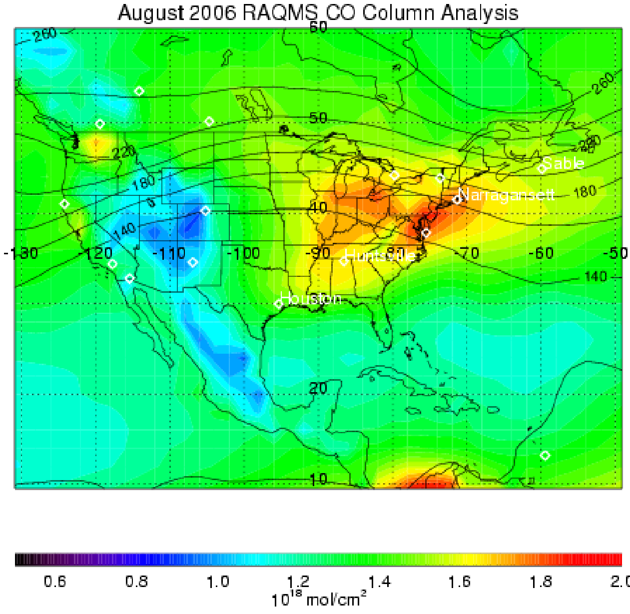
Column increment

OMI O3 Column (OMIDAPS)

