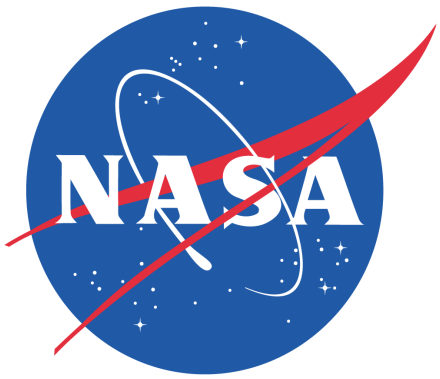
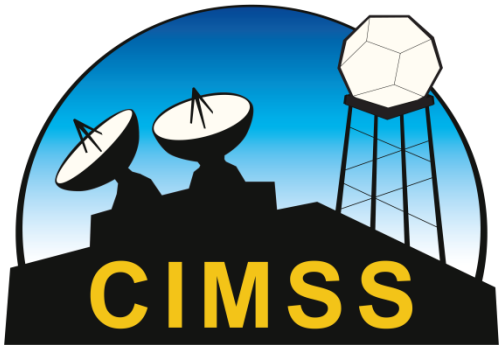
# Chemical Reanalysis in support of Air Quality Applications


**R. Bradley Pierce (NOAA/NESDIS), Allen Lenzen, Todd Schaack, Nadia Smith, Elisabeth Weisz, Bill Smith, James Davies, Kathy Strabala, Rebecca Cintineo, Marek Rogal, and Andrew Wentland (UW-Madison, CIMSS/AOS)**

***Data provided by: Ryan Spackman (NOAA/ESRL), Anne Thompson, (PSU/GFSC), the Aura Science Team, and JPSS CSPP***

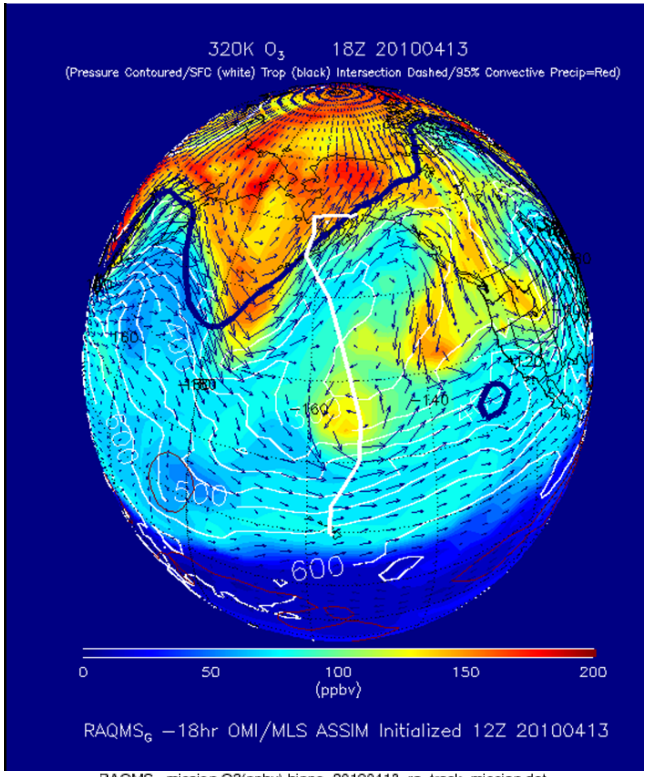



# New activity funded by the NASA ROSES-2013 call for an Applied Science representative on the Aura Science Team

## Focus

- **Provide the air quality community with a multi-year global chemical and aerosol reanalysis using NASA Aura and A-Train measurements.**
- Conduct regional chemical data assimilation experiments to quantify the influences in changes in NOx emissions on US air quality during the Aura period.
- Collaborate with International, Federal, State and Local air quality management communities in the utilization of the Aura and A-Train measurements and reanalysis for air quality assessment activities.

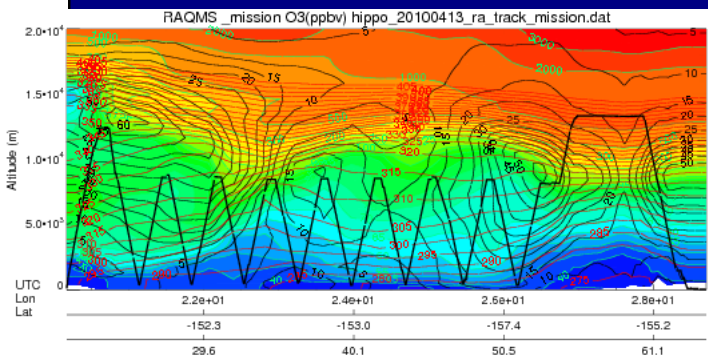

1. **Online global chemical and aerosol assimilation/ forecasting system**

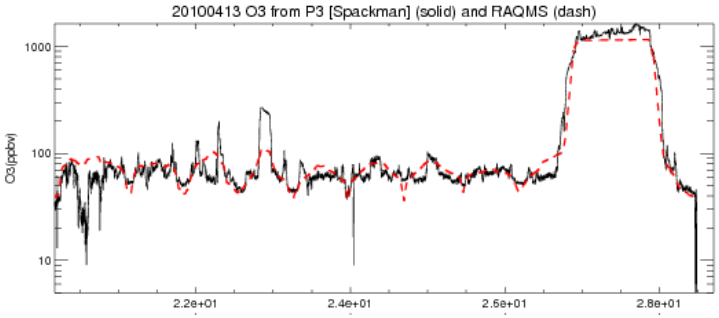
2. **UW-Madison sigma-theta hybrid coordinate model (UW-Hybrid) dynamical core**

3. **Unified stratosphere/troposphere chemical prediction scheme (LaRC-Combo) developed at NASA LaRC**

4. **Aerosol prediction scheme (GOCART) developed by Mian Chin (NASA GSFC).**

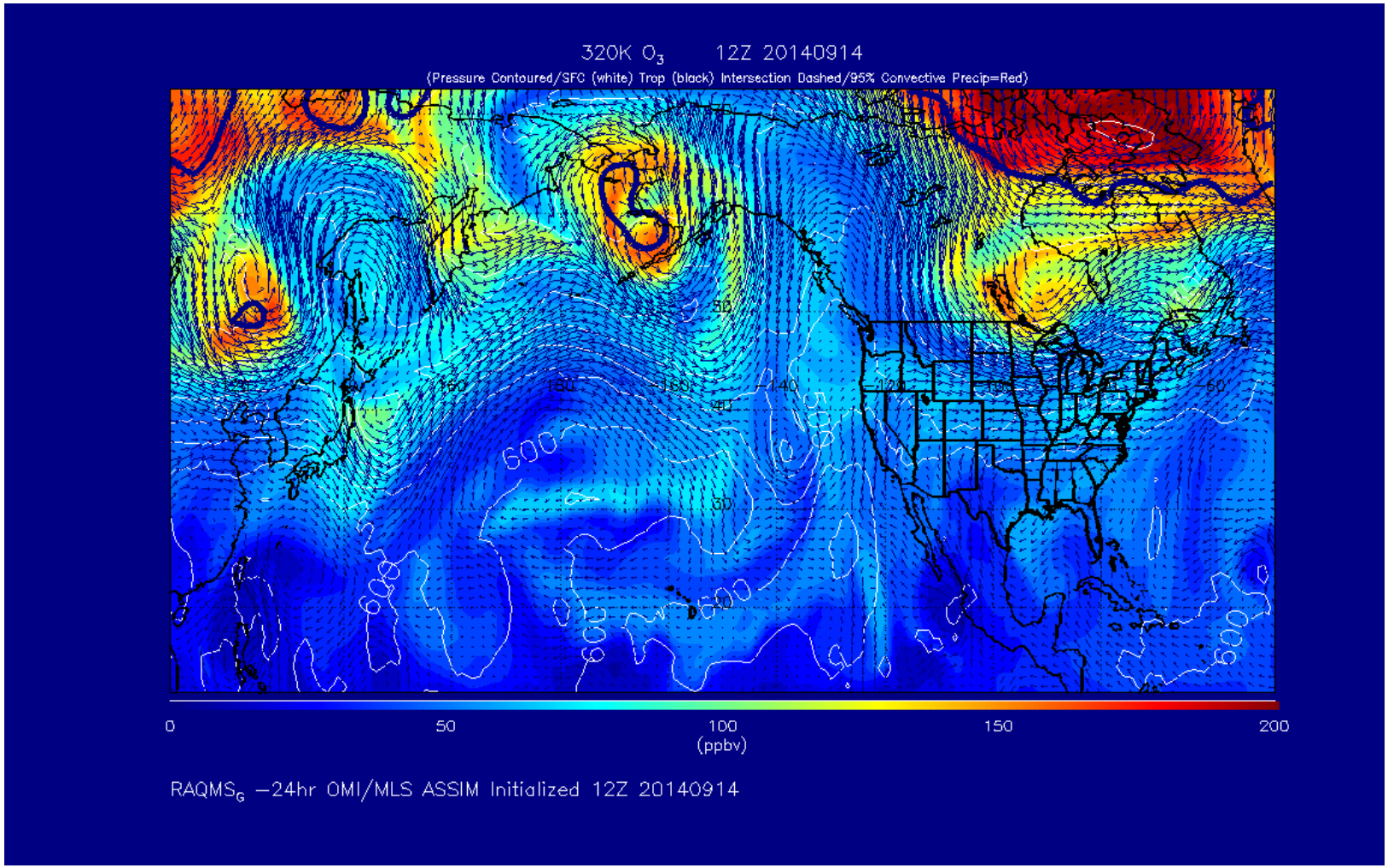
5. **Statistical Digital Filter (OI) assimilation system developed by James Stobie (NASA/GFSC)**



