

2 The author would like to thank Dr. Glen Jaross for the constructive and helpful suggestions on  
3 this manuscript. We replied 4 specific comments from this reviewer.

4

5 **General Comment:** I found this paper to be well written and organized, and the scientific  
6 relevance clearly indicated. The scientific arguments are substantiated through analysis and  
7 presented in a fashion that is mostly understandable. Since this paper reports on a technique  
8 that has already been published, its value is in describing how the performance varies with  
9 different instruments. The paper accomplishes this objective. It also provides an important  
10 independent evaluation of OMPS Level1 product performance. I do have several technical  
11 questions/criticisms. I don't think they represent major problems, but I would like to see the  
12 addressed in some way prior to publication.

13 **Specific Comment**

14 C1. Section3.1 it is not entirely obvious that the discussion in this section is necessary. The  
15 authors fail to provide an estimate of their sensitivity to slit function shape that justifies the  
16 investigation. Given that they use sun-normalized radiances in their retrievals, much  
17 sensitivity to the shape goes away in the ratio. While some sensitivity remains, it is not clear  
18 that this represents an error comparable to other error sources. For example, the large OMPS  
19 foot print means that most scenes are partially cloudy. The resulting signal gradient across the  
20 slit width not only shifts the weighted mean of the function, but also distorts its shape. The  
21 effects of this distortion do not cancel in the sun normalization. Surely this is a larger source  
22 of error than small shape errors, one that the authors have not accounted for.

23 ➔ In this section we would like to figure out if OMPS-NM preflight slit functions are still  
24 suitable for representing instrument line shapes after launch for ozone fitting window because  
25 it has not been shown in literature, and to determine which analytic function works best to  
26 simulate on-orbit instrument line shapes that deviate from the preflight-measured slit  
27 functions due to instrument degradation or thermal-induced variation. For this purpose, we  
28 justified that super Gaussian slit functions better represent OMPS irradiances than standard  
29 Gaussian and even slightly better than preflight measured slit functions. However the fitting  
30 accuracy of sun-normalized radiances with different slit functions show insignificant  
31 differences due to the differences between the slit functions derived from solar irradiances  
32 and slit functions derived from earth radiances caused by scene heterogeneity as also  
33 mentioned by this reviewer, differences in stray light between irradiance and radianc. In  
34 conclusion OMPS measured slit functions are used in our OMPS ozone fitting retrievals  
35 because they take account of the slight wavelength dependence of slit functions. It is worth to

36 know that OMPS measured slit functions work well for ozone fitting window when compared  
37 to the use of analytic slit functions.

38 C2. Lines225-226 this is not a correct assumption. OMPS NM is known to have slit widths that  
39 change with temperature. The result is Earth-view slit functions that are broader at the swath  
40 edges than their irradiance counter parts, by about 4percent.

41 ➔ We agree that this is not exactly true. But we would like to mention here that in practice,  
42 slit functions are typically analytically derived from irradiance spectrum through cross-  
43 correlation using high resolution solar reference spectrum and then used to convolve high-  
44 resolution cross sections in RT simulation of radiance spectrum if accurate preflight slit  
45 function measurements are unavailable. This implicitly assumes that the instrument line shape  
46 is similar for both radiance and irradiance. For more clarification, the relevant sentence have  
47 been edited as following:

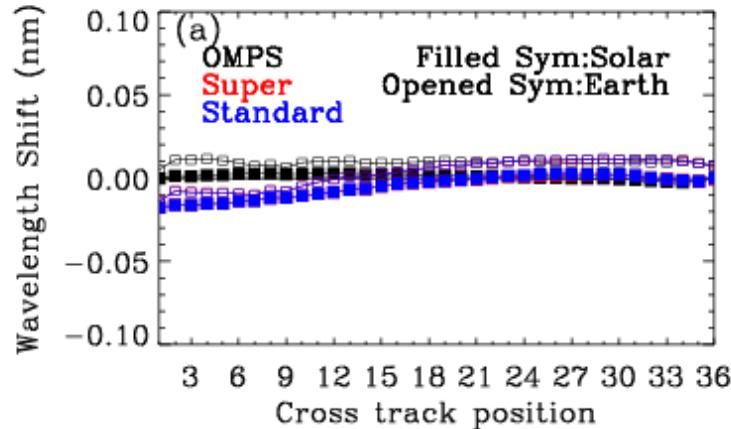
48 (Before revising) In general, the instrument line shape is assumed to be the same for both  
49 radiance and irradiance measurements from satellite observation and determined from  
50 irradiances due to lack of atmospheric interference.

51 (After revising) In general, when accurate measurements of slit functions are not available, the  
52 instrument line shape of satellite observation is typically assumed to be the same for both  
53 radiance and irradiance measurements, and then can be better determined from irradiances due  
54 to lack of atmospheric interference.

55 C3. Lines 263 and 268 these two lines of text seem contradictory. In the v2 L1B product  
56 separate wavelength scales are reported for radiance and irradiance data. These scales differ  
57 by almost 0.05 nm. Line263 implies that the reported radiance band centers are in error by  
58 0.05 nm on average, which is a very large number. But Line268 states that the derived  
59 difference between radiance and irradiance scales is 0.05 nm. Both of these statements cannot  
60 be true unless the authors are using the irradiance wavelength scale to represent radiance data.  
61 At the very least, the authors should state which parts of the L1B product are in error.

62 ➔ Yes, the wavelength errors shown in this study are larger than those reported in L1B  
63 product, due to the fitting window implemented for the wavelength calibration. OMPS team  
64 uses 350-380 nm where prominent solar Fraunhofer absorption lines exist and the  
65 interference with ozone absorption lines are negligible, compared to the used spectral region  
66 300-340 nm in this study. As shown in the following figure, the wavelength errors in the 340-  
67 380 nm range are reduced to ~ 0.02 nm or less for earthshine measurements and ~ 0.0 nm  
68 for solar measurements so that the shifts between solar and earthshine spectra become

69 similar to one reported in Seftor et al. (2014),  $\sim 0.015$  nm at tropics. We have added some  
70 sentence in the revised manuscript to notice this fact.



71  
72 Same as Figure 4.a in the manuscript, but for 340-380 nm.

73 (Reversed sentence) This analysis indicates that the accuracy of wavelength registration in  
74 ozone fitting wavelengths is 0.03-0.06 nm for earthshine measurements and  $< 0.02$  nm for  
75 solar measurements with consistent variation over all cross-track pixels. These wavelength  
76 errors are larger than those reported by Seftor et al. (2014), due to different fitting windows.  
77 They use 350-380 nm where prominent solar Fraunhofer absorption lines exist and the  
78 interference with ozone absorption lines are negligible.

79 C4. Section3.3 I fail to understand what is gained from the common mode correction described  
80 here. It appears that the end objective is to reduce fitting residuals and standard deviations  
81 along the orbit. When this is done independently for each spectrum, without identifying and  
82 correcting the underlying cause of these residuals, it's not clear there are any gains in product  
83 accuracy. It would be beneficial if the authors can discuss up front the objectives for these  
84 corrections. What types of physical errors will this correction address? Also, I would  
85 appreciate a clearer description of how the correction is derived (the explanation in the  
86 conclusions is better than in this section).

87 ➔ The soft calibration spectrum is derived from fitting residuals under tropical clear sky  
88 condition on March and applied independently on time and spatial. This eliminates fitting  
89 residuals very well for mild solar zenith angles, but noticeable systematic biases still remain  
90 over high latitude region after soft calibration (Figure 8 left vs right) so that we implement  
91 “common mode correction” to correct these fitting residuals, especially for polar region. The  
92 idea of common mode correction is to 1) characterize the systematic component of fitting  
93 residuals existing after soft calibration as a function of every month and three latitude bands  
94 (Southern/Northern high latitude and tropics), which is called “common mode spectrum”. 2)

95 The amplitude of this common mode spectrum is adjusted to massage OMI radiances during  
96 iterative ozone fitting. Both soft calibration and common mode correction account for errors  
97 that could be not explained by any physical meaning, such as forward model/parameter errors  
98 and uncorrected measurement errors. We show benefit of applying “common mode correction  
99 “on the fitting accuracy (figs 10 and 11) and on the smoothness of the cross-track dependent  
100 noises of the tropospheric ozone retrievals over the polar region (Figs 7b and 15a). As  
101 mentioned in conclusion, we will also evaluate algorithm implementation and retrieval  
102 accuracy using independent ozone measurements such as ozonesonde and other satellite  
103 product.

104 **Editorial comments.**

105 Line22 ...resulting in serious...

106 Line29 (and throughout document) the typical phrase is “noise floor” rather than “floor noise.”  
107 Line188 The OMPS preflight slit functions were characterized for each CCD pixel... (They  
108 were not measured for each pixel)

109 Line207 “super” instead of “supper”

110 ➔ We have accepted all editorial suggestions. Thanks.

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122 **Response to referee #2's comments**  

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123 The author would like to thank for the constructive and helpful suggestions on this  
124 manuscript.

125 We replied 5 specific comments from this reviewer.

126 **General comments and recommendation:** This paper demonstrates the need for better  
127 retrieving tropospheric ozone from space-borne instrument, OMPS Nadir Mapper. Out of 3  
128 OMPS sensors, the authors explained why OMPS NM is the most suitable for this. More detail  
129 description on the retrieval algorithm has been demonstrated on OMI instrument (Liu et al  
130 2010). In this paper, the authors focused on better optimizing OMPS NM L1B measurements  
131 by introducing additional tuning methods. This is a very well-written and well-structure paper  
132 and is highly relevant to the community. I only have several technical questions/criticisms.

133 **Specific comments:**

134 C1. p2 in the Introduction: Line 53-54: I could only find one reference for Huang et al 2017 in  
135 the Reference.

136 ➔ We have added another reference, “Huang, G., Liu, X., Chance, K., Yang, K., and Cai, Z.:  
137 Validation of 10-year SAO OMI Ozone Profile (PROFOZ) Product Using Aura MLS  
138 Measurements, Atmos. Meas. Tech. Discuss., <https://doi.org/10.5194/amt-2017-92>, in review,  
139 2017b” in the list of reference.

140 C2. Fig 2c.1: It'd be nice to have shown scaling factor on the second Y-axis, as shown in Fig  
141 2a.1 and 2b.1

142 ➔ Super Gaussian function is determined with slit width and shape factor (k), but standard  
143 Gaussian function has only one free parameter (slit width) so we don't need to add scaling  
144 factor in Fig 2c.1

145 C3. p10, in Soft Calibration Line 296: Figure 5 compares out preliminary tropospheric and  
146 stratospheric ozone column retrievals with collocated OMI retrievals. Can you elaborate more  
147 on how you collocated OMI and OMPS in this case?

148 ➔ We did not collocate OMI and OMPS based on pixel by pixel because quantitative  
149 comparison is not performed. We compare preliminary OMPS retrievals with OMI on same  
150 day (timely collocated). For more clarification, we have removed “collocated” in this sentence.

151 C4. p11 in Common Mode Correction You did not have CMC mentioned anywhere in the  
152 context, but Figure 10 and 11 use with CMC and without CMC experiments.

153 ➔ We have added “CMC” when we first mention Common Mode Correction in section 3.3.

154 C. p13 where you have comparison between Fig 15a and Fig 7b. Maybe it is just the color  
155 scheme that gives visual illusion. I found the higher value in pinkish color off west Atlantic  
156 shown in Fig. 7b, whereas in Fig 15a the max value seems to be shifted to east side of Atlantic  
157 in Fig 15a and it seems there is a strong gradient in Fig 15 in the middle of Atlantic.

158 ➔ Thank for your detailed analysis on this comparison. Calibration and Correction schemes  
159 presented by this study clearly demonstrate improvements with respect to spectral fitting  
160 accuracy and we will evaluate each scheme with respect to ozone retrieval accuracy using  
161 ozonesonde dataset as mentioned in conclusion.

