TEMPO Ozone Profile and Tropospheric Ozone Retrievals

Xiong Liu
xliu@cfa.harvard.edu

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Introduction

OMI Ozone Profile Retrieval

Validation of OMI Retrievals with Ozonesonde and MLS

Adaption of OMI Algorithm for TEMPO
  - Perform synthetic UV/visible retrievals
  - UV/visible retrievals from GOME-2 data

Summary and Future Outlook

Demonstrated retrievals of tropospheric $O_3$ from GOME, GOME-2, OMI UV data by various groups (Munro et al., 1998; Hoogen et al., 1999; Hasekamp and Landgraf, 2001; van der A et al., 2002; Liu et al., 2005, 2010; Cai et al., 2012; van Peet et al., 2014; Miles et al., 2015).

However, UV only retrievals provide limited retrieval sensitivity to lower tropospheric ozone.
GEOCAPE multispectral sensitivity studies: combine UV with visible and/or TIR can greatly improve sensitivity to 0-2 km O$_3$ (Natraj, Liu et al., 2011).

TEMPO: UV (Hartley/Huggins bands) + Visible (Chappuis bands) to distinguish boundary layer O$_3$ from free tropospheric and stratospheric O$_3$.
Visible retrievals: shown to improve tropospheric O₃ column from SCIAMACHY data by neural network algorithms (Sellitto et al., 2012a,b).

Challenges: weak visible O₃ absorption, strong interferences from surface reflectance and aerosols/clouds, consistent radiometric calibration across the spectral range.

We have used GOME-2 data to test this UV/visible approach. But GOME-2 are not ideal for testing this algorithm: peak of Chappuis bands is split into bands 3 and 4, radiometric calibration inconsistency.

1a: 240-307/283* nm, 0.25 nm FWHM  * changed in December 2008
1b: 307/283-315 nm, 0.25 nm FWHM
2: 311-403 nm, 0.25 nm FWHM
3: 401-600 nm, 0.5 nm FWHM
4: 590-790 nm, 0.5 nm FWHM

UV/visible O₃ profile retrieval using physically based algorithm has yet to be demonstrated from real data.

We identified this as an instrument project science risk for TEMPO.
Given that TEMPO's technique of combining UV and visible radiances for retrieving lower tropospheric (0-2 km) O$_3$ concentration has never been validated using existing nadir satellite measurements, and that TEMPO will attempt to make such measurements at finer spatial resolution than previous satellites, there is a possibility that TEMPO may not achieve 10 ppbv precision for 0-2 km O$_3$ concentrations during Phase E, which can result in a degradation of the TEMPO Instrument baseline science performance for the lower tropospheric O$_3$ product but higher than threshold.

<table>
<thead>
<tr>
<th>Response Plan Step</th>
<th>Start Date</th>
<th>End Date</th>
<th>Expected L x C</th>
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</thead>
<tbody>
<tr>
<td>1) Develop wavelength-dependent and angle dependent surface albedo/BRDF database at high spatial resolution over the TEMPO field of regard by combining MODIS albedo/BRDF product, ASTER spectral library and land cover types.</td>
<td>1/2014</td>
<td>11/2014</td>
<td>3 x 3</td>
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<tr>
<td>2) Perform non-linear ozone profile retrievals from simulated radiances, utilizing the developed albedo/BRDF database, and verify that the retrievals are self-consistent with the input profiles to within calculated retrieval uncertainties, to demonstrate the TEMPO approach can work theoretically for selected surface scenes.</td>
<td>1/2016</td>
<td>1/2016</td>
<td>2 x 3</td>
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<td>3) Apply the developed Albedo/BRDF database to GOME-2 retrievals, and perform empirical radiometric calibrations to GOME-2 data to improve the consistency among Huggins bands and two parts of Chappuis bands in different channels, to demonstrate the TEMPO approach can work at coarse resolution and over various scenes. In process.</td>
<td>1/2014</td>
<td>6/2017</td>
<td>2 x 2</td>
</tr>
<tr>
<td>4) Assess the quality of ACAM/GEO-TASO data and demonstrate high spatial resolution combined UV/Visible ozone retrievals over a variety of scenes from ACAM and GEO-TASO aircraft measurements. In process (ACAM &amp; GeoTASO measurements obtained during July-Aug deployment to Denver with DISCOVER-AQ have acquired the data for this response – progressing on schedule).</td>
<td>1/2014</td>
<td>9/2017</td>
<td>2 x 1</td>
</tr>
<tr>
<td>5) Use TEMPO as-built instrument characterization database and high spatial/spectral resolution reflectance database in retrieval simulations to verify expected on-orbit retrieval performance.</td>
<td>1/2016</td>
<td>2/2018</td>
<td>1 x 1</td>
</tr>
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</table>
SAO OMI Ozone Profile Retrieval Algorithm

