Joint AIRS+OMI Ozone Profile data for KORUS-AQ:
Updates on Validation and Science Applications

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04 NOAA/NESDIS Center for Satellite Applications and Research, USA

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A new generation of geostationary and low-earth orbiting (LEO) sounders will form a new composition-climate constellation.

- Geostationary sounders including GEO-CAPE, TEMPO, Sentinel-4, GEMS will provide an unprecedented number of composition observations at high spatial resolution.
- LEO sounders including IASI, CrIS, S5p provide the global picture and thread the geostationary observations together.

How does the constellation improve knowledge of global air quality?
Measurements from TIR (LW) are sensitive to the free-tropospheric trace gases. Measurements from UV-Vis-NIR (SW) are sensitive to the column abundances of trace gases. Joint LW/SW or ultra-high spectral resolution measurements can distinguish upper/lower troposphere.
Connecting remote sensing to assimilation

Optimal estimation (OE) techniques and error diagnostics (e.g., Bowman et al, 2002, 2006; Worden et al, 2004; Kulawik et al, 2006, 2008) for remote sensing along with the development of instrument operators for evaluation against models and assimilation are critical (Jones et al, 2003, Miyazaki et al, 2015).
This work combines AIRS single footprint L1B radiances to OMI measured radiances for retrieving O$_3$ profiles.
AIRS/OMI O$_3$ Compare well with TES Global Survey Mode

Fu et al., Submit to AMT 2018.

<table>
<thead>
<tr>
<th>Joint AIRS+OMI</th>
<th>316 hPa</th>
<th>510 hPa</th>
<th>750 hPa</th>
</tr>
</thead>
<tbody>
<tr>
<td>May 2006</td>
<td>A1</td>
<td>A2</td>
<td>A3</td>
</tr>
<tr>
<td>TES v6</td>
<td>B1</td>
<td>B2</td>
<td>B3</td>
</tr>
</tbody>
</table>

Miyazaki et al., Submit to JGR 2018

- **May 2016; 510 hPa**
- CHASER-DA system assimilated OMI (NO$_2$), GOME-2 (NO$_2$) MLS (HNO$_3$ and O$_3$), MOPITT (CO)
Comparisons to WOUDC Ozonesondes

<table>
<thead>
<tr>
<th>Pressure (hPa)</th>
<th>Spring Mean (ppb)</th>
<th>Spring Mean (%)</th>
<th>Spring RMS (ppb)</th>
<th>Spring RMS (%)</th>
<th>Summer Mean (ppb)</th>
<th>Summer Mean (%)</th>
<th>Summer RMS (ppb)</th>
<th>Summer RMS (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>316 hPa</td>
<td>AIRS+OMI</td>
<td>TES</td>
<td>AIRS+OMI</td>
<td>TES</td>
<td>AIRS+OMI</td>
<td>TES</td>
<td>AIRS+OMI</td>
<td>TES</td>
</tr>
<tr>
<td>Spring</td>
<td>2.8</td>
<td>6.1</td>
<td>0.7</td>
<td>13.4</td>
<td>4.2</td>
<td>6.6</td>
<td>17.0</td>
<td>23.8</td>
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<tr>
<td>Summer</td>
<td>1.3</td>
<td>8.6</td>
<td>2.2</td>
<td>6.6</td>
<td>6.6</td>
<td>7.3</td>
<td>10.6</td>
<td>17.9</td>
</tr>
<tr>
<td>510 hPa</td>
<td>AIRS+OMI</td>
<td>TES</td>
<td>AIRS+OMI</td>
<td>TES</td>
<td>AIRS+OMI</td>
<td>TES</td>
<td>AIRS+OMI</td>
<td>TES</td>
</tr>
<tr>
<td>Spring</td>
<td>1.3</td>
<td>3.6</td>
<td>-0.8</td>
<td>17.2</td>
<td>3.5</td>
<td>17.4</td>
<td>17.9</td>
<td>25.3</td>
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<tr>
<td>Summer</td>
<td>3.8</td>
<td>7.0</td>
<td>1.6</td>
<td>17.2</td>
<td>7.3</td>
<td>17.4</td>
<td>17.9</td>
<td>25.3</td>
</tr>
<tr>
<td>750 hPa</td>
<td>AIRS+OMI</td>
<td>TES</td>
<td>AIRS+OMI</td>
<td>TES</td>
<td>AIRS+OMI</td>
<td>TES</td>
<td>AIRS+OMI</td>
<td>TES</td>
</tr>
<tr>
<td>Spring</td>
<td>2.4</td>
<td>1.7</td>
<td>-2.2</td>
<td>21.1</td>
<td>2.6</td>
<td>16.2</td>
<td>18.8</td>
<td>25.3</td>
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<tr>
<td>Summer</td>
<td>8.0</td>
<td>3.4</td>
<td>-2.0</td>
<td>21.1</td>
<td>6.6</td>
<td>6.9</td>
<td>8.6</td>
<td>12.5</td>
</tr>
</tbody>
</table>

