OMPS Limb Profiler Ozone Product O3:
Version 2.5 Data Release Notes

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1. Instrument Introduction

The Ozone Mapping and Profiler Suite (OMPS) Limb Profiler (LP) on the Suomi National Polar-orbiting Partnership (NPP) satellite views the Earth's limb looking backwards along the orbit track, using three parallel vertical slits. One slit is aligned with the orbit track, and the other two slits are pointed 4.25° to each side, giving an effective cross-track separation of approximately 250 km at the tangent point. Each profile measurement takes approximately 19 seconds to complete, corresponding to along-track sampling of approximately 125 km. OMPS LP uses a 2-dimensional CCD detector that records atmospheric spectra covering the wavelength range 290-1000 nm at 1 km altitude intervals between 0 km and 80 km. These spectra are primarily used to retrieve vertical profiles of ozone and aerosol extinction coefficient. Additional description of the LP instrument is given in *Jaross et al*. [2014].

2. Retrieval Algorithm

The OMPS Limb Profiler (LP) Version 2.5 (V2.5) daily ozone product is created using a modified version of the ozone retrieval algorithm described in *Rault and Loughman* [2013]. The algorithm generates ozone density *vs.* altitude profiles at 1 km intervals, with a vertical resolution of ~1.6-2.8 km in the central portion of each retrieval, increasing to 3-4 km at lower and higher altitudes. The V2.5 algorithm uses altitude-normalized radiances to make the retrievals insensitive to both instrument calibration errors and to the diffuse upwelling radiation (DUR) produced by surface reflection and scattering of sunlight by clouds and aerosols located below the tangent point. Table 1 provides a summary of the Level 2 (L2) algorithm-specific changes from the original algorithm that are applied for V2.5 retrievals.

Separate retrievals are performed for the middle and upper stratosphere (using UV wavelengths) and for the upper troposphere and lower stratosphere (using visible (VIS) wavelengths).

1. The UV algorithm retrieves profiles between 29.5 km and 52.5 km, using radiances measured at three wavelengths (302, 312, 322 nm) normalized at 55.5 km. Each wavelength is paired with 353 nm to make the algorithm insensitive to errors in the assumed pressure *vs.* altitude profiles p(z) used in calculating the radiances.

2. The VIS algorithm retrieves profiles from cloud top to 37.5 km, using radiances measured at 600 nm and normalized at 40.5 km. Cloud detection is based on the algorithm described by *Chen et al*. [2016]. If no cloud is identified, the VIS retrieval lower limit is set to 12.5 km. These radiances are combined with 510 nm and 675 nm to form a triplet. In addition to making the algorithm insensitive to p(z), the triplet formulation greatly reduces the sensitivity of the algorithm to aerosols. An additional correction for aerosol scattering effects is calculated

using the concurrent aerosol extinction coefficient profile retrieval from the LP-L2-AER675 data product [*Johnson and DeLand*, 2017].

Table 1. Summary of key algorithm changes implemented in Version 2.5 compared to the base OMPS LP ozone algorithm described in *Rault and Loughman* [2013].

Key changes	Version 2.5
Cloud Height Detection	Use algorithm described in *Chen et al*. [2016]
Altitude Registration	Absolute adjustment applied in Level 1B (L1B) data Intra-orbital and seasonal adjustment applied in L2 processing [*Moy et al*., 2017]
Stray Light Correction	Empirical correction applied for VIS wavelengths
Wavelength Selection	**UV:** 302 nm, 312 nm and 322 nm paired with 353 nm (3 pairs) **VIS:** 600 nm combined with 510 nm and 675 nm to form a single triplet
Radiance Normalization Altitude	**UV:** 55.5 km **VIS:** 40.5 km
Aerosol Correction	Use aerosol extinction coefficient profiles retrieved from LP measurements for same event
Vertical Smoothing	2nd order Twomey-Tikhonov regularization term replaced with Rodgers minimum variance solution

Atmospheric pressure and temperature profiles used for forward model radiance calculation in this retrieval algorithm are derived from NASA GSFC Global Modeling Assimilation Office (GMAO) Forward Processing-Instrument Team (FP-IT) GEOS 5.12.4 data. The nearest spatial grid point (Δlatitude = 0.5°, Δlongitude = 0.625°) to each LP profile is identified, and the temperature and pressure profiles for time steps bracketing the LP measurement (Δt = 3 hours) are interpolated to the observation time. While the LP ozone retrieval algorithm is insensitive to p(z) profiles, these profiles are used for altitude registration analysis [*Moy et al.*, 2017]. We provide these data in the LP-L2-O3-DAILY files for the convenience of users who want to convert ozone profiles from our retrieval coordinates (number density *vs*. altitude) to mixing ratio *vs*. pressure profiles.