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# Characterization and Correction of OMPS

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## Nadir Mapper Measurements for Ozone Profile Retrievals

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### Abstract

188 This paper verifies and corrects the Ozone Mapping and Profiler Suite (OMPS) Nadir Mapper (NM)  
 189 Level 1B v2.0 measurements with the aim of producing accurate ozone profile retrievals using an  
 190 optimal estimation based inversion method to fit measurements in the spectral range 302.5-340 nm. The  
 191 evaluation of available slit functions demonstrates that preflight-measured slit functions well represent  
 192 OMPS measurements compared to derived Gaussian slit functions. Our initial OMPS fitting residuals  
 193 contain significant wavelength and cross-track dependent biases, resulting ~~into~~ in serious cross-track  
 194 striping errors in the tropospheric ozone retrievals. To eliminate the systematic component of the fitting  
 195 residuals, we apply “soft calibration” to OMPS radiances. With the soft calibration the amplitude of  
 196 fitting residuals decreases from ~1 % to 0.2 % over low/mid latitudes, and thereby the consistency of  
 197 tropospheric ozone retrievals between OMPS and the Ozone Monitoring Instrument (OMI) is  
 198 substantially improved. A common mode correction is also implemented for additional radiometric  
 199 calibration; it improves retrievals especially at high latitudes where the amplitude of fitting residuals  
 200 decreases by a factor of ~2. We estimate the ~~floor~~-noise floor error of OMPS measurements from  
 201 standard deviations of the fitting residuals. The derived error in the Huggins band (~0.1 %) is twice the

202 OMPS L1B measurement error. OMPS ~~floor~~-noise floor errors better constrains our retrievals, leading  
203 to improving information content of ozone and reducing fitting residuals. The final precision of the  
204 fitting residuals is less than 0.1 % in the low/mid latitude, with ~1 degrees of freedom for signal for the  
205 tropospheric ozone, meeting the general requirements for successful tropospheric ozone retrievals.

## 206 1. Introduction

207 Atmospheric ozone has very different roles depending upon its altitude. About 90 % of the total  
208 ozone is in the stratosphere, protecting the Earth's life from harmful solar ultraviolet (UV) radiation  
209 that can cause skin cancer and immune system suppression. The remaining 10 % in the troposphere  
210 shows dangerous effects as a major component of photochemical smog at surface level and as a short-  
211 lived greenhouse gas in the upper troposphere, whereas in the middle troposphere it plays a beneficial  
212 role in chemically cleaning the atmosphere as a precursor of hydroxyl radicals (OH). Therefore, vertical  
213 ozone profiles should be monitored to improve our understandings of the chemical and physical  
214 functions of this important trace gas. Space-based monitoring of ozone profiles including the  
215 troposphere from backscattered UV radiation has been available since the launch of Global Ozone  
216 Monitoring Experiment (GOME) (European Space Agency, 1995) on board the Second European  
217 Remote Sensing Satellite (ERS-2) in April 1995. Its successors continued the role of GOME for  
218 atmospheric ozone monitoring with Scanning Imaging Absorption SpectroMeter for Atmospheric  
219 ~~ChartographY~~ ChartographY (SCIAMACHY) (Bovensmann et al., 1999) aboard the Environmental  
220 Satellite (ENVISAT), GOME-2s (EUMETSAT, 2006) aboard the MetOp-A and MetOp-B, and Ozone  
221 Monitoring Instrument (OMI) (Levelt et al., 2006) flown on the EOS Aura spacecraft. The good  
222 performance of OMI ozone profile retrievals in both stratosphere and troposphere has been  
223 demonstrated through extensive validation efforts using ozonesondes, aircraft, satellite data, and  
224 ground-based total ozone data (Pittman et al., 2009; Liu et al., 2010b; Bak et al., 2013b; 2015; Huang  
225 et al., 2017a,~~b~~a,b). However, a portion of OMI radiance measurements has been affected by the partial  
226 blockage of the instrument's entrance slit, a problem termed the row anomaly, which started in 2007  
227 and grew serious in January 2009 (Schenkeveld, 2017). The Ozone Mapping and Profiler Suite (OMPS)  
228 aboard the Suomi National Polar-Orbiting Partnership (NPP) satellite launched in 2011 (Flynn, et al.,  
229 2014) represents the next generation of US instruments to continue the role of OMI in monitoring total  
230 ozone and ozone vertical profiles, together with the TROPOspheric Monitoring Instrument (TROPOMI)  
231 to be launched on board the Sentinel-5 Precursor satellite in 2017 (Veefkind et al., 2012). OMPS is a  
232 sensor suite which consists of three instruments, the Nadir Mapper (OMPS-NM), the Nadir Profiler

(OMPS-NP), and the Limb Profiler (OMPS-LP). The OMPS-NM is designed to measure the daily global distribution of total column ozone with an  $110^{\circ}$  cross-track field of view (FOV), similar to OMI and the Total Ozone Monitoring Spectrometer (TOMS) series (Bhartia and Wellemeyer, 2002). OMPS-NP is an ozone profiler sensor, measuring the vertical ozone profiles in the upper stratosphere, similar to the Solar Backscatter Ultraviolet (SBUV/2) series (Bhartia et al., 2013). The OMPS-LP is designed to measure ozone profiles in the stratosphere and upper troposphere at high vertical resolution, similar to the Microwave Limb Sounder (MLS). Both OMPS-NP and OMPS-LP are ozone profile sensors, but lack sensitivity to the troposphere due to the spectral coverage of 250-290 nm and the viewing geometry, respectively. Therefore, OMPS-NM is the only candidate for global monitoring of ozone profiles down to the troposphere even though its spectral resolution of 1.0 nm does not fully resolve the ozone absorption band features in the Huggins band and its spectral coverage of 300-380 nm is insufficient to retrieve stratospheric ozone profiles. The retrieving of ozone profiles including tropospheric ozone from OMPS-NM measurements has not yet been presented in the literature. The present effort fills the gap between OMI and upcoming satellite observations.

The final goal of this study is to demonstrate the successful performance of ozone profiles and tropospheric ozone retrievals from only OMPS-NM measurements. Thus, we refer to OMPS-NM simply as OMPS hereafter. The retrieval algorithm used in this study is based on the Smithsonian Astrophysical Observatory (SAO) ozone profile algorithm that was developed for GOME (Liu et al., 2005) and OMI (Liu et al., 2010a). The SAO OMI algorithm is based on an optimal estimation inversion (Rodgers, 2000) combined with accurate wavelength/radiometric calibration, forward model simulation, and good a priori knowledge. This algorithm has been implemented for ozone profile and  $\text{SO}_2$  retrievals from GOME-2 instrument (Cai et al., 2011; Nowlan et al., 2011) and will be adapted to ozone profile retrievals from upcoming geostationary UV/VIS spectrometers including the Geostationary Environmental Monitoring Spectrometer (GEMS) (Bak et al 2013a) and Tropospheric Emissions: Monitoring of Pollution (TEMPO) instrument (Chance et al., 2013, Zoogman et al., 2017) for monitoring air quality over North America and East Asia, respectively. OMPS has a similar instrument concept to OMI, GEMS, and TEMPO and hence the application of the similar retrieval algorithms to these measurements will provide an excellent opportunity for long-term trend analysis of ozone profiles, especially in the troposphere. The OMI algorithm is very similar to our OMPS algorithm, but it needs additional optimization for OMPS. In this paper we focus largely on characterizing OMPS measurements (1) through the cross-correlation between OMPS irradiances and a high-resolution solar reference to be used in the verification of OMPS slit function measurements and the characterization of the wavelength registration and (2) through extracting the systematic and random components of fitting

266 residuals between measured and calculated normalized radiances to be used in radiometric and  
267 measurement error calibrations, respectively. Several companion papers to follow will deal with the  
268 detailed error analysis, retrieval characteristics of the retrieved ozone profiles, and validation of  
269 retrievals.

270 The paper is divided into four sections: First, we give a description of OMPS-NM Level 1B (L1B)  
271 v2.0 data (Jaross, 2017) and the ozone profile algorithm in Sect. 2. Section 3 discusses the  
272 wavelength/slit function calibrations and measurement corrections for radiance and measurement error,  
273 respectively. Conclusions are in Sect. 4.

274

## 275 **2. Data and Method**

### 276 **2.1 OMPS measurements**

277 The Suomi NPP satellite is a NOAA/NASA scientific partnership, launched in 2011 into a 824 km sun-  
278 synchronous polar orbit with ascending node equator-crossing time at 13:30 local time. Routine  
279 operations began in 2012. Suomi NPP carries five instruments: The Visible/Infrared Imager Radiometer  
280 Suite (VIIRS), the Cross-track Infrared Sounder (CrIS), the Advanced Technology Microwave Sounder  
281 (ATMS), the Ozone Mapping and Profile Suite (OMPS), and the Clouds and the Earth Radiant Energy  
282 System (CERES). OMPS is a key instrument on Suomi NPP. The sensor suite has both nadir and limb  
283 modules. The nadir module combines two sensors: The Nadir Mapper for measuring total column ozone,  
284 and the Nadir Profiler for ozone vertical profile. The Limb Profiler module is designed to measure  
285 vertical ozone profiles with high vertical resolution from the upper troposphere/lower stratosphere to  
286 the mesosphere. The OMPS-NM employs a 2-D CCD that samples spectrally in one dimension and  
287 spatially in the other, similar to OMI. It has a 110 ° cross-track field of view, resulting in 2800 km  
288 instantaneous swath coverage at the earth's surface; this is sufficient to provide daily global coverage.  
289 It makes 400 swath lines per orbit with 36 cross-track measurements per swath line, resulting in a nadir  
290 footprint of 50 km × 50 km in its nominal configuration. Note that OMPS L1B data used in this  
291 investigation contain 36 cross-track pixels, because the L1B processing in the NASA Ozone SIPS  
292 retains the two central (near-nadir) instantaneous fields of views (IFOVs, 30 km × 50 km and 20 km ×  
293 50 km), without aggregating them into the nominal 50 km × 50 km pixel. The spectral coverage is from  
294 300 to 380 nm with a spectral resolution of ~ 1.0 nm and a sampling of 0.42 nm. The OMPS level 0 to  
295 1b processor was recently updated from version 1.0 to 2.0. The satellite measurements from the OMPS-  
296 NM instrument used in this study are from version 2 of the NMEV-L1B data product (Jaross, 2017)

297 available from the NASA Goddard Earth Sciences Data and Information Services Center (GES)  
298 DISC). The data consist of calibrated Earth-view radiance and solar irradiance data measured by the  
299 instrument between 300-380 nm. Seftor et al. (2014) documented many aspects of the previous version  
300 of the dataset that remain the same, but a number of changes for the V2 dataset do reflect advances in  
301 the characterization of the NM sensor (Seftor and Jaross, 2017) which are relevant to this study. These  
302 are summarized as follows: 1) recalculation of instrument band-pass functions in the 300-310 nm region  
303 affected by the dichroic element of the nadir instrument, 2) improved wavelength registration, 3) an  
304 update to the instrument radiance calibration, and 4) improvement to the stray light correction. The  
305 wavelengths below 302 nm are not used in this study, according to the recommendation of the OMPS  
306 science team.

## 307 **2.2 OMPS simulations**

308 We use the Vector LInearized Discrete Ordinate Radiative Transfer (VLIDORT) model (Spurr, 2006;  
309 2008) to simulate OMPS radiances. VLIDORT is also able to simulate the analytic derivatives of  
310 radiance with respect to any atmospheric or surface parameter due to its full linearization capability.  
311 The polarization of light is taken into account in VLIDORT calculation, but the Ring spectrum is  
312 modeled using a single scattering RRS model (Sioris and Evans, 2000). We consider only Rayleigh  
313 scattering (no aerosol) and ozone absorption (no other trace gases), with Lambertian reflectance  
314 assumed for the surface and for clouds. Clouds are treated as a Lambertian reflector at cloud top, with  
315 a fixed albedo of 0.8 unless it is fully cloudy so that the cloud albedo ( $>0.80$ ) can be derived. Cloud  
316 fraction is required to simulate partial clouds as the weighted average between clear and cloudy scenes  
317 using the Independent Pixel Approximation (IPA). The forward model inputs used in VLIDORT are  
318 listed in Table 1.