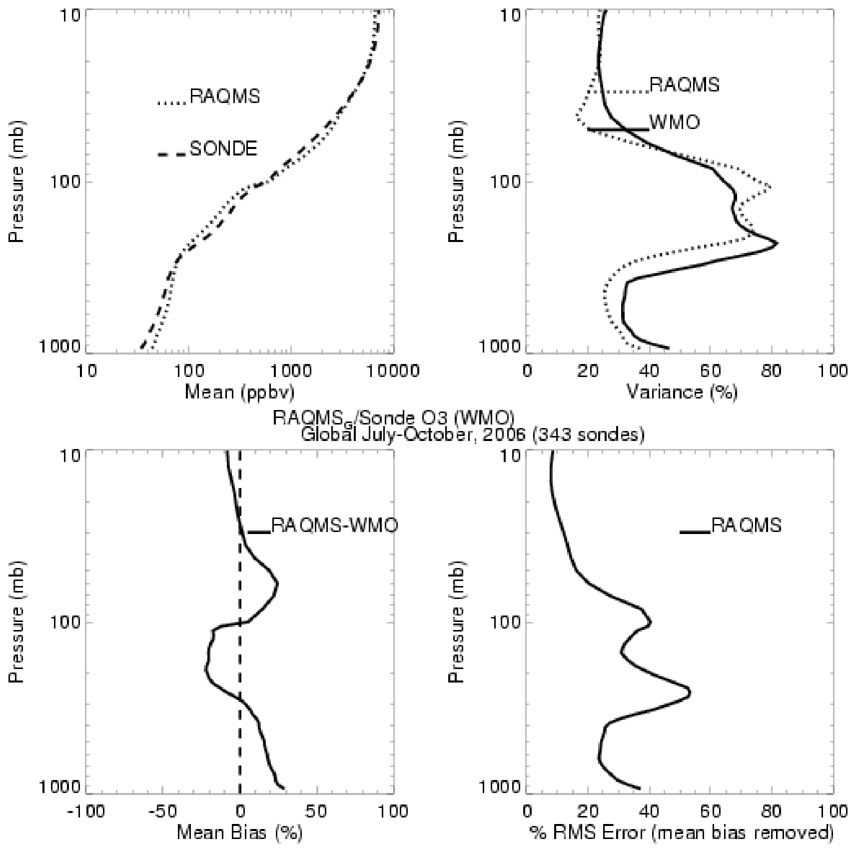


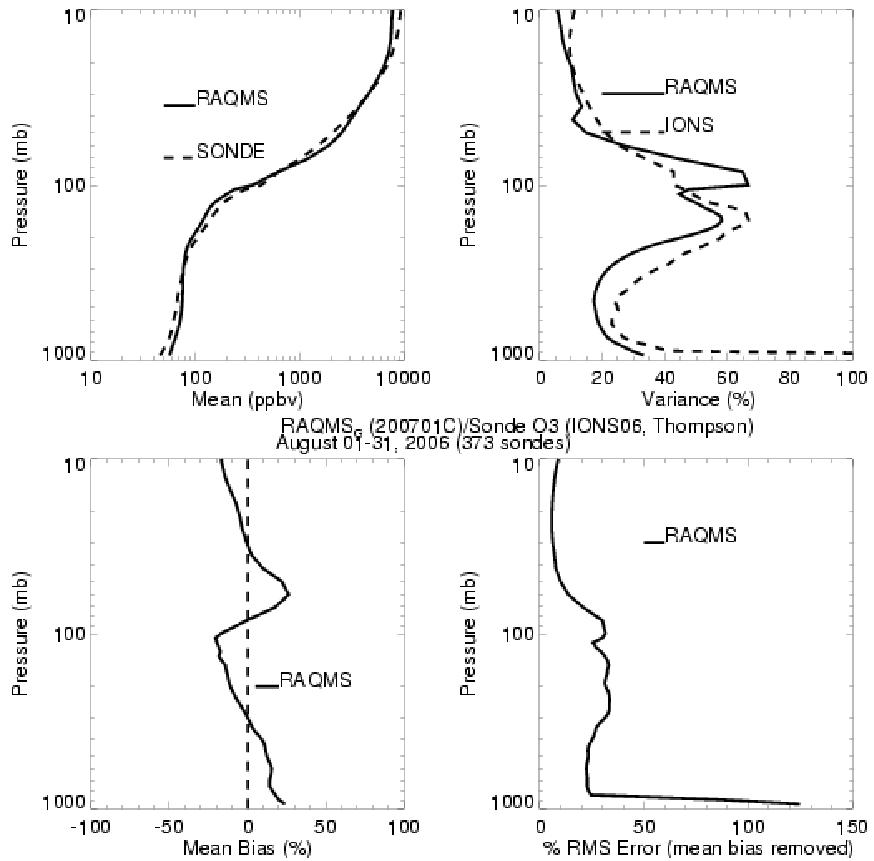


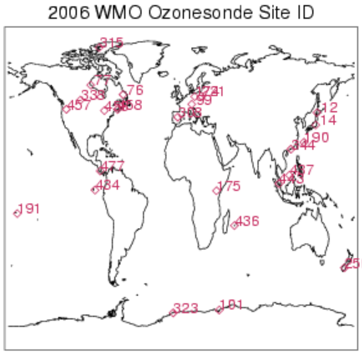
2006 Reanalysis includes OMI Column O3 and TES O3/CO profiles



RAQMS 2006 Reanalysis vs WMO and IONS Ozonesondes 2006


RAQMS$_G$/Sonde O3 (WMO)
Global July-October, 2006 (343 sondes)

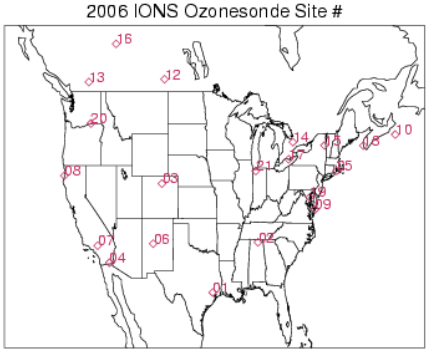

RAQMS$_G$ (200701C)/Sonde O3 (IONS06, Thompson)
August 01-31, 2006 (373 sondes)



ID Name

99= Hohenpeissenberg, Germany
77= Churchill, Canada
76= Goose Bay, Canada
477= Heredia, Costa Rica
458= Yarmouth, N.S.(CAN)
457= Kelowna, Brit Columbia (CAN)
456= Egbert, Ontario (CAN)
443= Sepang Airport, Malaysia
437= Java, Indonesia
436= Reunion Isl., Fr
434= San Christobal, Galapagoes
344= Hong Kong, China
338= Bratts Lake, CAN
323= Neumayer, Antarctica
315= Eureka, Canada
308= Barajas (Madrid), Spain
256= Lauder, New Zealand
221= Legionowo, Poland
191= American Somoa (USA)
190= Naha/Kagamizu, Japan
175= Nairobi, Kenya
174= Lindenberg, Germany
14= Tateno, Japan
12= Sapporo, Japan
101= Syowa, Antarctica (Japan)