Number of WOUDC Sonde Sites: 20 25 27 30
Number of Satellite/Sonde Coincident: 131 197 134 171

Coincident criteria:
- Passed retrieval quality check
- Distance within 300 km
- Time diff. within 4 hours
- Day Time; March, April, May (MAM) 2006
- Day Time; June, July, August (JJA) 2006

Fu et al., Submit to AMT 2018.
Joint AIRS/OMI ozone profiles have been assimilated into CHASER system.

CHASER system assimilated the OMI (NO$_2$), GOME-2 (NO$_2$) MLS (HNO$_3$ and O$_3$), MOPITT (CO) for KORUS-AQ, recently assimilated AIRS/OMI ozone profile data.
### Differences in comparison to AIRS+OMI Obs. (ppb)

<table>
<thead>
<tr>
<th>Differences in comparison to AIRS+OMI Obs. (ppb)</th>
<th>GL SH: 55°-15°S</th>
<th>GL TR: 15°S-15°N</th>
<th>GL NH: 15°-55°S</th>
<th>RE</th>
</tr>
</thead>
<tbody>
<tr>
<td>Model</td>
<td>Bias</td>
<td>RMSE</td>
<td>Bias</td>
<td>RMSE</td>
</tr>
<tr>
<td>510 HPa</td>
<td>4.0</td>
<td>8.3</td>
<td>-12.2</td>
<td>14.4</td>
</tr>
<tr>
<td>Reanalysis</td>
<td>4.5</td>
<td>6.0</td>
<td>-1.8</td>
<td>6.5</td>
</tr>
<tr>
<td>AIRS/OMI assim</td>
<td>-0.2</td>
<td>3.7</td>
<td>-5.3</td>
<td>7.1</td>
</tr>
</tbody>
</table>

Phase 1: May 1-16
Phase 2: May 17-22
Phase 3: May 25-31 (OMI instrument issue)
Phase 4: June 1-6 (OMI instrument issue)
The AIRS/OMI O₃ retrievals have been configured in two modes.

- **Global survey (GS) mode**
  - Provides profile data with a spatial sampling similar to TES global survey
  - 28-month data have been processed including
    - 2006 Jan – Dec
    - 2016 Mar – Jun
    - 2007 Jan – Dec
  - **Year 2006 and Mar-June 2016** GS data are available via the link ([AIRS-OMI combined products](https://tes.jpl.nasa.gov/data/)) at [https://tes.jpl.nasa.gov/data/](https://tes.jpl.nasa.gov/data/)

- **Regional mapping (RE) mode**
  - Processes all available measurements for flight campaigns including
    - **KORUS-AQ, Apr – Jun 2016**
    - **ORACLES, Aug, Sept 2016**
    - **POSIDON, Sept, Oct 2016**
  - **KORUS-AQ (Apr-June 2016) RE** data are available via the link ([AIRS-OMI combined products](https://tes.jpl.nasa.gov/data/)) at [https://tes.jpl.nasa.gov/data/](https://tes.jpl.nasa.gov/data/)

Data products have been saved in Hierarchical Data Format, a common format used in the NASA Earth Observation System level 2 products.
In October 13, 2017, ESA Sentinel 5 Precursor (S5P) launched successfully, forming a satellite constellation with Suomi-NPP satellite.

It provides an unique opportunity to extend and improve the MOPITT joint TIR/NIR CO data, via combining CrIS/TROPOMI measurements [Fu et al., AMT, 2016]

**XCO maps:** near surface partial column averaged VMR [surface to ~750 hPa]
Hazard of Thomas Fire
Location: near Los Angeles, California, USA
Date: Dec 4, 2017 - Jan 12, 2018
Burn Area: 281,893 acres; ~1,140 km²
Buildings Destroyed: 1,063
Fatalities: 1 firefighter, 1 civilian (20 indirectly)

SNPP Synergic Observations
December 12, 2017
[A] VIIRS image of fire plume
[B1-4] CrIS Carbon monoxide VMR
[B1] Day time; 316 hPa
[B2] Day time; 510 hPa
[B3] Night time; 316 hPa
[B4] Night time; 510 hPa