3. Data Summary

The LP-L2-O3-DAILY data files represent a subset of the L2 orbital file information, concatenated into a single HDF file for each day. These files contain two ozone density profiles (UV and VIS) for each event, along with geolocation information and informational flags. More details about the contents are given in the O3-DAILY Product Description document.

3.1. Changes Between Version 2 and Version 2.5 Data Product [June 2017]

Several changes have been implemented for the LP V2.5 ozone product compared to the V2 product previously released in 2014. The summary listing provided below complements the L2 algorithm changes summarized in Table 1.

- The L2 algorithm now uses Sun-normalized radiances for all retrievals. The effect of this change is relatively small, since the algorithm uses altitude-normalized radiances.
- We do not combine UV and VIS ozone profiles because of unresolved bias issues in the altitude range where they overlap.
- Only center slit data are provided in the daily product, since data from the left and right slits have some quality issues.
- The VIS retrieval radiances are corrected for the effects of aerosols. The aerosol extinction coefficient profile for each event is taken from the LP-L2-AER675 product retrieved for the same event.
- The UV retrieval wavelength selection has been reduced from 43 wavelengths in V2 (all available values between 289-325 nm, excluding 306.5-311.0 nm) to three wavelengths in V2.5 (302, 312, 322 nm). Each wavelength is paired with 353 nm and used from 52.5 km down to a specific lower altitude level (44.5 km, 38.5 km, 29.5 km respectively). This change simplifies the evaluation of radiance error effects by reducing the size of the measurement vector by approximately a factor of 20.
- The VIS retrieval wavelength selection has been reduced from 17 wavelengths in V2 (all available values between 549-633 nm) to one wavelength in V2.5 (600 nm). This wavelength is combined with 510 nm and 675 nm in a triplet. As with the UV algorithm, this reduction in the number of wavelengths simplifies the error analysis.
- The UV retrieval normalization altitude has been changed from 65.5 km to 55.5 km to reduce possible effects from PMC contamination.
- The VIS retrieval normalization altitude has been changed from 45.5 km to 40.5 km to reduce possible effects from residual stray light.
- An empirical stray light correction for visible wavelength data was developed from radiance measurements. High altitude non-zero signals were extrapolated down to 76 km, and the adjustment required to produce agreement with the prelaunch stray light model was calculated. These spectrally dependent scale factors are applied to L1B radiances.
- L1B data contain new adjustments for altitude registration: A static correction of 1.37 km is applied to all center slit data, and an additional +0.1 km adjustment is applied on 25 April 2013 to correct for a S-NPP spacecraft pitch maneuver, as described in *Moy et al*. [2017]. A separate adjustment of +0.1 km is made in L2 processing on 5 September 2014.
- Analysis of ARRM data presented by *Moy et al*. [2017] indicates a remaining altitude registration error that varies by approximately 300-400 m along each orbit, with additional seasonal components. We have developed a correction function that is applied in Level 2 processing. The specific dependence on event number and day of year is shown in Figure 1.