20-30% mean Bias
20-50% RMS errors

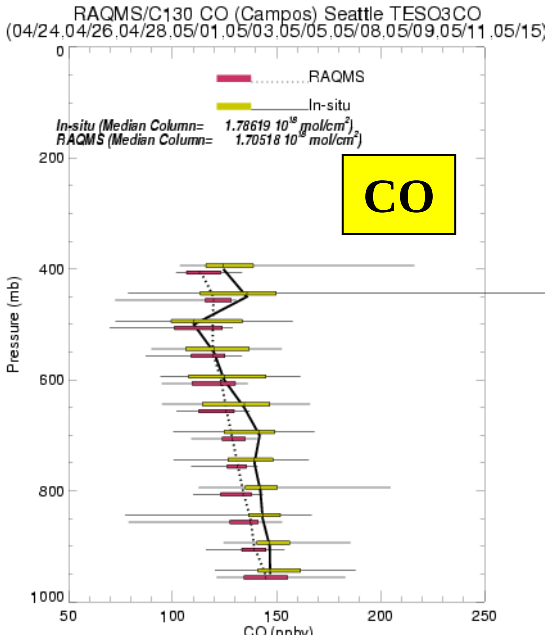


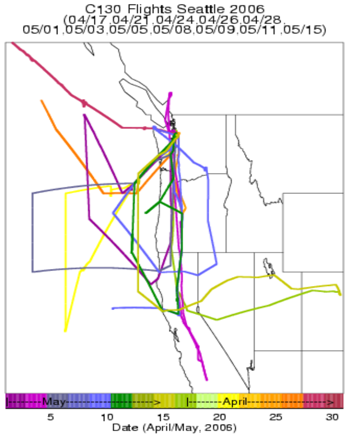
Site # Name

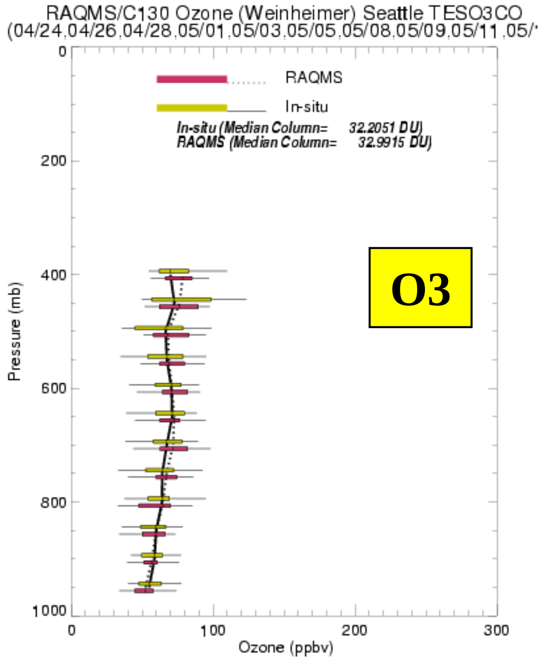
01= Houston, TX
02= Huntsville, AL
03= Boulder, CO
04= Holtville, CA
05= Narragansett, RI
06= Socorro, NM
07= Table Mountain, CA
08= Trinidad Head, CA
09= Wallops Is, VA
10= Sable Is, NS
12= Bratts Lake, SK
13= Kelowna, BC
14= Egbert, ONT
15= Paradox, NY
16= Edmonton, AB
17= Walsingham, ONT
18= Yarmouth, NS
19= Beltsville, MD
20= Richland, WA
21= Valparaiso, IN