- CO volume mixing ratio profiles (VMR) retrieved using JPL multi-spectra, multi-Species, multi-sensors (MUSES) [Fu et al, 2013, 2016]
- Provides retrieved profiles and observation operators
- 9X finer spatial resolution than the operational AIRS/CrIS products
- Algorithm heritage of TES, OMI, OCO-2, have been applied to TES, AIRS, CrIS, TROPOMI, OMI, OMPS, OCO2 for a suite of species including CO, O3, CH4, H2O, HDO, CH3OH, PAN, NH3, CO2

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MUSES retrieval algorithm can combine radiances measured from long wavelength (TES, AIRS, CrIS) and short wavelength (OMI, OMPS, TROPOMI) space sensors to retrieve the vertical concentration profiles of primary gaseous pollutants including O$_3$ and CO.

- Joint AIRS/OMI and CrIS/OMPS retrieved O$_3$ profiles can distinguish the abundances in the upper troposphere from the lower troposphere.
- Joint CrIS/TROPOMI would help in extending the MOPITT CO profile data.

The observation operators of joint AIRS/OMI data products enable data assimilation, e.g., “CHASER-DA”, demonstrating the significant impacts on ozone distributions.

The O$_3$ and CO data products from MUSES algorithm could help in the quantitative attribution of anthropogenic emissions and natural influences of pollutants for NASA KORUS-AQ and NOAA FIREX.
The differences are within the estimated uncertainty.

<table>
<thead>
<tr>
<th></th>
<th>316 hPa</th>
<th></th>
<th></th>
<th></th>
<th>510 hPa</th>
<th></th>
<th></th>
<th></th>
<th>750 hPa</th>
<th></th>
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</thead>
<tbody>
<tr>
<td></td>
<td>Mar</td>
<td>Apr</td>
<td>May</td>
<td>Jun</td>
<td>Mar</td>
<td>Apr</td>
<td>May</td>
<td>Jun</td>
<td>Mar</td>
<td>Apr</td>
<td>May</td>
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<tr>
<td>Pearson Correlation Coefficient</td>
<td>0.85</td>
<td>0.84</td>
<td>0.84</td>
<td>0.84</td>
<td>0.87</td>
<td>0.88</td>
<td>0.89</td>
<td>0.86</td>
<td>0.90</td>
<td>0.90</td>
<td>0.90</td>
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<tr>
<td>Mean (ppb)</td>
<td>-7.3</td>
<td>-6.9</td>
<td>-8.1</td>
<td>-6.0</td>
<td>-2.9</td>
<td>-3.3</td>
<td>-3.6</td>
<td>-4.1</td>
<td>4.9</td>
<td>4.2</td>
<td>4.2</td>
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<tr>
<td>RMS (ppb)</td>
<td>21.5</td>
<td>21.6</td>
<td>22.6</td>
<td>19.8</td>
<td>8.6</td>
<td>8.9</td>
<td>9.2</td>
<td>9.5</td>
<td>5.0</td>
<td>5.0</td>
<td>5.0</td>
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<tr>
<td>Mean (%)</td>
<td>9.8</td>
<td>7.3</td>
<td>7.3</td>
<td>-5.0</td>
<td>4.9</td>
<td>4.2</td>
<td>4.2</td>
<td>-4.5</td>
<td>17.3</td>
<td>18.2</td>
<td>16.4</td>
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<td>RMS (%)</td>
<td>24.2</td>
<td>25.7</td>
<td>24.7</td>
<td>23.8</td>
<td>19.6</td>
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<td>19.5</td>
<td>22.4</td>
<td>22.9</td>
<td>24.1</td>
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<tr>
<td>Total Uncertainty</td>
<td>28.6</td>
<td>28.9</td>
<td>28.5</td>
<td>28.0</td>
<td>28.6</td>
<td>28.9</td>
<td>28.5</td>
<td>28.0</td>
<td>28.6</td>
<td>28.9</td>
<td>28.5</td>
</tr>
<tr>
<td>AIRS+OMI O₃ (%)</td>
<td>22.5</td>
<td>23.0</td>
<td>22.9</td>
<td>22.1</td>
<td>22.5</td>
<td>23.0</td>
<td>22.9</td>
<td>22.1</td>
<td>22.5</td>
<td>23.0</td>
<td>22.9</td>
</tr>
<tr>
<td>TES V6 O₃ (%)</td>
<td>22.5</td>
<td>23.0</td>
<td>22.9</td>
<td>22.1</td>
<td>22.5</td>
<td>23.0</td>
<td>22.9</td>
<td>22.1</td>
<td>22.5</td>
<td>23.0</td>
<td>22.9</td>
</tr>
</tbody>
</table>