- **Initial OMI algorithm (Liu et al., 2010):** adapted from GOME
  - Spectral fitting + full radiative transfer simulation (VLIDORT)
  - Retrieve $O_3$ partial columns at 24 layers from surface to $\sim$60 km, total, stratospheric, tropospheric ozone columns are integrated with the use of NCEP tropopause
  - Fitting windows: 270-309, 311-330 nm
  - 3-year mean solar irradiance spectra + soft radiometric correction
  - Ill-posed problem: non-linear optimal estimation (Rodgers, 2000) with zonal mean $O_3$ profile climatology (McPeters et al., 2007)

\[
\chi^2 = \left\| \frac{1}{S_y^2} \{ K_i (X_{i+1} - X_i) - [Y - R(X_i)] \} \right\|^2 + \left\| \frac{1}{S_a^2} (X_{i+1} - X_a) \right\|^2
\]

\[
X_{i+1} = X_i + (K_i^T S_y^{-1} K_i + S_a^{-1})^{-1} \{ K_i^T S_y^{-1} [Y - R(X_i)] - S_a^{-1} (X_i - X_a) \}
\]

- $Y$: Measurement vector (e.g., radiances)
- $X, X_i, X_{i+1}$: State vector (e.g. ozone profile)
- $X_a$: a priori state vector
- $K$: Weighting function matrix, sensitivity of radiances to ozone
- $S_a$: A priori covariance matrix
- $S_y$: Measurement error covariance matrix
**SAO OMI Ozone Profile Retrieval Algorithm**

- **Measurement L1b, I, F, SZA, VZA, AZA**
- **Measurement Constraint**
- **λ selection, Wavelength & Radiometric calibration**
- **Calibrated Measurements**
- **Optimal Estimation**
  - State vector: partial ozone column at 24 layers, trace gases (e.g., SO₂, SO₂ plume altitude, BrO), cloud fraction, λ-dependent surface albedo, wavelength shifts, Ring parameters

- **Forward model simulation (VLIDORT+ RRS model)**
- **Simulated radiances and Weighting functions**
- **Climatological Constraint**
- **Converge**
  - No
  - Yes

**Keys to retrievals:** accurate calibration and forward model simulations, fit the radiance spectra to ~0.1% in the 310-330 nm
Empirical Radiometric Calibration (OMI)

- Calibrate OMI data using daily zonal mean MLS profiles and McPeters climatology in the tropics (20°S-0)
- Significant wavelength and X-track dependent biases, large discontinuity
- Correction is derived from 2 days’ residuals & applied independent of time & location
It is implemented in OMI SIPS: based on Liu et al. (2010) with 2 major modifications:
- 4x binning along the track to speed up processing $52 \times 48 \text{ km}^2$ @ nadir
- A minimum floor noise of 0.4% in UV1 and 0.2% in UV2 is used to stabilize retrievals, but reduces retrieval sensitivity.

It produces PROFOZ: available at Aura AVDC for the entire period: http://avdc.gsfc.nasa.gov/index.php?site=1389025893&id=74
Examples of Retrievals (OMI, 2006m0826)
Most of the information is in the stratosphere.

Tropical and mid-latitude summer: tropospheric $O_3$ information generally peaks in the 500-700 hPa layer, retrievals are effectively sensitive to ozone down to ~800 hPa.

6-7.3 DFS, 5-6.5 in the stratosphere, 0-1.2 in the troposphere, 2-3 below the ozone density peak.
Averaging kernels based on Liu et al. (2010). Retrieval sensitivity especially in the troposphere is reduced by ~0.2 in PROFOZ.

Well resolved in the stratosphere with ~7-10 km FWHM, and ~10-14 km in the troposphere

Significant retrieval interferences from other auxiliary parameters in the lower troposphere, and the use of 0.2% floor noise: otherwise: up to 1.8 DFS, effectively sensitive to ozone at 900-950 hPa.
Retrieval Errors ($\sigma$ Random-Noise + Smoothing Errors)

- **Random-noise (R) errors:**
  - 0.6-2.5% in the middle strat., generally within 12% below

- **Smoothing (S) errors usually dominate solution errors**

- **Solution (R+S) errors:**
  - 1-7% in the middle strat.
  - generally up to 10% in the upper stratosphere
  - generally within 7-38% in the lower stratosphere and troposphere
Retrieval Errors (1σ Random-Noise + Smoothing Errors)

Errors (SZA < 80°):  
- **TOZ**: 0.5-3 DU, OMTO3 and OMDOAO3 errors are a few times larger  
- **SOC**: 1.5-4 DU, better than limb measurements (e.g., MLS on Aura)  
- **TOC**: 2-5 DU  

Validation shows that total ozone retrieval performance is better than the three operational products (Bak et al., 2015).
With 10+ years of data, what is the data quality and long-term stability? ➔ Evaluate the need to perform time-dependent soft calibration for next version.