RAQMS 2006 Reanalysis vs NSF C130 and NOAA P3 O3/CO

NSF C130: Seattle, Apr-May 2006

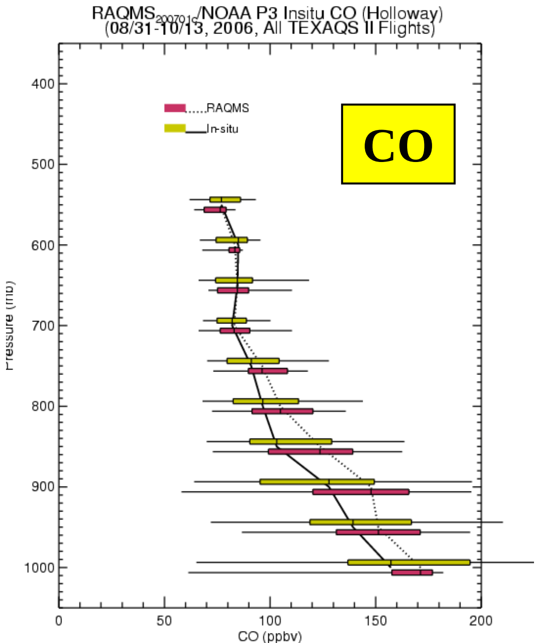


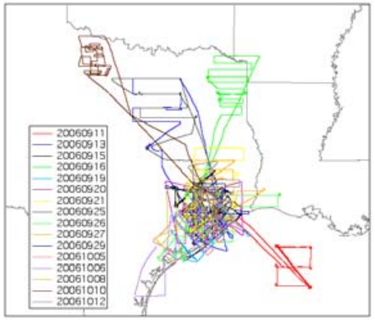


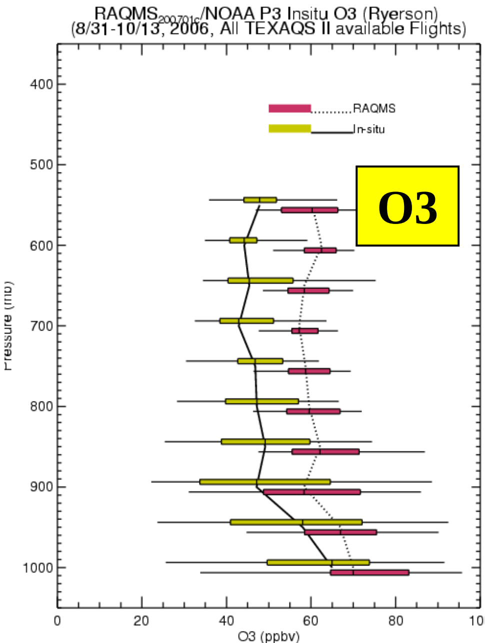


Spring trans-pacific transport

NOAA P3: Houston, Sep-Oct 2006





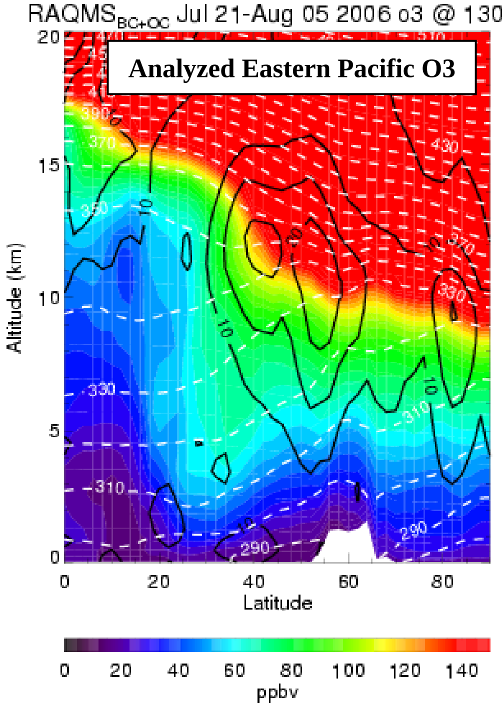


Summer urban air quality

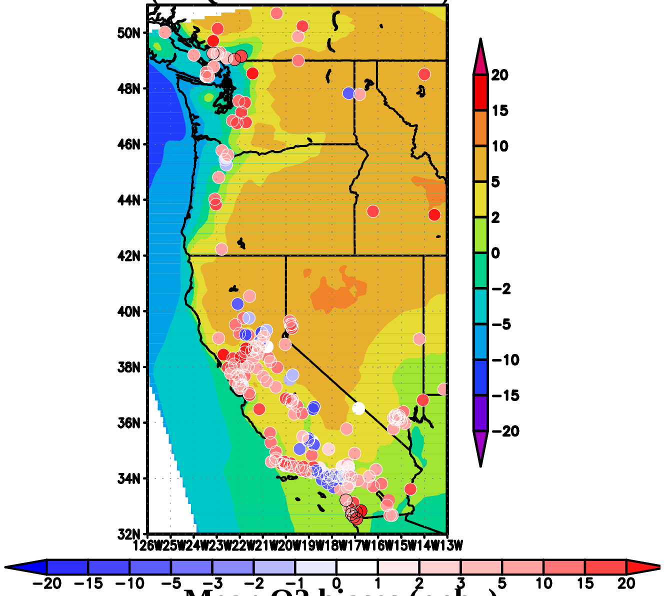
Impact of Global BC on regional AQ Prediction

Assessment using pre-operational NOAA/NWS NAM-CMAQ 12km forecast[1]

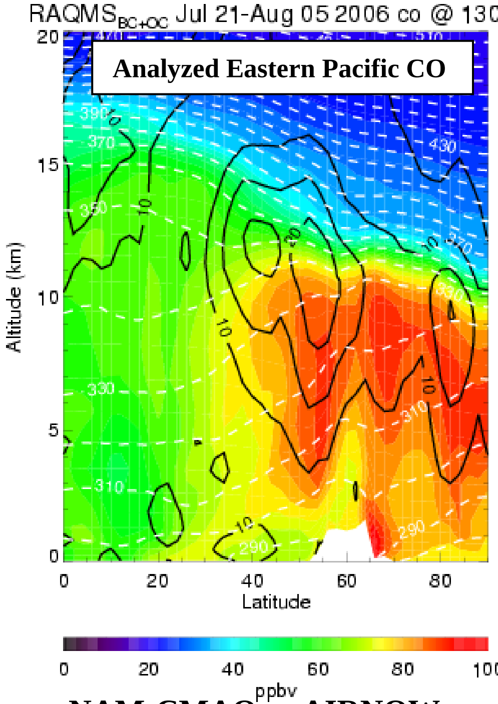
(July 21-August 5, 2006)