## 319 **2.3 OMPS ozone profile retrievals**

320 The inversion from Backscattered UV measurements to the state of the atmosphere is performed  
321 using the well-known optimal estimation method (Rodgers, 2000). It calculates the a posteriori solution  
322 by iteratively and simultaneously minimizing the cost function consisting of the sum of the squared  
323 differences between measured and simulated radiances and between retrieved and a priori state vectors,  
324 constrained by measurement error covariance matrix and a priori error covariance matrix. The a  
325 posteriori solution and cost function can be written:

326 
$$X_{i+1} = X_i + (K_i^T S_y^{-1} K_i + S_a^{-1})^{-1} [K_i^T S_y^{-1} (Y - R(X_i)) - S_a^{-1} (X_i - X_a)] \quad (1)$$

327 
$$\chi^2 = \left\| S_y^{-\frac{1}{2}} \{ K_i (X_{i+1} - X_i) - [Y - R(X_i)] \} \right\|_2^2 + \left\| S_a^{-\frac{1}{2}} (X_{i+1} - X_a) \right\|_2^2. \quad (2)$$

328 The inputs to the optimal estimation are defined as follows.  $\mathbf{X}$  is the state vector to be retrieved,  
 329 consisting of ozone profiles as well as other geophysical parameters and spectroscopic parameters  
 330 affecting the observed radiances and hence the retrieval of ozone profile. The 24 partial columns of  
 331 ozone in DU are retrieved at 25 pressure levels that are initially set to be  $P_i = 2^{-i/2}$  atm for  $i =$   
 332  $0, 1, \dots, 23$  (1 atm = 1013.25 hPa) with the top of the atmosphere at 0.087 hPa for  $P_{24}$ . The geophysical  
 333 parameters include effective surface albedo and cloud fraction. The calibration parameters consists of  
 334 two wavelength shift parameters between radiances and irradiances and between radiances and ozone  
 335 cross sections and two scaling parameters for the Ring effect that account for filling-in of Fraunhofer  
 336 lines in the solar spectrum due to rotational Raman scattering and mean fitting residuals that may not  
 337 be accounted for properly in radiometric calibration. The a priori data for ozone is one of the key optimal  
 338 estimation inputs because the retrieval solution comes mainly from a priori information rather than  
 339 measurement information where the instrument sensitivity to the true ozone profile is insufficient. The  
 340 a priori value ( $X_a$ ) and a priori error covariance ( $S_a$ ) of ozone is taken from the tropopause-based ozone  
 341 profile climatology that is optimized to represent the dynamical ozone variability in the upper  
 342 troposphere and lower stratosphere (Bak et al., 2013b). The measurement vector  $Y$  is defined as the  
 343 logarithm of the earthshine radiances normalized to the daily solar irradiance.  $S_y$  is a measurement  
 344 error covariance matrix that is assumed to be a diagonal matrix with diagonal elements being the squares  
 345 of the assumed measurement errors. We use OMI ~~floor~~-noise ~~floor~~ errors (0.4 % below 310 nm, 0.2 %  
 346 above, Huang et al., 2017a) as our preliminary measurement constraint and then derive OMPS ~~floor~~  
 347 noise ~~floor~~ errors specified in Section 3.4.  $R(X)$  is the calculated radiances corresponding to  $X$ .  $K$  is  
 348 a weighting function matrix representing partial derivatives of the forward model with respect to the  
 349 atmospheric parameters,  $K_{ij} = \partial R_i(X) / \partial X_j$ . More detailed descriptions can be detailed in Liu et al.  
 350 (2010a).

351

352 **3. Results**

353 **3.1 Slit Function and Wavelength Calibration**

354 It is essential to investigate the best knowledge of the instrument slit function to convolve a high-  
355 resolution solar reference spectrum for wavelength calibration as well as to convolve high-resolution  
356 trace gas cross sections for simulation of earthshine spectra. A triangular bandpass with a fixed  
357 bandwidth of 1.1 nm has been typically used for Total Ozone Monitoring Instrument (TOMS), SBUV,  
358 and SBUV/2 monochromators. Slit functions of spectrometers such as OMI and GOME1/2 have been  
359 measured prior to launch using a tunable laser or analytically derived assuming a Gaussian-type shape  
360 if measured slit functions are unavailable or inaccurate. The OMPS preflight slit functions were  
361 measured characterized for each CCD pixels (196 band centers and 36 cross-track positions), which has  
362 been adopted and modified for OMPS trace-gas retrievals such as in Yang et al. (2013; 2014) and  
363 Gonzalez Abad et al. (2016). The slit function modification is accomplished in the previous works  
364 (Yang et al., 2013, 2014) by stretching and shrinking the slit widths, i.e., by applying a wavelength-  
365 dependent scaling factor to the OMPS measured slit functions. According to Yang et al. (2013; 2014),  
366 we fit the scaling factor as a slit parameter so that variations in measured slit functions before and after  
367 launch could be taken into account.

368 Figure 1a shows an example of measured OMPS slit functions at 320 nm, illustrating that their  
369 shapes seem to be Gaussian and vary considerably over cross-track pixels, especially near the wings.  
370 Note that the 36 cross-track positions are denoted from 1 at the left edge and 36 at the right edge. The  
371 slit function shapes at 17<sup>th</sup> cross-track position are nearly consistent over wavelengths that we are  
372 focusing on for ozone retrievals (Fig. 1.b). Figure 1c displays the full width at half maximum (FWHM)  
373 including dependencies in both dimensions of the detector arrays. The spectral variation of the slit  
374 widths is insignificant (FWHMs vary by less than 0.01 nm), whereas average slit widths vary  
375 significantly across track by over 0.1 nm. This characteristic of measurement slit functions confirms  
376 that we should consider their cross-track dependence for OMPS slit functions, but their wavelength  
377 dependence is ignorable so that we can avoid the time-consuming convolution process.

378 We evaluate the usefulness of these measured slit functions for fitting both OMPS radiance and  
379 irradiance against the analytical slit functions assusing both standard Gaussian and ~~upper~~ Gaussian  
380 distributions. We note all the Gaussian shapes used in this analysis are assumed to be symmetric. The  
381 Gaussian slit function is expressed as

382

$$S(\lambda) = \frac{k}{2w\Gamma\left(\frac{1}{k}\right)} \exp\left[-\left|\frac{\Delta\lambda}{w}\right|^k\right], \quad (3)$$

383 where  $k$  is the shape factor and  $w$  is the slit width, with relative wavelength to band center wavelength,  
 384  $\Delta\lambda$ . This function can describe a wide variety of shapes just by varying  $k$ ; for  $k=2$  it becomes the  
 385 standard Gaussian and  $w$  represents the half width at 1/e intensity (FWHM =  $2\sqrt{\ln 2} w$ ). Compared  
 386 to the standard Gaussian, the super Gaussian has broader peaks at the top and thinner wings if  $k$  is larger  
 387 than 2 whereas it has sharper peaks and longer tails if  $k$  is smaller than 2.  $w$  of the super Gaussian  
 388 function represents the half-width at 1/e<sup>th</sup> intensity (FWHM =  $2^k\sqrt{\ln 2}$ ). The symmetric or asymmetric  
 389 standard Gaussian has been commonly assumed to derive OMI, GOME, and GOME-2 slit functions  
 390 (Liu et al., 2005;2010; Nowlan et al., 2011; Cai et al., 2012; Munro et al., 2016). Recently the hybrid  
 391 combination of standard and flat-top Gaussian functions has been implemented for characterizing OMI  
 392 laboratory measurements of slit functions (Dirksen et al., 2006) and deriving airborne instrument slit  
 393 functions (Liu et al., 2015a;2015b; Nowlan et al., 2016). The concept of this hybrid Gaussian function  
 394 is very similar to the super Gaussian, but is a rather complex with more slit parameters. The super  
 395 Gaussian function was introduced and tested as an analytical slit function by Beirle et al. (2017) and  
 396 Sun et al. (2017a;b).

397 In general, when accurate measurements of slit functions are not available, the instrument line shape  
 398 of satellite observation is typically assumed to be the same for both radiance and irradiance  
 399 measurements, and then can be better determined from irradiances due to lack of atmospheric  
 400 interference. In general, the instrument line shape is assumed to be the same for both radiance and  
 401 irradiance measurements from satellite observation and determined from irradiances due to lack of  
 402 atmospheric interference. We simultaneously and iteratively determine the wavelength and slit  
 403 calibration parameters through cross-correlation of the measured OMPS irradiances to simulated solar  
 404 irradiances from a well calibrated, high-resolution solar irradiance reference spectrum (Chance and  
 405 Kurucz, 2010). The simulation of solar irradiance,  $I_s$  is described as

406

$$I_s(\lambda) = AI_o(\lambda + \Delta\lambda) \times \sum_{i=0}^2 P_i(\lambda - \lambda_{avg})^i, \quad (4)$$

407 where  $I_o$  is the convolved high-resolution solar reference spectrum with assumed slit functions,  $A$  is  
 408 the scaling parameter for  $I_o$ .  $\lambda + \Delta\lambda$  Indicates the process of wavelength calibration (e.g. shift and  
 409 squeeze); only the wavelength shift is considered in this study.  $P_i$  represents the coefficients of a scaling  
 410 polynomial (third order in this study). This approach was firstly introduced by Caspar and Chance

411 (1997), and is widely used for wavelength and slit function calibrations in trace gas retrievals from  
412 UV/visible measurements.

413 In this experiment, the slit parameters,  $w$  and  $k$  or slit scaling are fitted from daily measured  
414 OMPS irradiances over the wavelength range 302-340 nm at each cross-track position. Note that this  
415 slit calibration ignores the wavelength dependence for deriving analytic slit functions and slit scaling to  
416 the measured slit functions; this is a good approximation based on Fig. 1b as the wavelength dependence  
417 of the slit functions is small. But the variation of the slit shape with wavelength could be considered  
418 with OMPS preflight measured slit functions given for every CCD dimension if it becomes necessary.  
419 The left panels of Fig. 2 compare the derived slit parameters from OMPS irradiances using different  
420 functions. The red line of Fig. 2.a.1 shows that a slight change of the preflight-measured slit functions  
421 is required to model the OMPS irradiance measurements, by up to 4% at both edges. Therefore the  
422 benefit of fitting measured slit functions over fixing them is found to be trivial ( $\sim 0.001\%$ ) at nadir  
423 cross-track pixels (12-30<sup>th</sup>); for edge pixels, the improvement in fitting residuals is more noticeable, up  
424 to 0.18%. The shape factor ( $k$ ) of the derived super Gaussian functions is found to be  $\sim 2.3$  for left swath  
425 and  $\sim 2.5$  for right swath (Fig. 2.b.1), implying that they have broader peaks and thinner wings compared  
426 to the standard Gaussian if slit widths are equal. The slit widths of three different slit functions show  
427 similar variations with respect to cross-track positions. The FWHMs vary from widest at  $\sim 12^{\text{th}}$  cross-  
428 track position to narrowest at the edges, but they are significantly narrower at the rightmost cross-track  
429 positions than at the leftmost ones. Compared to the standard Gaussian slit widths, the super Gaussian  
430 slit widths show a much better agreement with measured slit widths; the average difference of slit widths  
431 between measured and super (standard) Gaussian functions is  $\sim 0.01$  (0.05) nm. In Fig. 3, an example  
432 of the derived slit functions and fitted preflight slit functions shows that the shapes are very similar.

433 The wavelength calibrations using different slit functions are characterized for the ozone fitting  
434 window and are shown in Fig. 4b. The shift parameter is determined from irradiance and radiance at  
435 second cross-correlation step after slit parameters are determined from irradiances at first cross-  
436 correlation step. Note that the wavelength shifts fitted between first and second steps are very similar,  
437 indicating little correlation between slit and wavelength calibration parameters. This analysis indicates  
438 that the accuracy of wavelength registration in ozone fitting wavelengths is 0.03-0.06 nm for earthshine  
439 measurements and < 0.02 nm for solar measurements with consistent variation over all cross-track  
440 pixels. These wavelength errors are larger than those reported by Seftor et al. (2014), due to different  
441 fitting windows. They use 350-380 nm where prominent solar Fraunhofer absorption lines exist and the  
442 interference with ozone absorption lines are negligible. This analysis indicates that the accuracy of  
443 wavelength registration in level 1b data is on average 0.05 nm for earthshine measurements and within

444 0.02 nm for solar measurements with consistent variation over all cross-track pixels.

445 HoweverFurthermore, the wavelength calibration results using OMPS measured slit functions show  
446 different characteristics from those using both Gaussian-type slit functions, especially over left cross-  
447 track pixels. The different wavelength shifts are likely because the original OMPS slit functions show  
448 slight asymmetry and are used in the wavelength calibration of L1B data. There exists a  $\sim 0.07$  nm shift  
449 between irradiances and radiance. In ozone retrieval algorithm we shift neither radiance nor irradiance  
450 to a reference spectra before retrievals, but the shift between irradiance and radiance is adjusted during  
451 ozone retrievals to account for the on-orbit variations of wavelength shifts as mentioned in Sect. 2.3.