OMI has Row Anomaly (RA) problem: first started in 2007 at a few positions, become serious in Jan. 2009, affecting > 1/3 positions.

How is the retrieval quality affected by RA? It was suggested that RA likely affects UV 1 data (therefore stratospheric ozone) at all cross-track positions.

Validate using ozonesonde & MLS.
  ➢ Pre RA (2004-2008)
  ➢ Post RA (2009-2014)
Validation with Ozonesonde

- Ozonesonde data (~27,000 profiles) over the globe (2004-2014).
- ~100 ozonesonde stations, including those from field campaigns, was obtained from Aura AVDC, WOUDC, SHADOZ, DISCOVER-AQ, etc.
- TOC Mean biases (MBs) mostly < 3 DU and 1σ < 6 DU except for large MBs/1σ at several N. high latitude locations, and in India due to the use of different type of sonde (India sondes).
### Validation with Ozonesonde Data

#### Key Thresholds

<table>
<thead>
<tr>
<th>Threshold</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Distance</td>
<td>&lt; 100 km (nearest coincident pair)</td>
</tr>
<tr>
<td>Time</td>
<td>&lt; 6 hours</td>
</tr>
<tr>
<td>R.M.S.</td>
<td>&lt; mean + 2σ</td>
</tr>
<tr>
<td>Cloud Fraction</td>
<td>&lt; 0.3</td>
</tr>
<tr>
<td>Cross-Track</td>
<td>4-27</td>
</tr>
<tr>
<td>SZA</td>
<td>&lt; 75°</td>
</tr>
</tbody>
</table>

- **Fitting RMS increases with time due to increase noise and Row anomaly**
Profile Comparison

- Better agreement in the mid-latitudes and tropics than in the high latitudes.
- Biases are within 6% in mid-latitudes and tropics, with standard deviations of up to 20-25%.
- Low mean biases (<10%) above 20 km at high latitudes.
- Pre-RA results show better comparison than post-RA with smaller standard deviations.
Solar Zenith Angle and Cloud Fraction Dependence

- Poorer comparison (larger biases or altitude dependence, larger standard deviations) at larger SZAs (>75°) due to weaker signals and larger other sources of calibration errors.
- Poorer comparison at large cloudiness (e.g., > 0.3).
Cross-track Dependence

- Poorer comparison (larger biases or alt. dependence, larger std. dev.) for extreme off nadir positions (e.g., 1-4, 28-30)
Tropospheric Ozone Column Comparison

- Surface to tropopause
- Much better correlation after applying OMI AKs
- In the tropics and middle latitudes, Mean Biases (MBs) are within 1.5 DU (6%) with standard deviations (STDs) within 15%.
- At high latitudes, MBs are within 2.5 DU with STDs of 30%.
- Smaller STDs and better correlations during the Pre-RA period (2004-2008).
Comparison of Lower Tropospheric Ozone Columns

Smaller slopes, correlations, larger standard deviations for layers closer to the surface due to reduced retrieval sensitivity down to the atmosphere
Bias Trends

- Significant trends in mean biases vs. ozonesonde at individual layers or in Tropospheric Ozone Column especially during the post-RA period.

- Need to improve OMI's radiometric calibration vs. time especially during the post-RA period to maintain the long-term stability of the product.
Validation with MLS

- MLS V4 O₃
- During post-RA period, no OMI/MLS collocation, use nearest MLS data.
- For pre-RA period, comparisons with either collocated MLS or post-RA masked MLS are similar.