Mean O_3 Difference (ppbv)
(RAQMS-BC – Fixed-BC)



Mean O3 biases (ppbv)



NAM-CMAQ vs AIRNOW

	West of -115°W
Static BC	S=0.804 R=0.691 MB=4.7 ppbv
RAQMS BC	S=0.914 R=0.703 MB=7.1 ppbv
MOZART BC	S=0.872 R=0.730 MB=2.2 ppbv
GFS BC (above 10km)	S=0.820 R=0.697 MB=4.8 ppbv

- RAQMS lateral Boundary Conditions (BC) show enhanced O3 and CO between the Sub-tropical and Polar Jets

- RAQMS lateral Boundary Conditions lead to 10-15 ppbv reductions in off-shore surface ozone and 5-10 ppbv increases in surface ozone over mountain regions of the western US.

- Comparison with EPA AIRNow surface ozone west of -115°W shows RAQMS results in improved slope and correlations but increased positive bias.

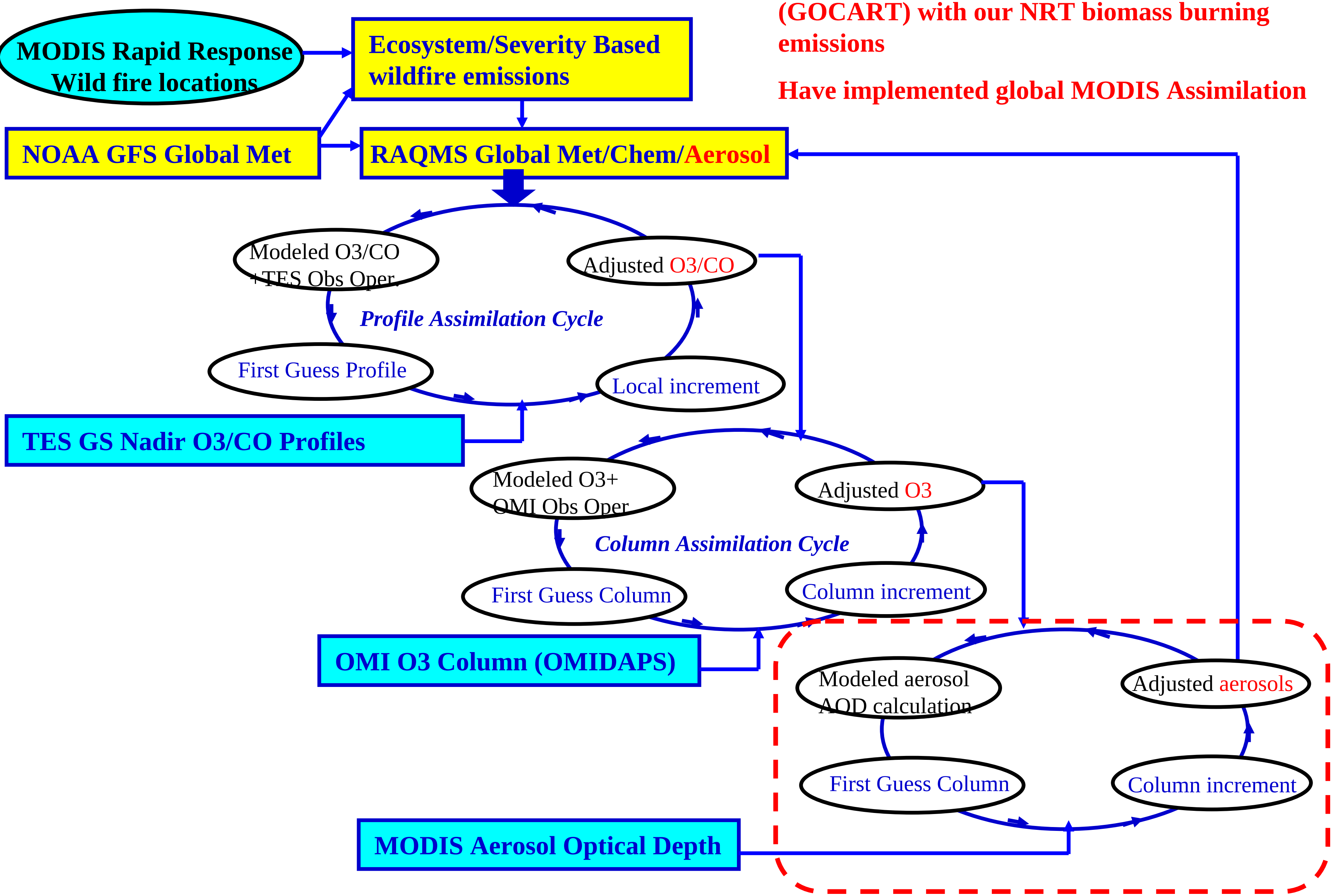
---

[1] **Tang, Y., et al., (2007) The Impact of Lateral Boundary Conditions on CMAQ Predictions over the Continental US: a Sensitivity Study Compared to Ozonsonde Data, extended abstract submitted to the 6th Annual CMAS Conference, UNC-Chapel Hill, NC**