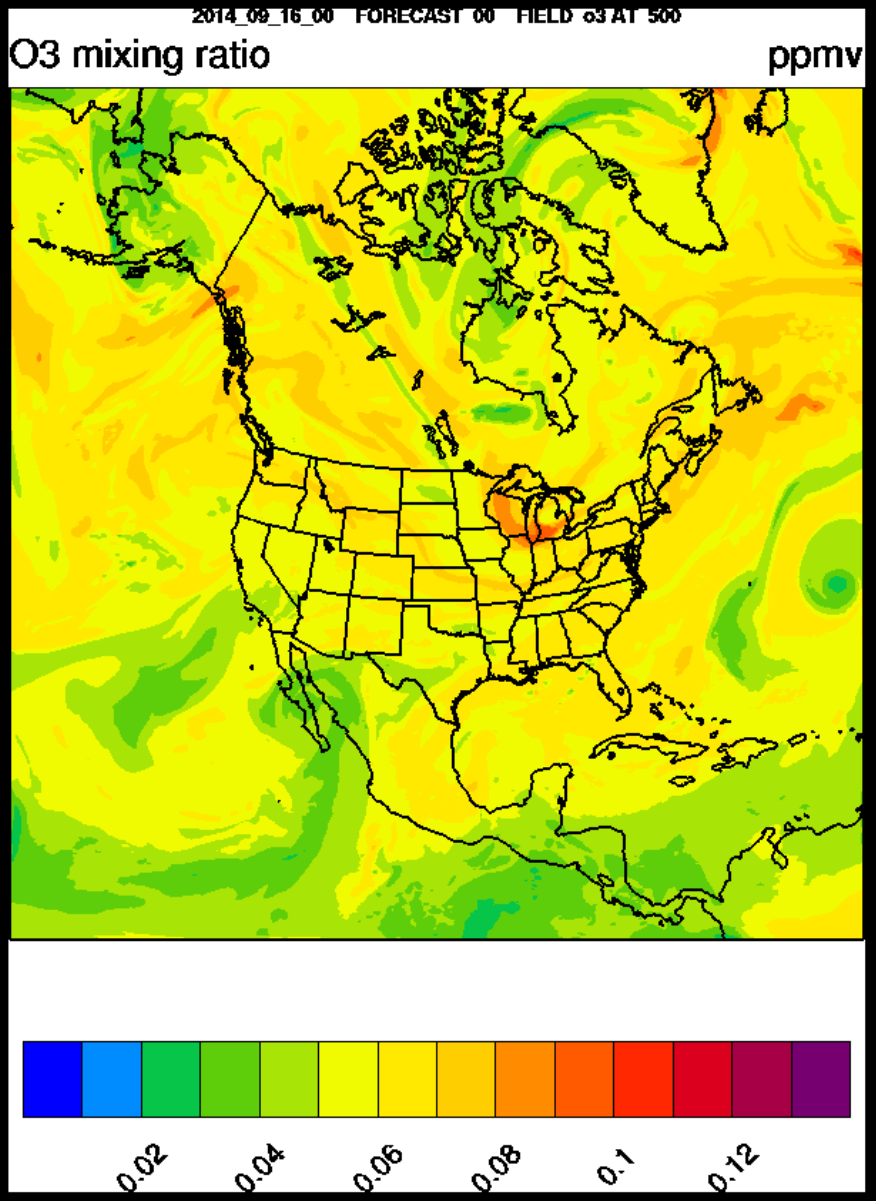

**HIPPO March-April 2010, Mission scientist: Steve Wofsy (Harvard), O3 PI: Ryan Spackman (NOAA/ESRL)**

# Current real-time RAQMS/Rapid Refresh with Chemistry (RR-Chem) air quality forecasts




**In collaboration with Georg Grell and Steven Peckham (NOAA/ESRL/GSD)**

RAQMS/RR-Chem
500mb O3 Forecast
00Z September 16 –
00Z September 18, 2014




**http://ruc.noaa.gov/wrf/WG11_RT/**


***The RAQMS real-time assimilation/forecast system has been running continuously since January 2012 (N Amer: http://raqms-ops.ssec.wisc.edu/, CONUS: http://raqms.ssec.wisc.edu/)***

# Chemical Reanalysis assimilation configuration:

**NOAA Grid-point Statistical Interpolation (GSI) 3D variational analysis of:**

- **Aura Microwave Limb Sounder (MLS)**
  - **O3, H2O, HCL, HNO3, N2O, and CO (?) profiles**
- **Aura Ozone Monitoring Instrument (OMI)** → **Transition to OMPS**
  - **Total Column (profile ?) O3, NO2, and HCHO (?)**
- **Aura Tropospheric Emission Spectrometer (TES)**
  - **O3, CO, CH4, and N2O**
- **Aqua Atmospheric Infrared Sounder (AIRS)**
  - **O3, CO, CH4, and N2O**

**Transition to CrIS**

Need to evaluate impact of reduction in TES Global Survey sampling

- **Terra/Aqua Moderate Resolution Imaging Spectroradiometer (MODIS)** → **Transition to VIIRS**
  - **Aerosol Optical Depth (AOD), fire detection**

# RAQMS TES and OMI+TES 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)

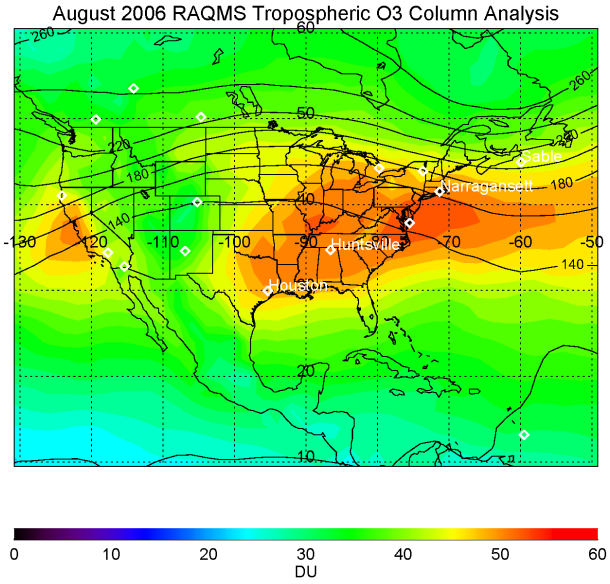
Meteorological Analysis: GFS/GSI

Chemical Analysis:

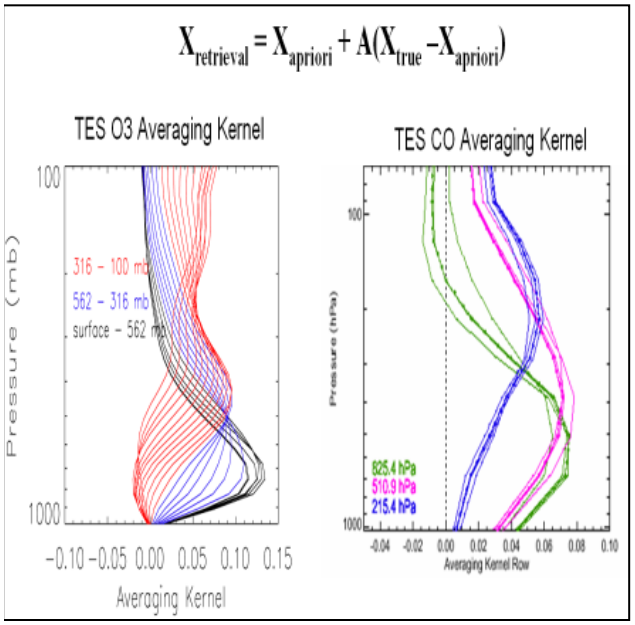
- Optimal Interpolation (IO) univariate (Pierce et al., 2007)
- unified online troposphere/stratospheric chemistry for first guess

Procedure:
Compare RAQMS analyses with ozonesonde

1) No Assimilation
2) TES (O3&CO) only
3) TES (O3&CO)+OMI (Cloud Cleared)



# RAQMS OMI/TES Reanalysis O3/CO Assimilation Procedure




NOAA GFS Global Met → RAQMS Global Met/Chem

Modeled O3/CO+ TES Obs Operator

Adjusted O3/CO

***TES***

***Profile Assimilation Cycle***

First Guess Profile

Local increment

Modeled O3+ OMI Obs Operator

Adjusted O3

***OMI***

***Column Assimilation Cycle***

First Guess Column

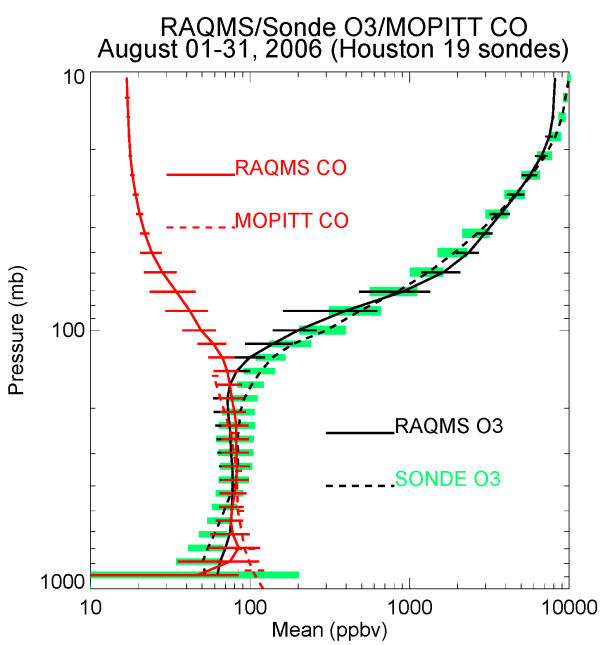
Column increment

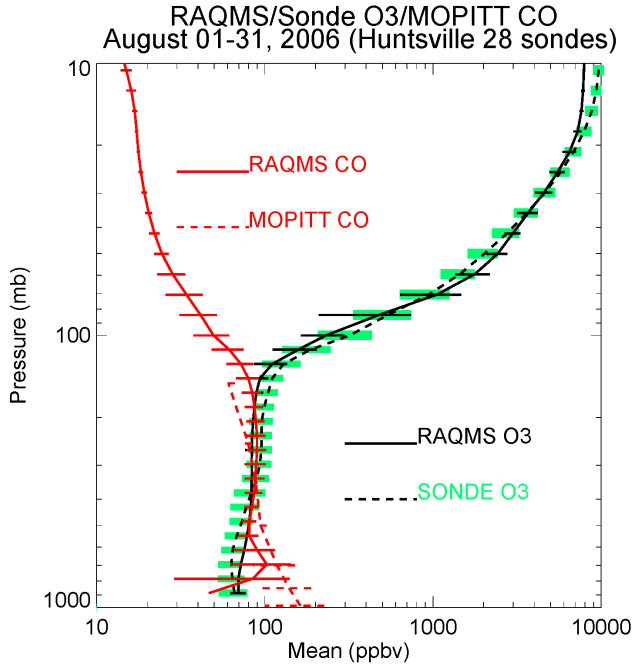
**Pierce, R. B., et al. (2007) Chemical data assimilation estimates of continental US ozone and nitrogen budgets during the Intercontinental Chemical Transport Experiment-North America. J. Geophys. Res. doi:10.1029/2006JD007722**