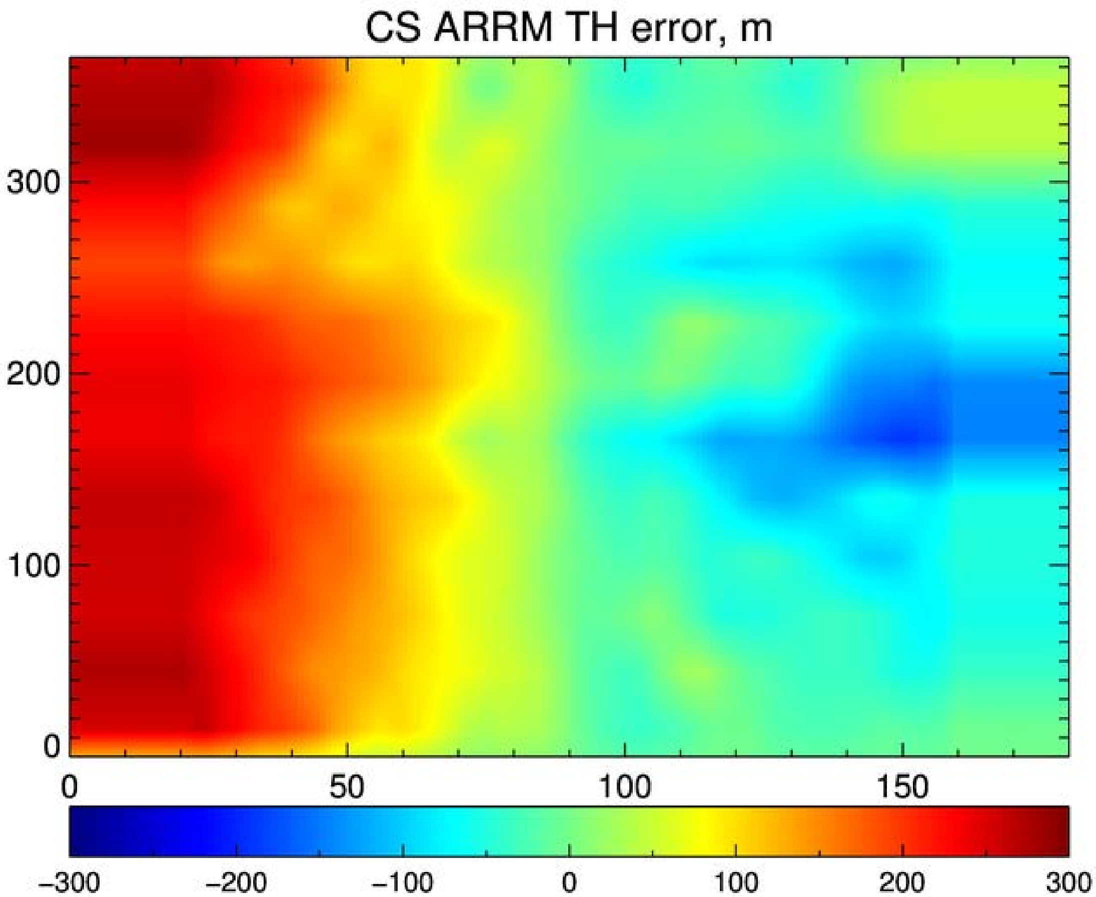

Figure 1. Altitude registration correction applied in V2.5 Level 2 processing as a function of event number and season. The X-axis scale shows event number along the orbit, and the Y-axis scale shows day of year. The Southern Hemisphere terminator crossing occurs at event 0. The color scale shows calculated tangent height error, ranging from -300 m [*blue*] to +300 m [*red*].

4. V2.5 Data Quality

We have made uncertainty estimates for LP V2.5 ozone retrievals, based on our evaluation of the retrieval algorithm and radiance residuals. We have verified that these estimates are reasonable, based on comparisons of the LP V2.5 ozone data product against other data sets (*e.g.* Aura MLS, Odin OSIRIS, ACE FTS). Our initial assessment of LP data quality is given in this section, followed by a discussion of specific features that users should be aware of.

4.1. Accuracy

The accuracy of LP retrieved ozone profiles depends on the combination of many individual factors. The relationship between uncertainty of any factor and a corresponding ozone profile error may depend on altitude, latitude, season, wavelength, or other parameters. A summary of known uncertainties is given below. Table 2 lists estimated ozone profile errors at selected altitudes due to these uncertainties.

