Data assimilation applications of sounder composition products

Kazuyuki Miyazaki, Kevin Bowman, Vivienne Payne, Jet Propulsion Laboratory, California Institute of Technology
What is the impact of IR soundings in regional and global models?

What is the optimum latency for regional and global models?

Impact of IR sounders on reanalysis for climate studies

Do you use IR soundings for both retrievals as well as direct assimilation in operations? How are retrievals used?
1. Emissions

-3 TgN/yr = 10% of global total emissions
≈ Europe (4.1 TgN/yr), US (4.2 TgN/yr), India (3.4 TgN/yr)

Miyazaki et al., 2020a
MDA8 ozone and PM2.5 response to the COVID emission anomaly

2. Concentrations

- Up to +16 ppb for MDA8 ozone
- Up to 23 µgm⁻³ for PM2.5 for a single day

(Feb 15-25, 2020)

3. Health Impacts

- 2,100 more ozone-related and at least 60,000 fewer PM2.5-related morbidity incidences,
- Augmented efforts to reduce hospital admissions

Miyazaki et al., 2020a
MOMO-Chem (Multi-mOdel Multi-cOnstituent Chemical) Data Assimilation System

Tropospheric Chemical Reanalysis

- 16 years (2005-present), two-hourly, global, surface to lower stratosphere chemical concentrations of 35 species, including $O_3$, NOx, OH, $SO_2^+$, VOCs
- Anthropogenic, biogenic, biomass burning, and lightning emissions (NOx, CO, $SO_2$)
- Used in various science applications, including validation of NASA satellite products
- Able to support OSSE activities in support of mission formulation

Satellite Observations Assimilated in MOMO-Chem

Models Used for Assimilation

Validation against in-situ & aircraft measurements

Satellite Observations: (O3, CO, NO$_2$, HNO$_3$, CO)

Model: (4 models)
Multi-constituent multi-satellite chemical data assimilation

MLS (O₃,HNO₃)

TES

AIRS/OMI (O₃)

OMI, SCIAMACHY, GOME-2, TROPOMI (NO₂)

Stratosphere

Troposphere

from IGAC TOAR report

MOPITT (CO)

Monitoring

CrIS (O₃,PAN)

CrIS

(O₃,NH₃)

Monitoring

 Assimilation

SO₂ emissions

NOx emissions

CO emissions

Anthropogenic & Natural Emissions

NMVOCs

CO

CH₄

NO

NO₂

O₃

OH

H₂O

O₂

PAN

H₂O

O₃

Chemical Production

Aerosol-cloud chemistry

Advection

Mixing

Deposition

Chemical Destruction

Land

Ocean
Decadal tropospheric chemistry reanalysis: TCR-2

<table>
<thead>
<tr>
<th>Assimilation</th>
<th>2005</th>
<th>2010</th>
<th>2015</th>
<th>Year</th>
<th>2020</th>
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<tr>
<td>OMI NO₂</td>
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<td>TES O₃</td>
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<td>MLS O₃/HNO₃</td>
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<tr>
<td>MOPITT CO</td>
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<tr>
<td>OMI SO₂</td>
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<tr>
<td>TROPOMI NO₂</td>
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</tbody>
</table>

| Monitoring            |      |      |      |      |      |
| AIRS/OMI O₃           |      |      |      |      |      |
| TES/OMI O₃            |      |      |      |      |      |
| CrIS CO, PAN, O₃     |      |      |      |      |      |
IGAC TOAR-II chemical reanalysis Focus Working Group

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Dylan Jones, WG co-lead, Univ. of Toronto, Canada
Helen Worden, TOAR-II SC, NCAR, USA

Overview and Goals in support of TOAR-II

• Evaluation of chemical reanalyses with TOAR-II observations will assess the potential of using reanalysis data for studying spatial gradients at both regional and global scales and trends in areas with sparse in-situ observations.

• Assess the relative importance of individual observations to improve surface ozone analyses and help to design observing systems that better capture the distribution and regional trends in tropospheric ozone.

• Inter-comparisons of top-down precursor emissions from reanalyses, and their impacts on surface/tropospheric ozone and subsequent radiative effects will facilitate evaluation of emission scenarios and environmental policy in realistic conditions.