**Table 1.** Results of OSE Studies of the Impact of TES and Combined TES+OMI Ozone Assimilation on the RAQMS Chemical Analysis[a]

| | No Assimilation | TES Assimilation | TES+OMI Assimilation |
|---|---|---|---|
| Column bias (%) | −8.47 | −3.46 | +0.30 |
| Stratospheric bias (%) | −12.87 | −12.17 | +0.06 |
| Middle stratosphere bias (%) | −17.63 | −17.60 | −5.18 |
| Lower stratosphere bias (%) | −4.31 | −2.40 | +9.51 |
| Tropospheric bias (%) | −5.05 | +3.32 | +0.49 |
| Upper troposphere bias (%) | −3.65 | +2.21 | −11.31 |
| Lower troposphere bias (%) | −6.44 | +4.42 | +12.29 |

[a]Biases are determined with respect to August 2006 IONS ozonesonde data. [*Thompson et al.*, 2007, 2008], consisting of more than 370 profiles during TexAQS-II. The accuracy of the sondes in the troposphere is ~5–7% [*Smit et al.*, 2007].




**Pierce, R. B., et al., 2009 Impacts of background ozone production on Houston and Dallas, TX Air Quality during the TexAQS field mission, J. Geophys. Res., 114, D00F09, doi:10.1029/2008JD011337**

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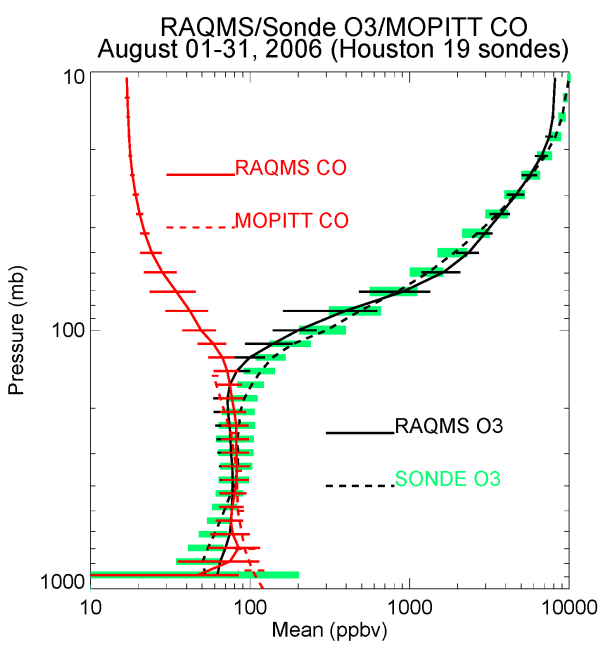


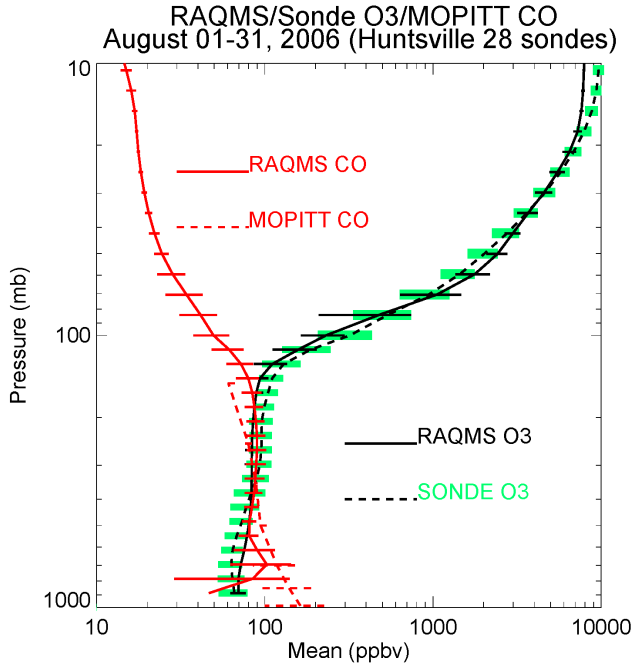


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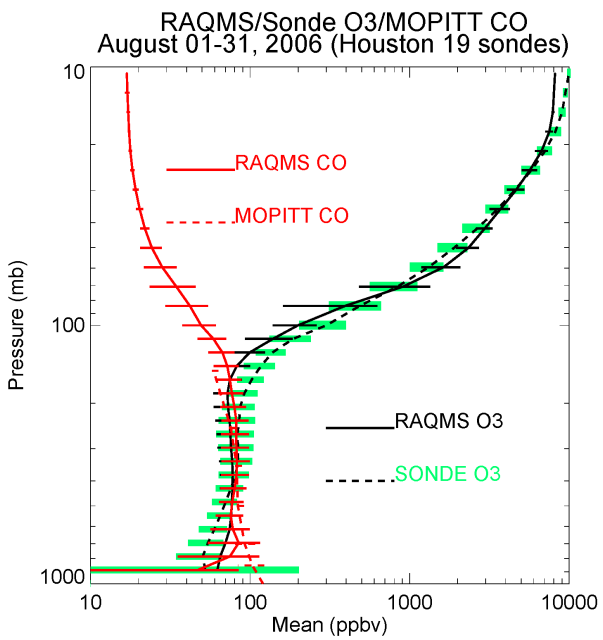


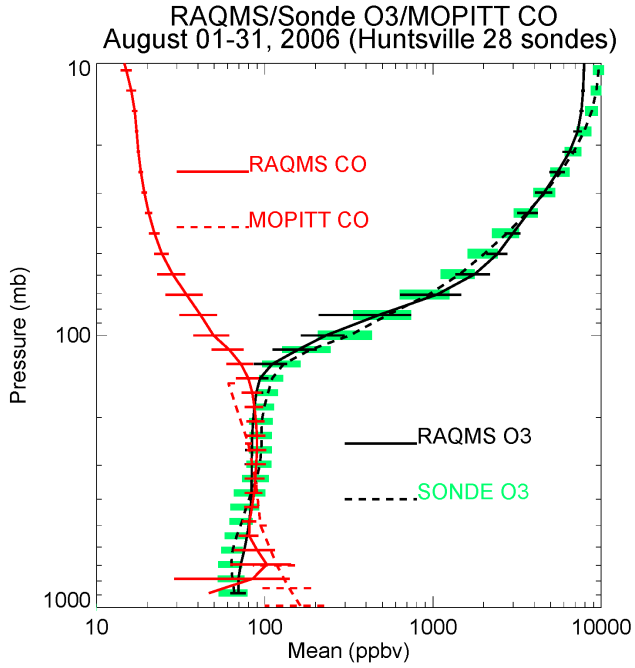


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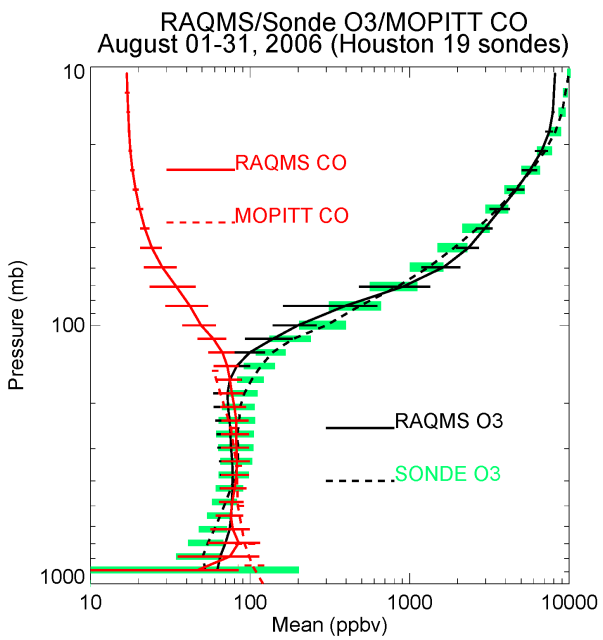


