An assessment of the value of IR sounder trace gas retrievals in chemical data assimilation

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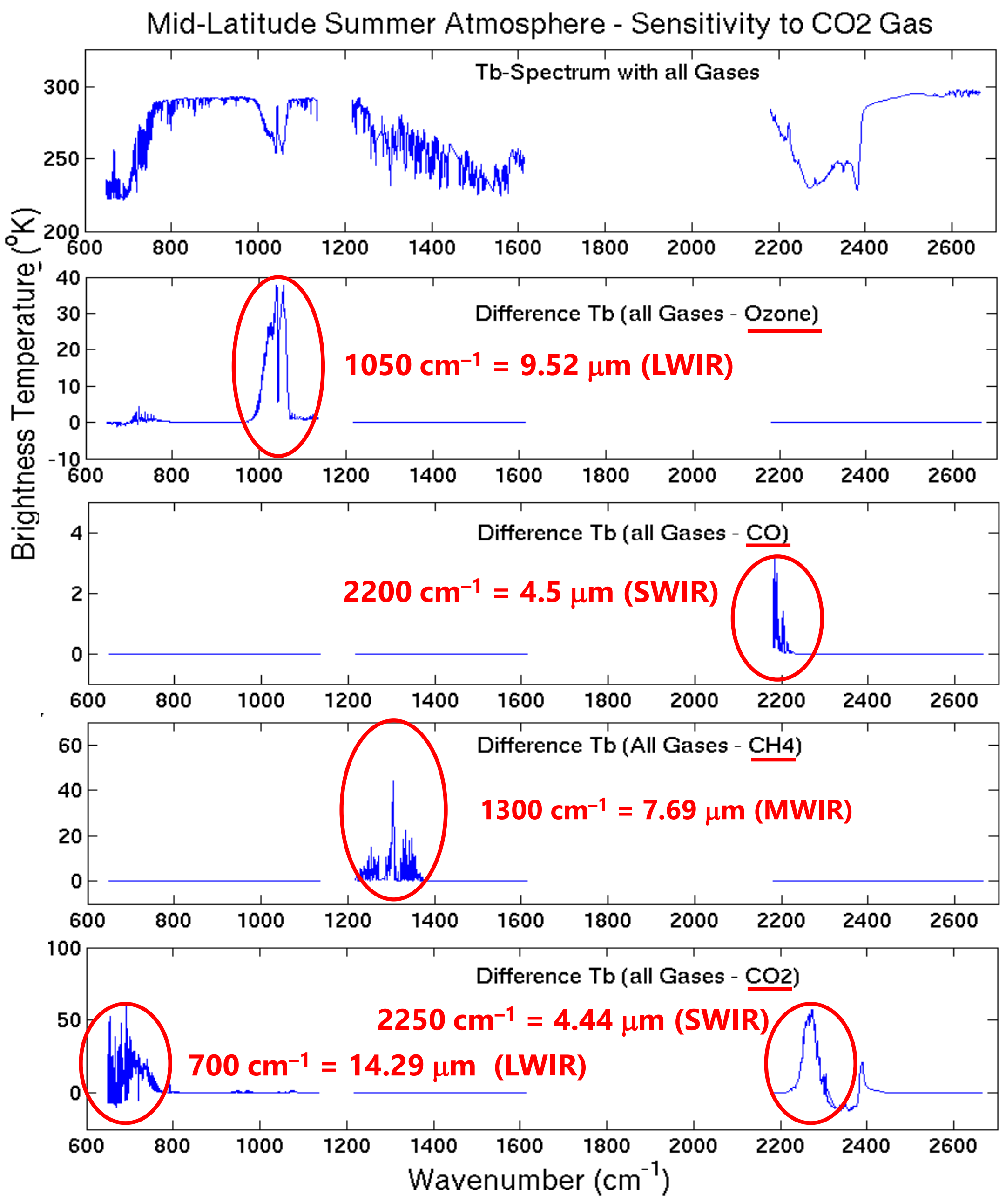
UW-Madison
Space Science and Engineering Center

NOAA INFRARED SOUNDER WORKSHOP, MONDAY, DEC. 6, 2021

CrIS Specs for Baseline Reference

	SWIR	MWIR	LWIR
Reference Range (microns)	3.7-6.6	6.6-8.6	8.6-15.38
Desired Range (gaps/ no gaps)	3.92-4.64	5.71-8.26	9.14-15.38
Desired Spectral Resolution	0.625 cm-1	0.625 cm-1	0.625 cm-1
NEDN/NEDT	CrIS noise levels	CrIS noise levels	CrIS noise levels
Horizontal Resolution/ GSD at Nadir	14 km @ 832 km altitude	14 km @ 832 km altitude	14 km @ 832 km altitude
Swath (km)	2200 km @ 832 km altitude	2200 km @ 832 km altitude	2200 km @ 832 km altitude

Trace Gas Infrared Radiative Signatures



Infrared Radiative influences of Ozone, CO, CH4, CO2, N2O and other GHG are <u>significant</u>

Temporal/spatial variability should be accounted for in forward radiative transfer modeling

Question: What is the ideal configuration for an IR sounder backbone?

- **SWIR (CO, CO2), MWIR (CH4) and LWIR (O3) are all critical for supporting global Air Quality and Climate services.**

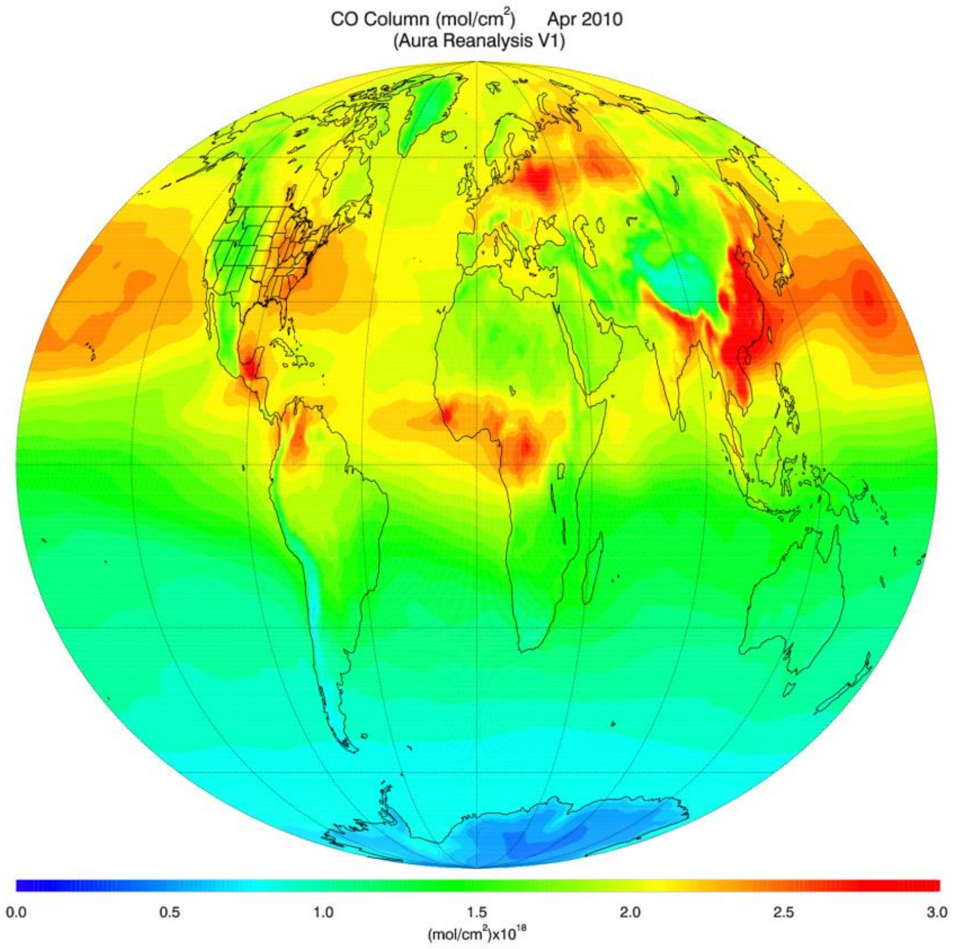
Figure provided by Tim Schmit, NESDIS/STAR

Demonstration of the impact of assimilating hyperspectral IR CO and O3 retrievals within a global chemical reanalysis

Aura Chemical Reanalysis 2006-2016

- Project Summary

  Utilize the Real-time Air Quality Modeling System (RAQMS) in conjunction with the Operational Gridpoint Statistical Interpolation (GSI) 3-dimensional variational data assimilation (DA) system to conduct a multi-year global chemical and aerosol reanalysis using NASA Aura and A-Train measurements.



- Earth Observations

  OMI: Total Column O_3 , Tropospheric NO_2 Column

  MLS: Stratospheric and upper tropospheric O_3

  AIRS: Stratospheric and Tropospheric CO

  MODIS: Aerosol Optical Depth, Fire Detection

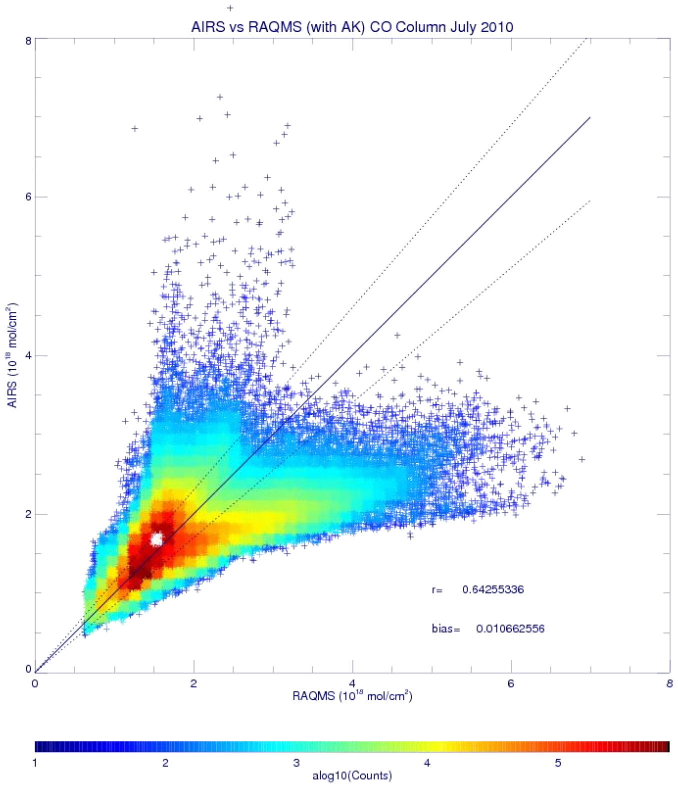
Funded by the NASA Aura Science Team and Health and Air Quality Program

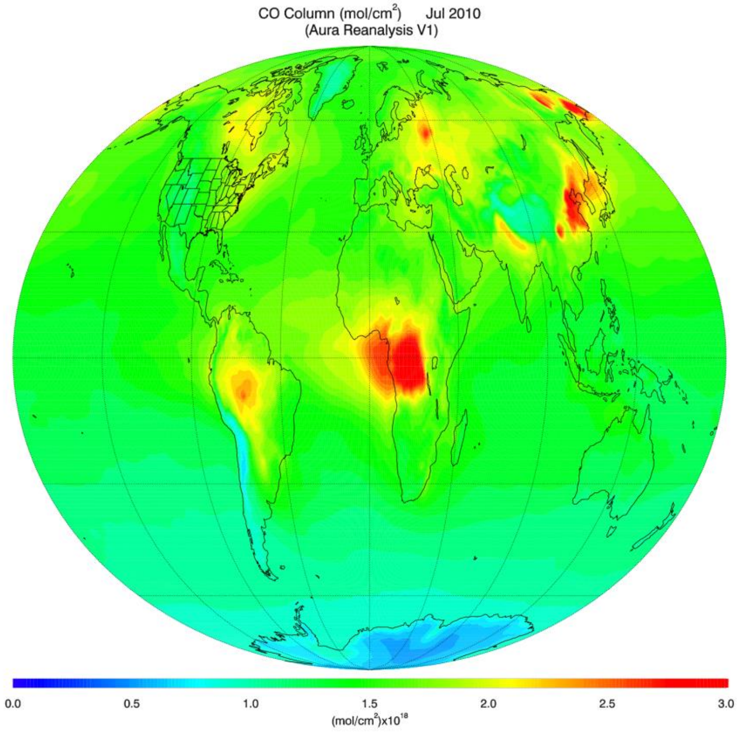
RAQMS/GSI AIRS CO Data Assimilation (July 2010)

Observation-Background (O-B):
(Instantaneous comparisons)

r=0.643
Bias=0.011x10^{18}mol/cm^2

With Averaging Kernels





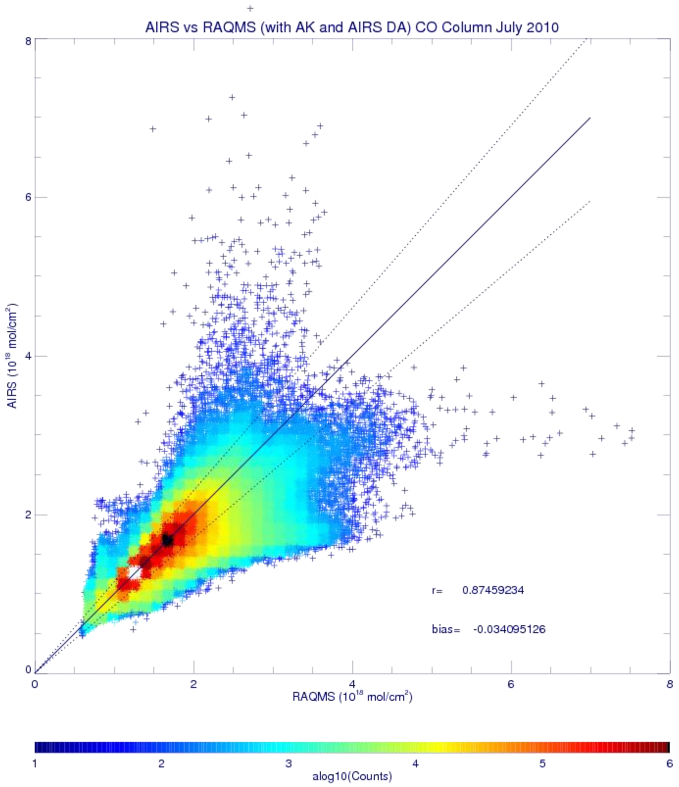
AIRS CO averaging kernels and apriori profiles are used for forward operator and applied to RAQMS CO predictions, tangent linear observation operator implemented within GSI inner loop. ***Based on GMAO MOPITT DA***