• Improve the TOAR-II observation quality control processes and representativeness
Ozone reanalysis inter-comparisons

<table>
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<tr>
<th>Products</th>
<th>Model</th>
<th>DA</th>
<th>Period</th>
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<td>CAMS-iRA</td>
<td>IFS (CB05) T159 (1.1)</td>
<td>4D-VAR</td>
<td>2003-2018</td>
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<tr>
<td>CAMS-RA</td>
<td>IFS(CB05)+Aerosol T255 (0.7)</td>
<td>4D-VAR</td>
<td>2003-present</td>
</tr>
<tr>
<td>TCR-1</td>
<td>CHASER-EnKF T42 (2.8)</td>
<td>EnKF</td>
<td>2005-2016</td>
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<tr>
<td>TCR-2</td>
<td>MIROC-Chem-EnKF T106 (1.1)</td>
<td>EnKF</td>
<td>2005-2018</td>
</tr>
</tbody>
</table>

RMSE (ppbv)

- CAMS-iRA: 4.9
- CAMS-RA: 3.2
- TCR-1: 5.0
- TCR-2: 3.4

Huijnen et al., 2020
Towards an Air Quality Constellation

How does the constellation improve knowledge of global air quality?

➢ GEO sounders (GEO-CAPE, TEMPO, Sentinel-4, GEMS) will provide an unprecedented number of composition observations at high spatial resolution.

➢ LEO sounders (IASI, CrIS, S5p) provide the global picture and thread the GEO observations together.
AIRS/OMI ozone monitoring and assimilation

Joint LW/SW or ultra-high spectral resolution measurements distinguish upper/lower troposphere.

➢ TIR observations are sensitive to the free-tropospheric trace gases.
➢ UV-Vis-NIR observations are sensitive to the column abundances of trace gases.

How are retrievals used?

MUlti-SpEctra, MUlti-SpEcies, MUlti-Sensors (MUSES) Retrieval Algorithm

\[
\| y - F(x_a) \|_{S^{-1}}^2 + \| x - x_a \|_{S^{-1}}^2
\]

\[
\hat{x} = x_a + A(x - x_a) + G_n
\]

NASA Retrieval Algorithm

Ozone Profiling

Operational Data Processing

Data Assimilation

\[
\sum_i \left\| \hat{x}_i - H_i(x) \right\|_{(G_i S_i G_i^T)^{-1}}^2 + \left\| x_0 - x_B \right\|_{B^{-1}}^2
\]

Fu et al., 2019
**EnKF:** The forecast error covariance is advanced by the model itself (flow-dependent forecast error covariance), which allow us to fully take advantage of the CTM.

**Background error covariance**
(assuming that background ensemble perturbations sample the forecast errors)

\[ P^b = X^b(X^b)^T. \]

\[ \bar{x}^b = \frac{1}{k} \sum_{i=1}^{k} x_i^b; \quad X_i^b = x_i^b - \bar{x}^b. \]

**Analysis ensemble mean and its perturbation**

\[ \bar{x}^a = \bar{x}^b + X^b \tilde{P}^a (Y^b)^T R^{-1} (y^o - \bar{y}^b), \]

- **The observation operator** \( (H) \) converts the model profiles \( (x) \) to the profile that would be retrieved from satellite measurements \( (y^b) \).

\[ y^b = H(x) = x_a + A(S(x) - x_a). \]

- The model-satellite difference is not biased by the retrieval a priori profile.

\[ y^o - y^b = A(x_{true} - S(x)) + \epsilon, \]  
(Rodgers, 2000; Eskes and Boersma, 2003)
What is the impact of IR soundings in regional and global models?

**Mean ozone profile**

- **OMI + GOME-2 NO₂ →** Improved the lower tropospheric ozone
- **MLS O₃/HNO₃ →** Additional important corrections throughout the troposphere.
- **Multi-constituent (Reanalysis) →** correct the entire tropospheric ozone profile

**Ozone biases to DC-8 (ppb)**

- During stagnant condition

**Miyazaki et al., 2019a**
Comparisons against KORUS-AQ DC8 ozone at 650 hPa

- AIRS/OMI ozone retrievals provided the largest corrections for dynamic weather conditions (P1), whereas the improvement was limited just after stagnant conditions (P3).
- Combining precursors’ emission optimization and direct ozone assimilation is an effective method to obtain sufficient corrections on ozone for any meteorological condition.
Free tropospheric and surface ozone validation

700-300 hPa: against TES (China)

700-500 hPa: against AIRS/OMI (China)

Surface ozone changes: 2005-2014

Gridded Surface Obs (TOAR)

TES/OMI multispectral ozone products have also been used to infer surface ozone (Colombi et al., 2021)
Regional model boundary conditions: Evaluation using AIRS/OMI

What is the impact of IR soundings in regional and global models?