452 The right columns of Fig. 2 compare the impact of different slit functions on spectral fitting residuals  
453 of solar irradiances, together with the average fitting residuals as a function of cross-track position in  
454 Fig.4.a.4. a. Measured solar spectra are mostly within an average of  $\sim 1\%$  of modeled solar spectra,  
455 except for the first few wavelengths. Based on these fitting results, we revise the fitting window to  
456 302.5-340 nm. The fitting residuals using a derived standard Gaussian function are the worst for all  
457 cross-track positions. On the other hand, the super Gaussian slit function similarly represents the  
458 measured slit function, but slightly improves the fitting accuracy at the 6~18 cross-track positions (Fig.  
459 4.a). However, the benefit of using the super Gaussian function for fitting OMPS radiances over the  
460 standard Gaussian function is insignificant within 0.02 % (not shown here). These results agree well  
461 with Beirle et al. (2017), who demonstrated the similar benefit of using Standard and Super Gaussian  
462 slit functions on OMI and GOME-2 measurements. Moreover, the impact of using different slit  
463 functions could be less important for OMPS than OMI and GOME-2 due to its coarser spectral  
464 resolution.

465 In summary, super Gaussian functions are recommended for the OMPS instrument slit functions  
466 than the standard Gaussian functions if the on-orbit instrument slit functions largely deviate from the  
467 preflight-measured slit functions due to instrument degradation or thermal-induced variation. In the rest  
468 of this paper, the measured slit function is used for the analysis of OMPS measurements.

## 470 3.2 Soft Calibration

471 The OMPS instrument 2-D CCD detector array could be susceptible to artificial cross-track  
472 dependent errors that are commonly seen in OMI trace gas retrievals. To eliminate this impact on the  
473 OMI L2 product, soft calibration and post-processing cross-track smoothing have been typically  
474 implemented: the first correction removes the systematic wavelength and cross-track dependent

475 component in measured radiances (Liu et al., 2010; Cai et al., 2012), whereas the second correction  
476 removes cross-track dependent biases in retrievals (Kurosu et al., 2004; Hormann et al., 2016). Figure  
477 5 compares our preliminary tropospheric and stratospheric ozone column retrievals with ~~collocated~~  
478 OMI retrievals on 14 March 2013. OMPS stratospheric retrievals show an excellent consistency with  
479 OMI even though OMPS measurements does not cover much of the Hartley ozone absorption  
480 wavelengths where most of the vertical information of stratospheric ozone comes from. This is because  
481 the separation of stratospheric ozone columns from tropospheric ozone columns is still mainly  
482 determined from wavelengths longer than 300 nm (Bak et al., 2013a). On the other hand, tropospheric  
483 ozone retrievals are positively biased with respect to OMI, by amounts largely dependent on the OMI  
484 cross-track position. Therefore, we decide to include a soft-calibration correction in our retrievals to  
485 eliminate wavelength and cross-track dependent errors in OMPS radiances. A general approach to the  
486 soft calibration is to characterize systematic differences between measured and computed radiances for  
487 scenes where we could assume that all parameters are known; the tropics were typically selected since  
488 ozone variability is relatively small (Liu et al., 2010). OMPS normalized radiances are simulated with  
489 collocated OMI ozone profiles averaged and interpolated onto  $5^\circ \times 5^\circ$  grid cells to fill in bad pixels  
490 mostly caused by the row anomaly. Other forward model inputs are described in Sect. 2. We use 25 days  
491 of data between 1 March 2013 and 25 March 2013 under the following conditions: latitude  $<15^\circ\text{N/S}$ ,  
492 solar zenith angle (SZA)  $< 40^\circ$ , cloud fraction  $< 0.1$ , and surface reflectivity  $< 0.1$ . The systematic and  
493 random components of measured-to-simulated radiance ratios are displayed in Fig. 6. Agreement is  
494 mostly at the  $\pm 2\%$  level below 310 nm, except at wavelengths shorter than  $\sim 302.5$  nm where the  
495 systematic biases increase sharply due to the overcorrection of straylight in OMPS v2.0 data processing.  
496 For wavelengths longer than 310 nm, OMPS observations show negative biases with maximum of  $\sim 3\%$   
497 at 315 nm. The standard deviations of mean differences steadily increase from longer wavelengths to  
498 302.5 nm (2-2.5%) and then sharply rise up to  $\sim 4\%$ . The abnormal features of fitting residuals below  
499 302.5 nm shown in Figs. 2 and 6 provide a basis for why we select the lower boundary of the ozone  
500 fitting window as 302.5 nm. The soft calibration is applied before the fitting starts by dividing OMPS  
501 radiances by the derived correction spectrum just at the initial iteration with the assumption that the  
502 systematic biases consistently exist independent of space and time. Figure 7 shows how our  
503 tropospheric ozone retrievals are improved with our soft calibration in comparison with retrievals  
504 shown in Fig. 5.b. The usefulness of our soft calibration implementation is also evaluated through  
505 comparisons of the accuracies of the spectral fitting residuals with and without soft calibration as shown  
506 in Fig. 8. The mean fitting residuals without soft calibration are  $\sim \pm 1\%$  at shorter wavelengths  $< 320$   
507 nm for all latitudes and sky conditions, whereas for longer wavelengths they increase from 0.3 % to

508 0.5 % with increasing latitudes. Our soft calibration dramatically improves the fitting accuracy for both  
509 clear and cloudy pixels, especially over the tropics and mid-latitude regions; fitting residuals are mostly  
510 within 0.2 % at longer wavelengths  $> 310$  nm. In high latitudes, improvements can be identified, but  
511 large remaining systematic biases can still be found.

### 512 **3.3 Common Mode Correction**

513 In previous section, it is shown that our soft calibration effectively eliminates systematic biases of  
514 measurements relative to VLIDORT simulations for most cases, except for high latitudes/SZAs where  
515 there still exists a distinct wavelength-dependent pattern in fitting residuals because the soft calibration  
516 spectrum is derived only under small SZA conditions. In order to verify and correct such systematic  
517 biases remaining after soft calibration, we characterize spectral fitting residuals at the final iteration  
518 classified into 3 latitude/SZA regimes (southern polar region/SZA $>60^\circ$ , tropical region/ SZA $<40^\circ$ ,  
519 northern polar region/ SZA $>60^\circ$ ) for each cross-track position and for one day (14<sup>th</sup> or 15<sup>th</sup>) of each  
520 month. The remainder is called the common residual spectrum. Examples of derived common spectra  
521 are presented in Fig. 9 for March and August 2013. The main peak positions of residuals of all common  
522 residual spectra are well matched to each other. The amplitude of tropical residuals is very similar  
523 between two months, whereas the variation of the amplitude at high latitudes seems to be associated  
524 with snow/ice cover and SZA variations such that the amplitude is maximized during the polar winter  
525 season. Applying the common mode correction ([CMC](#)) means subtracting the common spectrum with  
526 amplitude determined iteratively along with the rest of state vector components from the measured  
527 spectrum. Fig. 10 compares the fitting residuals at high SZAs for one orbit of data on 02 March 2013  
528 with and without the common mode correction. It is evident that wavelength dependent fitting residuals  
529 are greatly reduced even for the first few wavelengths, with amplitude of spectral residuals reduced  
530 from  $\sim 1$  % to 0.5 %. Moreover, the common mode correction slightly reduces the standard deviations  
531 of residuals. The improvement is seen everywhere as shown in Fig. 11 where RMS of relative fitting  
532 residuals (ratio of fitting residuals to measurements error) is displayed for all individual pixels within  
533 one orbit.

### 534 **3.4 Measurement Error Correction**

535 The measurement error covariance matrix  $S_y$  is one of the essential inputs in an OE based algorithm,  
536 because it significantly affects the stability of retrievals and retrieval sensitivities. OMPS L1B v2.0 data

537 contain the relative errors of radiance measurements, but these measurement errors ( $\sim 0.04\%$  @ 320  
538 nm) were too small to regularize our ozone fitting process so that many retrievals fail due to negative  
539 or large positive ozone values as a result of over fitting. Ideally, the measurement errors need to include  
540 not only photon shot noise but also other kinds of random noise errors caused by readout, straylight,  
541 dark current, geophysical pseudo-random noise errors due to sub-pixel variability and motion when  
542 taking a measurement, forward model parameter error (random part), and other unknown errors.  
543 However, OMPS measurement errors reported in the L1B only include photon shot noise and read-out  
544 errors, which underestimate the overall measurement error. For this reason, OMI ~~noise-noise floor (NF)~~  
545 errors instead of OMPS random-noise errors are imposed on our preliminary retrievals, as mentioned  
546 in Sect 2.3. However, better signal-to-noise ratios (SNRs) could be expected for OMPS than OMI due  
547 to OMPS's coarser spectral and spatial resolutions, as shown from the improved detection limit of  
548 OMPS H<sub>2</sub>CO retrievals compared to OMI as discussed in Gonzalez Abad et al. (2016). Fig. 11 also  
549 implies that there is room for increasing the Degrees of Freedom for Signals (DFS) to current ozone  
550 retrievals by regularizing them using the improved measurement error instead of using OMI ~~floor noise~~  
551 ~~NFerror~~; the ideal value of RMS is one, but our RMS is mostly within 0.4 at low and mid-latitudes. The  
552 random-noise component of measurements could be derived from standard deviations of spectral fitting  
553 residuals (Cai et al., 2012; Liu et al. 2015b). Fig. 12 shows how we derive the measurement errors to  
554 improve our retrievals. We first characterize the minimum measurement errors from fitting residuals  
555 under nearly clear-sky condition at SZAs  $< 40^\circ$  and cross-track pixels between 4 and 33; note that no  
556 radiometric calibration is applied to these fitting residuals. The standard deviations of fitting residuals  
557 are nearly invariant at longer wavelengths  $> 310$  nm and show a significant increase from  $\sim 0.1\%$  at  
558 310 nm to  $\sim 0.3\%$  at 302 nm as plotted with the red dashed line in Fig. 12.a. We eliminate the low-  
559 frequency portion of the noises with a 4<sup>th</sup> order polynomial fit to define the minimum OMPS ~~floor noise~~  
560 ~~(FN)NF~~ errors as plotted with the red solid line in Fig. 12.a. The derived ~~FN-NF~~ errors are  $\sim 2$  (1.5-  
561 4) times smaller than OMI ~~floor noise~~~~NF~~ errors above (below) 310 nm and thereby could increase the  
562 measurement information in our retrievals. We impose the minimum ~~FN-NF~~ errors as a measurement  
563 constraint in our algorithm when SZAs are smaller than  $\sim 20^\circ$ , whereas they are multiplied by a SNR  
564 scaling factor to increase measurement errors as a function of SZAs. Figure 12.b shows an example of  
565 how derived measurement errors increase with SZA at the boundary wavelengths of the ozone fitting  
566 window, with errors from 0.24 % to 0.45 % for 302.5 nm and from 0.097 % to 0.19 % for 340 nm.

567 Figure 13 shows the effect of using the derived ~~FN-NF~~ errors on our retrievals. The RMS of fitting  
568 residuals increases from 0.2-0.4 to 0.4-0.8 in swath lines 50-350, where SZAs are within  $\sim 60^\circ$ , due to  
569 SNR increases, whereas the average fitting residuals slightly improves by 0.015 %. Using the new ~~FN~~

570 NF errors slightly increases the number of iterations; one or more iterations are required for  $\sim 24\%$  of  
571 the total retrieved pixels and hence our fitting process converges mostly within 3-4 times, except for  
572 thick clouds where the number of iterations increases to 6. Using the derived FN-NF errors significantly  
573 increases the retrieval information content. Both stratospheric and tropospheric DFSs are improved by  
574 0.2-0.4 under mild SZAs and by up to 0.2 under high SZAs as shown in Fig. 14, so that tropospheric  
575 ozone retrievals demonstrate  $\sim 1$  DFS in low/mid latitudes, which is similar to OMI retrievals (Liu et  
576 al., 2010a). Fig 15.a shows the retrieved tropospheric ozone column distribution with two radiometric  
577 calibrations (soft, CMC) and OMPS NFFN errors. Compared to Fig 7.b without CMC and OMI FN-NF  
578 errors, the cross-track dependent noises over the polar region are smoothed due to CMC and the columns  
579 are enhanced in the tropics and the northern mid-latitudes due to OMPS NFFN errors. Successful  
580 tropospheric retrievals typically require better than 0.2-0.3 % fitting accuracy between measured and  
581 modeled radiances in the Huggins band (310-340 nm) (Munro et al., 1998). Our fitting algorithm meets  
582 this requirement after carefully applying empirical calibrations as shown in Fig 15.b; the average fitting  
583 residuals are within 0.1 % for moderate SZAs, with insignificant dependence on cross-track position.