- Altitude Registration (absolute). Since the ozone profile varies by up to 30%/km at some altitudes, small errors in altitude registration of radiances can produce large errors in retrieved ozone. Since the shape of the ozone profile changes considerably with altitude, latitude, and season, this error pattern can be quite complex. However, for any given ozone profile, or zonally averaged profile, this uncertainty can be estimated accurately if the altitude registration uncertainty is known. Our current best estimate is that our altitude registration accuracy is ±200 m [*Moy et al.*, 2017], which can produce up to 6% uncertainty in ozone density in the upper stratosphere, reducing to zero uncertainty near the density peak, and reversing in sign below the peak.
- Altitude Registration (drift). Analysis of V2.5 data suggests that there may be a small drift (16 m/year) in LP altitude registration. This produces about +0.5%/year drift in ozone in the upper stratosphere, decreasing to zero near the density peak. This drift has been observed in MLS comparisons.
- Bias at Normalization Altitude. Ozone values assumed by the V2.5 algorithm show a bias of -10% compared to MLS data at 55.5 km, where UV radiances are normalized. If MLS data are assumed to be correct, this bias will produce a small bias in LP retrieved ozone at nearby altitudes (48-52 km).
- Systematic Errors. LP radiances show quasi-systematic errors of 1-3% that vary between CCD pixels. These errors produce approximately ±3% errors in retrieved ozone that vary with altitude, latitude, and season. The cause of these systematic errors is under investigation. Some errors appear to be caused by small uncorrected wavelength shifts with altitude.
- Precision. Random noise in LP measured radiances is much smaller than the quasi-systematic errors discussed in the previous item, so we do not consider this effect here.
- Aerosol Correction. Our experience with the LP V2 data product, where no explicit aerosol correction was applied in the retrieval algorithm, suggests that any remaining errors due to aerosols in V2.5 retrieved ozone profiles are quite small.
- Polar Mesospheric Cloud (PMC) Contamination. While these clouds exist at 80-85 km and high latitudes (> 50°), they can affect the measured radiances as low as 50 km if they are in the line of sight (LOS) of the LP instrument. Although lowering the UV normalization altitude has reduced the overall impact, Northern Hemisphere measurements can still be affected because forward-scattered PMC photons have not passed through the ozone molecules in the LOS. This leads to an underestimate of the ozone profile (see also Section 4.5).

Table 2. Summary of estimated OMPS LP ozone profile errors due to uncertainties discussed in Section 4.1.

Altitude	16.5 km	24.5 km	32.5 km	40.5 km	48.5 km	52.5 km
Alt. Reg. (abs.)	5%	0%	3-4%	6%	6%	6%
Alt. Reg. (drift)	0.6%/yr	< 0.2%/yr	0.5%/yr	0.5%/yr	0.5%/yr	0.5%/yr
Bias at 55.5 km	–	–	–	-0.5%	-3%	-5%
System. Error	±3%	±3%	±3%	±3%	±3%	±3%

4.2. LP UV Profiles and MLS Comparisons

- The mean differences between LP and MLS ozone profiles are within ±5% between 29.5 km and 43.5 km. This agreement is well within the combined uncertainty of LP retrievals and MLS retrievals (quoted accuracy of 5-7%).
- Average LP ozone values tend to be 5-15% smaller than MLS above 45 km, with clear seasonal biases. These biases are still within the combined systematic error bars for MLS and LP instruments. Possible causes of these larger biases are discussed in Section 4.1, and are currently under investigation.
- Relative drift between LP and MLS ozone time series of ~0.3-0.8%/year is observed at altitudes above 33 km. The vertical pattern of the observed ozone drift is consistent with possible altitude registration drift in one of these instruments.

4.3. LP VIS Profiles and MLS Comparisons

- Biases between LP and MLS ozone profiles are generally less than ±5% for all altitudes between 18-30 km. Larger biases observed at Northern Hemisphere high latitudes (> 50°N) may be caused by residual errors in the LP stray light correction at VIS wavelengths.
- Significant negative LP biases of ~10-30% are observed in the lower stratosphere (< 18 km) in the southern mid-latitudes (40°S-60°S).
- Larger ozone differences between LP and MLS are observed in the tropical upper troposphere/lower stratosphere (UT/LS), with negative LP biases (up to -30%) in the upper troposphere and smaller positive biases (~10%) in the lower stratosphere. LP and MLS ozone variability are also higher in this region.
- Negative drifts of 0.3-0.6%/year in LP VIS data are consistent with the altitude registration drift errors described in Section 4.1. Selected altitude and latitude regions can exhibit positive drifts in LP ozone.

