Promises and Challenges in Assimilating Aura/OMI Satellite Data to Study Global Air Quality

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Ozone Hole
1st generation Instruments

Backscattered UV (BUV, SBUV, SBUV/2)
- 12 discrete λs (250-340 nm), 1nm bandpass
- Nadir only, 11° IFOV (~200 km)
- Product: O\textsubscript{3} profile at 6-25 km vert resolution

Total O\textsubscript{3} Mapping Spectrometer (TOMS)
- 6 discrete λs (312-380 nm), 1 nm bandpass
- 102° x-track scan (2600 km swath), 3° IFOV (~50 km).
- Designed for total column O\textsubscript{3} only but yielded unexpected dividends.
40 Years of BUV Observations

<- 8 flights of SSBUV on Space Shuttle ->

Nimbus-4 BUV
Nimbus-7 SBUV
Nimbus-7 TOMS
NOAA-9 SBUV-2
NOAA-11
Meteor-3 TOMS
NOAA-14
GOME
Earth Probe TOMS
NOAA-16
SCIAMACHY
EOS Aura OMI
GOME-2
OMPS

Ozone Proc. Team formed
1977 Amendment of Clean Air Act
Discovery of Polar O$_3$ Depletion
The Afternoon Constellation consists of 7 U.S. and international Earth Science satellites that fly within approximately 30 minutes of each other to enable coordinated science. The joint measurements provide an unprecedented sensor system for Earth observations.
EOS AURA

- Orbit: Polar: 705 km, sun-synchronous, 98° inclination, ascending 1:45 PM +/- 15 min. equator crossing time.
- Launch Vehicle: Delta 7920 from VAFB, July 15, 2004
- AURA follows AQUA in the same orbit by 15 minutes.
- Six Year Spacecraft Life
OMI

Ozone Monitoring Instrument

- Joint Dutch-Finnish Instrument with Dutch/Finish/U.S. Science Team
  - PI: P. Levelt, KNMI
  - Hyperspectral wide FOV Radiometer
    - 270-500 nm
    - 13x24 km nadir footprint
    - Swath width 2600 km
  - Radicals: Column O$_3$, NO$_2$, BrO, OCIO
  - O$_3$ profile ~ 5-10 km vert resolution
  - Tracers: Column SO$_2$, HCHO
  - Aerosols (smoke, dust and sulfates)
  - Cloud top press., cloud coverage
  - Surface UVB
  - Tropospheric ozone

2-dimensional CCD

- ~ 580 pixels wavelength
- ~ 780 pixels viewing angle ± 57 deg
- flight direction » 7 km/sec
- 13 km
- 2600 km (~2 sec flight)
- 12 km/24 km (binned & co-added)
Typical OMI Spectrum
Ozone Products from OMI

1. Total $O_3$ Column (3)
2. Partial $O_3$ columns (2)
3. $O_3$ MR vs pressure (2)
4. Trop $O_3$ column (3)

*Numbers in the parenthesis are the number of different algorithms that currently exist. Additional algorithms are being planned!
OMI Total O$_3$ Column Algorithms

- **TOMS Version 8.5**
  - Based on TOMS V8. Uses cloud optical centroid pressure derived from Raman filling-in (Ring effect), instead of IR-based climatology.

- **DOAS**
  - Developed at KNMI/NL. Uses cloud effective pressure derived from O$_2$-O$_2$ absorption. Differs from MetOp/GOME-2 DOAS algorithm.

- **Optimal Estimation**
  - By integrating retrieved O$_3$ profiles. Similar to SBUV.
Data Assimilation Issues

- What information does total $O_3$ contain?
- How important is the knowledge of $O_3$ profile to retrieve total $O_3$?
- How do clouds affect the retrieval?
- How do aerosols affect the retrieval?
- Can we assimilate radiances instead and avoid all these problems?
What information does total $O_3$ column contain?