Fu et al., Submit to AMT 2018.
Performances of GS and RE mode joint AIRS/OMI data

- Diff. (Reanalysis without Joint AIRS+OMI – Joint AIRS+OMI Obs.) < (Model - Joint AIRS+OMI Obs.)
- Reanalysis without Joint AIRS+OMI closely agree to joint AIRS+OMI ozone with a mean bias of
  - 0.9 ppbv for RE mode
  - 4.2 ppbv in the northern extratropics
  - -1.8 ppbv in the tropics
  - 4.5 ppbv in the southern hemisphere
Joint AIRS/OMI $O_3$ Maps for KORUS-AQ Campaign

- Korea-US Air Quality study (KORUS-AQ) - International Cooperative Air Quality Field Study
- Joint AIRS/OMI $O_3$ profile data
  - Total ozone shows strong latitudinal dependence, dominated by stratospheric ozone.
  - The pattern of enhancement (Upper tropospheric $>$ Lower tropospheric) over Korean peninsula $<$ Japan suggests either lofting and transport of pollution from the surface or the influence of stratosphere-troposphere exchange.

Three-day averaged May 18-20, 2016.
ARIS/OMI vs. TES v6 GS Trop DOFS

April 2006
Corr. R = 0.65;
Mean(TES/Joint) = 1.10
Mean(TES-Joint) = 0.04

May 2006
Corr. R = 0.58;
Mean(TES/Joint) = 1.10
Mean(TES-Joint) = 0.03

June 2006
Corr. R = 0.51;
Mean(TES/Joint) = 1.14
Mean(TES-Joint) = 0.07

Fu et al., Submit to AMT 2018.
**Fire Influence on Regional and Global Environments Experiment (FIREX)** is to study the impact of biomass burning of western North America fires on climate and air quality.

**JPL/UW-Madison team** will combine high vertical/spatial resolution $O_3$ and CO data with chemical data assimilation to provide a critical synoptic context for quantifying the role of fires on atmospheric composition and air quality.

**JPL MUSES algorithm will provide**

- CrIS CO profile data
  - nine times higher spatial resolution vs. the CrIS operational data products
- Joint CrIS/OMPS $O_3$ profile data
  - could distinguish upper/lower troposphere, similar to AIRS/OMI $O_3$, but 3X spatial coverage
- Both CO and $O_3$ profile data products provide full observation operators readily for data assimilation/model evaluation

**UW-Madison Real time Air Quality Modeling System (RAQMS) will provide**

- Real-time assimilation
  - Aura-MLS stratospheric ozone profiles (>50mb)
  - Aura-OMI total ozone column (cloud cleared)
  - MODIS aerosol optical depth
- Real-time fire detection via MODIS data
- Will assimilate JPL CrIS CO and joint CrIS/OMPS $O_3$ profile data
Plume of biomass burning observed on August 5, 2017

CrIS CO profiles were retrieved using single footprint CrIS full spectral resolution data.

MUSES algorithm retrieves trace gases profiles, cloud optical depths, surface properties and temperature profiles.
Comparisons of MUSES-CrIS and RAQMS CO Data

- Used CrIS single footprint full spectral resolution L1B radiances in the retrievals
- MUSES CrIS CO data show agreement to the RAQMS model fields that were applied the observation operators of CrIS CO.
- Collaborating with Dr. Pierce at UW-Madison for assimilating CrIS CO data into the RAQMS model

<table>
<thead>
<tr>
<th>Applying MUSES CrIS CO Observation Operator to RAQMS Predicted CO Fields</th>
<th>Correlation Coefficient</th>
<th>Mean Diff</th>
<th>RMS</th>
</tr>
</thead>
<tbody>
<tr>
<td>With</td>
<td>0.68</td>
<td>-0.15</td>
<td>6.9</td>
</tr>
<tr>
<td>Without</td>
<td>0.40</td>
<td>-0.15</td>
<td>6.6</td>
</tr>
</tbody>
</table>
JPL MUSES algorithm delivers both retrieved trace gas concentration profiles and observation operators needed for trend analysis, climate model evaluation, and data assimilation.

E.g., a data assimilation system applies an observation operator (H)

\[ y^s = H(x) = x_a + A(x_{model} - x_a) \]

\( y^s \) is the model profiles; \( x_a \) is a priori profiles used in the retrievals; \( A \) is the averaging kernels of satellite observations.

After applying observation operator to model profiles, the satellite-model differences (\( y^o - y^s \)) is not biased by the a priori used in the retrievals.

\[ \Delta y = y^o - y^s = A(x_{true} - x_{model}) + \epsilon \]