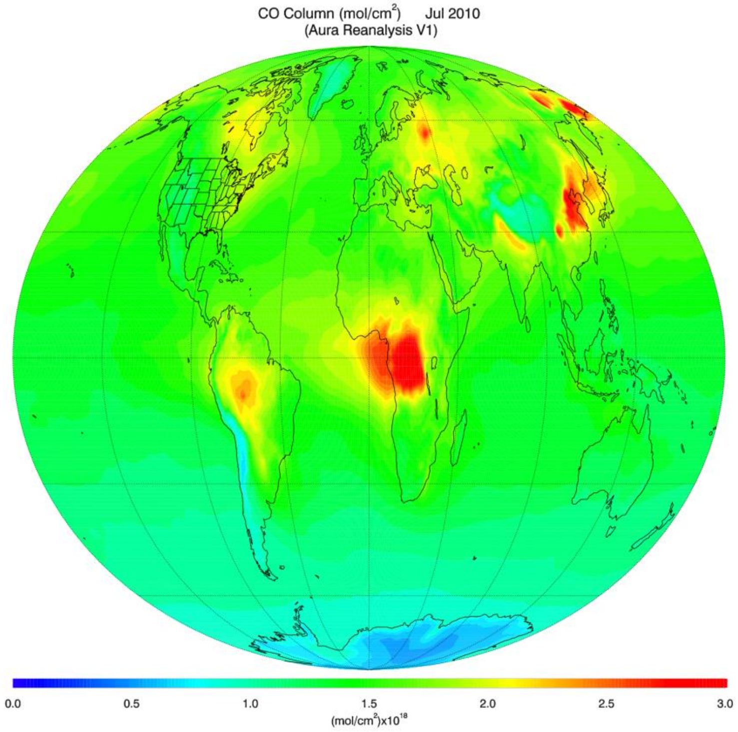
RAQMS/GSI AIRS CO Data Assimilation (July 2010)

Observation-Analysis (O-A):
(Instantaneous comparisons)

r=0.875
Bias=-0.034x10^{18}mol/cm^2

With Averaging Kernels





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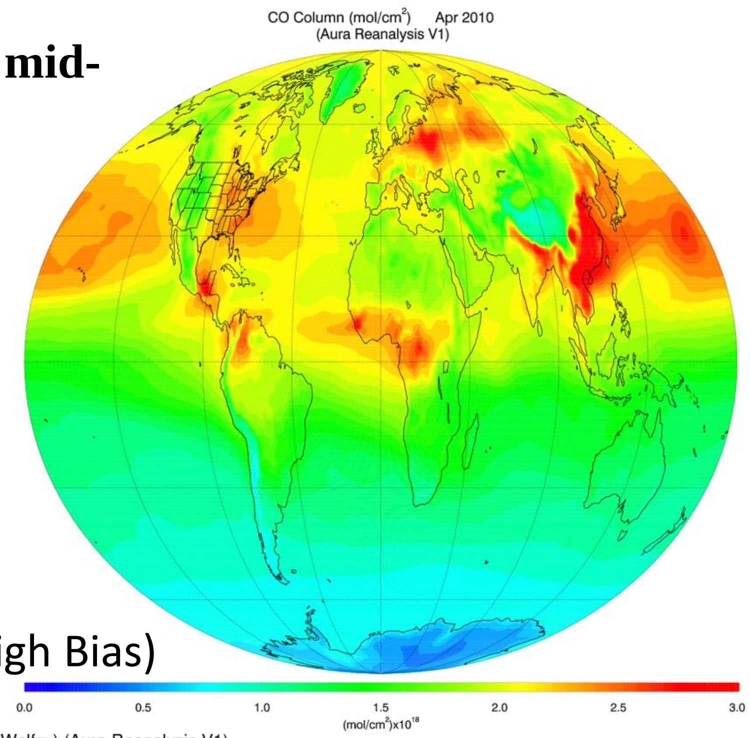
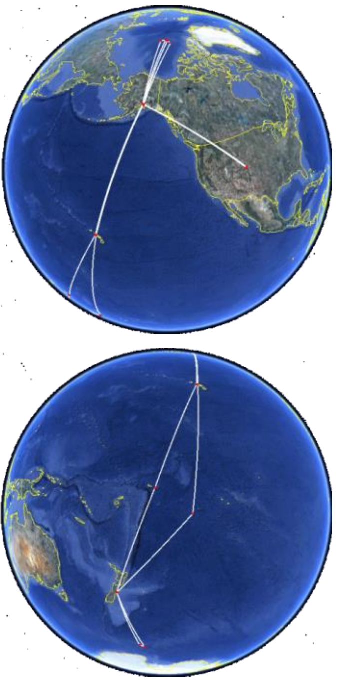
The NSF HIAPER Pole-to-Pole Observations (HIPPO) measured pole-to-pole cross sections of atmospheric concentrations from the surface to the tropopause across the mid-Pacific ocean.



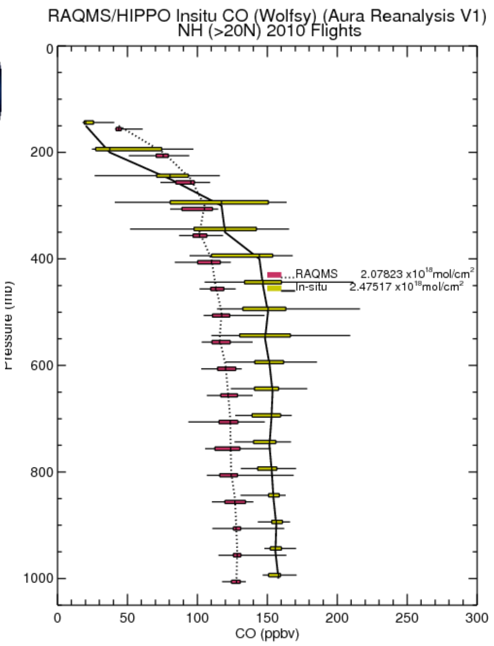
HIPPO III Flight Tracks
Mar 20 –Apr 20, 2010



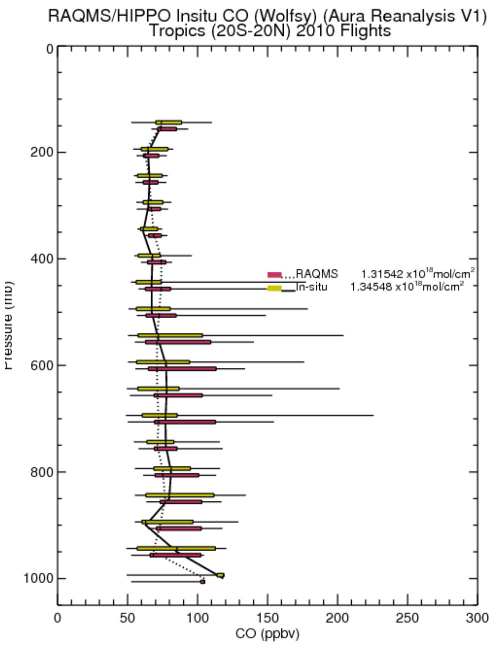
Verification of the RAQMS AIRS CO Reanalysis during NH Spring shows:

- **Underestimates CO concentrations in the NH troposphere**
- **Overestimates CO concentrations in the NH and SH lower stratosphere**

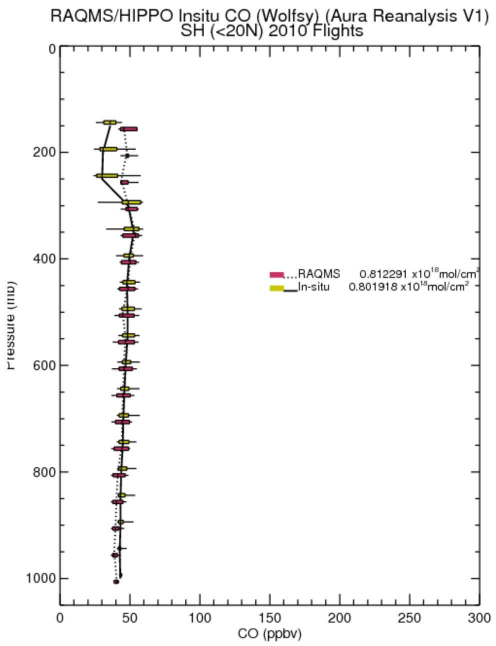
NH (16% Low Bias)



Tropics (2% Low Bias)



SH (1% High Bias)



HIPPO
HIAPER Pole-to-Pole Observations

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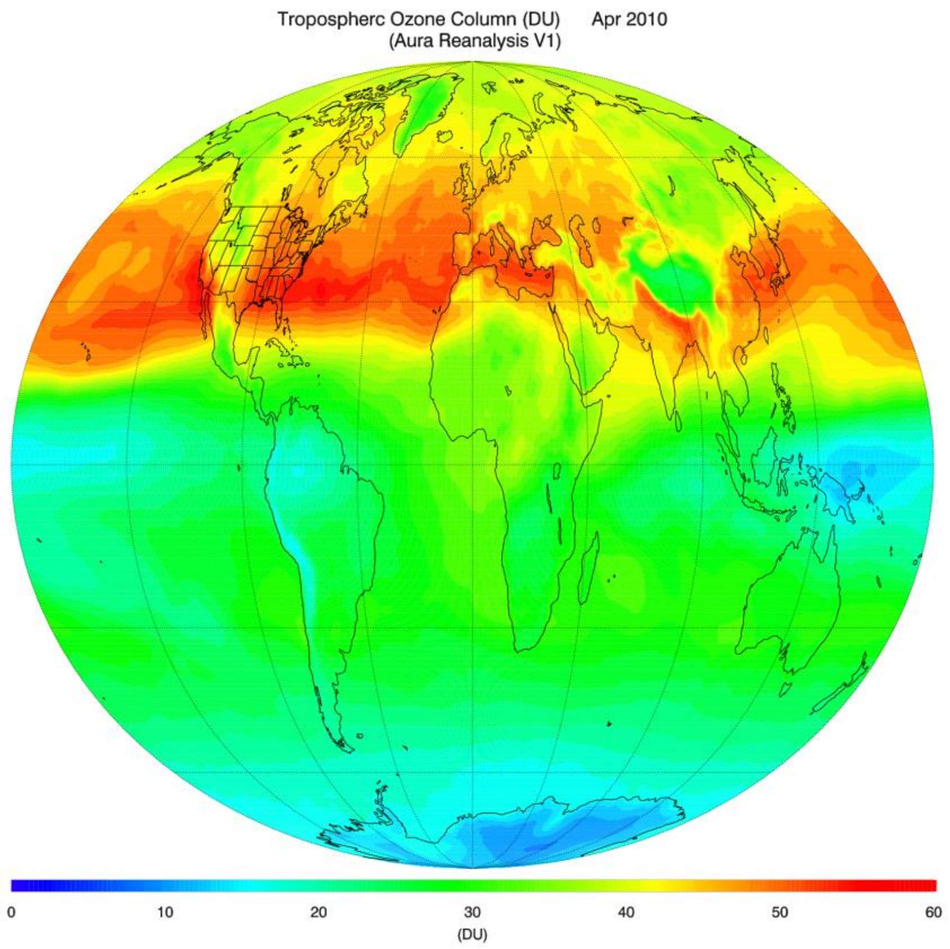