- Pre-RA: Global mean biases generally within 5%, with 1σ of 3-5% at 2-30 hpa, increasing to 10% above 1 hPa and to 20% at 261 hPa.
- Post-RA: slightly larger 1σ/ biases below 3 hPa, much larger 1σ at higher altitudes, suggesting UV1 is affected by RA for non-flagged pixels.
Validation with MLS

SOC down to 100 hPa
SOC down to 215 hPa
SOC down to 261 hPa

Excellent agreement with MBs typically within 2 DU (0.7%) and $1\sigma$ of ~1.9-2.3% for collocated OMI/MLS, $1\sigma$ 0.3-0.6% larger for 2004-2008 with post-RA mask or 2009-2014.
Post-RA: a few periods with very large biases, larger variation, significant trend
Adaption of OMI Algorithm for TEMPO

- Adapted from GOME (Liu et al., 2005), OMI (Liu et al., 2010), GOME-2 (Cai et al., 2012): Spectral fitting + VLIDORT + OE
- Fitting windows: 290-345 nm (UV), 540-650 nm (Visible)
- O₃ profile at > 24 layers (add several 1 km layers near the surface) from surface to ~60 km, derive 0-2 km ozone column in addition to total, stratospheric, and tropospheric ozone columns
- Tropopause-based O₃ profile climatology (Bak et al., 2013): further improvement to account for diurnal variation
- Meteorological data (temperature profiles, surface pressure, and tropopause pressure): North American Mesoscale (NAM) Forecast System grid 227 with 5-km resolution
- Speedup radiative transfer calculation: look-up table correction and/or fast Principal Component Analysis (PCA) LIDORT
Important to account for the temperature-dependence of the O$_2$-O$_2$ cross sections using cross sections by Thalman et al. (2013).

Line-by-line calculations of O$_2$ and H$_2$O cross sections from HITRAN 2012 accounting for T- and P-dependence with solar $I_0$ correction, with additional O$_2$ delta band, empirical correction (O$_2$ line mixing)
Ozone has weak spectral features in the Chappuis band

But retrieval is very sensitive to errors in surface reflectance

- Spectral variation
- Dependence on land cover
- Changes with viewing geometry
Developed visible surface albedo spectrum (Zoogman et al., 2016)

- Lab spectra (400-900 nm) of possible ground cover including vegetation, soils, rocks, manmade, water, snow, from ASTER, USGS, MPI/Wagner’s group

- Empirical Orthogonal Function (EOF) analysis of shows that first 4 EOFs can explain more than 99.5% of the variance over land

- Mean snow/ice (ASTER) and water over ocean spectra (USGS)

- Combine EOFs+snow/ice+water with 10-year (2002-2011) average high resolution (30 arc s) MODIS BRDF climatology (466, 555, 645, 859 nm over land only) or GOME-2 surface albedo climatology (15 wavelengths in 400-900 nm, both water & land)
Assumption of Lambertian surface

- UV: initialize albedo from climatology at 342 nm, and fit constant albedo in band 1a and albedo polynomials in band 2b (e.g., 2\textsuperscript{nd})

- Visible over land: Combine land EOFs and MODIS (blue sky albedo) to initialize visible surface reflectance spectrum and further fit surface spectra using 2 approaches as follows

\[
a_\lambda = a_\lambda^0 \sum_{i=0}^{n} c_i (\lambda - \lambda_{av})^i
\]

1. Albedo scaling:

\[
a_\lambda = a_\lambda^0 + \sum_{i=0}^{n} c_i \text{EOF}_i
\]

2. Fit EOFs:

Visible over snow/ice or water surface: scale average snow/ice spectrum or water albedo spectrum

- Key: use fewer surface albedo parameters that increase O\textsubscript{3} retrieval sensitivity while adequately fit radiance spectra
Perform Synthetic Retrievals to verify

UV/Visible O$_3$ Profile Algorithm

- Verify the algorithm: iterative nonlinear retrievals (simultaneous fitting of surface parameters) from simulated radiances to show that retrievals are self-consistent with true profiles to within retrieval uncertainty
- Tested nonlinear retrievals under clear-sky conditions
  - 3 vegetation, 3 soil/desert, snow/ice, water with diff. TEMPO viewings, O$_3$ amounts for both UV only (290-345 nm) and UV + visible (290-345, 540-650 nm) retrievals
  - Each test consists of the same simulated radiance added with 101 different sets of TEMPO random noise

Fitting RMS (ratio of fitting residuals to measurement precisions) is almost 1 for both UV, and visible regions.
Example of Synthetic Nonlinear Retrievals: Vegetation, UV/VIS vs. UV

Fitting 1st-order albedo polynomial in UV and 3 EOFs in the visible.

Both UV only and UV/visible retrievals are verified for all the cases.

UV/visible retrievals show enhanced retrieval sensitivity to lower tropospheric ozone, better agreement, smaller retrieval errors (~15% vs. ~10%) but larger retrieval precision in the bottom layers.
Both UV only and UV/visible retrievals show agreement with true columns to within retrieval precision.