Ozone at 680 hPa April 21-30, 2016

Free Running Model  Assimilation

FR Model - Assim -

AIRS/OMI  AIRS/OMI  AIRS/OMI

Δ Ozone (ppb)

30 33 36 39 42 45 48 51 54 57 60 63 66 69 72

Ozone (ppb)

The assimilation improves the representation of plume transport across the Pacific relative to AIRS/OMI.

Further improvements may be seen with assimilation of AIRS/OMI O₃.

Neu et al., 2020
Environmental policy to reduce human health risk from air pollution

COVID-19 natural experiment

Human activity and technology

Air pollutant emissions (NOx etc)

Complex chemical mechanisms

Air pollution level (Ozone, PM2.5)

Human health & Climate

Implications for effective policy making

Answer!! (observables)

Can be inferred

Miyazaki et al., Science Adv. 2021
Laughner et al., PNAS 2021
Global anthropogenic emission reductions in 2020: 7% (CO$_2$) 8% (NO$_x$)

1. Emissions (NO$_x$, SO$_2$, CO)

2. Concentrations

3. Health and climate Impacts
Figure 1: Schematic diagram of the methodology used in this study. (1) (a) The top-down 2010-2019 emissions obtained from the chemical data assimilation (green lines) were used to (b) evaluate relative temporal emission changes from the base date (February 1, January 10 for China only) through July 31 each year. (c) The calculated relative temporal emission changes were averaged over the ten years (2010-2019) to obtain climatological relative emission variations (solid blue line). (d) The climatological variations were applied to the 2020 emission (solid red line) values on the base date to obtain the BAU emissions for 2020 (solid blue line) and then compared with the 2020 emissions to estimate the COVID emission anomaly. (2) The COVID-19 ozone response through February to July 2020 and monthly OPE estimated from the beginning to end of each month were estimated from model simulations by replacing the BAU emissions with the 2020 emissions for each region or globally. (3) The evaluated ozone response were compared with the observed changes from the CrIS satellite and surface observations.
Estimated NOx emissions

In April-May 2020
- Europe, North America, the Middle East and West Asia: -18-25%
- Africa and South America: -5-10%
- Global total: -5 TgN/year
Global ozone response: Comparisons against CrIS satellite

CrIS (JPL TROPESS) ozone 700 hPa: 2020 minus 2019

2. Concentrations
Primary pollutants
SO₂, NOₓ, CO, VOCs, NH₃,
Primary aerosols (dust, carbon)

Secondary pollutants
Ozone, PAN,
Secondary aerosols
( nitrate, sulfate, ammonium)

Chemistry

Assimilation
OMI, TROPOMI (SO₂,NO₂)
CrIS (NH₃)
MOPITT (CO)

Validation
VIIRS (AOD)
CrIS (O₃,PAN)
OMPS (SO₂,NO₂)
Summary

• The chemical reanalysis data, combined with suborbital and ground-based measurements, has been used to improve our understanding of atmospheric composition and to evaluate new satellite data products including AIRS/OMI and CrIS.

• **Answers to the meeting questions**: (1) IR soundings have a big impact on global and regional studies as well as climate. (2) Low data latency would be important for predictions (e.g., wildfire impacts) while attribution analysis w/o low data latency is also important. (3) Assimilation of retrievals are efficient and sufficient for science applications.

• New LEO and GEO measurements and multi-spectral retrievals of composition provide much-improved spatial and temporal resolution and coverage in conjunction with the chemical reanalysis. They should lead to greater usefulness of satellite measurements for climate and air quality applications. E.g., GEMS NO₂ with CrIS/TROPOMI O₃ would better isolate sources and attribute sectors and their influences on ozone at daily scales.