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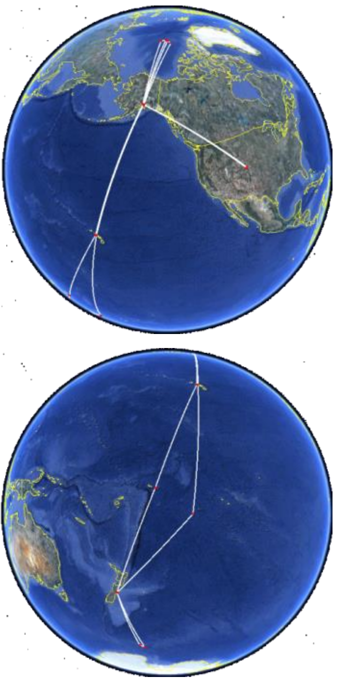
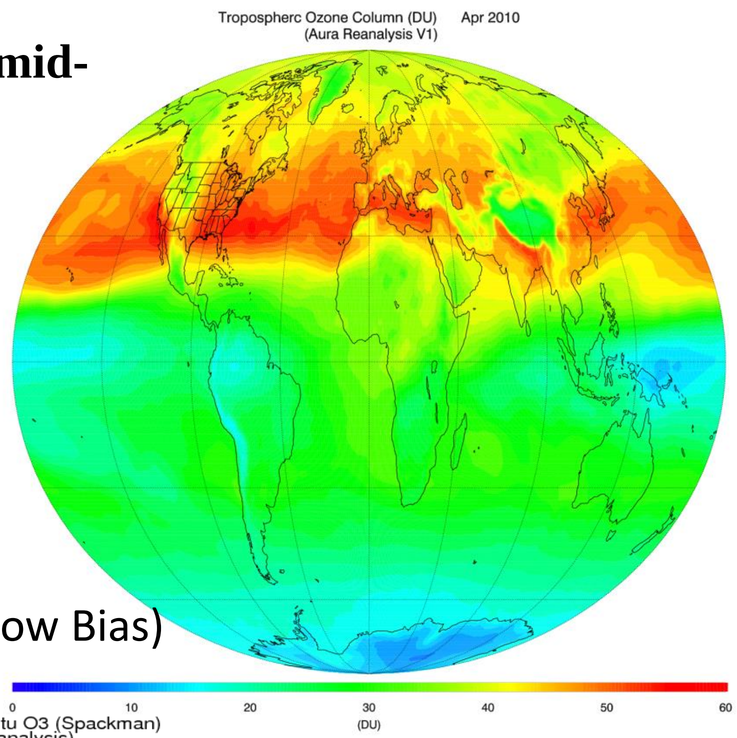
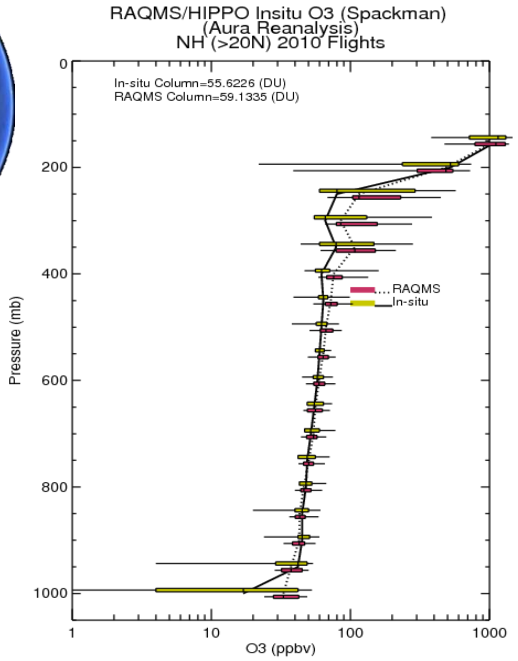


Verification of the RAQMS OMI/MLS O3 Reanalysis during NH Spring shows:

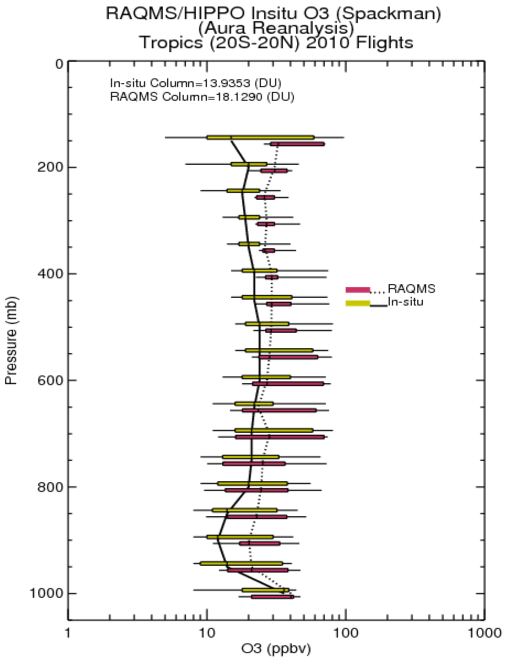
- **Overestimates in O3 concentrations in the NH upper troposphere**
- **Overestimates in O3 concentrations in the Tropics**
- **Good agreement in the SH**



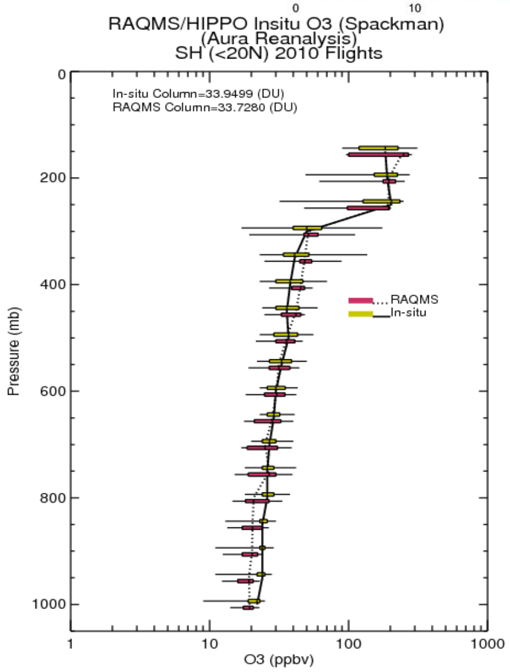
NH (6% High Bias)
~4DU



Tropics (30% High Bias)
~4DU



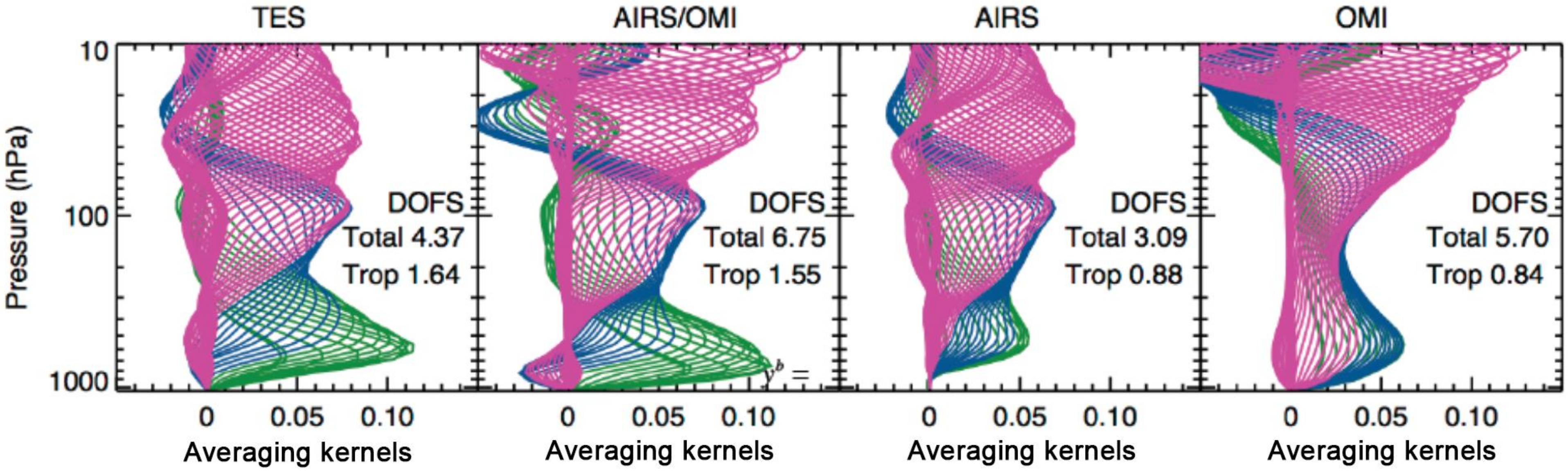
SH (<1% Low Bias)



HIPPO
HIAPER Pole-to-Pole Observations

Multi-Spectral MUSES UV+LWIR O3 Data Impact Assessments

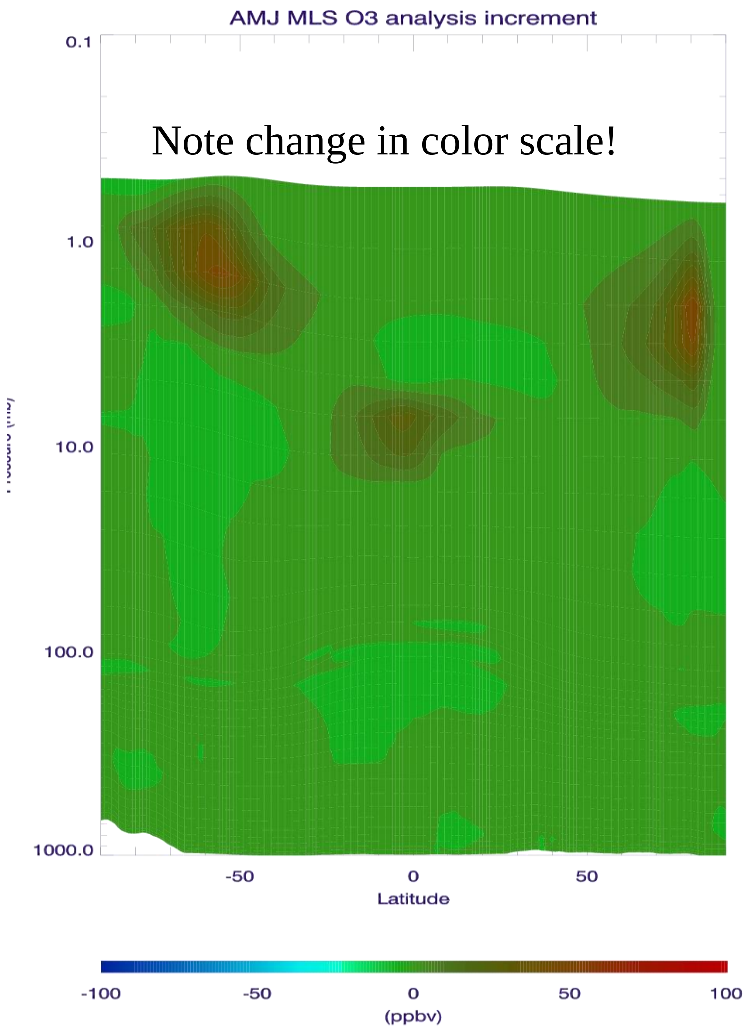
- April-June 2016 RAQMS Aura Reanalysis data impact studies assess the impacts of assimilation of joint AIRS/OMI O3 retrievals processed through the MUlti-SpEctra, MUlti-SpEcies, MUlti-SEnsors (MUSES) retrieval algorithm.

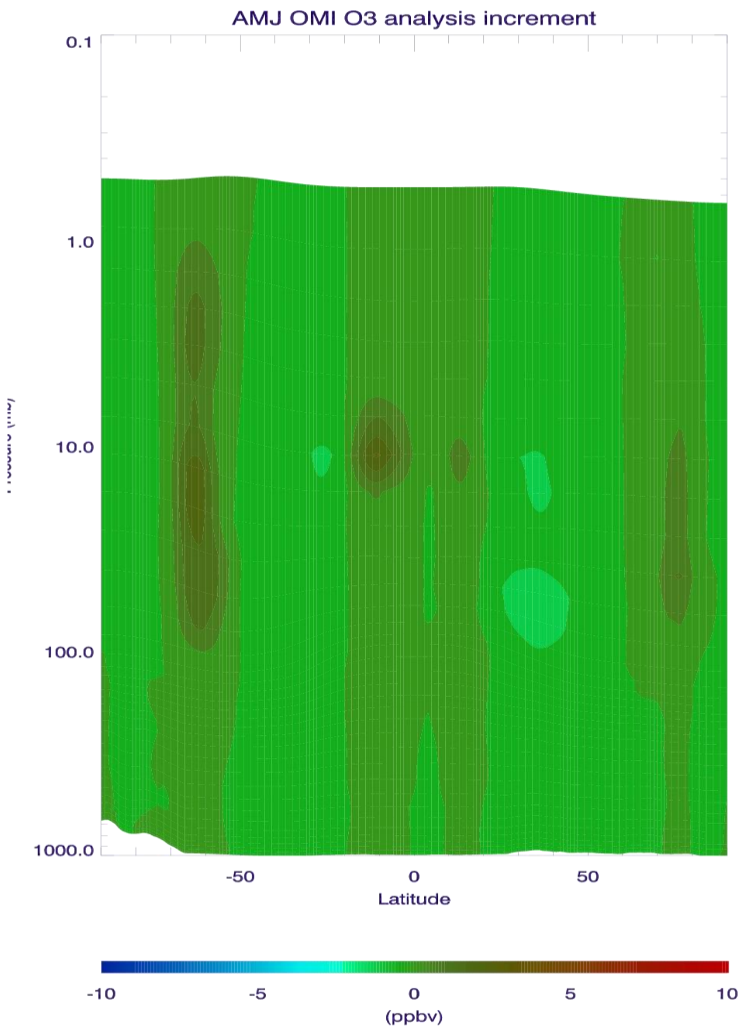


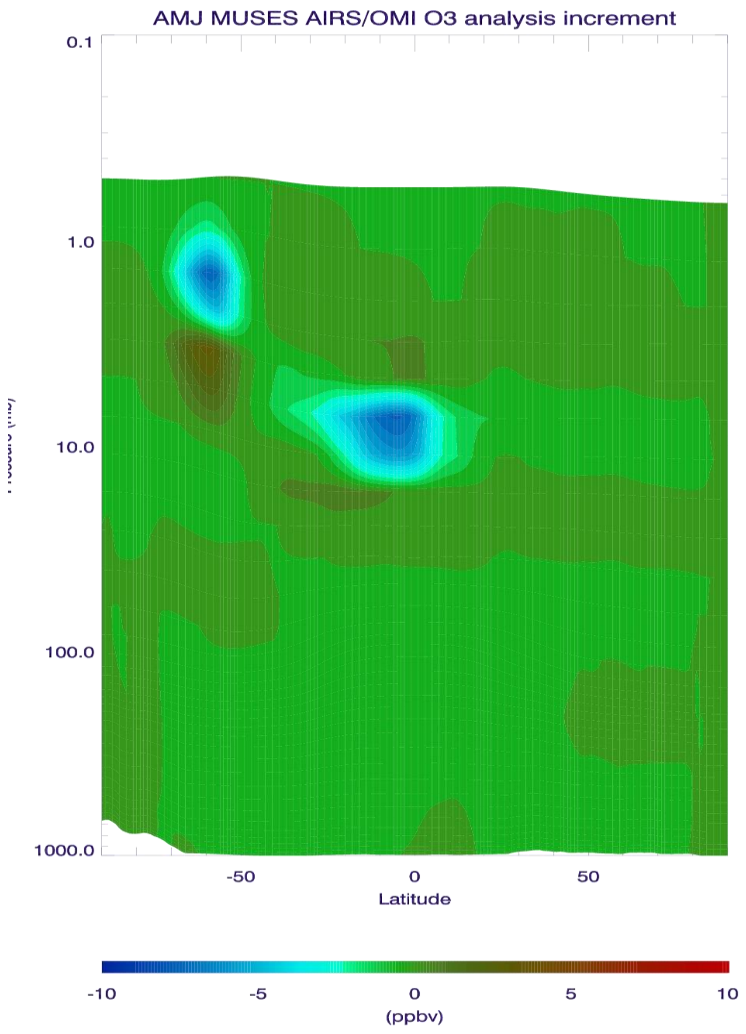
Dejian Fu et al. (2018) Retrievals of tropospheric ozone profiles from the synergism of AIRS and OMI: methodology and validation, Atmos. Meas. Tech., 11, 5587–5605, 2018, https://doi.org/10.5194/amt-11-5587-2018