4.4 LP UV/VIS Bias

- LP UV and VIS ozone retrievals overlap between 29.5 km and 35.5 km. We find that VIS and UV retrievals agree quite well (±3-5%) between ~30-33 km in the tropics (30°S-30°N). At mid- and high latitudes, UV retrievals systematically give larger ozone values than VIS retrievals (~5-7% differences in the Southern Hemisphere, up to 10-20% differences in the Northern Hemisphere). Comparisons with MLS also confirm that VIS retrievals are lower.

4.5. Data Product Features

1. Inter-Slit Differences. Internal analysis shows that radiances measured in the left slit and right slit still contain some biases relative to center slit data. These biases show a complex dependence on multiple factors (event number, tangent height adjustment, stray light). The center slit data show essentially no tangent height offset when evaluated using the ARRM method described by *Moy et al*. [2017]. Based on these results, we provide only center slit data in the V2.5 LP-L2-O3-DAILY product.

2. Profile Quality Flag. The LP retrieval algorithm creates radiance residuals (difference between measurement vector and forward model calculation) at each altitude level for every event. We define a profile quality flag (Q_UV, Q_VIS) based on the root-sum-square (RSS) of all residuals for that profile. Q_retrieval = 0, which we believe represents the best profiles, corresponds to an RSS residual < 0.05. A typical day has 90-95% of all profiles with Q_UV = 0, most of the remainder with Q_UV = 1, and less than 1% with Q_UV ≥ 2. Figure 2 shows the geographic distribution of Q_UV = 1 profiles for a single day. Almost all VIS profiles achieve the best quality flag. A typical day has < 0.2% of profiles with Q_VIS ≥ 1.

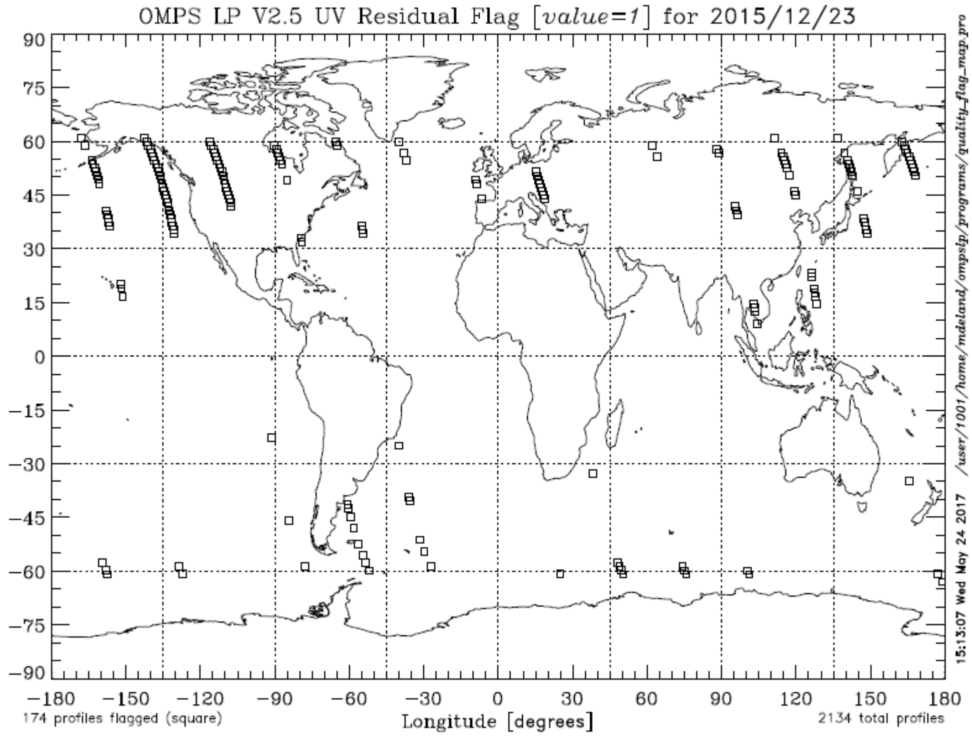

Figure 2. Geographic distribution of UV profile residual quality flag Q_UV = 1 for 23 December 2015.