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

Have implemented Carbonaceous Aerosol (GOCART) with our NRT biomass burning emissions

Have implemented global MODIS Assimilation



MODIS Rapid Response Wild fire locations

Ecosystem/Severity Based wildfire emissions

NOAA GFS Global Met

RAQMS Global Met/Chem/Aerosol

Modeled O3/CO +TES Obs Oper.

Adjusted O3/CO

Profile Assimilation Cycle

First Guess Profile

Local increment

TES GS Nadir O3/CO Profiles

Modeled O3+ OMI Obs Oper

Adjusted O3

Column Assimilation Cycle

First Guess Column

Column increment

OMI O3 Column (OMIDAPS)

Modeled aerosol AOD calculation

Adjusted aerosols

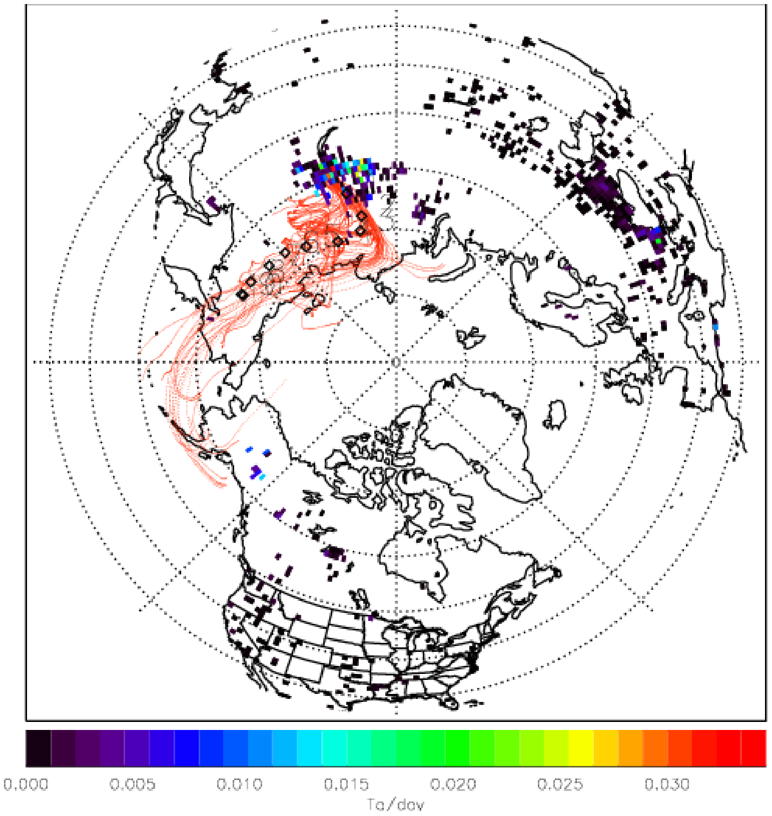
First Guess Column

Column increment

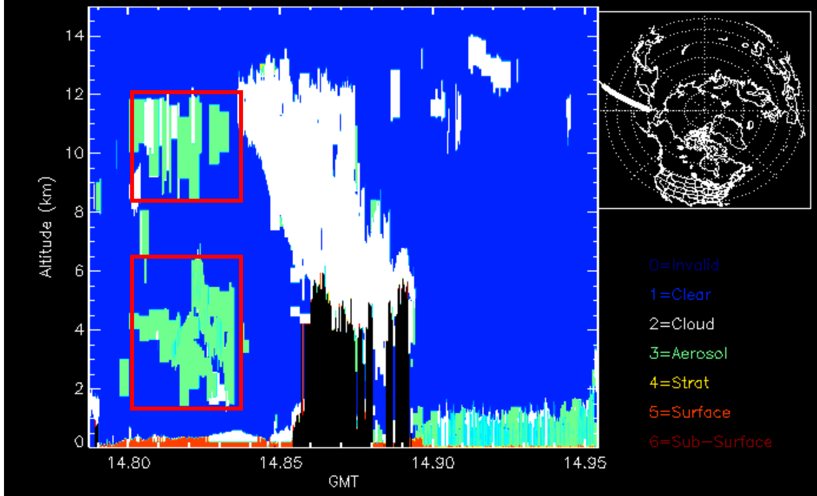
MODIS Aerosol Optical Depth

Long-range transport of Siberian Wild Fire emissions

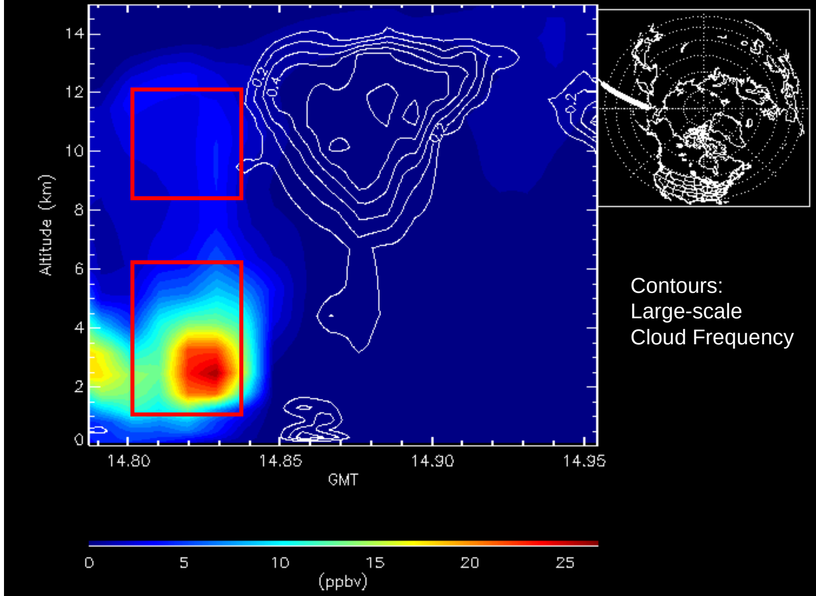
July 24, 2006 Wild fire emissions
10-day forward trajectories



July 31, 2006 CALIPSO Feature Mask



July 31, 2006 RAQMS BC+OC Analysis



Contours:
Large-scale
Cloud Frequency

RAQMS Reduced (strat/trop) chemistry