With Co-PI Kevin Bowman (JPL) Funded by the NOAA CPO/AC4 Program

April-May-June (AMJ) 2016 RAQMS Aura Reanalysis (MLS+OMI)
plus
AIRS/OMI MUSES O3 assimilation

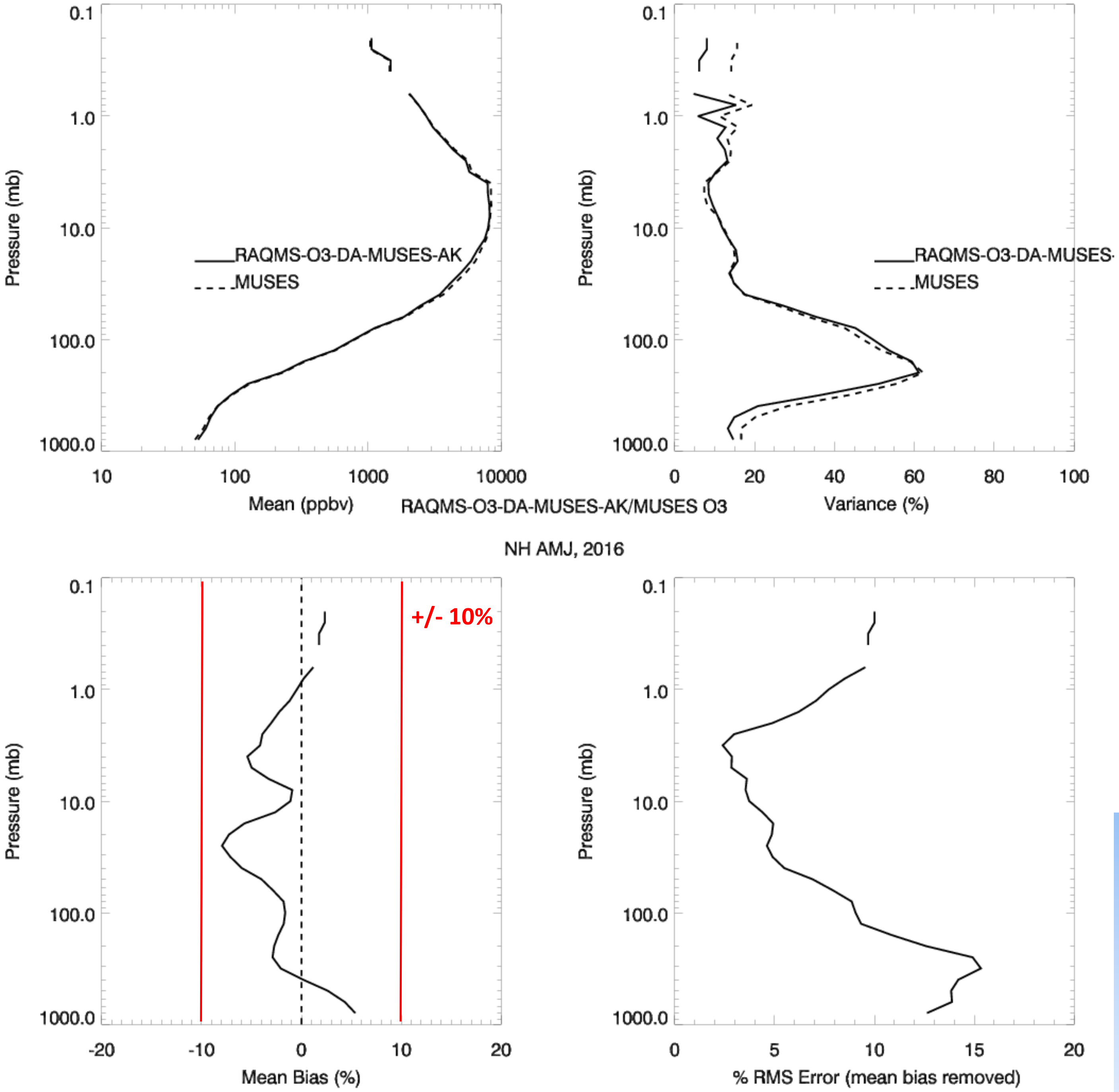


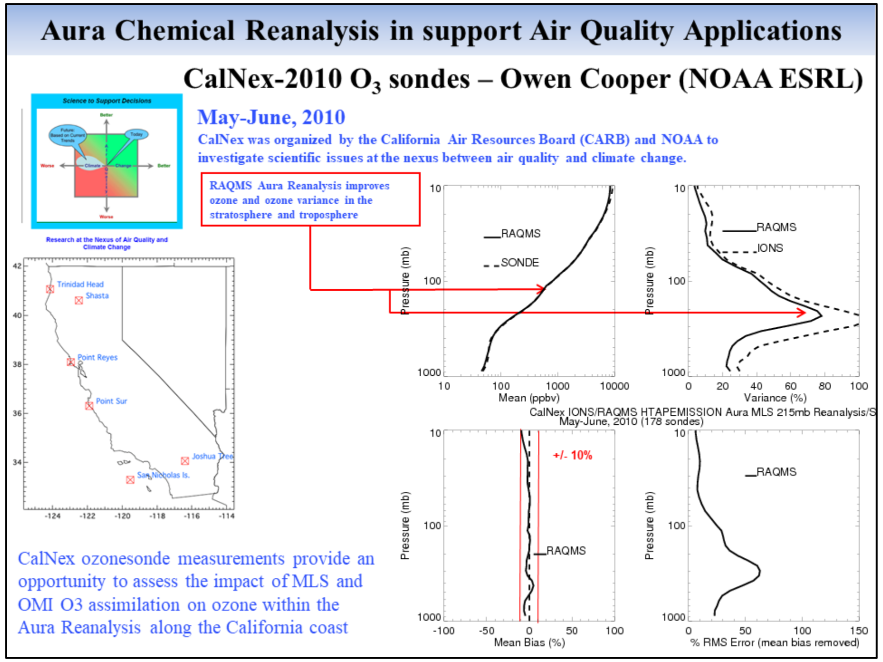




MUSES adjustments are small (<10ppbv), primarily in the Stratosphere, and tend to appose the larger MLS adjustments

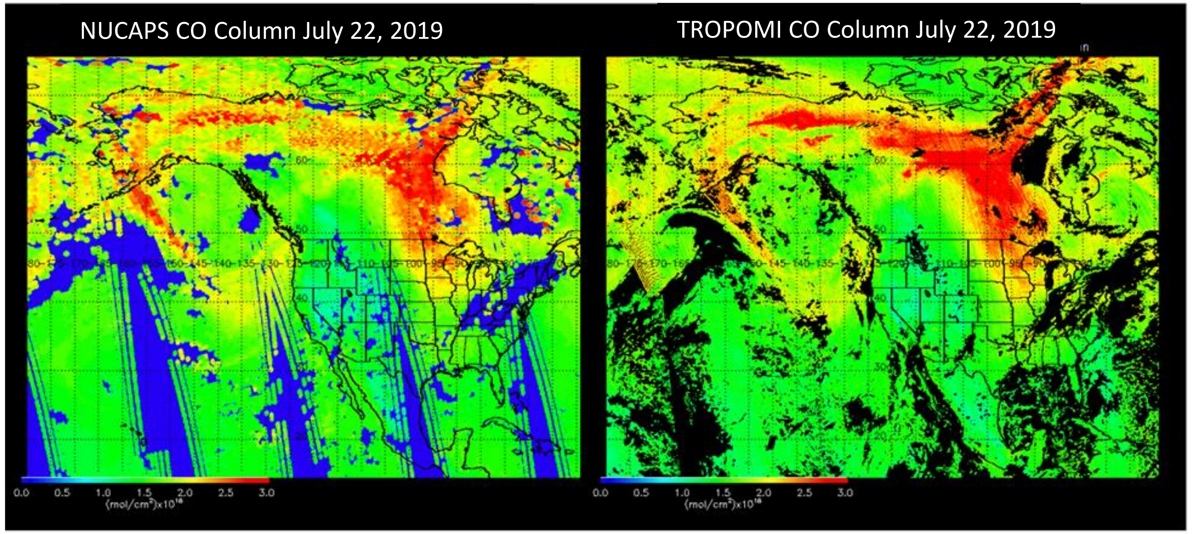
RAQMS Aura Reanalysis (MLS+OMI+MUSES AIRS/OMI) NH (>20N) April-June, 2016





Impact of MUSES AIRS/OMI is small since:

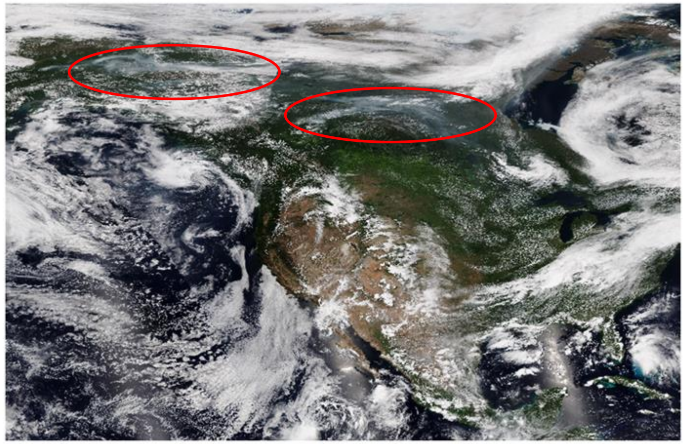
- MUSES AIRS/OMI retrieval is fully consistent with RAQMS Aura Reanalysis
- RAQMS Aura Reanalysis O3 is already well constrained with MLS/OMI



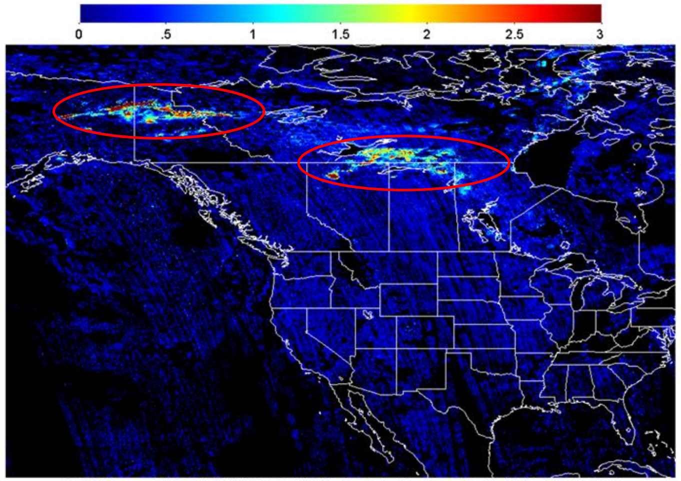
Question: What additional IR measurements would be ideal to augment the backbone?