## 584 4. Conclusions

585 The OMI ozone profile algorithm has been adapted and modified to retrieve tropospheric ozone and  
586 ozone profiles from OMPS-NM L1B 2.0 product. To verify the best knowledge of OMPS instrument  
587 slit functions, we evaluate OMPS preflight measured slit functions and analytical slit functions  
588 assuming standard and super Gaussian distributions through cross-correlation using a high-resolution  
589 solar reference spectrum. We also adjust preflight measured slit functions to post-launch OMPS  
590 measurements by broadening/squeezing them by up to 4%, which slightly improves the fitting residuals  
591 at nadir cross-track pixels, but by up to 0.18% (e.g., from 0.75% to 0.6% at the first cross-track position)  
592 at edge pixels. The super Gaussian slit functions better represent OMPS irradiances than the standard  
593 Gaussian and even the preflight measured slit functions, but the fitting residuals of radiances with  
594 different slit functions show insignificant differences. OMPS measured slit functions are finally  
595 implemented in our OMPS ozone fitting retrievals because they take account of the slight dependence  
596 of slit functions on wavelengths.

597 We perform two kinds of radiometric calibrations to eliminate the systematic components of fitting  
598 residuals. First, we apply “soft calibration” to OMPS radiance before retrievals. This correction  
599 spectrum is derived as a function of wavelength and cross-track position by averaging the ratio of  
600 measured radiances to simulated radiances using collocated OMI ozone profile retrievals in the tropics

601 under nearly clear-sky conditions for 25 days of May 2013. Applying soft calibration to OMPS radiance  
602 dramatically improves the spectral fitting residuals, especially under low to moderate SZA. The  
603 amplitude of fitting residuals decreases from 1 % to 0.2 %. Therefore, the significant cross-track striping  
604 pattern shown in preliminary OMPS tropospheric ozone retrievals is mostly eliminated. Second, the  
605 CMC is implemented to compensate fitting residuals uncorrected by soft calibration, especially for high  
606 SZA retrievals. This correction spectrum is derived as functions of wavelength and cross-track position  
607 by averaging one day's fitting residuals over the tropics and northern/southern high latitude regions,  
608 respectively. The amplitude of the correction spectrum is iteratively and simultaneously adjusted with  
609 ozone. It is found that the amplitude of the fitting residuals decreases by a factor of 2 due to the CMC  
610 over high latitudes.

611 Our preliminary algorithm uses OMI ~~floor noise~~<sup>NF</sup> errors to represent measurement constraints  
612 because OMPS L1B random-noise errors are too tight to stabilize retrievals. However, we found that  
613 OMI ~~floor noise~~<sup>NF</sup> errors cannot sufficiently constrain our OMPS retrievals, indicating that there is  
614 room to increase the retrieval sensitivity to measurement information by improving measurement  
615 constraints. Therefore, we derive the minimum ~~floor noise~~ (~~FN~~)<sup>NF</sup> error corresponding to standard  
616 deviations of spectral fitting residuals over the tropics. The derived minimum ~~FN~~<sup>NF</sup> error is  $\sim 0.097\%$   
617 in 310-340 nm and increases to  $\sim 0.24\%$  at 302.5 nm, which is smaller than OMI error by a factor of  
618 1.5-4 below 310 nm and 2 above. We apply this OMPS ~~FN~~<sup>NF</sup> error at SZAs  $< \sim 20^\circ$  and those  
619 multiplied by a SNR scaling factor to take into account the decreasing SNR with increasing SZA at  
620 SZAs  $> \sim 20^\circ$ ; at SZA =  $90^\circ$  errors becomes 0.45 % at 302.5 nm and 0.19 % at 340 nm. Using OMPS  
621 ~~NFFN~~ errors as a retrieval constraint slightly improves the fitting residuals, by 0.015 % on average, and  
622 both stratospheric and tropospheric ozone retrieval sensitivity (DFS increases by 0.2-0.4), but requires  
623 1 or more additional iterations for convergence. In this study, we meet the requirement to achieve  
624 successful tropospheric ozone retrievals in terms of DFS ( $> 1$ ) and fitting residuals ( $< 0.2\text{-}0.3\%$ ) with  
625 empirical calibrations optimized to OMPS L1B measurements. In future work, we will characterize  
626 OMPS ozone profile retrievals, present error analysis, and validate retrievals using a reference dataset,  
627 to verify that the quality of OMPS ozone retrievals is adequate for scientific use.

628

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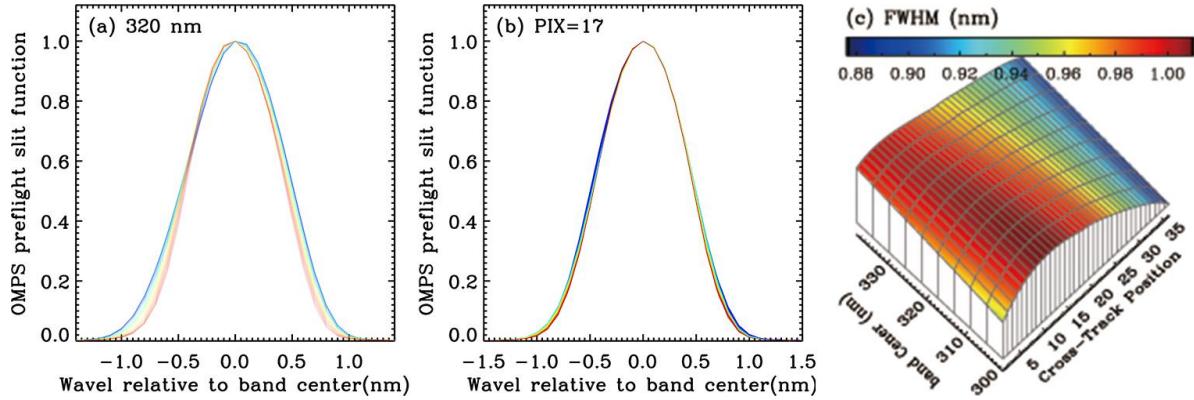
789 **Table1. Surface and atmospheric input parameters and cross section data used in forward model**  
790 **calculations.**

Forward model Parameters	Data Source
O <sub>3</sub> cross sections	Brion et al. (1993)
Ozone Profile <sup>a</sup>	OMI ozone profiles from Liu et al. (2010)
Temperature profile, surface/tropopause pressure	Daily National Centers for Environmental Prediction (NCEP) final (FNL) operational global analysis data ( <a href="http://rda.ucar.edu/datasets/ds083.2/">http://rda.ucar.edu/datasets/ds083.2/</a> )
Surface albedo	OMI surface climatology (Kleipool et al., 2008)
Cloud fraction	Derived at 347 nm
Cloud-top pressure <sup>b</sup>	OMPS Cloud Optical Centroid Pressures (OCPs) (Vasilkov et al., 2014)

791 <sup>a</sup>OMI ozone profiles retrieved at 48×52 km<sup>2</sup> with spatial coadding and then interpolated to 5° × 5° to fill  
792 bad pixels.

793 <sup>b</sup>OCPs retrieved from OMPS-NM L1B v1.0 measurements using a rotational Raman scattering cloud  
794 algorithm.

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797 **Figure 1.** (a) OMPS preflight slit function at 320 nm band center, with colors representing different cross-  
 798 track positions from 1 (blue) to 36 (red). (b) Same as (a), but for the 17<sup>th</sup> cross-track position, with colors  
 799 representing different wavelengths from 300 nm (blue) to 340 nm (red). (c) Full Width at Half Maximum  
 800 (FWHM) in nm as functions of cross-track positions (x-axis) and band center wavelengths (y-axis) ranging  
 801 from 300 to 340 nm.

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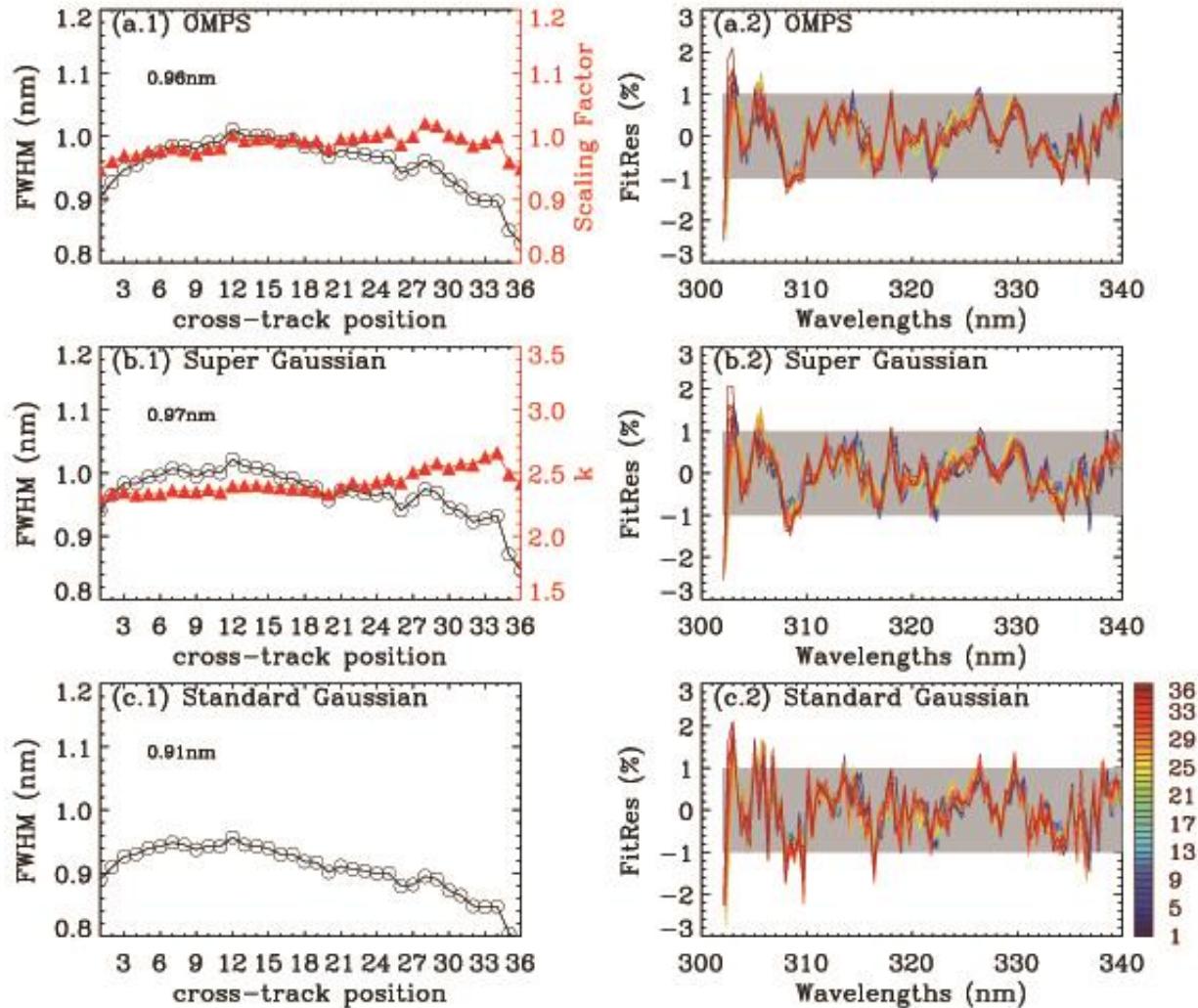
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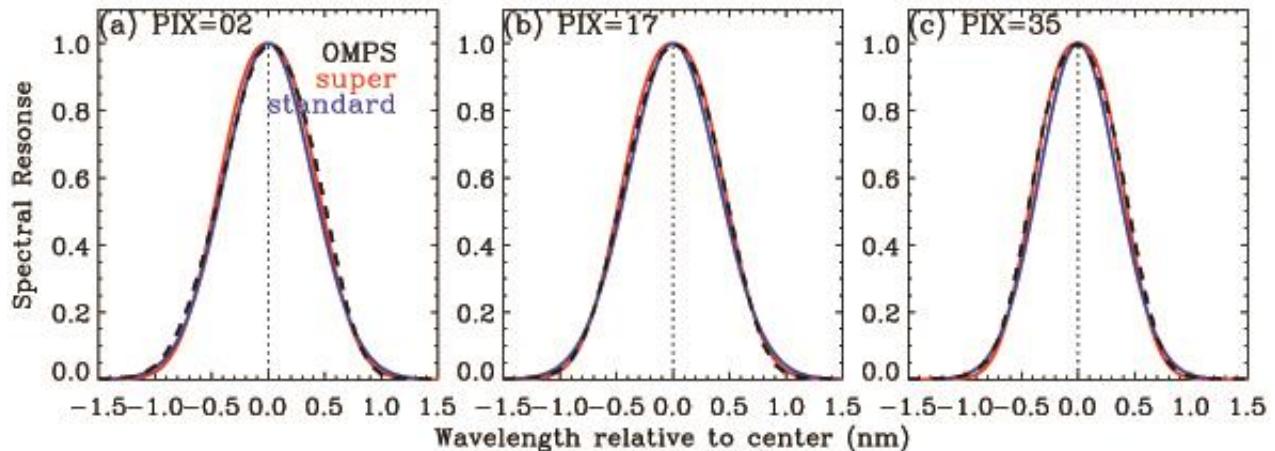
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822 **Figure 2.** (Left) Slit function parameters as a function of cross-track position (1<sup>th</sup>-36<sup>th</sup>) for three different  
 823 slit functions from OMPS irradiance measurements (302-340 nm) for orbit 7132 on 14 March 2013. The  
 824 legends represent the FWHM averaged over all spectral pixels. (Right) The corresponding relative fitting  
 825 residuals between measured and simulated irradiance spectra.