<u>3. Polar Mesospheric Clouds</u>. We include a flag in the V2.5 data product to identify the most significant instances of PMC contamination in the ozone retrieval. The occurrence frequency of this flag (primarily during June-August in NH data, and December-February in SH data) varies from 5-10% of events at 60°-65° latitude to 85-90% of events at 75°-80° latitude. We recommend that the measurements identified by the PMC flag should not be used in data analysis.

<u>4. Data Sampling</u>. Data rate limitations on the Suomi NPP satellite prevent collection of the full wavelength and altitude range observed by LP for every event. The selection of pixels to be downloaded is specified by the Sample Table, which can be reprogrammed on-orbit. Table 3 gives a list of the main sample tables used by the LP instrument since launch. During the time period covered by Sample Table (STB) v0.5 (11/26/2013 – 01/23/2014), the altitude coverage of short wavelength radiance data causes problems in the UV retrieval algorithm. As a result, we have replaced all UV retrieval density values with fill values during this period, and set the corresponding retrieval quality flag to -999. We do not believe that the VIS retrievals are impacted by this issue, but we have not fully verified this statement. We therefore set the VIS retrieval quality flag to 2 during the STB v0.5 period as a caution to users.

Table 3. OMPS LP Sample Table list as loaded on the Suomi NPP spacecraft for Earth view data collection. Note that during early instrument operations (through February 2012), there was more frequent switching between different sample tables.

Version	Orbits	Start Date	End Date	Comments
1.2	1-1581 3735-3737	10/28/2011	02/16/2012	BATC sample table
84.4	1043-1072	01/09/2012	01/11/2012	Initial sample table for regular science operations (ST 5A)
84.3	1279-1298	01/26/2012	01/27/2012	Left slit only (all pixels)
84.1	1299-1386	01/27/2012	02/03/2012	Right slit only (all pixels)
84.2	1387-1438	02/03/2012	02/06/2012	Center slit only (all pixels)
84.5	1439-3734 3738-4658	02/06/2012	09/20/2012	Minor smear pixel revision to operational table
0.4	4659-10788	09/20/2012	11/26/2013	Minor revision to move wavelength registration columns
0.5	10789-11612	11/26/2013	01/23/2014	First revision for improved spectral coverage
0.6	11613-12010	01/23/2014	02/20/2014	Second revision for spectral coverage
0.7	12011-13101	02/20/2014	05/08/2014	Third revision for spectral coverage
0.8	13102-current	05/08/2014	current	Small changes to improve IR coverage

5. Data Coverage. The first OMPS LP measurements were taken on January 10, 2012. LP data for January-March 2012 have numerous gaps due to variations in instrument operations and changes in sample tables. Regular operations began on April 2, 2012. Note that there is very little or no LP data on days when the OMPS Nadir Mapper conducts high-resolution measurements. This sequence occurred approximately one day per week from April 2012 to June 2016.

6. Solar Intrusion. LP radiance data near the end of the orbit can show anomalous values at high altitude. This behavior begins at approximately event 170, and has a seasonal variation with maximum effects in July [minimum solar β angle] and minimum effects in November. We believe that this behavior is caused by solar radiation that enters the instrument when the Sun illuminates the spacecraft insulation at high solar zenith angle at the end of the orbit. Users should be cautious with data taken during these situations.

7. Measurement Flags. The O3-DAILY data product contains important information about spacecraft position and orientation for each measurement in the 'SwathLevelQualityFlags' dataset of the GeolocationFields group (see the O3-DAILY Product Description document for details). The 'SAA' value of this dataset indicates the probability of South Atlantic Anomaly (SAA) charged particle effects on raw CCD data. The 'NonNominalAttitude' value of this dataset indicates when the S-NPP spacecraft orientation is temporarily changed, such as during roll maneuvers for VIIRS lunar calibrations. Both flags indicate an increased possibility of abnormal ozone density profiles. Users should check these flags when selecting observations for their analysis to ensure maximum data quality.

5. Citation Format

Publications that reference these data should include the following citation:
"OMPS LP Version 2.5 ozone profile data are produced by the LP processing team (DOI 10.5067/X1Q9VA07QDS7)".

The LP AER675 aerosol extinction data product and documentation referenced here can be found at the NASA GES DISC using this link:

https://disc.gsfc.nasa.gov/uui/datasets/OMPS_NPP_LP_L2_AER675_DAILY_1/summary

6. References

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