- **Extending the SWIR down to 2.3µm would allow improved detection of boundary layer CO (wildfires) and CH4 (GHG emissions)**

VIIRS True Color Imagery July 22, 2019



TROPOMI-NUCAPS CO Column July 22, 2019

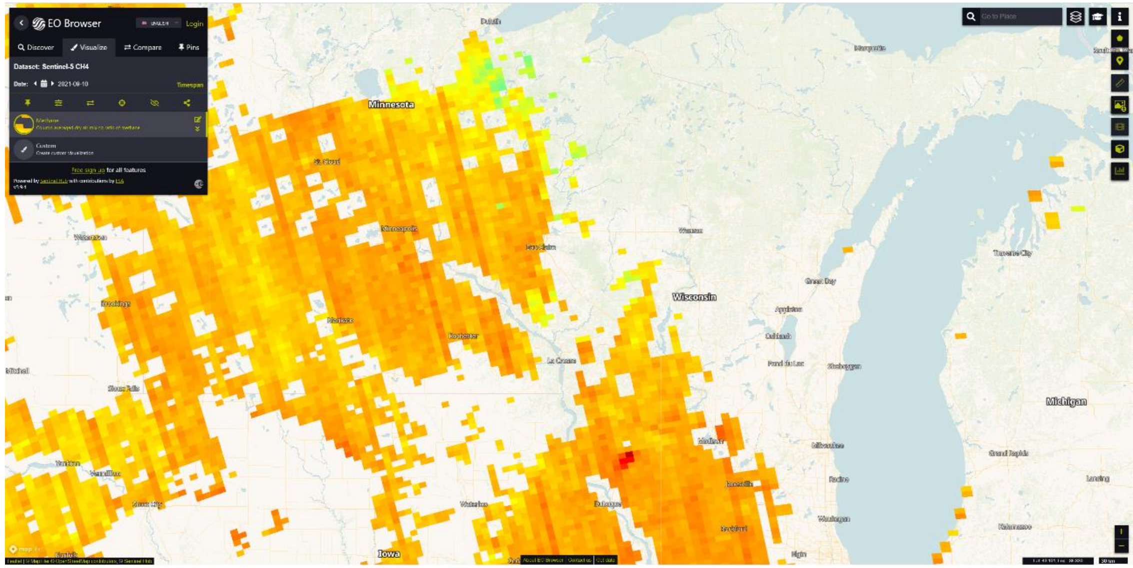


CO Difference (TROPOMI-NUCAPS) with Missing Data Check (mol/cm2)x10^18 - 2019-07-22

Addition of SWIR (2.3mm-3.7mm) band would allow for DOAS column retrievals using reflected solar

- Combination of mid-troposphere emitted and solar reflected could enhance boundary layer CO and CH4 sensitivities

TROPOMI CH4 Column, September 10, 2021



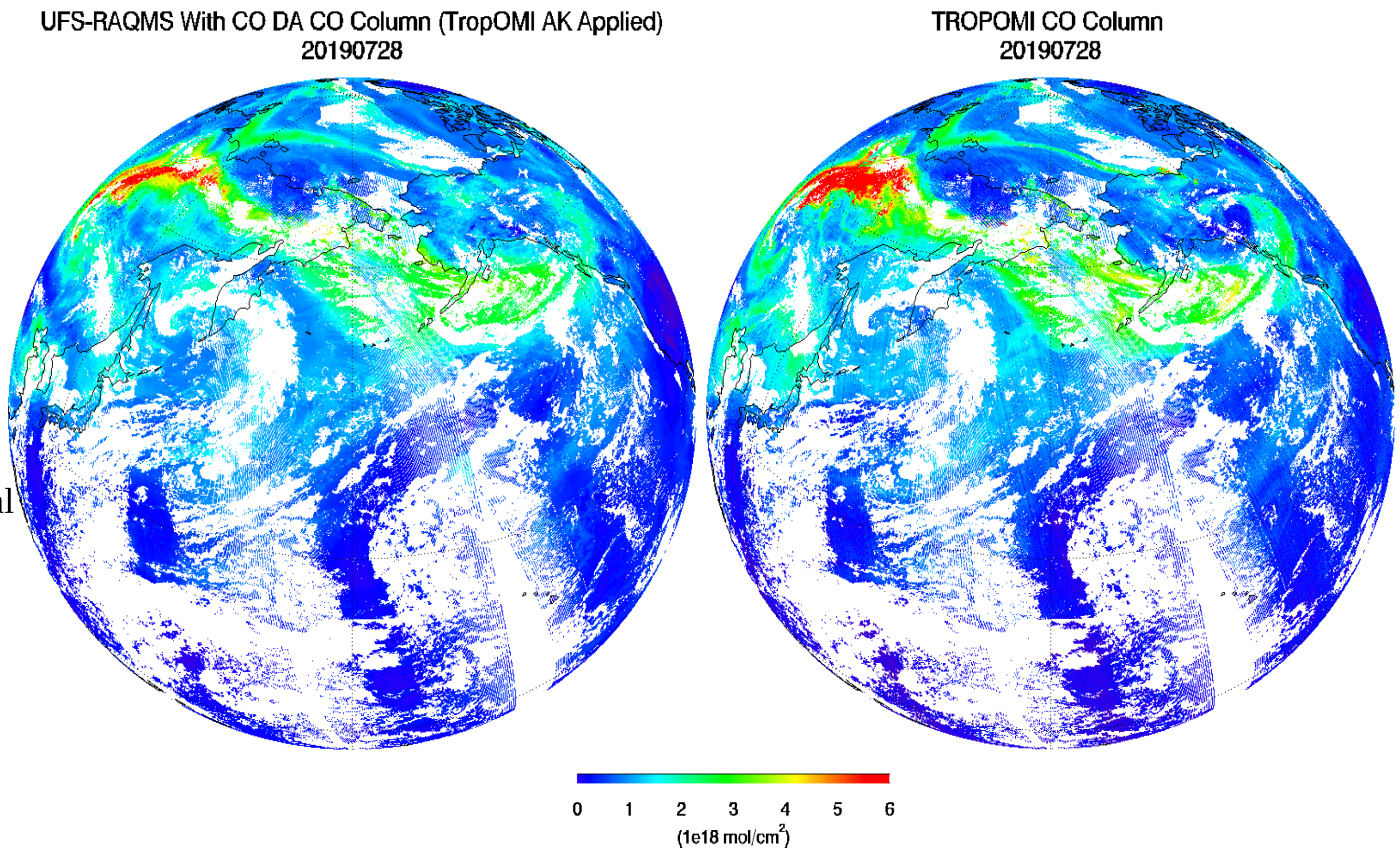
Demonstration of the impact of SWIR (2.3μm) CO within the UFS-RAQMS composition forecasting and analysis system

Unified Forecast System (UFS) Composition Forecasting

With Allen Lenzen (UW-Madison Space Science and Engineering Center), Margaret Bruckner (UW-Madison Atmospheric and Oceanic Sciences Department)

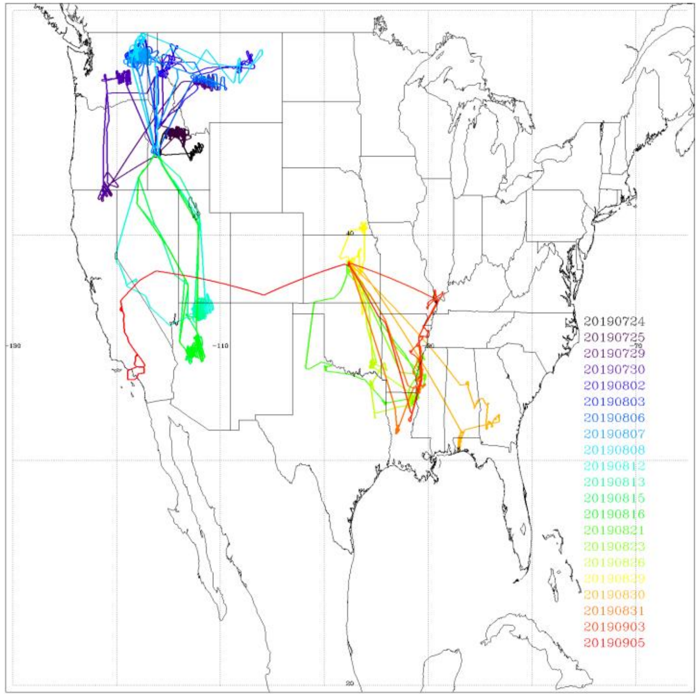
- **Real-time Air Quality Modeling System (RAQMS)** unified stratosphere/ troposphere chemical module incorporated into UFS under support from NOAA Research Transition Acceleration Program (RTAP)
  - *Supports global air quality and Seasonal to Sub-seasonal (S2S) forecasting*
- **Capabilities to assimilate composition** developed under support from NOAA Office of Projects, Planning, and Analysis (OPPA) Technology Maturation Program (TMP)
- **New JPSS Proving Ground/Risk Reduction Project** to develop capabilities for assimilation of JPSS Atmospheric Composition and Aerosol products and **transition to NOAA/ESRL** for pre-operational testing

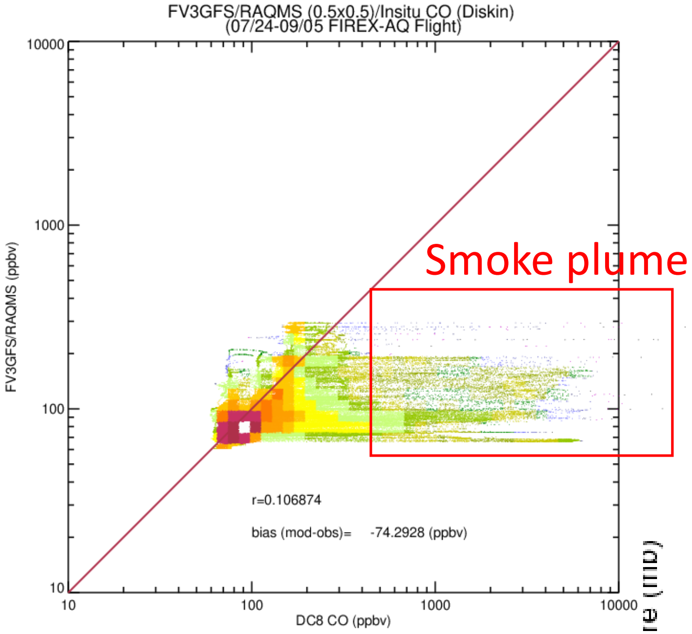
Assimilation of TROPOMI 2.3µm total CO column provides constraints on the impact of long-range transport of Siberian wildfire emissions on North American Air Quality



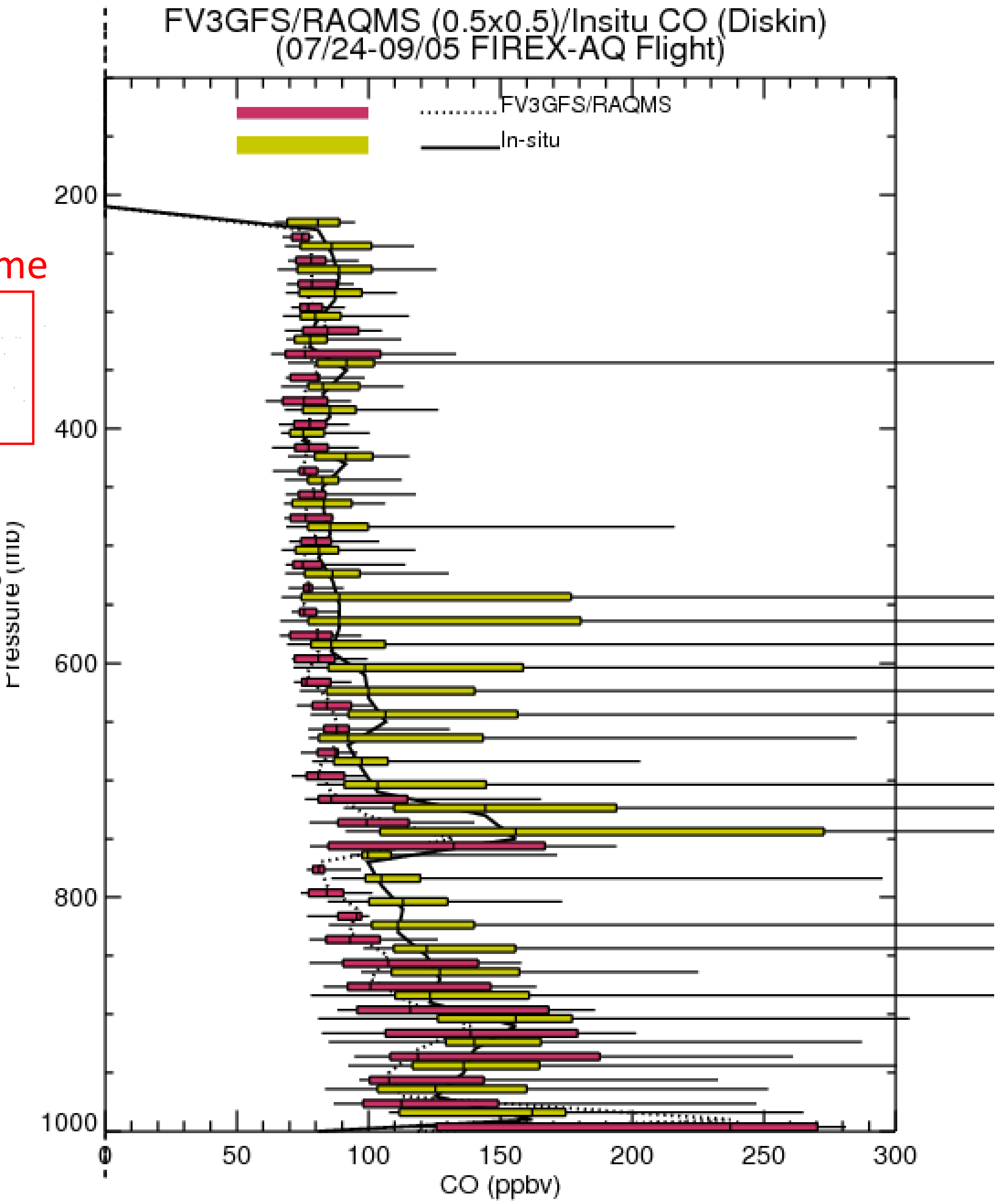
UFS-RAQMS (left) and TROPOMI (right) column carbon monoxide (1e^{18}mol/cm^2) on July 28, 2019

FIREX-AQ DC8 Flights
(July 24 –September 05,2019)





UFS-RAQMS (Control)