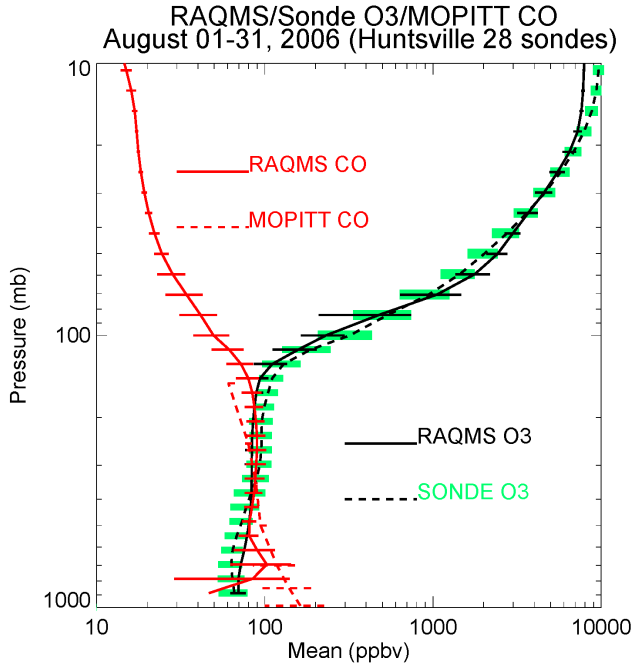


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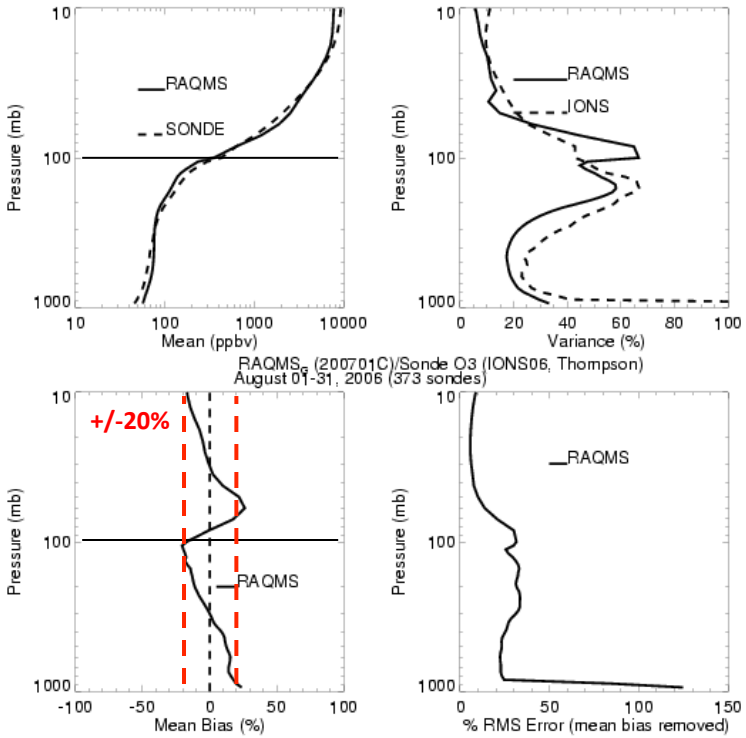
# Comparison of RAQMS OMI+TES reanalysis with ozonesondes during TEXAQS (373 sondes, August, 2006)




**RAQMS TES/OMI Data denial Studies**

| Bias (%) | No Assimilation | TES Assimilation | TES+OMI Assimilation |
|---|---|---|---|
| **Column** | **- 8.47** | **- 3.46** | **+ 0.30** |
| **Stratospheric** | **-12.87** | **- 12.17** | **+ 0.06** |
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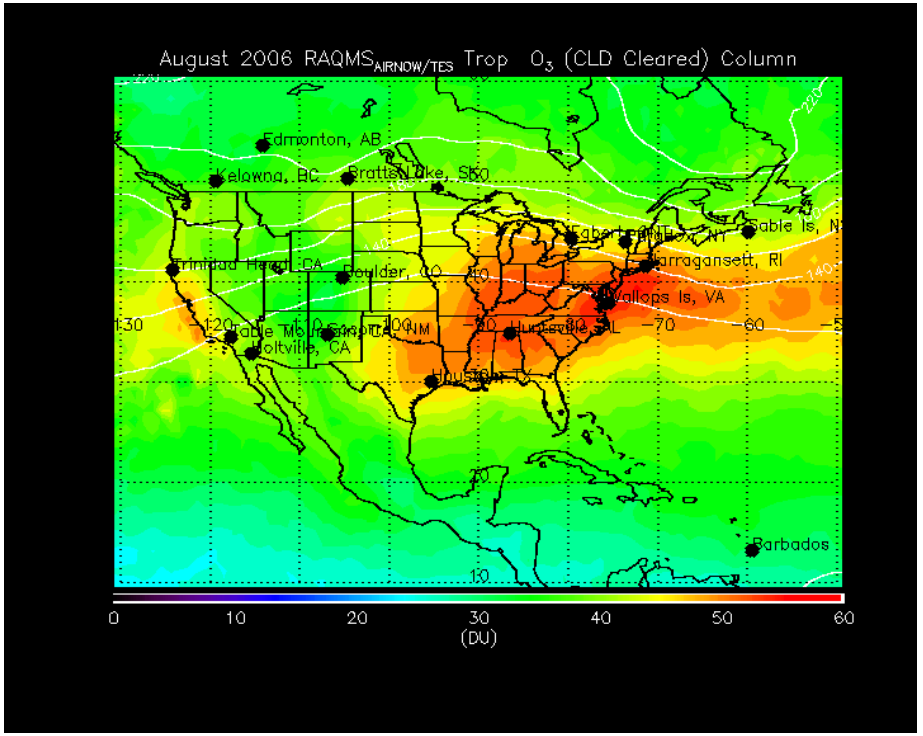
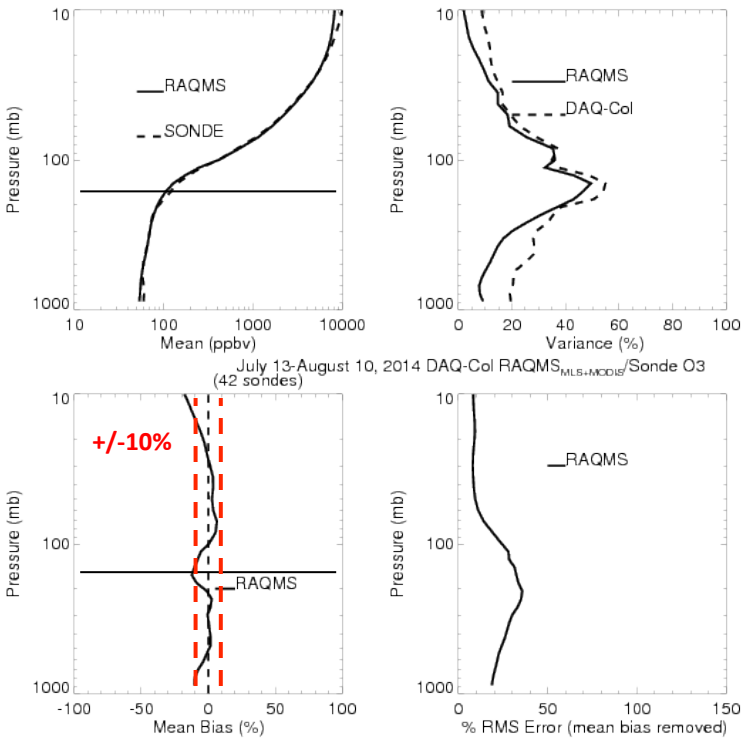
**PI: ANNE M. THOMPSON GSFC**

**RAQMS OMI+TES Tropospheric Ozone Column (August 01-31, 2006)**

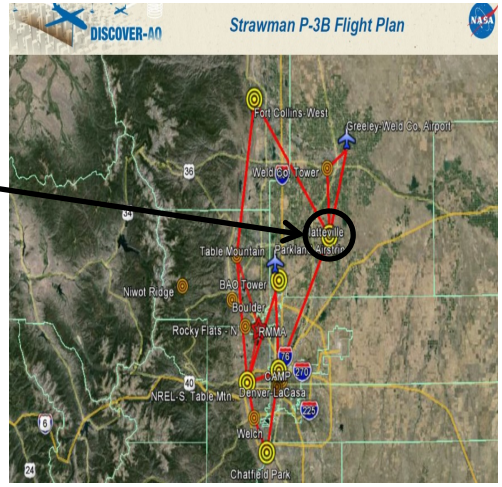



**Pierce, R. B., et al. (2009), Impacts of background ozone production on Houston and Dallas, Texas, air quality during the Second Texas Air Quality Study field mission, J. Geophys. Res., 114, D00F09, doi:10.1029/2008JD011337.**

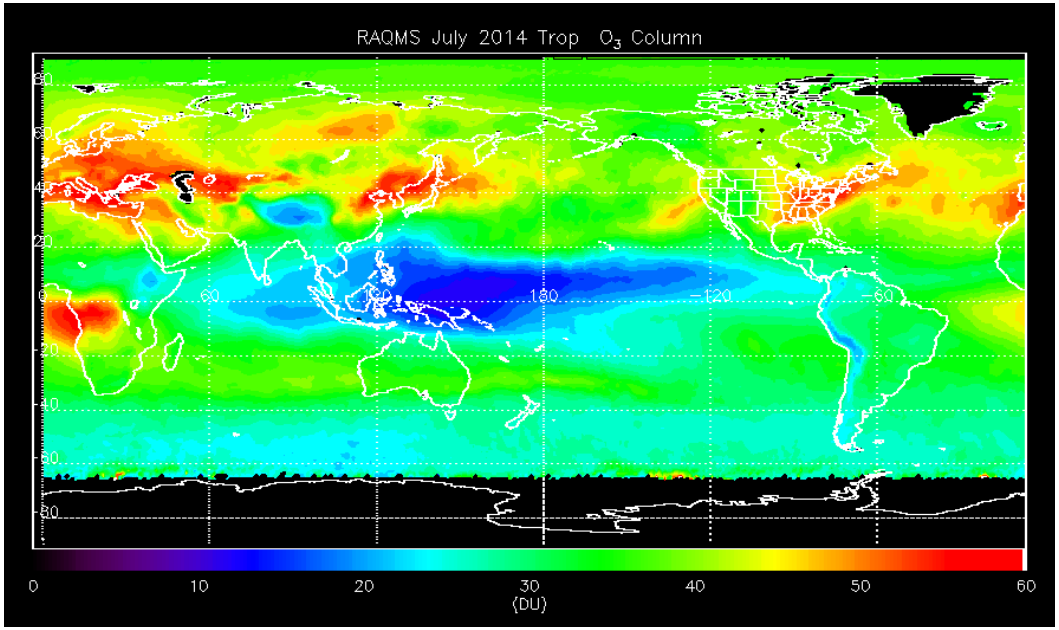
# Comparison of RAQMS NRT OMI+MLS analysis with ozonesondes during FRAPPE/DISCOVER-AQ (42 sondes, July-August, 2014)