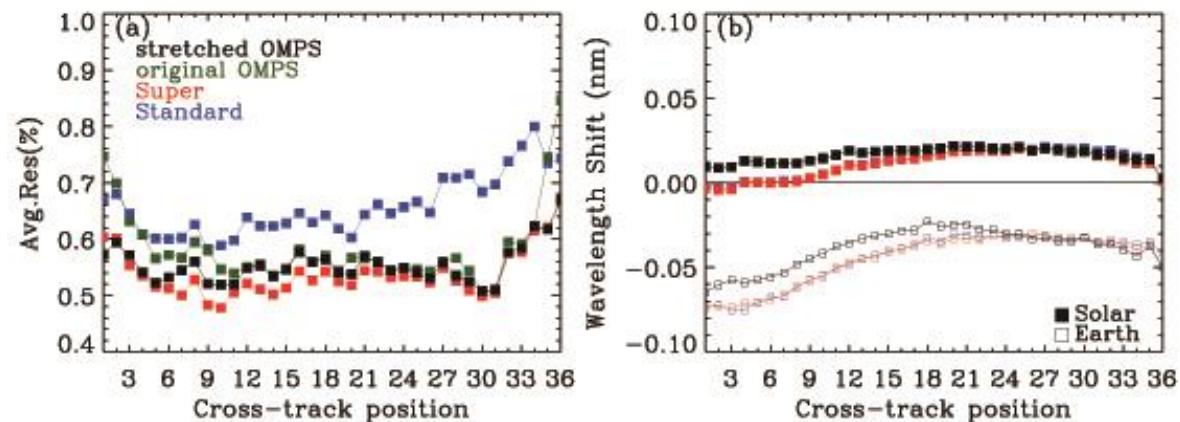
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835 **Figure 3.** Comparison of OMPS measured slit measurements (black) and derived slit functions assuming a  
836 standard Gaussian (red) and super Gaussian (blue) for orbit 7132.

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839 **Figure 4.** Same as Fig. 2, but for (a) average fitting residuals (%) as a function of cross-track positions. The  
840 green line represents the fitting residuals with measured OMPS slit functions without fitting a scaling factor.  
841 (b) Wavelength shifts between OMPS irradiance and reference spectrum (filled symbols) and between  
842 OMPS radiance at the middle swath line and reference spectrum (open symbols).

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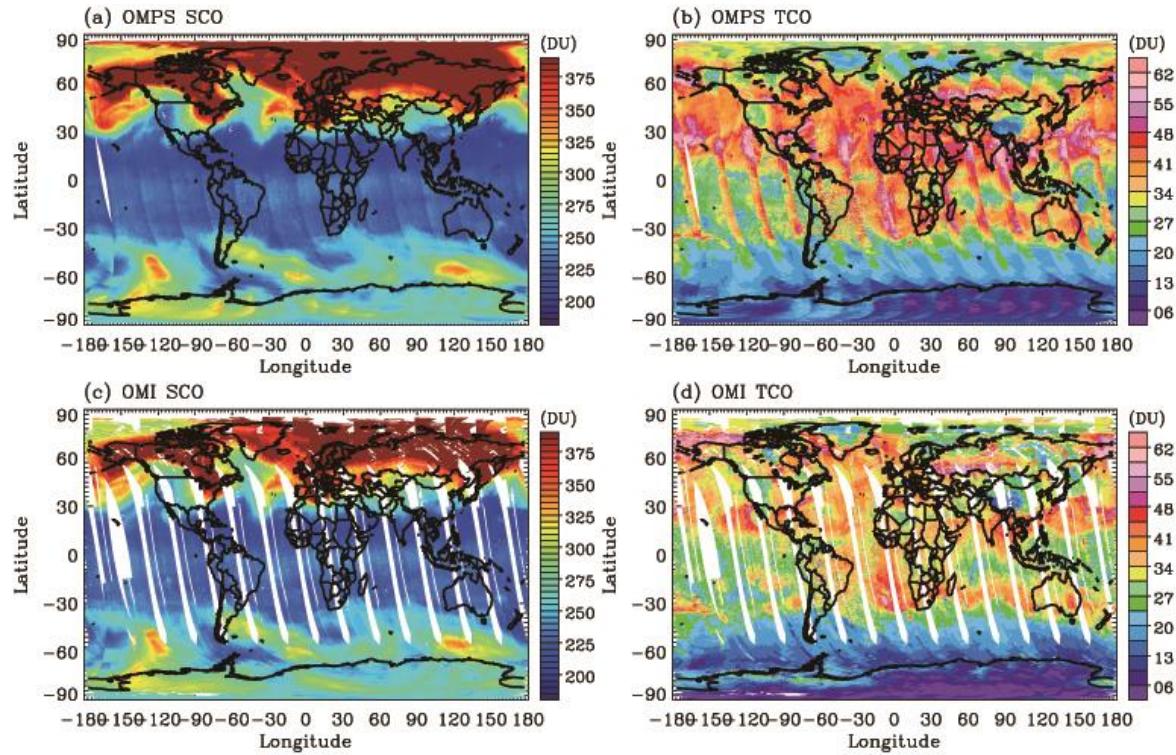
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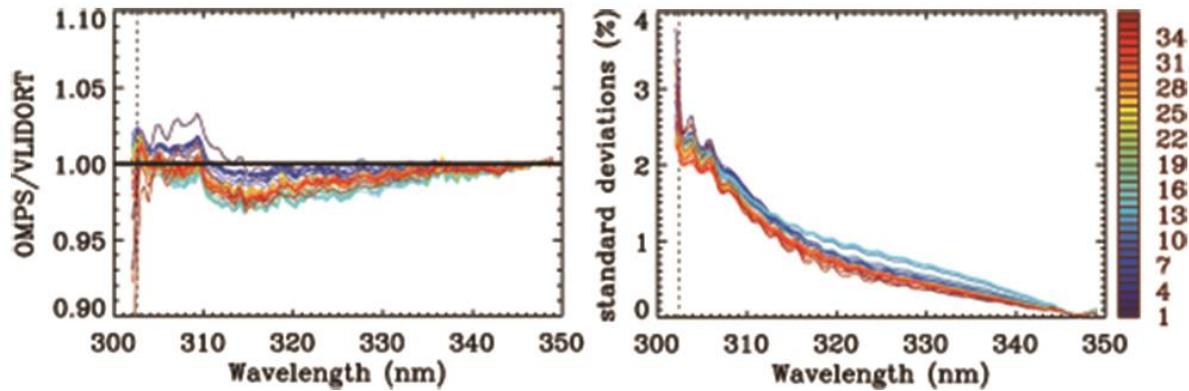
851 **Figure 5. Maps of stratospheric and tropospheric ozone column on 14 March 2013, retrieved from OMPS**  
852 **(top) without any correction and OMI (bottom) measurements, respectively.**

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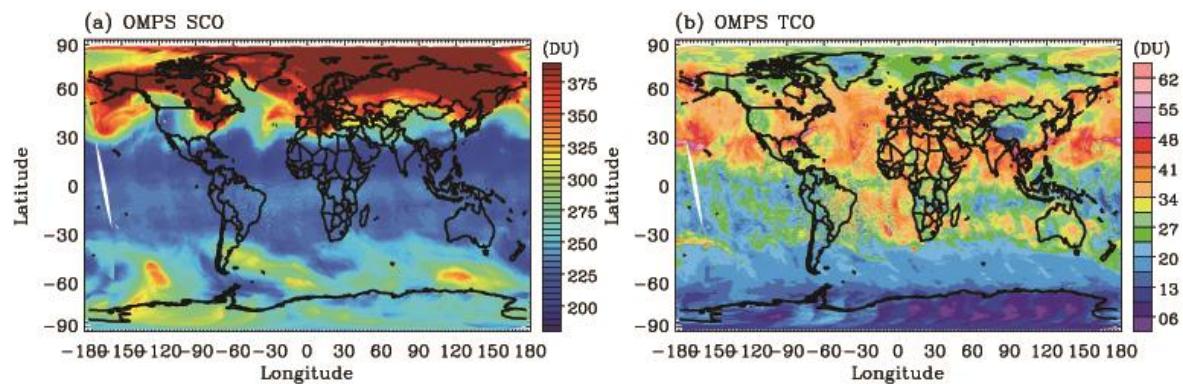
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858 Figure 6. (a) Soft calibration spectrum derived from OMPS measured to simulated radiance ratio at initial  
 859 iteration, as a function of wavelength ranging from 302 nm to 350 nm. The vertical dotted line indicates  
 860 302.5 nm. OMPS data used in this calculation is limited to tropical clear-sky conditions (latitude <  $\pm 15^\circ$ ,  
 861 cloud fraction < 0.1, surface reflectivity < 0.1) for 25 days between 1 March 2013 and 25 March 2013.  
 862 Forward model inputs listed in Table 1 are used for OMPS simulations. (b) Standard deviations of fitting  
 863 residuals. Different colors represent various cross-track positions.



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865 Figure 7. Same as Figure 5 (a) and (b), but for OMPS ozone retrievals with soft calibration.