- **Facts:**
  - Total $O_3$ is poorly correlated with $O_3$ at or above the altitude where the $O_3$ density peaks (~22 km), thought it contains ~50% of the total column.
  - Outside the tropics ~70% of the variation in total $O_3$ comes from 10-20 km that contains only ~25% of the column.
  - In the tropics ~50% of the variation in total $O_3$ is caused by the troposphere that contains only ~10% of the column.
KEY IDEAS

- Use Multiple Wavelengths Pairs
- Standard Ozone Profiles- defined by total $O_3$
- Treat Cloud and Aerosols as Opaque Lambertian Surface (LER model)
Total Ozone Dependent Standard Profiles

ORIGINAL VERSION

MODERN VERSION

low

mid

high
How important is the knowledge of profile to derive total O₃?

- Not very important (up to SZA ~80°) if one uses TOMS “standard” profiles that vary with total O₃ and latitude.
- Climatological profiles that vary with month/lat and are proportionally adjusted with total column can produce large errors @ SZA>60°.
- Use of TOMS standard profiles would very likely improve retrieval of total O₃ from IR sounders (TOVS, AIRS, IASI, CrIS).
Multi-phase/Multi-layer Cloud Effects

There are 5 different methods of estimating cloud height: 2 TIR, $O_2$-A, $O_2$-$O_2$, and Raman.

CloudsSat radar reflectivity

MODIS cloud-top press is insensitive to cloud vertical structure

Cloud Optical Centroid press calculated using OMI-measured Rot Raman Scattering is sensitive to cloud vert structure (ref: Vasilkov et al., JGR, '08)
Summary of Cloud Effects

- IR cloud heights can be used only when the clouds are single-layered and <1 km thick.
- In OMI pixels ~40% of the clouds are either multi-layered or vertically extended (ref: Joiner et al., 2009). GOME-2 and OMPS pixels are likely to be worse.
- Use of optical centroid press derived from Raman filling-in (Ring effect) is currently the best way to account for clouds in UV, though, strictly speaking, the method is accurate only if O\textsubscript{3} is well-mixed in the troposphere.
Effective Pressure (Efficiency Factor Method)  11 July 2006
Summary of Aerosol Effects

- Boundary layer aerosols have no significant effect. Elevated aerosols (primarily smoke and desert dust) greatly reduce the sensitivity to O$_3$ below the altitude where they are located.
- Primary reason is high UV absorption of these aerosols. These aerosols also have a large (up to 30%) impact on the estimation of surface UV radiation.
- To estimate and correct for these effects we need to know $\tau_{\text{abs}}$ and aerosol centroid press. (Surface UV is not affected by aerosol ht.) We are trying to estimate both using OMI data.
How do aerosols absorb in the UV?

\[ \tau_{\text{abs}} \propto \lambda^{-k} \]

- \( k = 1 \) for BC
- \( \approx 2 \) for OC
- \( \sim 3 \) for Desert Dust
Comparison of TOMS-derived UVB (symbols) with an accurate ground-based instrument (lines). The good clear-sky comparison (upper curve) was an expected result, but similar results under all-sky conditions (lower curve) were quite unexpected. Other comparisons show that aerosols can produce up to 30% errors due to their high UV absorption.
Alaska Fires, June 25-27, 2004

SeaWiFS June 27, 2004

TOMS Aerosol Index
Retrieving Aerosol Absorption in the near-UV

By means of an inversion algorithm AOD and SSA are derived
Radiance Assimilation

- Clouds and aerosols are by far the biggest issues in assimilating UV radiances. Assimilation will need to handle cloud vertical structure, aerosol absorption in UV somehow.

- Assimilation of radiance requires good knowledge of the uncertainty in the forecast profiles as a function of altitude. Lacking such information it may be better to assimilate the profiles we provide with our total O₃ data. The worst strategy is to assume that forecast profiles have the same fractional error at all altitudes.
Assimilation of OMI $O_3$ profiles

- Primary information OMI (also SBUV and GOME-2) provides is the column $O_3$ above pressure surfaces ($\sim 1$ hPa to surface). MR is derived by differentiating this curve, which increases the error and creates large dependence on *a priori* profiles, particularly below 30 km.