**Platteville ground site**



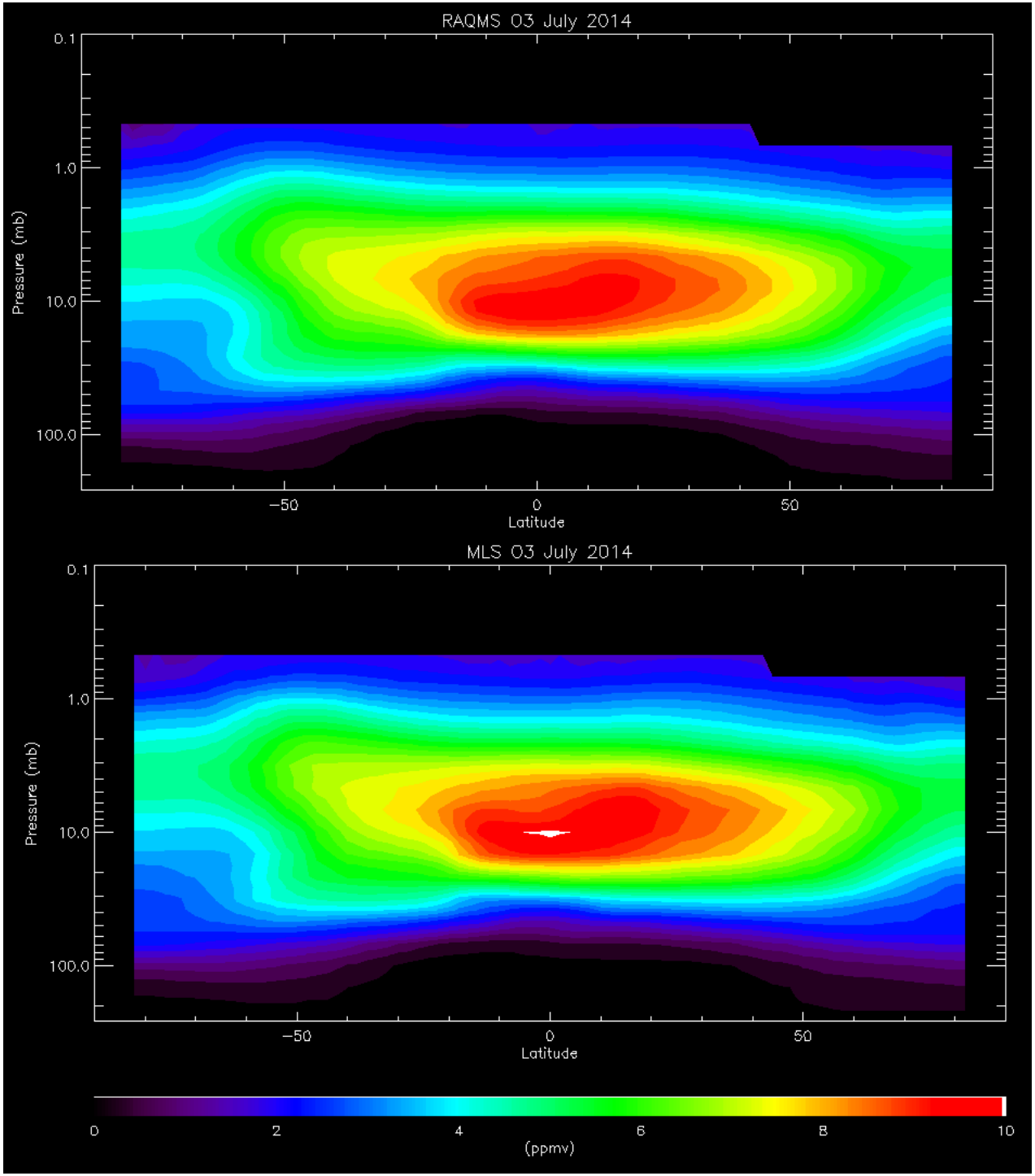

**RAQMS analyzed tropospheric ozone column (July 2014, OMI sampling)**




**PI:ANNE M. THOMPSON GSFC**

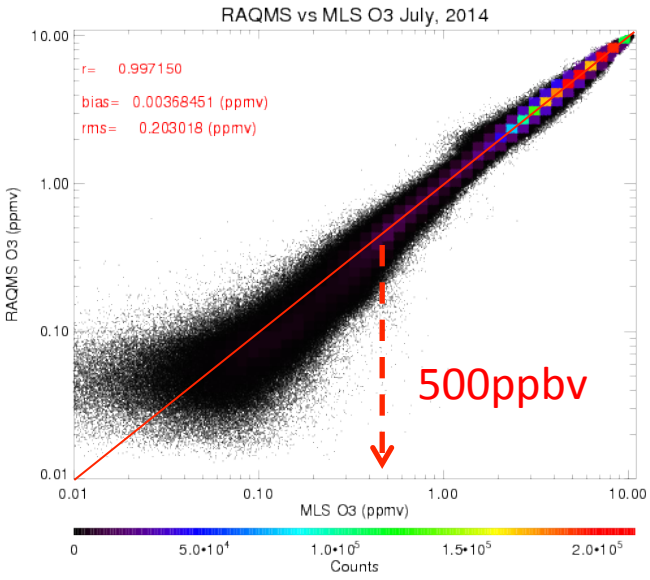
Assimilation of MLS+OMI O3 retrievals results in good agreement (within 10%) with Platteville ozonesondes during FRAPPE/DISCOVER-AQ

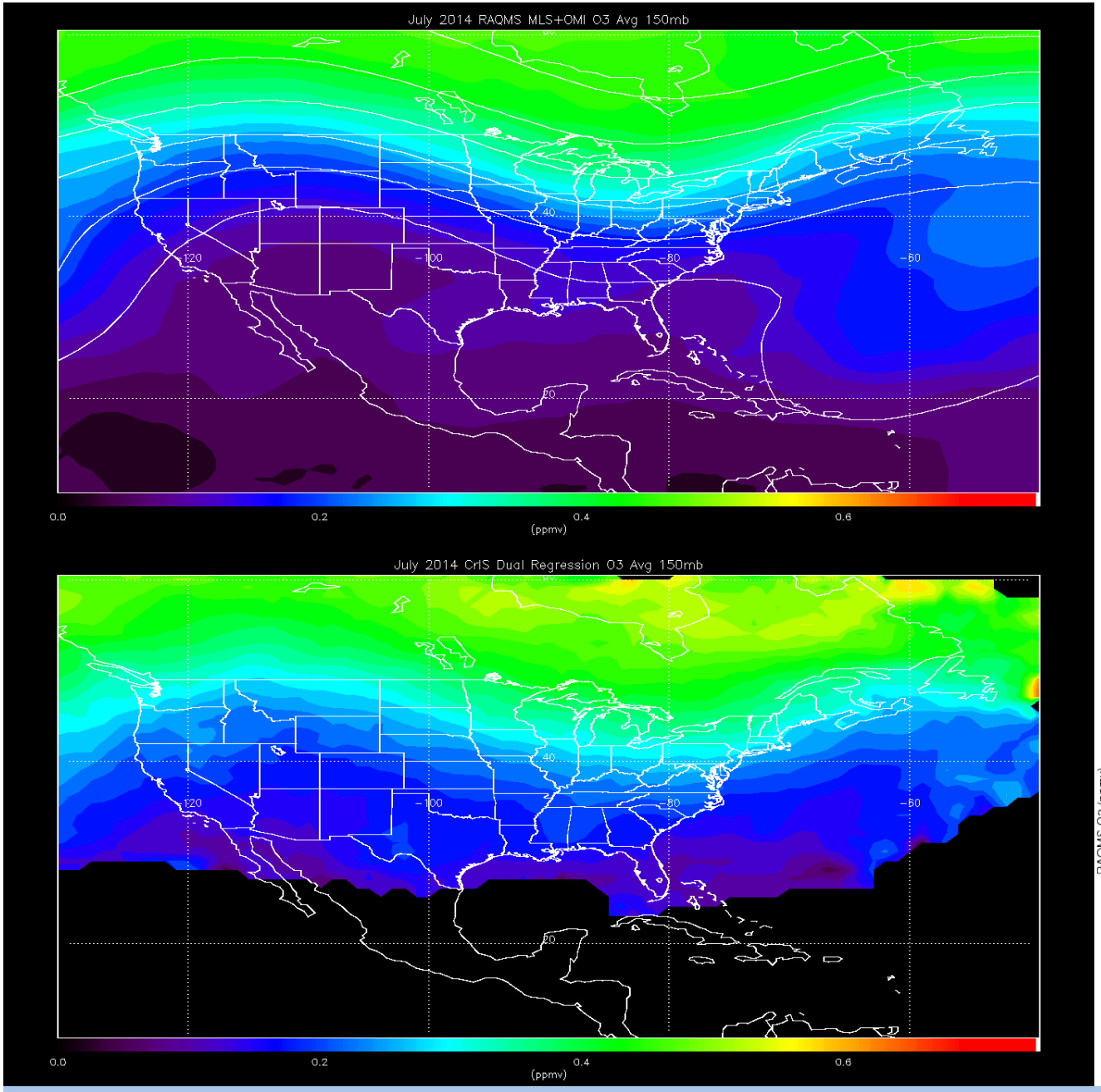
# Comparison of RAQMS with MLS Global O3 July 2014




Currently only assimilating NRT MLS O3 above 50mb

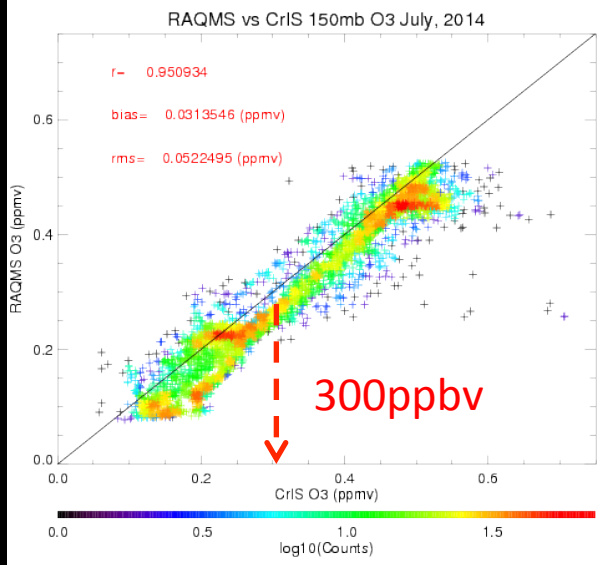
Need to determine minimum MLS O3 mixing ratio for reanalysis






# Comparison of RAQMS 150mb O3 with CrIS UWHS retrievals July 2014

Mean CrIS UWHS O3 is highly correlated (0.95) with RAQMS and is ~30ppbv higher than the RAQMS O3 analysis at 150mb



