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

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## CrIS Specs for Baseline Reference

<table>
<thead>
<tr>
<th></th>
<th>SWIR</th>
<th>MWIR</th>
<th>LWIR</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reference Range (microns)</td>
<td>3.7-6.6</td>
<td>6.6-8.6</td>
<td>8.6-15.38</td>
</tr>
<tr>
<td>Desired Range (gaps/ no gaps)</td>
<td>3.92-4.64</td>
<td>5.71-8.26</td>
<td>9.14-15.38</td>
</tr>
<tr>
<td>Desired Spectral Resolution</td>
<td>0.625 cm-1</td>
<td>0.625 cm-1</td>
<td>0.625 cm-1</td>
</tr>
<tr>
<td>NEDN/NEDT</td>
<td>CrIS noise levels</td>
<td>CrIS noise levels</td>
<td>CrIS noise levels</td>
</tr>
<tr>
<td>Horizontal Resolution/ GSD at Nadir</td>
<td>14 km @ 832 km altitude</td>
<td>14 km @ 832 km altitude</td>
<td>14 km @ 832 km altitude</td>
</tr>
<tr>
<td>Swath (km)</td>
<td>2200 km @ 832 km altitude</td>
<td>2200 km @ 832 km altitude</td>
<td>2200 km @ 832 km altitude</td>
</tr>
</tbody>
</table>
Infrared Radiative influences of Ozone, CO, CH4, CO2, N2O and other GHG are significant.

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

$r=0.643$
Bias=$0.011 \times 10^{18}\text{mol/cm}^2$

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)

\[ r = 0.875 \]
\[ \text{Bias} = -0.034 \times 10^{18} \text{mol/cm}^2 \]

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
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)
Aura Chemical Reanalysis 2006-2016

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• Earth Observations
  **OMI:** Total Column \(O_3\), Tropospheric \(NO_2\) Column
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HIPPO III Flight Tracks Mar 20 – Apr 20, 2010

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

Note change in color scale!

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

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
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
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 2.3 μm)** + MWIR + LWIR hyperspectral geostationary sounder would allow **hourly monitoring** of boundary layer O3, CO, CH4, and CO2 for regional Air Quality and Climate services.

Addition of SWIR (2.3 μm-3.7 μm) 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 Natraj¹, Allen Lenzen², Susan Kulawik³, Helen Worden⁴, Xiong Liu⁵, Mike Newchurch⁶

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 O₃ Retrievals

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

Assimilation of UV-VIS-SWIR O3 leads to improved correlation, reduced bias, lower RMSE
Impact of UV-VIS-LWIR Assimilation: Urban AIRNOW Sites

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.
A LEO hyperspectral IR Sounder with SWIR (CO, CO2), MWIR (CH4) and LWIR (O3) 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 CH4 (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 O3, CO, CH4, and CO2 for regional Air Quality and Climate services.
Extra Slides
OSSE Flow Chart
Nature
High Spectral Resolution Emissivity
Nature
High Spectral Resolution Emissivity