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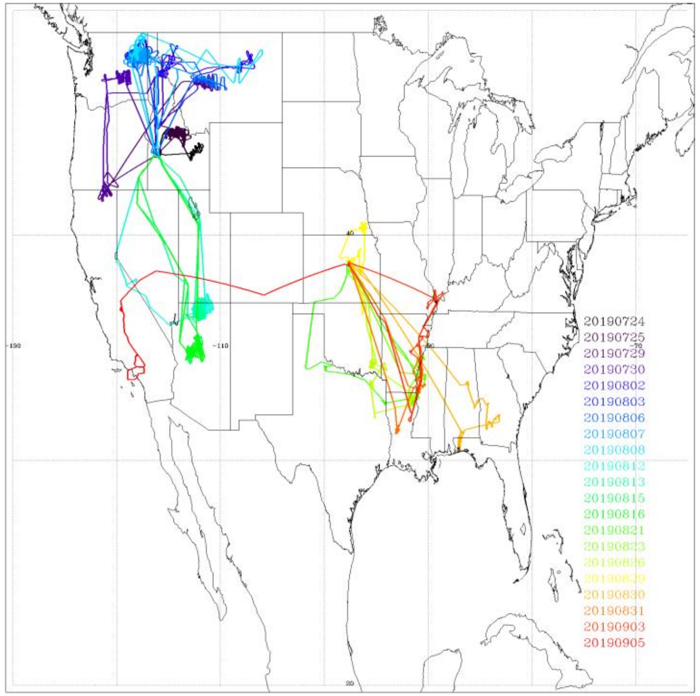
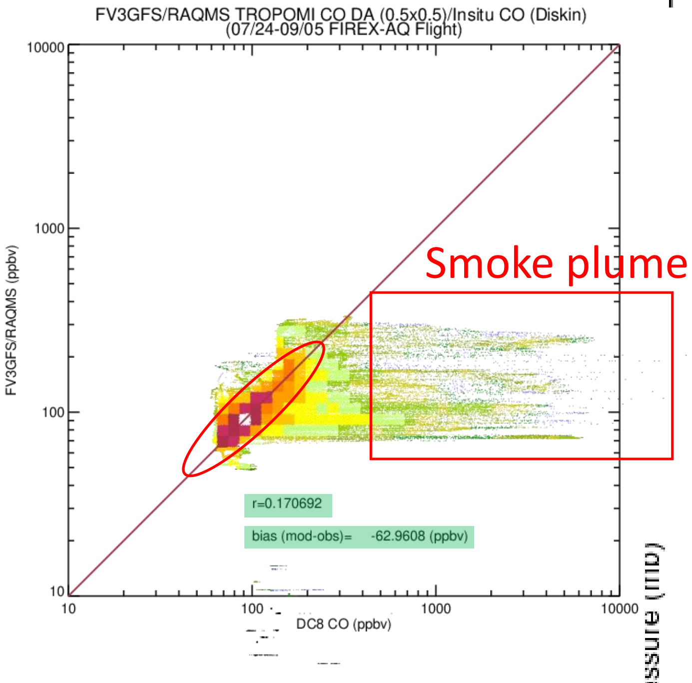
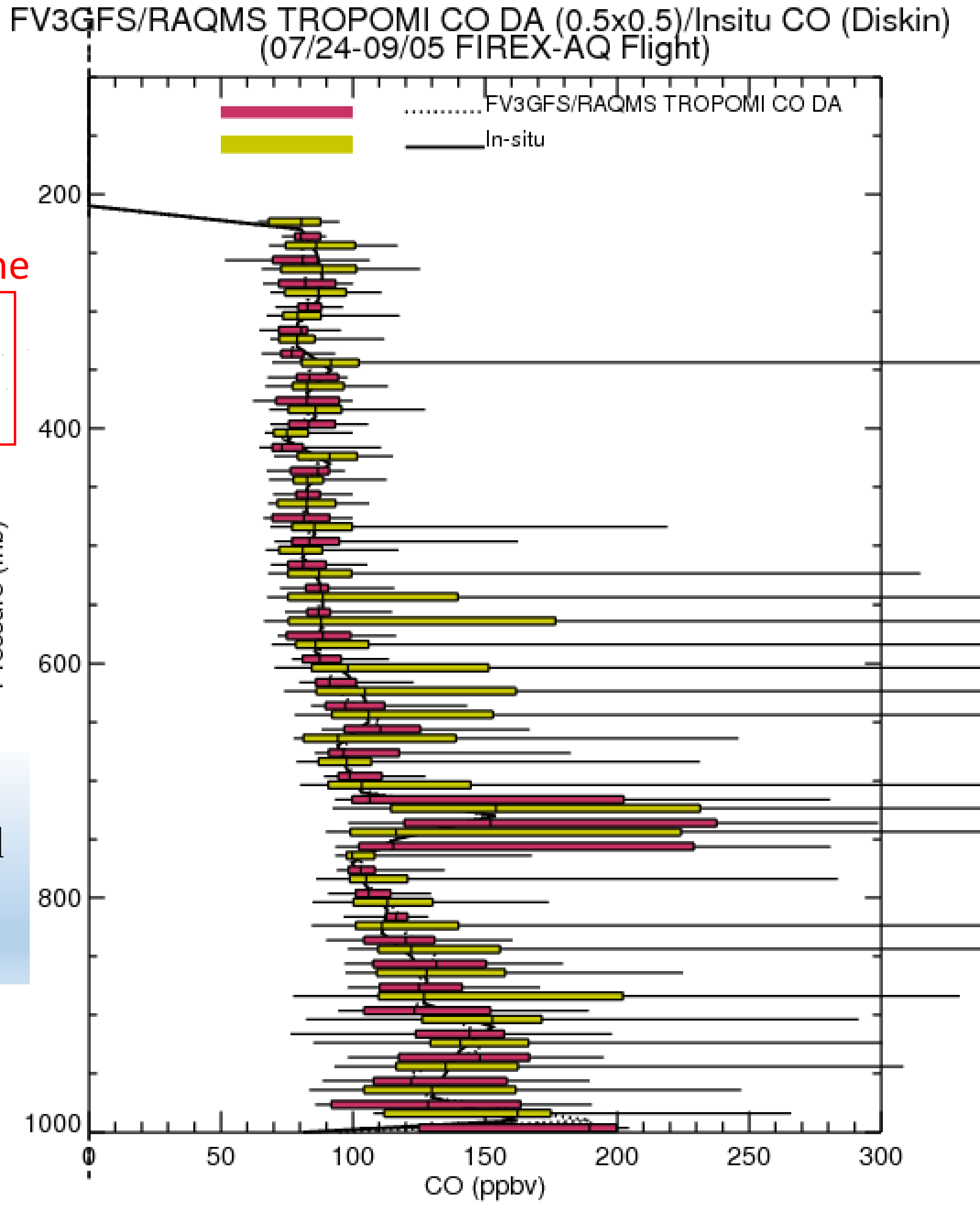
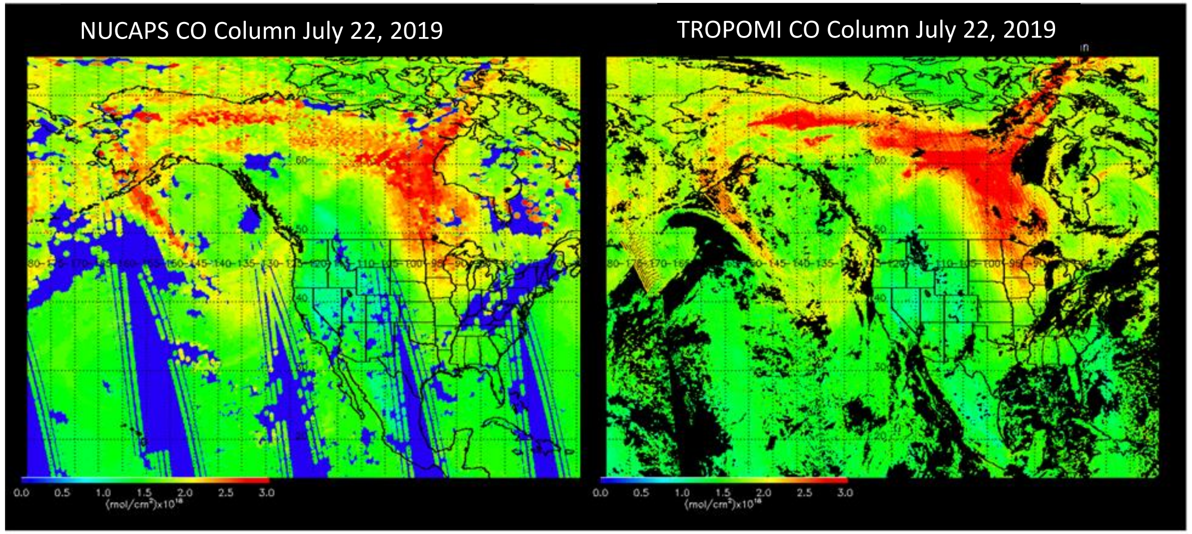




UFS-RAQMS (TROPOMI DA)

Comparison with airborne insitu CO measurements shows improved representation of background CO during FIREX-AQ

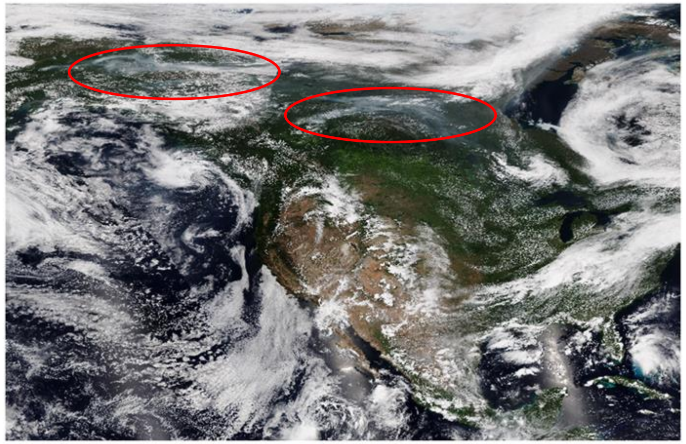




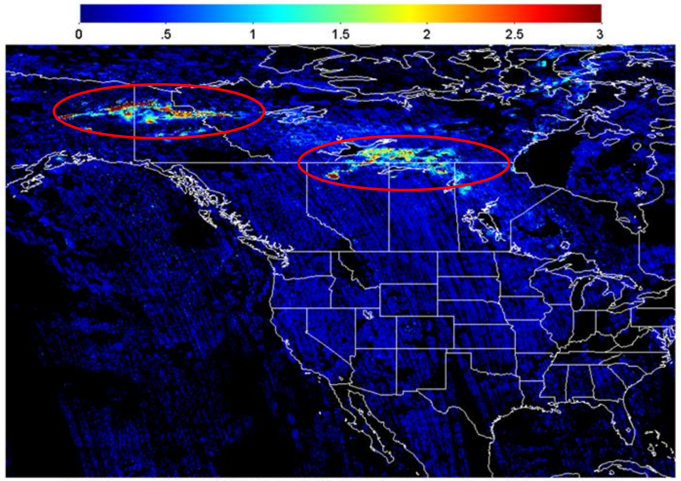
Question: What additional IR measurements would be ideal to augment the backbone?

- ***SWIR (to 2.3μm)+MWIR+LWIR hyperspectral geostationary sounder would allow <u>hourly</u> monitoring of boundary layer O3, CO, CH4, and CO2 for regional Air Quality and Climate services***

VIIRS True Color Imagery July 22, 2019



TROPOMI-NUCAPS CO Column July 22, 2019



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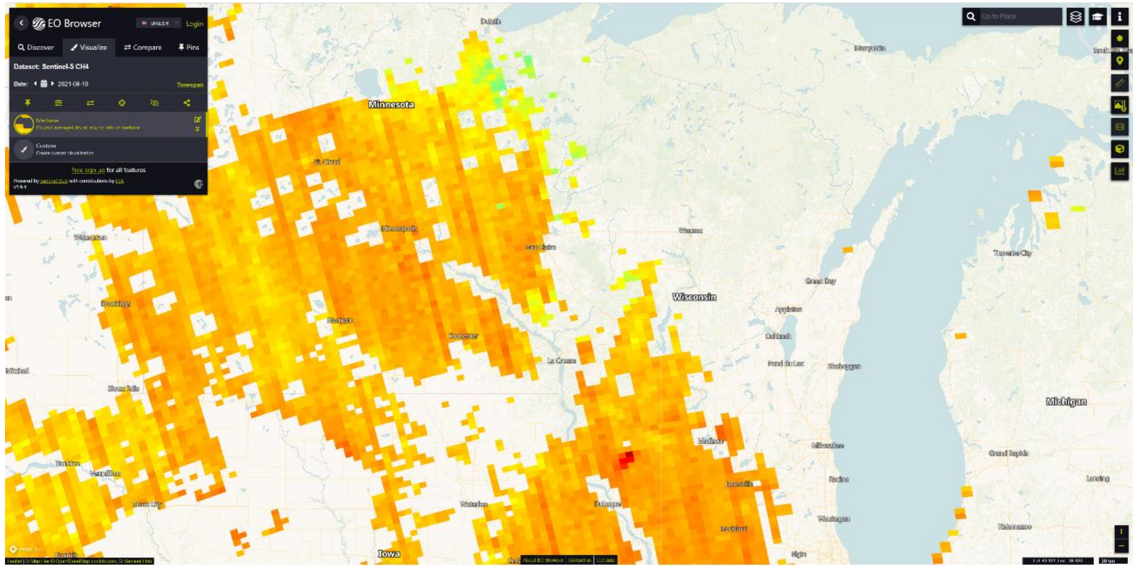
TROPOMI CH4 Column, September 10, 2021



Addition of SWIR (2.3μm-3.7μm) band would allow for DOAS reflected solar column CO and CH4 retrievals