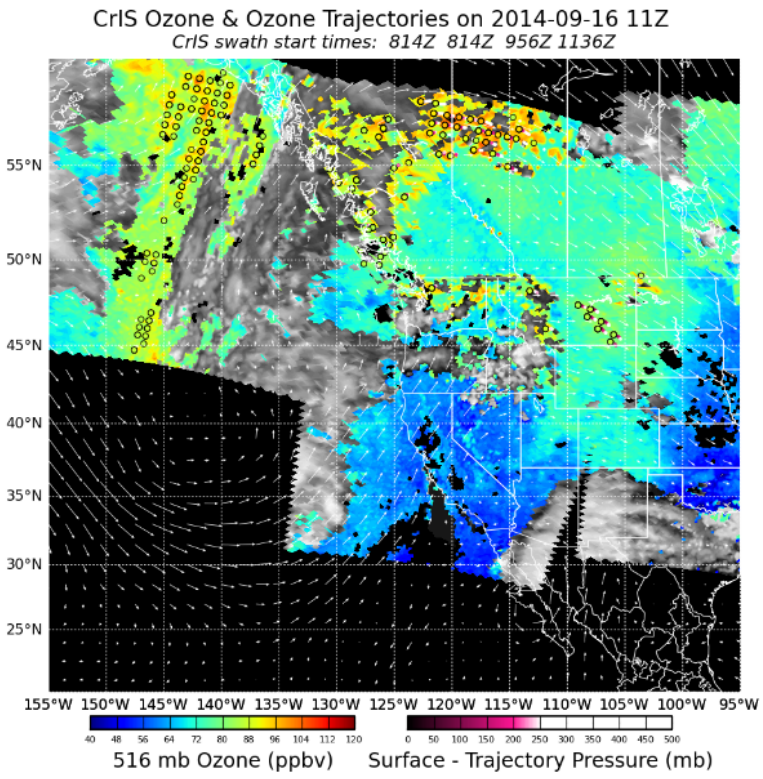

**The UW hyper-spectral retrieval package was released under the JPSS Community Satellite Processing Package (CSPP) in November 2012.**

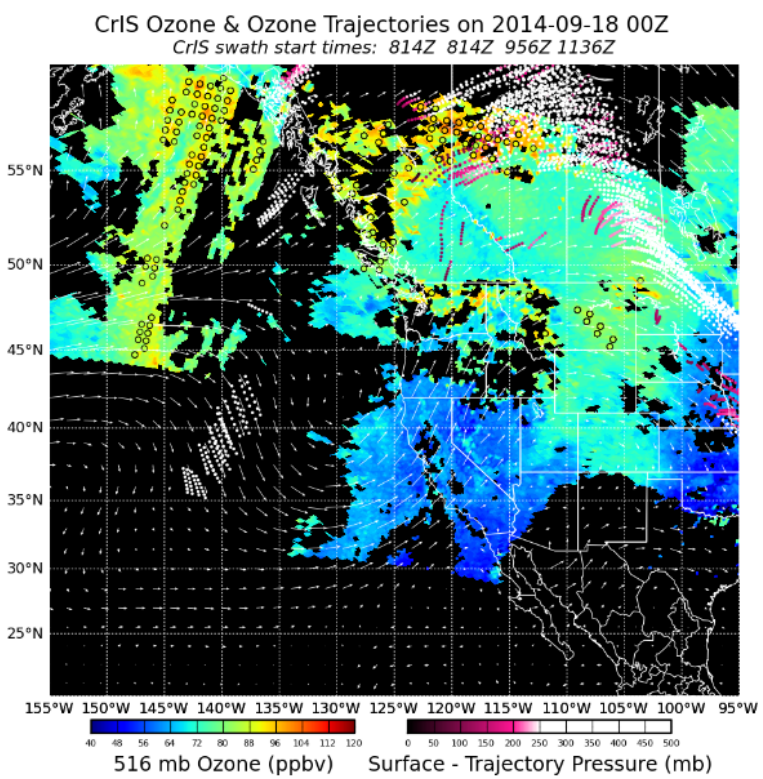
# NASA AQAST Tiger Team Project FY2013

## Satellite based support for Stratospheric Intrusion Exceptional Event Analysis

**<u>Objective:</u> Provide satellite based support to state and local air quality management for stratospheric intrusion (SI) related exceptional event analysis. (Gail Tonnesen and Pat Reddy POCs)**

**<u>Approach:</u> Add capabilities to IDEA-I (http://cimss.ssec.wisc.edu/imapp/ideai_v1.0.shtml) within the International AIRS/MODIS Processing Package (IMAPP) and the Community Satellite Processing Package (CSPP) to produce trajectory based SI forecasts initialized with real-time AIRS, IASI, and CrIS ozone retrievals.**



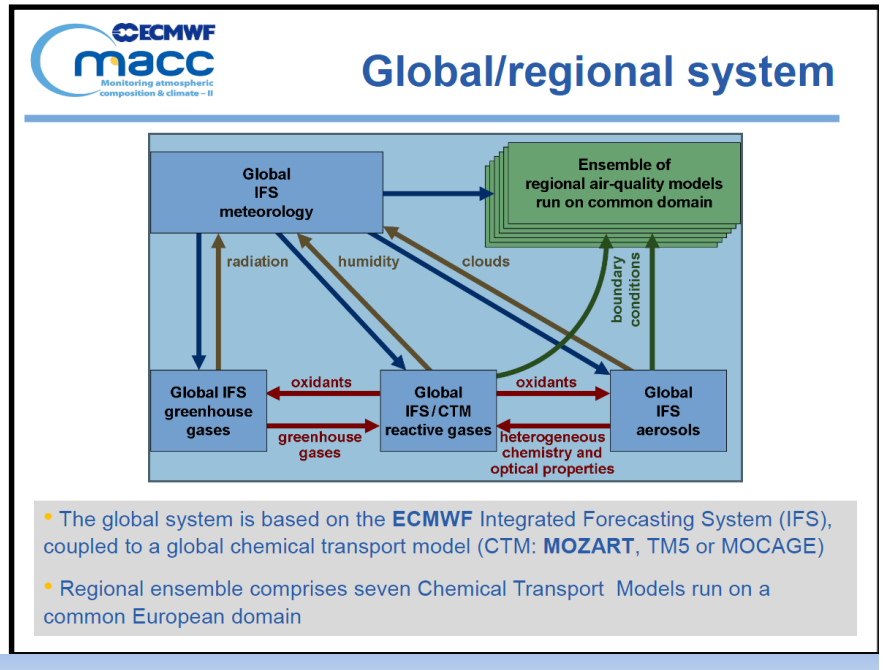

**The Infusing Satellite Data Into Environmental Applications - International (IDEA-I) Stratospheric Intrusion forecast (http://cimss.ssec.wisc.edu/idea-i/USozone/index.php)**

# Summary

- **Data denial experiments using Aura OMI, TES, and MLS O3 demonstrate the utility of assimilating UV and MW ozone and IR ozone/carbon monoxide retrievals for air quality applications – *improved constraints on lateral boundary conditions for regional AQ models* (Yates, et al. ACP, 2013, Huang et al, JGR, 2013, Fiore et al., EM, 2014)**

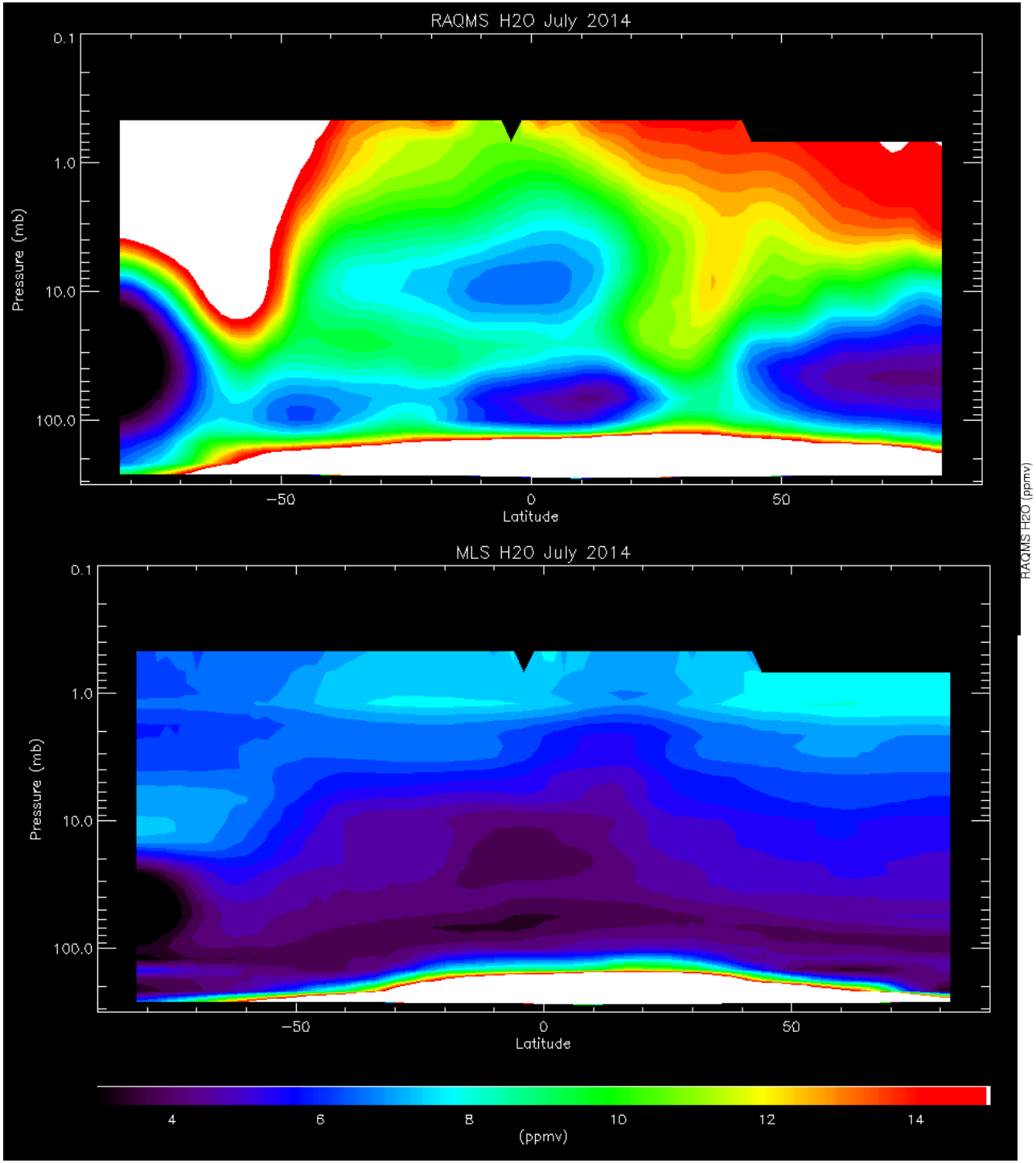
- **Under support from the NASA Aura Science team, we intend to extend this capability to other OMI, MLS, and TES (or AIRS) trace gas retrievals using the NOAA 3D variational analysis scheme (GSI) to provide the air quality community with a multi-year global chemical and aerosol reanalysis using NASA Aura and A-Train measurements.**