A “reduced” stratosphere/troposphere chemistry module is being developed to provide a capability of operational global AQ prediction.

- Transport of only 12 tracers (memory requirements)

- 30min time-steps (cpu requirements)

- Explicit stratospheric chemistry (limb+nadir assimilation)

- Neglects NMHC chemistry (no NOx via PAN decomposition)

- Initiated under NASA Applied Sciences Program

- Seeking JCSDA funding

RAQMS Reduced (strat/trop) chemistry

(12 species/families explicitly transported, PCE assumptions for “fast” species)

1) Ox
2) NOy
3) HNO3
4) N2O5
5) H2O2
6) HNO4
7) H2O
8) NO3
9) NO2
10) CH2O
11) CH3OOH
12) CO
13) CH4
14) ClONO2
15) N2O

Ox-HOx-NOx+CH4+CO oxidation

NOy partitioning relies on climatological ClNO3*

Stratospheric Bromine and Chlorine Ozone P-L from model* climatology

Chemical families

Ox=O(1D)+O(3P)+O3+NO2+HNO3+2(NO3)+3(N2O5)+HNO4
NOy=N+NO+NO2+NO3+2(N2O5)+HNO3+HNO4+ClNO3

Transported Species:

Ox, NOy, HNO3, N2O5, HNO4, H2O, NO3, NO2, CO, H2O2, CH2O, CH3OOH

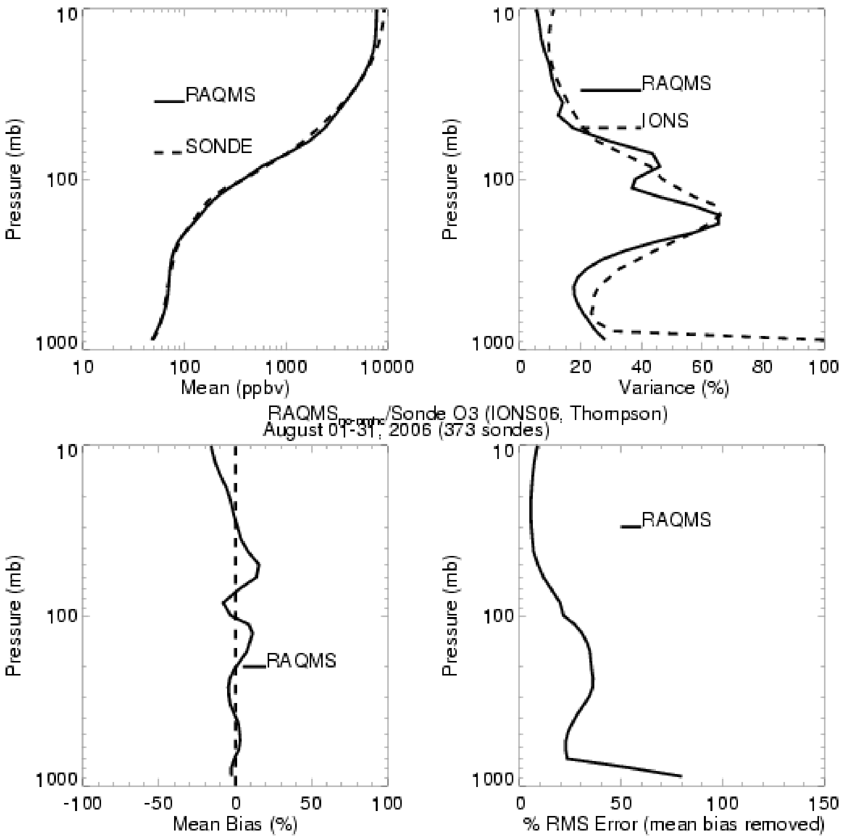
Climatological Species:

ClONO2, N2O, CH4

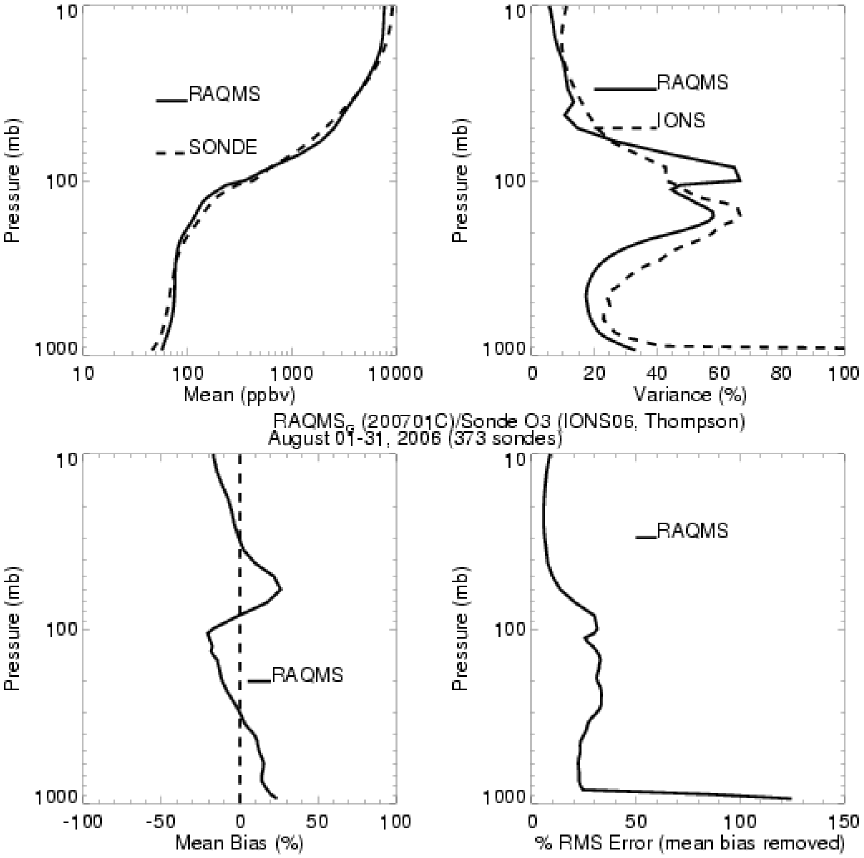
***LaRC IMPACT coupled chemistry/dynamics model (Al-Saadi et al., 2004, Pierce et al., 2000)**

August 2006 test of reduced chemistry: impact of NMHC

NO NMHC



With NMHC



Comparison between RAQMS chemical mechanism and the NASA Global Modeling Initiative (GMI) tropospheric chemistry (based on GEOS-CHEM) shows strong sensitivity in tropospheric ozone production to treatment of isoprene oxidation (RAQMS isoprene nitrates oxidized to NOx vs converted to HNO3 and rapidly scavenged) [David Considine, NASA/LaRC].

Closing Thoughts

- Global chemical model is appropriate framework for incorporation of satellite composition measurements into AQ forecasting system

- Coupling to NWP/Climate requires computationally efficient (CPU/Memory) online, unified trop/strat chemical mechanism

- “One atmosphere” coupled aerosol/chemistry/dynamics needed to model global air quality (long-range transport, episodic severe events such as wild-fires) and climate change

- Online approach simplifies ESMF coupler issues (1D “physics” not 3D “transport” coupler)

- Need to align EMC and JCSDA global AQ model development with OAR research activities