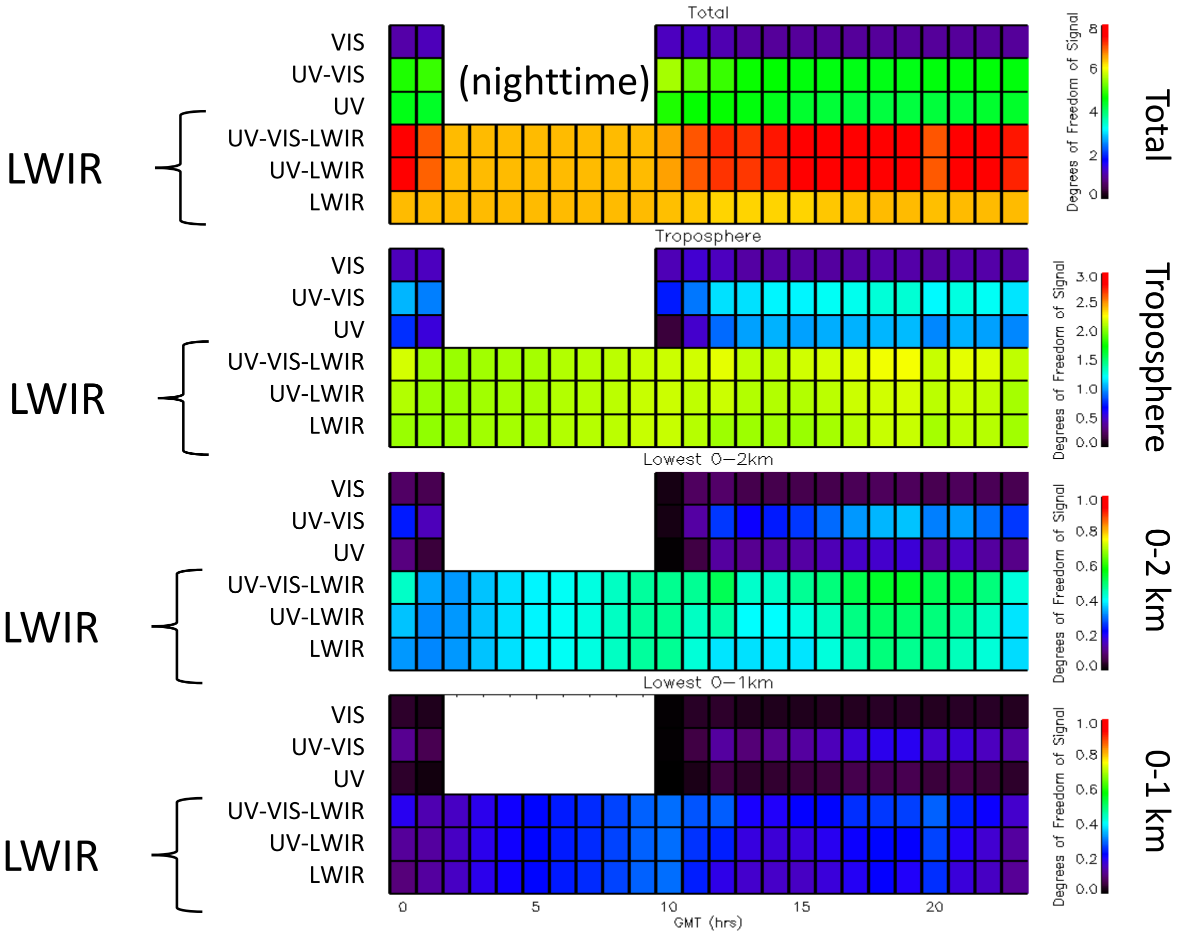
- Combination of mid-troposphere emitted and solar reflected could enhance boundary layer CO and CH4 sensitivities

Demonstration of the impact of assimilating geostationary UV, UV-VIS, and UV-VIS-LWIR ozone profile retrievals (Regional OSSE)

With Vijay Natraj[1], Allen Lenzen[2], Susan Kulawik[3], Helen Worden[4], Xiong Liu[5], Mike Newchurch[6]

1- Jet Propulsion Laboratory, California Institute of Technology
2- Space Science and Engineering Center, University of Wisconsin-Madison
3- Bay Area Environmental Research Institute
4- National Center for Atmospheric Research
5- Harvard-Smithsonian Center for Astrophysics
6- University of Alabama, Huntsville

Multispectral O_3 Retrievals



Full Optimal Estimation Retrievals
(UV, UV-VIS, UV-VIS-LWIR)

Diurnally resolved Degrees of Freedom for Signal (DOFS) for different pressure ranges and spectral combinations for all Regional OSSE sites (no VIS, UV, or UV/VIS retrievals between 02-09Z)

- **UV/VIS has the same spectral range and noise as TEMPO.**
- **TIR has same spectral range and noise as TES**

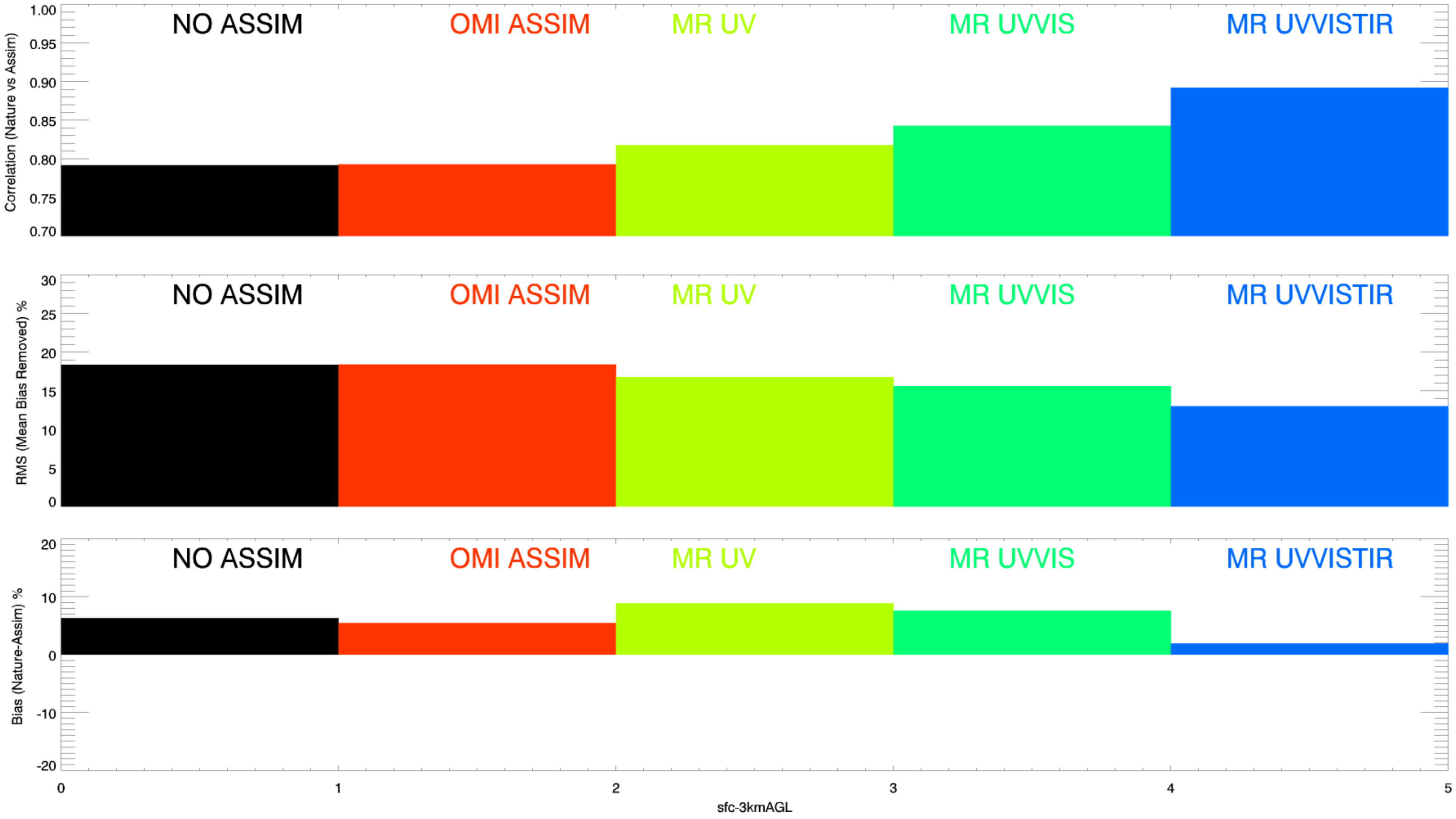
Data Assimilation

WRF-CHEM/GSI (3D-VAR) Regional/Urban O3 OSSE Study – July 2011

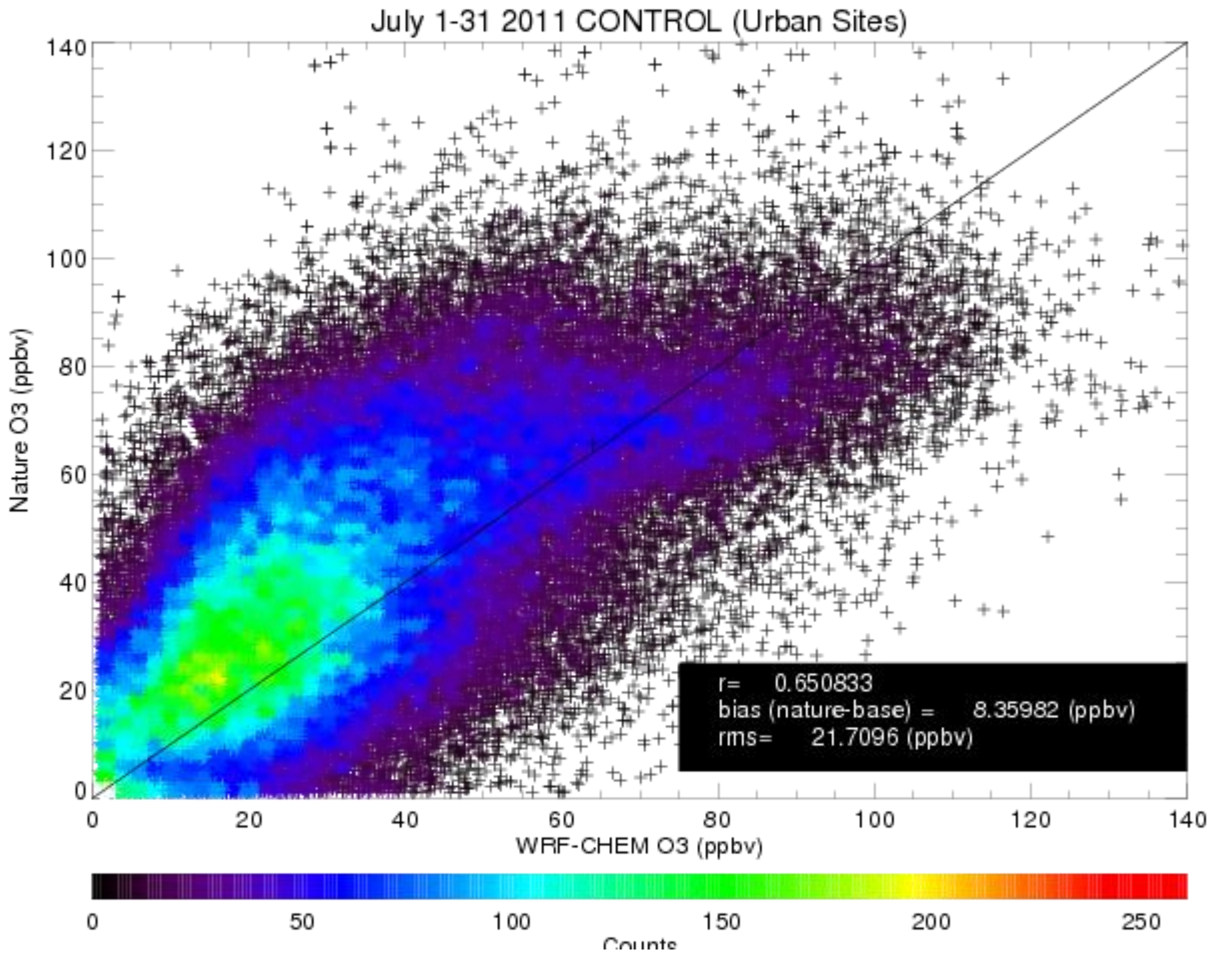
- Control
- Synthetic OMI (using retrieval efficiency factors and apriori)
- Multiple Regression UV-VIS-LWIR synthetic retrievals
- Multiple Regression UV-VIS synthetic retrievals
- Multiple Regression UV synthetic retrievals

- All DA experiments include:
  - 1 hour cycling
  - Inflation of background error covariances near surface
  - Application of tangent linear observation operator (AK) in GSI enter loop
- Results compared to nature run integrated over atmospheric layers and at AIRNow surface sites