- UV/visible retrievals show better agreement with true columns, smaller retrieval errors but larger retrieval precisions vs. UV retrievals all due to improved retrieval sensitivity.
One pixel at: 113.2°W, 32.7°N with an effective cloud fraction of 0.08

Fitting 2 EOFs in bands 3 & 4, respectively (4 parameters): UV+visible shows significant DFS increase mainly in the lower troposphere, but still with relatively large fitting residuals in the visible (0.1-0.15%)
Scaling albedo spectra (1\textsuperscript{st} & 2\textsuperscript{nd} orders) in bands 3 & 4, respectively (4 & 6 parameters): more parameters leads to better fitting but also less retrieval enhancement.
Scaling albedo spectra (2nd order) in visible (i.e., bands 3 + 4 together, 3 parameters): larger fitting residuals and very small tropospheric O₃ values.

Add a scaling parameter (4 parameters) in band 4 radiance can significantly reduce fitting residuals. This suggests calibration inconsistency across channels.
### Impact of surface albedo fitting parameters on the retrievals

<table>
<thead>
<tr>
<th>Options</th>
<th>Trop. DFS</th>
<th>TOC (DU)</th>
<th>Band 3 Res (%)</th>
<th>Band 4 Res (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>UV</td>
<td>1.27</td>
<td>38.5</td>
<td></td>
<td></td>
</tr>
<tr>
<td>UVVIS 2albspc, 2W</td>
<td>1.48</td>
<td>55.2</td>
<td>0.162</td>
<td>0.071</td>
</tr>
<tr>
<td>UVVIS 3albspc, 2W</td>
<td>1.35</td>
<td>44.0</td>
<td>0.147</td>
<td>0.066</td>
</tr>
<tr>
<td>UVVIS 3albspc, 1W</td>
<td>1.55</td>
<td>5.4</td>
<td>0.218</td>
<td>0.182</td>
</tr>
<tr>
<td>UVVIS 3albspc, 1W, scale band 4 rad.</td>
<td>1.47</td>
<td>47.8</td>
<td>0.148</td>
<td>0.066</td>
</tr>
<tr>
<td>UVVIS 2 EOFs, 2 W</td>
<td>1.56</td>
<td>41.6</td>
<td>0.152</td>
<td>0.098</td>
</tr>
<tr>
<td>UVVIS 3 EOFs, 2 W</td>
<td>1.39</td>
<td>47.4</td>
<td>0.141</td>
<td>0.076</td>
</tr>
<tr>
<td>UVVIS 3 EOFs, 1 W</td>
<td>1.83</td>
<td>84.9</td>
<td>0.217</td>
<td>0.160</td>
</tr>
<tr>
<td>UVVIS 3 EOFs, 1 W, scale band 4 rad.</td>
<td>1.82</td>
<td>79.9</td>
<td>0.138</td>
<td>0.100</td>
</tr>
</tbody>
</table>

* 2W: band 3, 4 separately, 1W: visible (band 3+4 together)
One orbit of GOME-2 data overpass North America on 1 July 2008. UV/visible retrievals still show frequent retrieval failures (mostly negative O$_3$ values or do not converge) and large band 3-4 residuals with some albedo options.
Some retrievals show clearly tropospheric DFS (>100 mb) increase of up to 0.30 and significant changes in tropospheric O₃ column over land under nearly clear-sky conditions especially with 2 EOF or 1st-order scaling option. Fitting higher order EOFs/albedo typically improves fitting residuals, but decreases DFS and tropospheric ozone column difference.


- **Summary and Future Outlook**

- UV only algorithm has been successfully implemented (e.g., GOME, OMI, and GOME-2, OMPS)
- Adapted our UV O<sub>3</sub> profile algorithm for joint UV/visible retrievals including the modeling of surface albedo spectrum
- Synthetic retrievals verify the retrieval enhancement to lower tropospheric ozone with additional visible.
- Preliminary retrievals demonstrate the potential of adding visible to improve ozone profile retrievals in the lower troposphere
- However, retrievals are very sensitive to the fitting of surface albedo parameters; relatively large fitting residuals still occur
- Near-term work to joint UV/visible retrievals will include:
  - Updated to use new version of GOME-2 data and account for provided view-angle dependent correction
  - Further improve surface albedo modeling and fitting
  - Refine the derivation of empirical calibration among different bands.
  - Account for aerosols and surface BRDF
  - Validate both UV/visible & UV only retrievals against ozonesonde observations, and examine retrievals in regions of pollution episodes.