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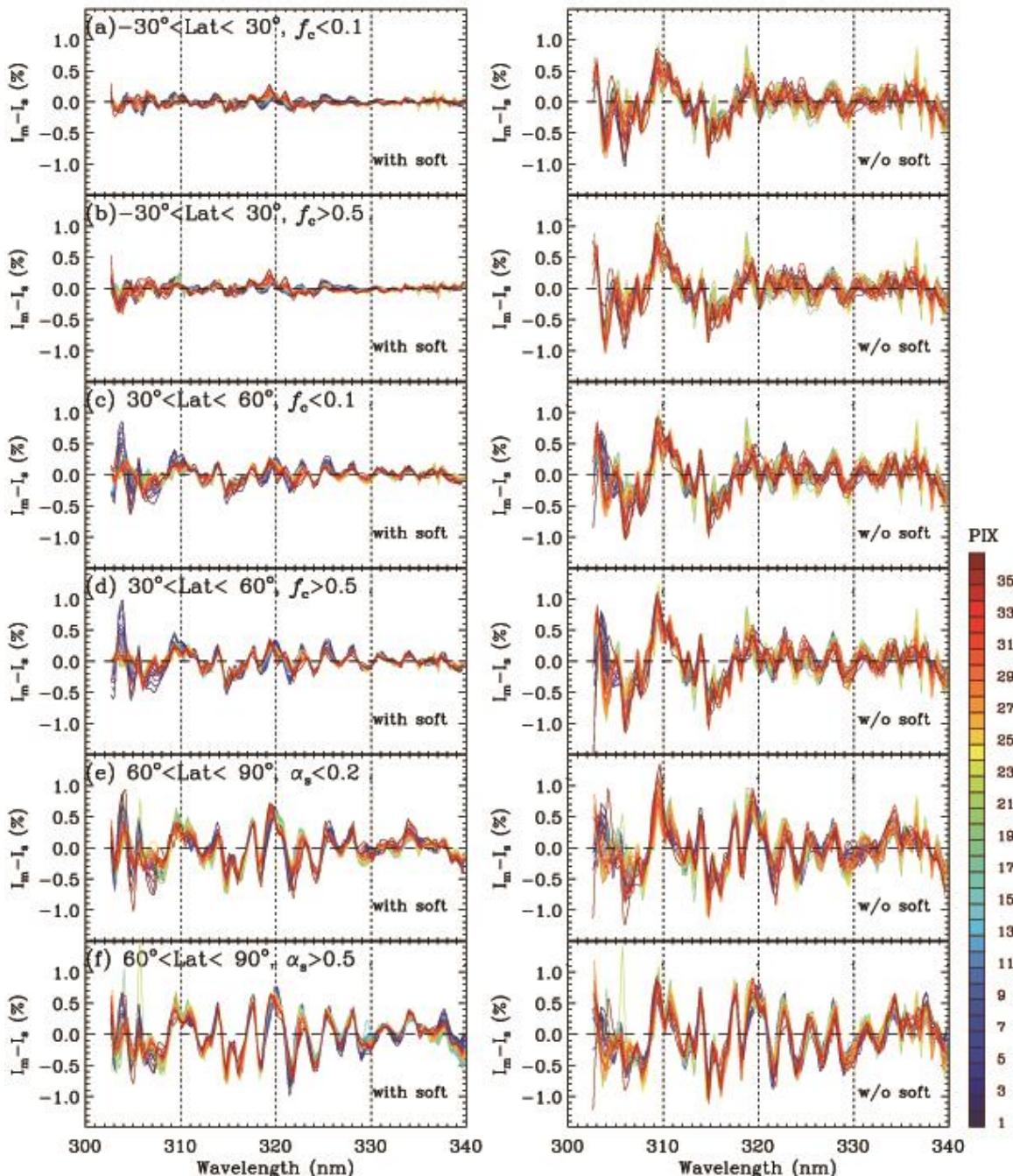
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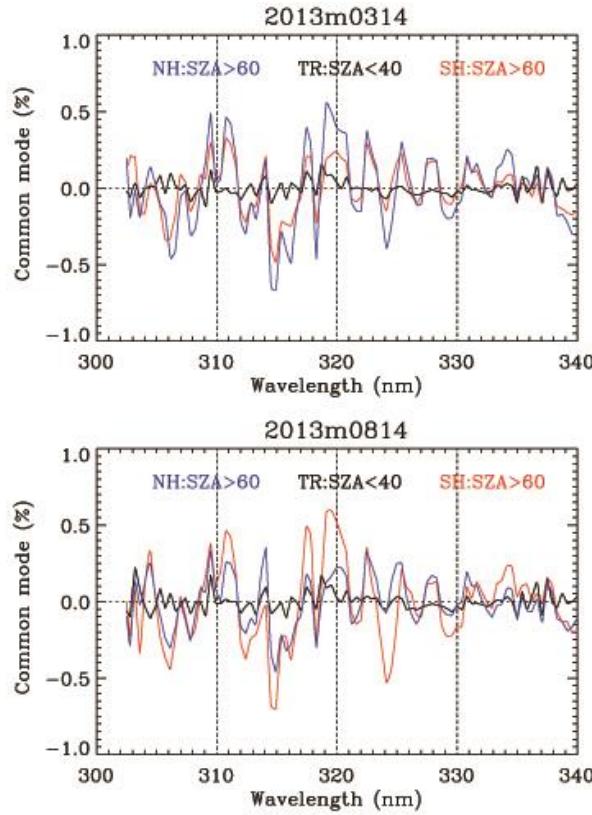
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875 **Figure 8. Comparison of fitting residuals on 14 March 2013 with (left) and without (right)**  
 876 **soft calibration for 6 cases: (a-b) Tropics and (c-d) mid-latitudes each for clear sky (effective**  
 877 **cloud fraction,  $f_c < 0.1$ ) and cloudy ( $f_c > 0.5$ ) conditions and (e-f) high-latitudes for snow-free and**  
 878 **snow-covered surface conditions. Different colors represent different cross-track positions.**



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880 **Figure 9. Common mode spectra derived from final fitting residuals at the 17<sup>th</sup> cross-track position using**  
 881 **one day of measurements in March (upper) and August (lower), respectively. Note that tropical residuals**  
 882 **are derived from nearly clear-sky conditions where SZA < 40°, cloud fraction < 0.1, and surface albedo <**  
 883 **0.1. No special data screening is applied for polar residual spectra, except for SZA > 60°.**

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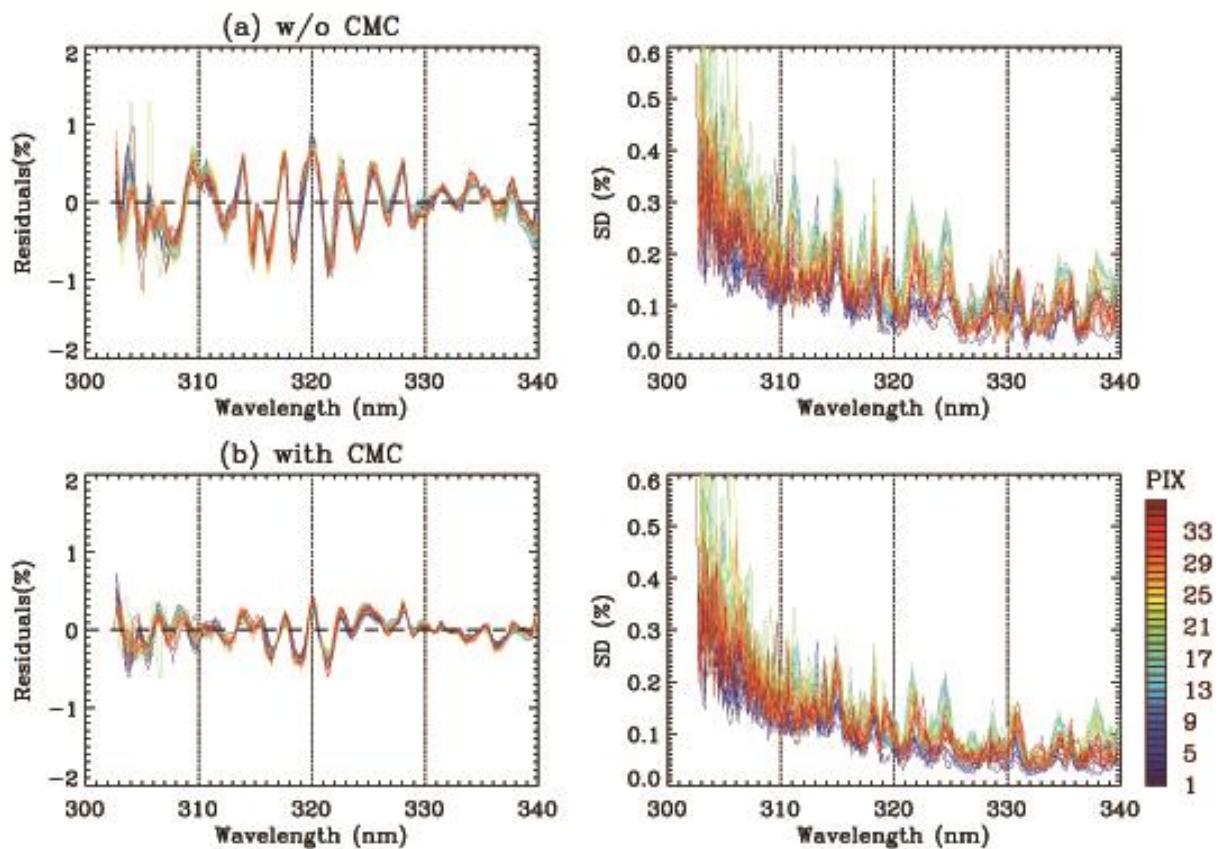
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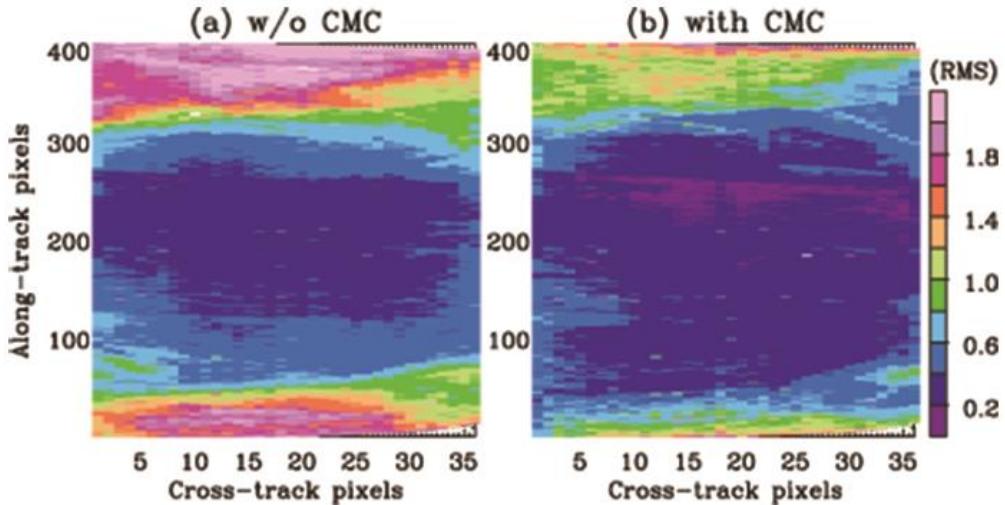


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 894 **Figure 10.** Comparisons of mean fitting residuals (%) and its standard deviations (%) for latitude  $> 60^\circ$ ,  
 895 with different cross-track positions in different colors for one orbit data (6962) on 02 March 2013, without  
 896 (a) and with (b) common residual-mode correction.