Impact of Assimilation: sfc-3km Results



Impact of UV-VIS-LWIR Assimilation: Urban AIRNOW Sites



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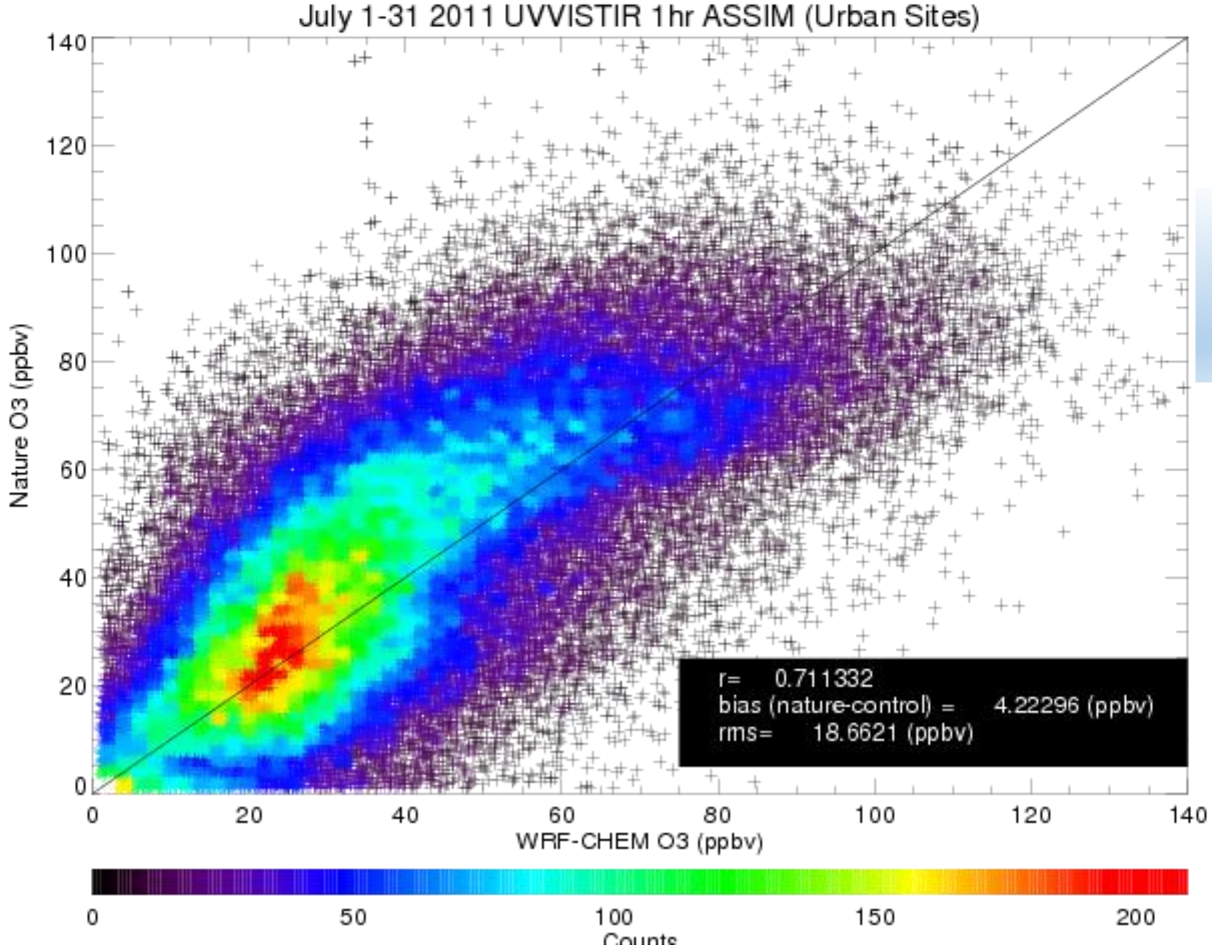
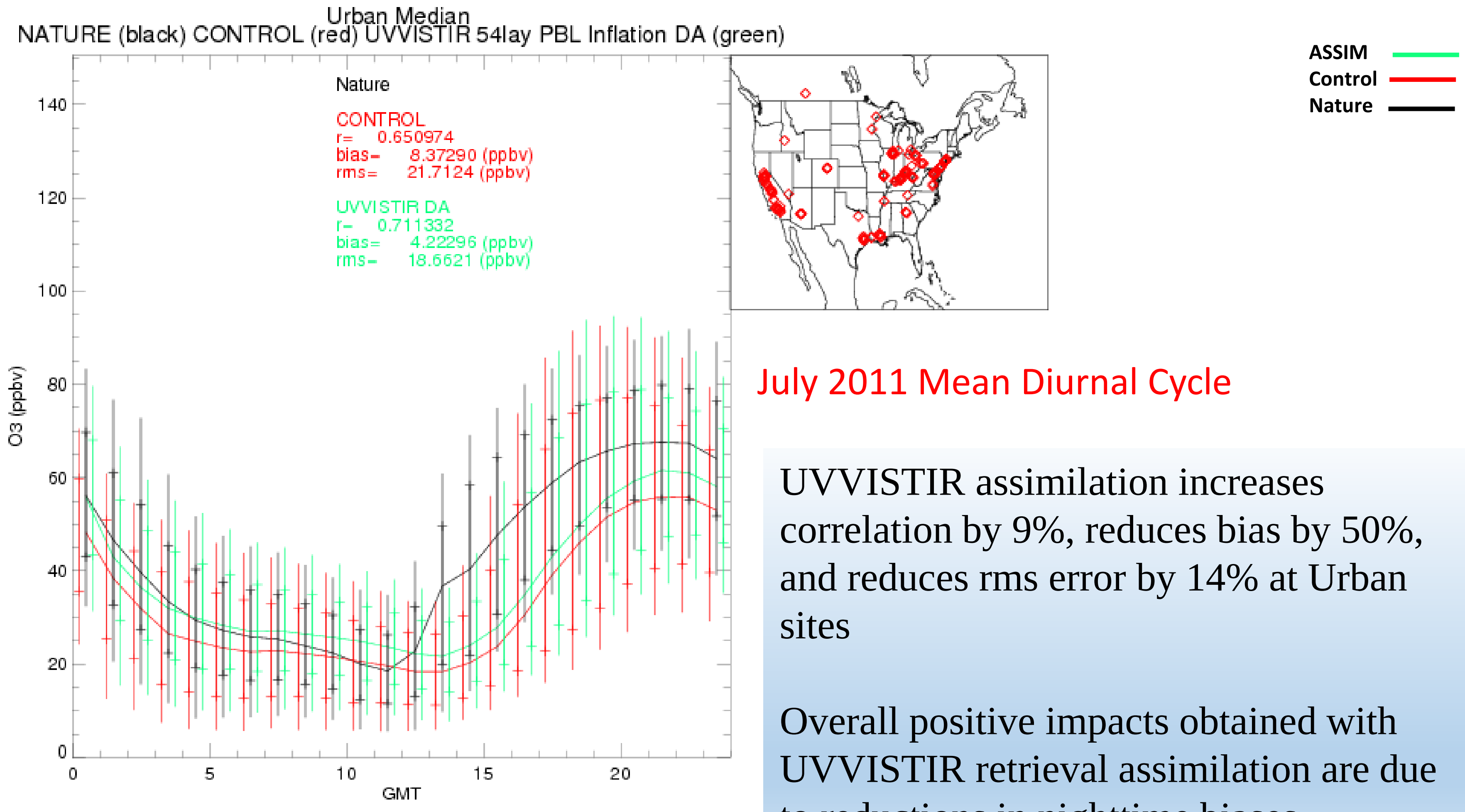


Assimilation of UV-VIS-SWIR O3 leads to improved correlation, reduced bias, lower RMSE

Impact of UV-VIS-LWIR Assimilation: Urban AIRNOW Sites



July 2011 Mean Diurnal Cycle

UVVISTIR assimilation increases correlation by 9%, reduces bias by 50%, and reduces rms error by 14% at Urban sites

Overall positive impacts obtained with UVVISTIR retrieval assimilation are due to reductions in nighttime biases.

Summary:

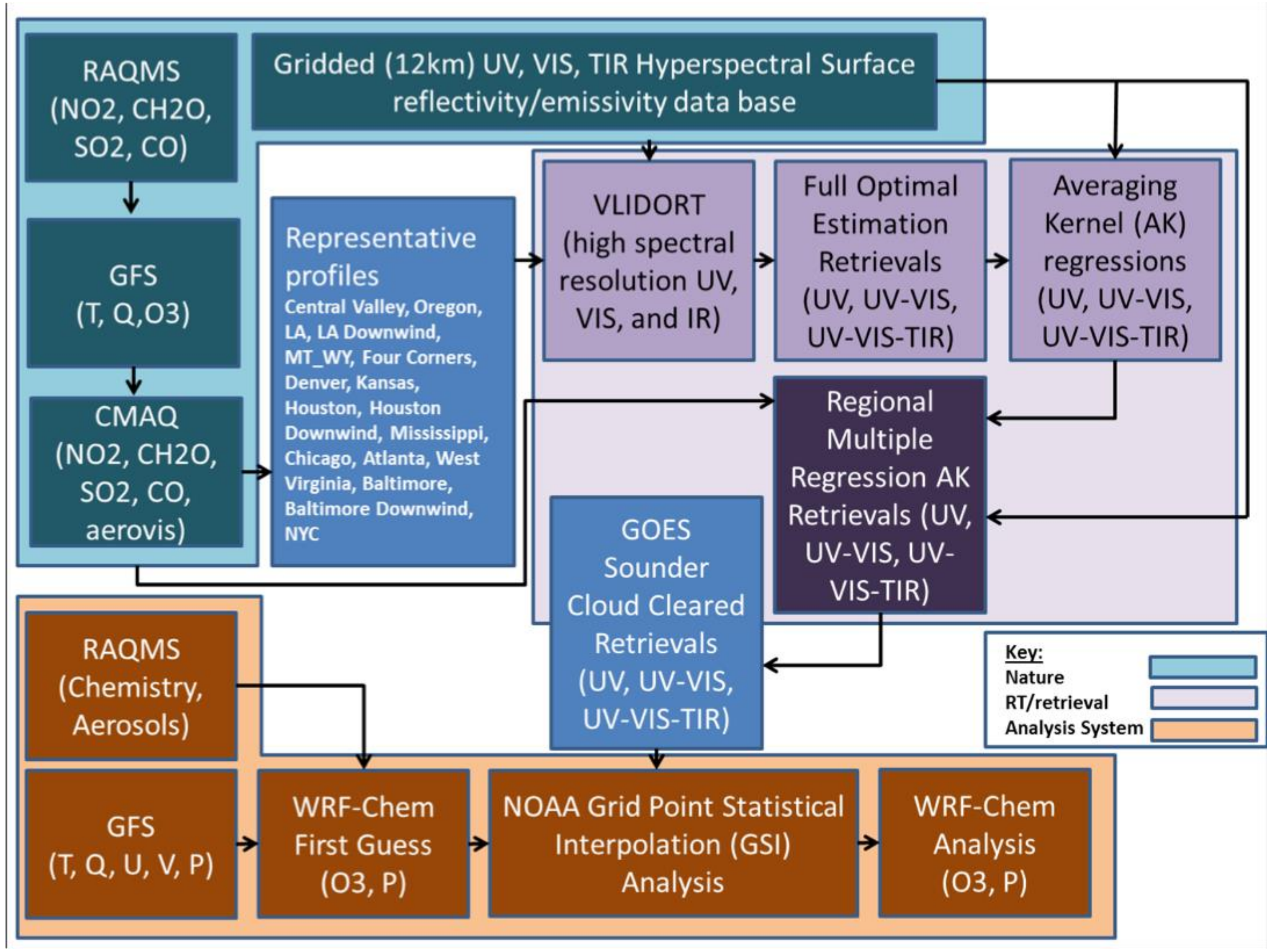
- A LEO hyperspectral IR Sounder with SWIR (CO, CO_2), MWIR (CH_4) and LWIR (O_3) capabilities is critical for supporting global Air Quality and Climate services.

- Extending the SWIR down to 2.3mm would allow improved detection of boundary layer CO (wildfires) and CH_4 (GHG emissions)

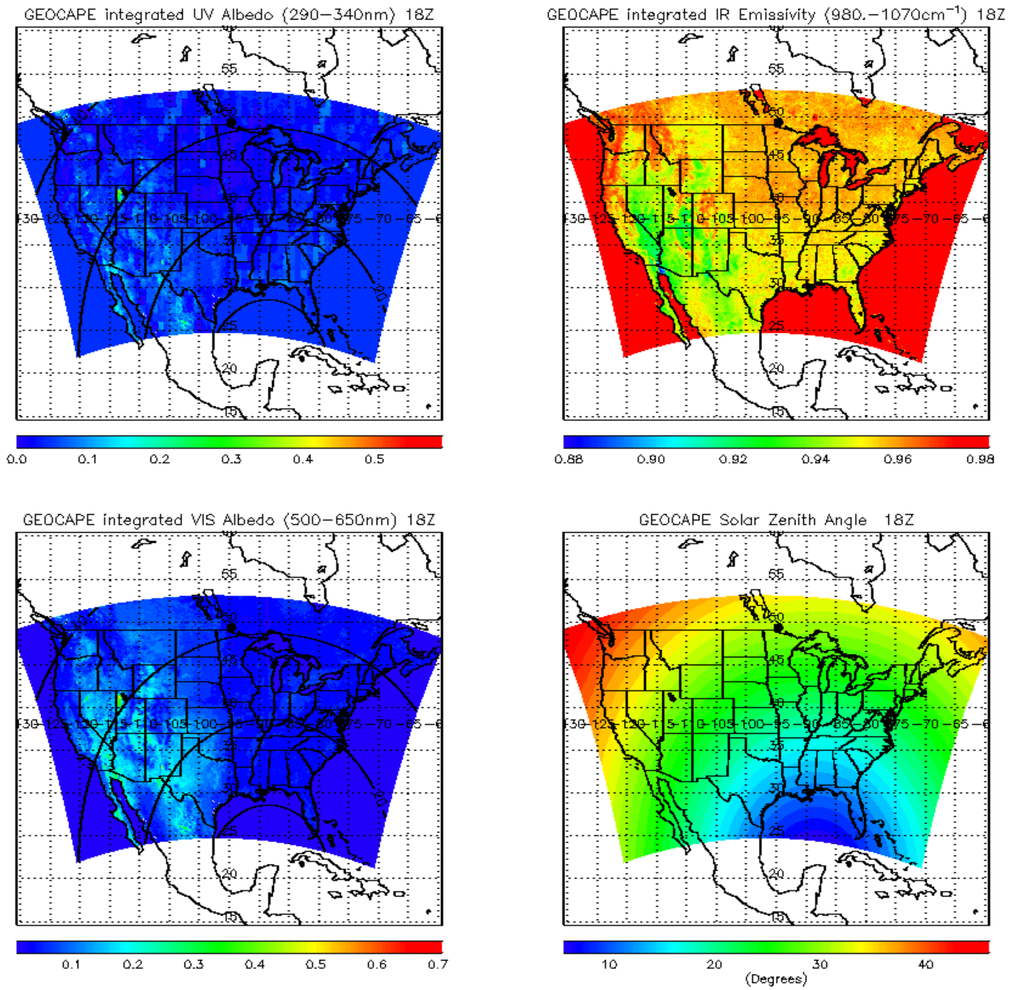
- SWIR (to 2.3mm)+MWIR+LWIR hyperspectral geostationary sounder combined with UV or UV-VIS (TEMPO like) instrument would allow hourly monitoring of boundary layer O_3, CO, CH_4, and CO_2 for regional Air Quality and Climate services

Extra Slides

OSSE Flow Chart



Nature
High Spectral Resolution Emissivity



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