- If these partial column $O_3$ amounts cannot be directly assimilated, they should, at least, be used for the validation of assimilated MR profiles.
Column $O_3$ profile

Desired information for scientific studies. Derived by differentiation. Precision varies with the slope of the upper curve. Worst in the troposphere.

Primary information in the bv radiances. OMI retrieval precision $\sim 1\%$ at all pressure levels.

$O_3$ MR profile
Retrieval of Trop O$_3$ column from OMI- Methods

- Cloud Slicing (aka the CCD method)
  - For monthly means only. Works best in the Pacific region. Data goes back to ‘79.

- OMI total Column - MLS strat column
  - Relatively noisy, best for weekly/monthly means.

- Partial O$_3$ column estimated from profile retrieval
  - Best for producing daily maps. Monthly means may be less accurate than the methods above.
Stratospheric O$_3$ Column by Cloud Slicing (aka the CCD method)

Can be used to estimate MM TOR in the Pacific and 15S-15N with high accuracy

Old paradigm
Ziemke et al., ‘98
O₃ mr in deep convective clouds in the Pacific is usually <10 ppbv. Method doesn’t work outside the Pacific since clouds are usually dirtier.
Changes in Tropical Trop O$_3$ Column over the past 30 years

Result is insensitive to instrument drift, since it is derived from the difference between cloudy and clear data.
June-Aug ‘08

Sept-Nov ‘07

Trop O$_3$ column from OMI-MLS

Images courtesy of Mark Schoeberl
Problems with Trop O$_3$ Column Concept

- Lower boundary of OMI-derived total O$_3$ column is not the surface, but the effective pressure (see slide #17). O$_3$ column below this altitude is estimated from climatology.
- O$_3$ Tropopause is often poorly known.
- Better concept: column-averaged MR
  - $\text{CMR} = (\Omega_1 - \Omega_2)/(p_1 - p_2) \times 1.27$, where $\Omega_i$ is the column above $p_i$, and $p_i$'s are chosen suitably.
Trop Column O$_3$ vs CMR

OMI/MLS Tropospheric Ozone (DU) September-November 2007

OMI/MLS Tropospheric Ozone (ppbv) September-November 2007
Direct Retrieval of O$_3$ column above 215 hPa from OMI vs MLS-derived column
Direct Retrieval vs MLS- Single Orbit Comparison

OMI is less noisy
Direct retrieval captures the variability of strat $O_3$ column seen by MLS in the tropics.
AQ related products from OMI

- NO$_2$
- Aerosols
- SO$_2$
- Formaldehyde (HCHO)
- BrO
- Glyoxol (CHOCHO)
OMI AQ Products- Sources of Error

- **Sub-pixel clouds**
  - Cloud effect is enhanced since clouds are much brighter than the boundary layer. Most serious for aerosols, moderately serious for NO₂, less serious for O₃ and SO₂.

- **Surface BRDF**
  - Currently assumed to be Lambertian

- **Vertical profile**
  - Based on models

- **Aerosols**
  - Absorbing aerosols reduce the sensitivity
OMI NO$_2$ Western US + Cities
OMI NO$_2$ Western US + Cities + Power Plants

Differentiating between stationary & mobile sources
Cloud interference on a single day

Tropospheric NO₂ from OMI for June 6, 2005
Issues with Assimilation of Atm Composition Data to Study AQ

- Lifetime is short so system resets itself in hours and days, i.e., there is less dependence on initial conditions that make met data assimilation a fundamental necessity.
- Sparse or non-existent vertical profile information (getting better for aerosols).
- No information below clouds. Convective clouds change composition discontinuously.
- A very ill-posed mathematical problem, particularly for aerosols.
- Short lifetime and point emission sources require high temporal and spatial resolution data that are not currently available.
Issues for the Audience

• Given the issues that I have identified in this talk, is assimilation of OMI data worthwhile?
• What is the best way to assimilate data that provide column amounts in relatively thick layers?
• Can an assimilation system be designed to use cloudy data to improve assimilation rather than discarding cloudy pixels?
• How does one account for clouds and aerosols in a pure radiance assimilation?
• Is a hybrid assimilation approach—half way between product and radiance assimilation—more useful?