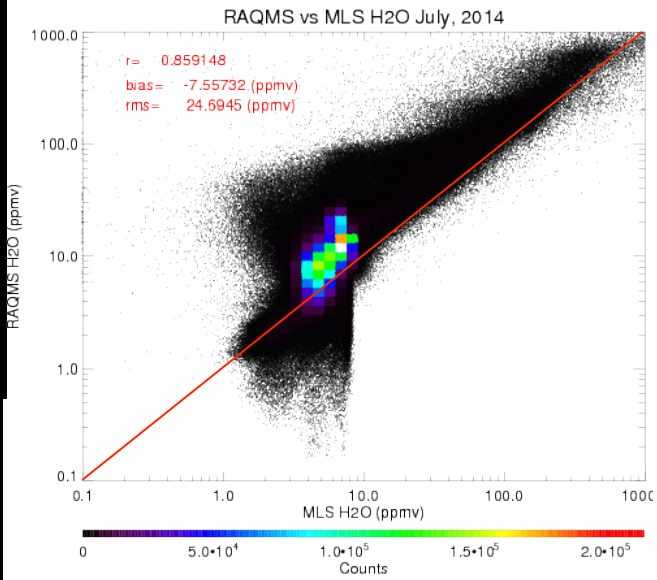
  - **This Aura analysis can serve as a "proof of concept" for future global operational trace gas and aerosol data assimilation/ forecasting at NOAA (following EU GEMS/MACC path)**

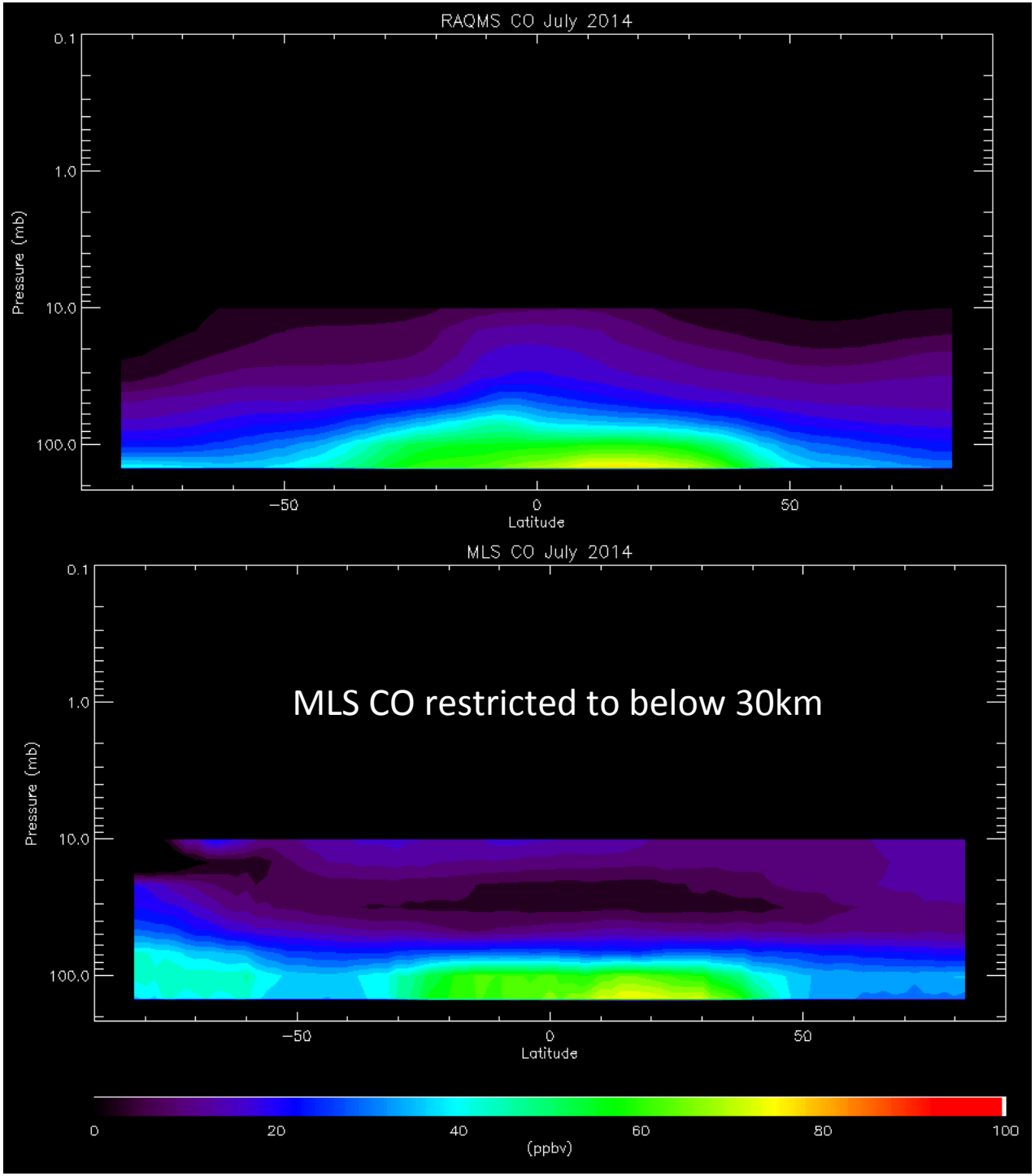


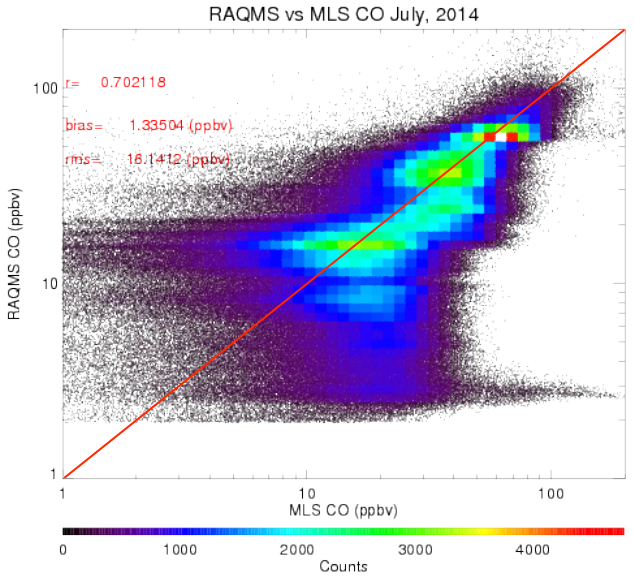

**http://www.copernicus-atmosphere.eu/services/aqac/**

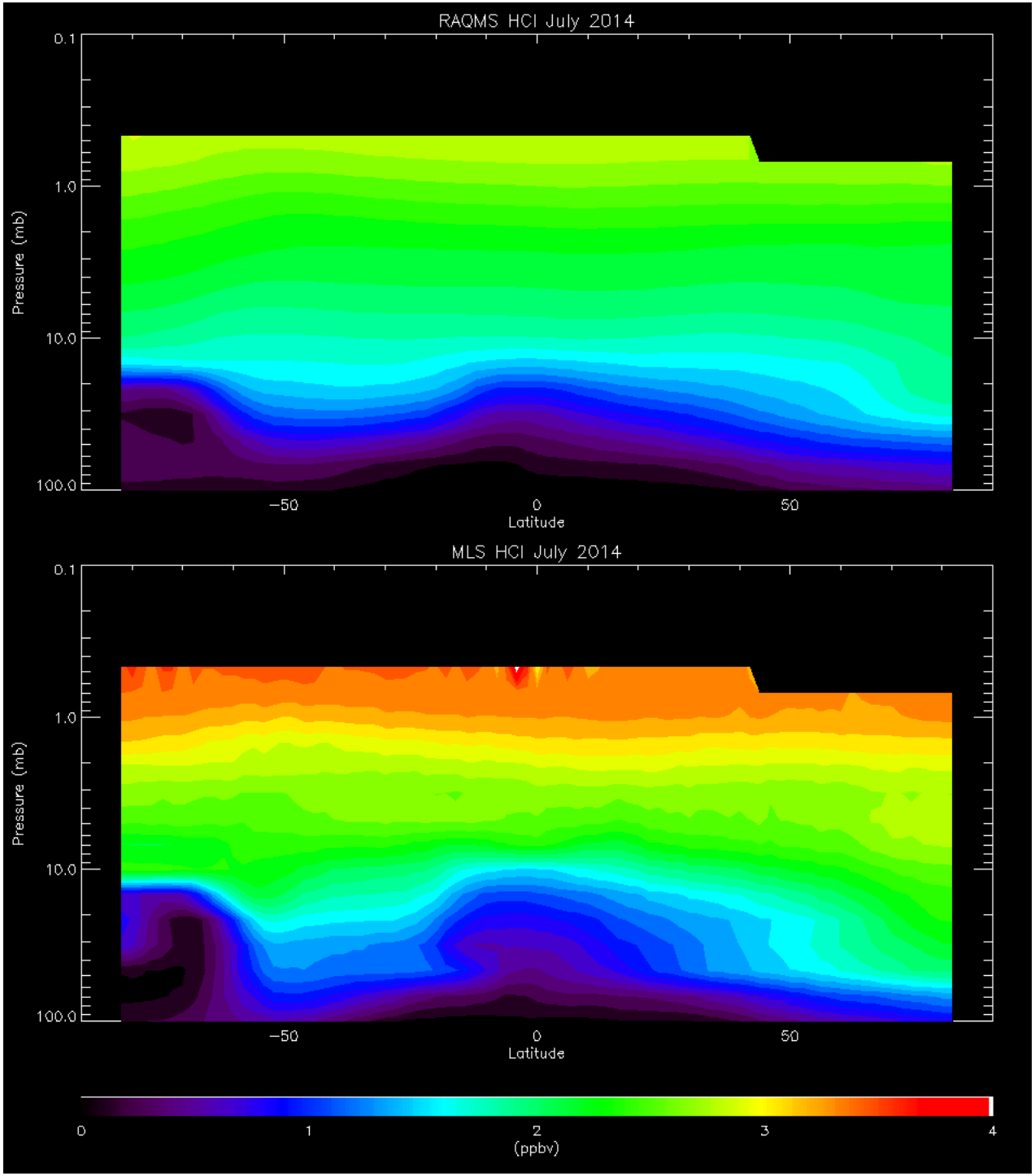
Extra Slides

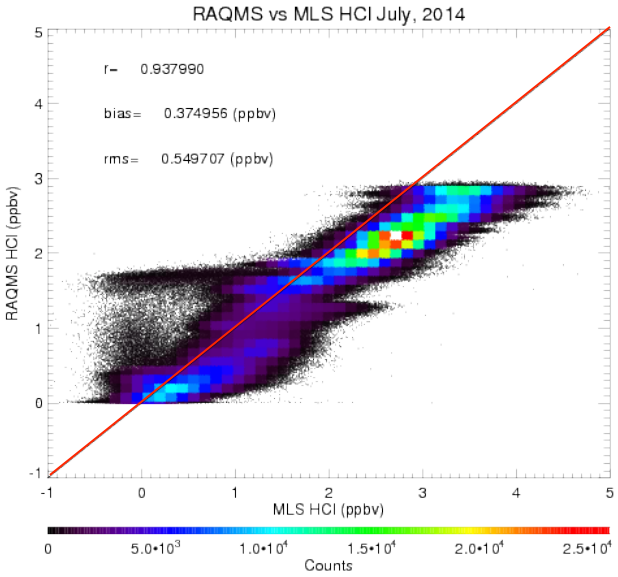

RAQMS H2O July 2014
Pressure (mb)
0.1
1.0
10.0
100.0
−50
0
50
Latitude
MLS H2O July 2014
Pressure (mb)
0.1
1.0
10.0
100.0
−50
0
50
Latitude
4
6
8
10
12
14
(ppmv)

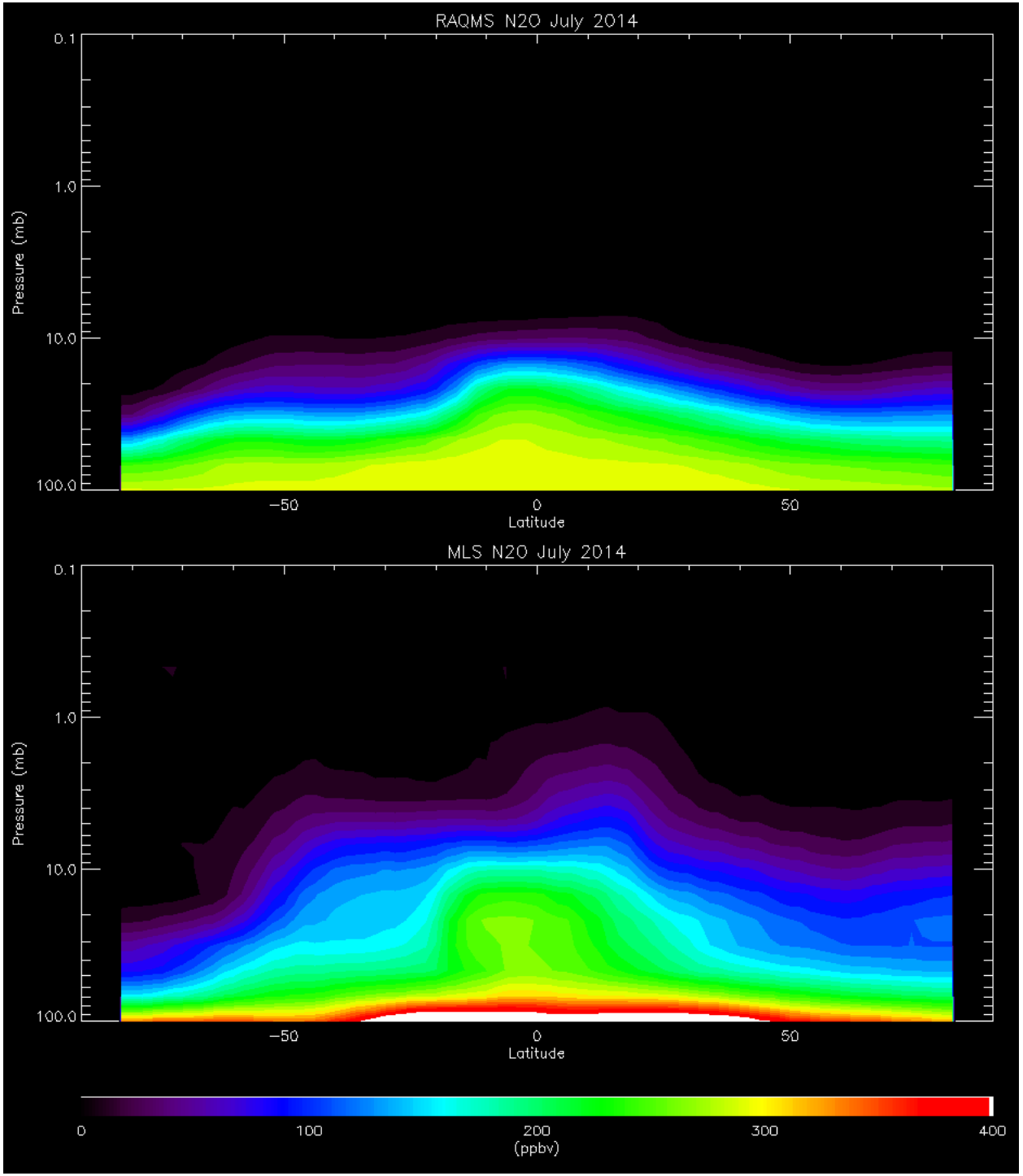

RAQMS vs MLS H2O July, 2014
r= 0.859148
bias= -7.55732 (ppmv)
rms= 24.6945 (ppmv)
RAQMS H2O (ppmv)
1000.0
100.0
10.0
1.0
0.1
0.1
1.0
10.0
100.0
1000
MLS H2O (ppmv)
0
5.0•10^4
1.0•10^5
1.5•10^5
2.0•10^5
Counts

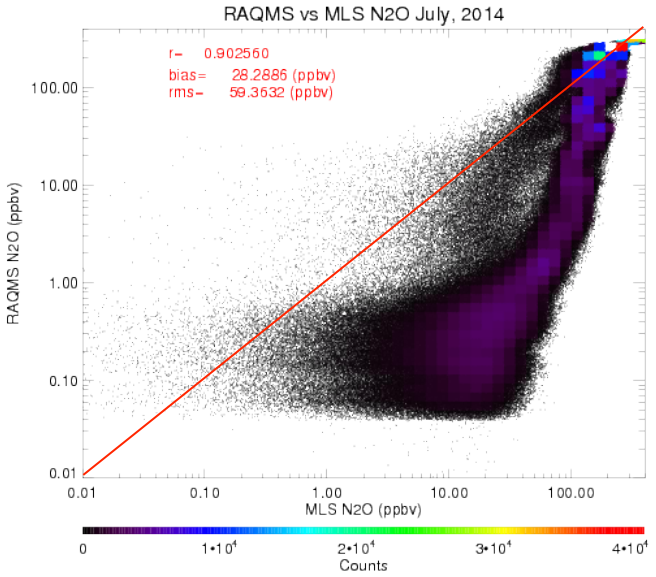

RAQMS CO July 2014
Pressure (mb)
0.1
1.0
10.0
100.0
−50
0
50
Latitude
MLS CO July 2014
MLS CO restricted to below 30km
0
20
40
60
80
100
(ppbv)


RAQMS vs MLS CO July, 2014
r= 0.702118
bias= 1.33504 (ppbv)
rms= 16.1412 (ppbv)
RAQMS CO (ppbv)
100
10
1
1
10
100
MLS CO (ppbv)
0
1000
2000
3000
4000
Counts


RAQMS HCl July 2014
Pressure (mb)
0.1
1.0
10.0
100.0
−50
0
50
Latitude
MLS HCl July 2014
Pressure (mb)
0.1
1.0
10.0
100.0
−50
0
50
Latitude
0
1
2
3
4
(ppbv)


RAQMS vs MLS HCl July, 2014
r= 0.937990
bias= 0.374956 (ppbv)
rms= 0.549707 (ppbv)
RAQMS HCl (ppbv)
MLS HCl (ppbv)
-1
0
1
2
3
4
5
0
5.0•10^3
1.0•10^4
1.5•10^4
2.0•10^4
2.5•10^4
Counts


RAQMS N2O July 2014
Pressure (mb)
0.1
1.0
10.0
100.0
−50
0
50
Latitude
MLS N2O July 2014
Pressure (mb)
0.1
1.0
10.0
100.0
−50
0
50
Latitude
0
100
200
300
400
(ppbv)


RAQMS vs MLS N2O July, 2014
r= 0.902560
bias= 28.2886 (ppbv)
rms= 59.3632 (ppbv)
RAQMS N2O (ppbv)
0.01
0.10
1.00
10.00
100.00
MLS N2O (ppbv)
0
1•10^4
2•10^4
3•10^4
4•10^4
Counts