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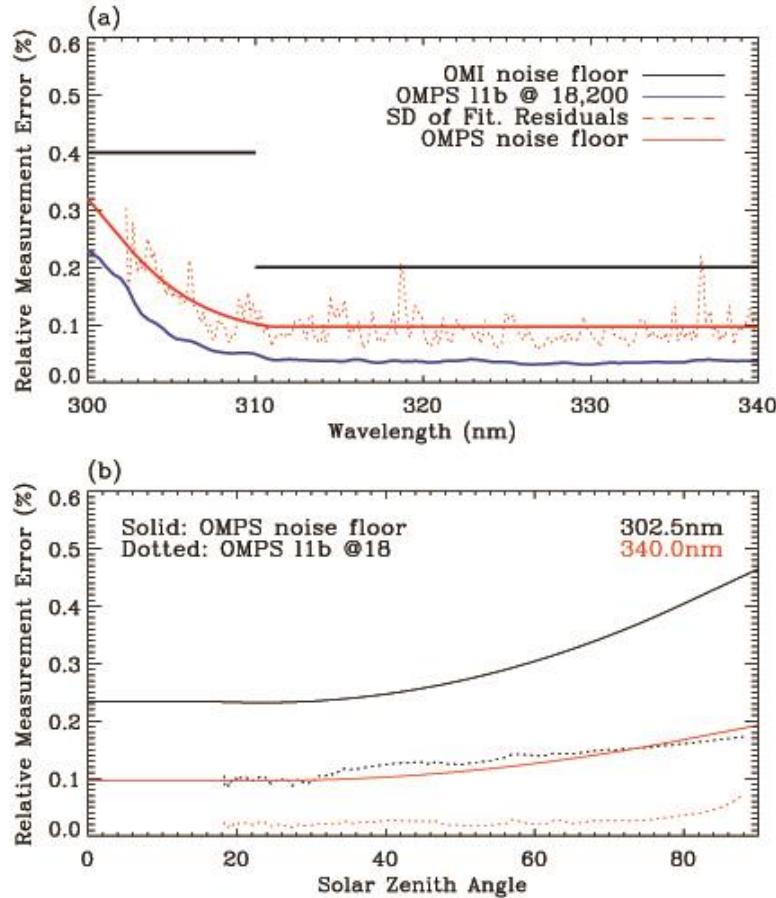
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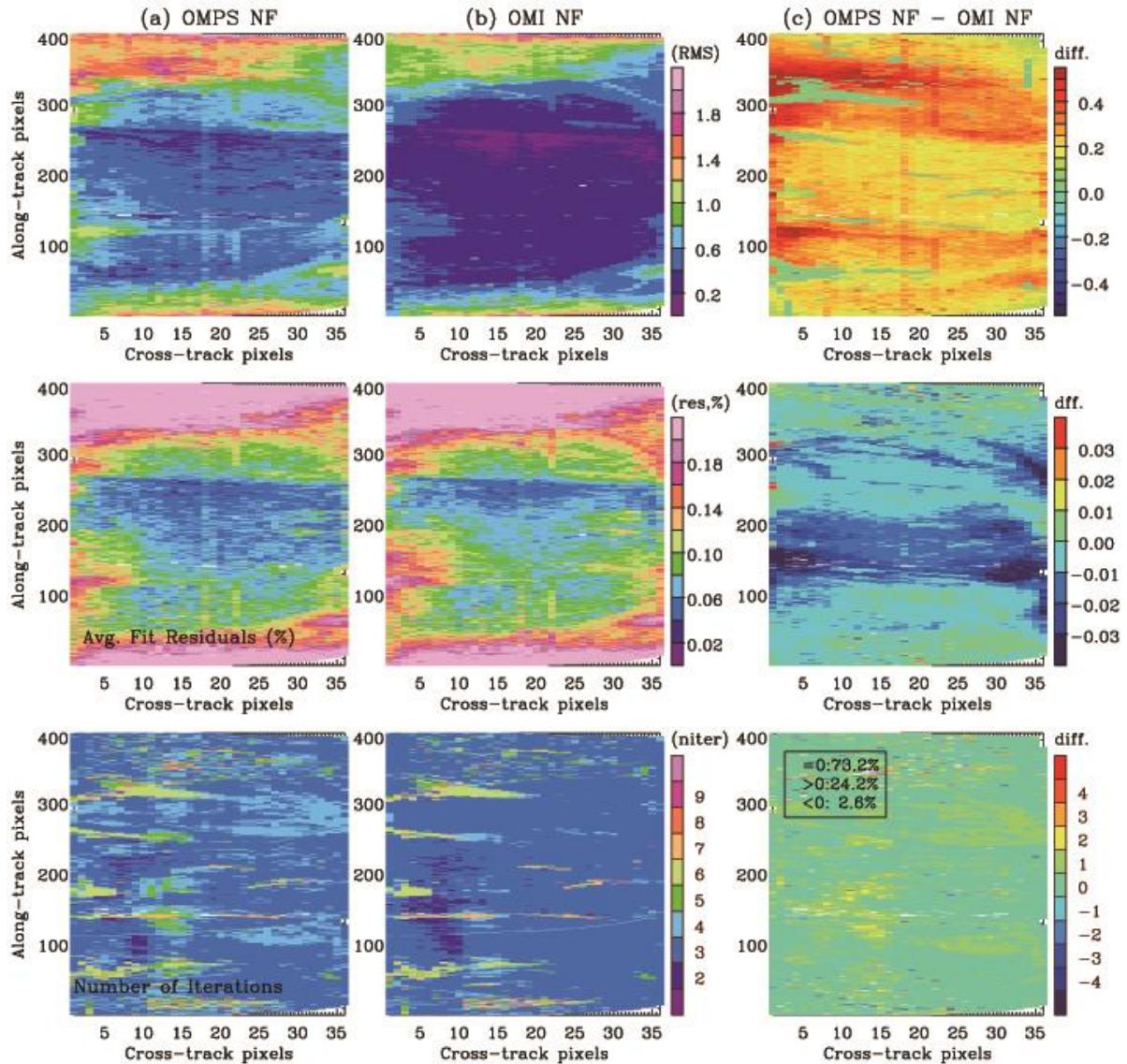
901 Figure 11. Same as Figure 10, but for Root Mean Square (RMS) of fitting residuals relative to the  
 902 measurement errors as functions of along- and cross-track pixels. The RMS is defined as  $\sqrt{\frac{1}{n} \sum_i^n \left( \frac{Y-R}{S_y^{1/2}} \right)^2}$ .  
 903 Note that OMI **floor**-noise **floor** errors (0.4% at wavelengths  $< 310$  nm, and 0.2% at wavelengths  $> 310$  nm)  
 904 are used to define RMS.



905

906 **Figure 12. (a)** Standard deviations of spectral fitting residuals for 14 March 2013 under clear-sky conditions  
 907 and for small SZAs  $< 40^\circ$  (red dotted line), with the 4<sup>th</sup> order polynomial fitting of them (red solid line)  
 908 called “OMPS noise noise floor (FNF) error”. This FNF error represents the minimum measurement  
 909 constraint implemented in OMPS ozone fitting process. OMI floor noise error (black line) and OMPS L1B  
 910 v2.0 random-noise error (blue line) (orbit: 7132, cross-track: 18, along-track: 200) are also shown for  
 911 comparison in the same panel. (b) OMPS NNF at 302.5 nm and 340 nm as a function of SZAs (solid line),  
 912 with the corresponding OMPS L1B v2.0 measurement error (dotted line).

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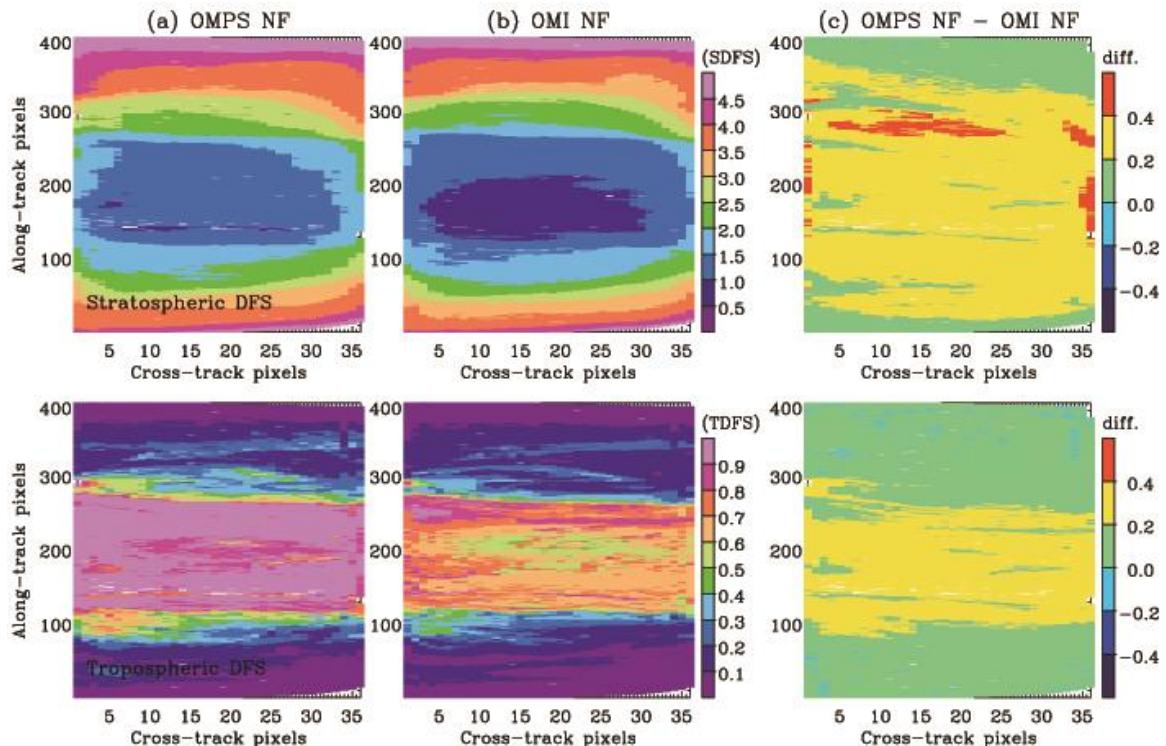
915 Figure 13. Top: Comparison of RMS of fitting residuals relative to the assumed measurement errors as  
916 functions of cross-track and along-track pixels for orbit 7132 with (a) OMPS NF (first column) and (b)  
917 OMI NF (second column), respectively, with (c) their absolute differences (third column). The definition  
918 of RMS is given in Fig. 11. Middle: Comparison of average fitting residuals relative to the simulated  
919 radiances (%), which are similar to RMS, except that radiance differences are normalized to measured  
920 radiances instead of measurement errors. Bottom: Comparison of the number of the retrieval iterations.

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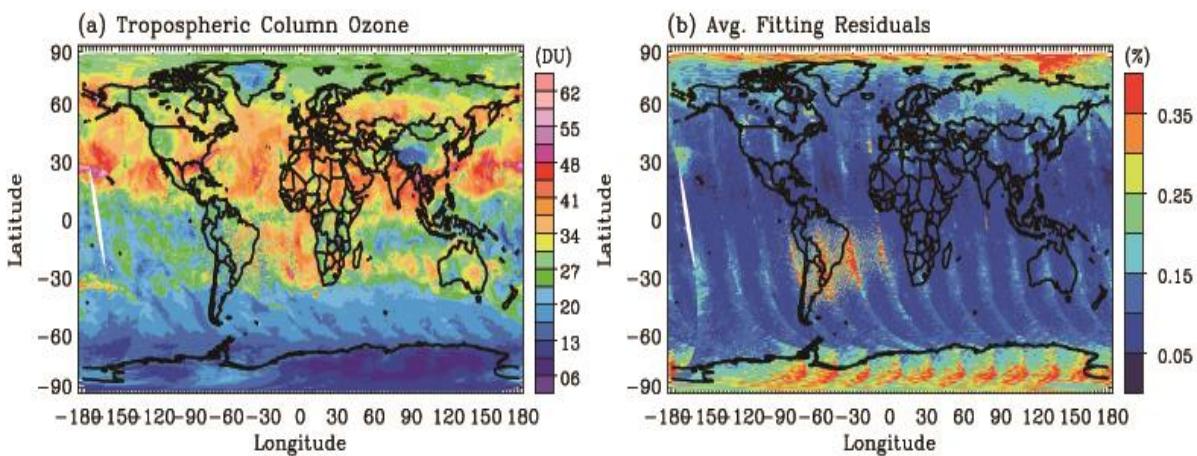
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927 **Figure 14.** Same as Fig. 13, but for the integrated Degrees of Freedom for Signal (DFS) in the stratosphere  
928 (top) and troposphere (bottom), respectively.

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931 **Figure 15.** (a) Same as Fig 7.b, but for improved retrievals with common mode correction and OMPS **floor**  
932 noise **floor** error, (b) corresponding average fitting residuals (%).

1      **Characterization and Correction of OMPS**

2      **Nadir Mapper Measurements for Ozone Profile**

3      **Retrievals**

4

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16      **Abstract**

17     This paper verifies and corrects the Ozone Mapping and Profiler Suite (OMPS) Nadir Mapper (NM)  
18     Level 1B v2.0 measurements with the aim of producing accurate ozone profile retrievals using an  
19     optimal estimation based inversion method to fit measurements in the spectral range 302.5-340 nm. The  
20     evaluation of available slit functions demonstrates that preflight-measured slit functions well represent  
21     OMPS measurements compared to derived Gaussian slit functions. Our initial OMPS fitting residuals  
22     contain significant wavelength and cross-track dependent biases, resulting ~~into-in~~ serious cross-track  
23     striping errors in the tropospheric ozone retrievals. To eliminate the systematic component of the fitting  
24     residuals, we apply “soft calibration” to OMPS radiances. With the soft calibration the amplitude of  
25     fitting residuals decreases from ~1 % to 0.2 % over low/mid latitudes, and thereby the consistency of  
26     tropospheric ozone retrievals between OMPS and the Ozone Monitoring Instrument (OMI) is  
27     substantially improved. A common mode correction is also implemented for additional radiometric  
28     calibration; it improves retrievals especially at high latitudes where the amplitude of fitting residuals  
29     decreases by a factor of ~2. We estimate the ~~floor~~-noise floor error of OMPS measurements from

30 standard deviations of the fitting residuals. The derived error in the Huggins band (~0.1 %) is twice the  
31 OMPS L1B measurement error. OMPS ~~floor~~-noise floor errors better constrains our retrievals, leading  
32 to improving information content of ozone and reducing fitting residuals. The final precision of the  
33 fitting residuals is less than 0.1 % in the low/mid latitude, with ~1 degrees of freedom for signal for the  
34 tropospheric ozone, meeting the general requirements for successful tropospheric ozone retrievals.

## 35 1. Introduction

36 Atmospheric ozone has very different roles depending upon its altitude. About 90 % of the total  
37 ozone is in the stratosphere, protecting the Earth's life from harmful solar ultraviolet (UV) radiation  
38 that can cause skin cancer and immune system suppression. The remaining 10 % in the troposphere  
39 shows dangerous effects as a major component of photochemical smog at surface level and as a short-  
40 lived greenhouse gas in the upper troposphere, whereas in the middle troposphere it plays a beneficial  
41 role in chemically cleaning the atmosphere as a precursor of hydroxyl radicals (OH). Therefore, vertical  
42 ozone profiles should be monitored to improve our understandings of the chemical and physical  
43 functions of this important trace gas. Space-based monitoring of ozone profiles including the  
44 troposphere from backscattered UV radiation has been available since the launch of Global Ozone  
45 Monitoring Experiment (GOME) (European Space Agency, 1995) on board the Second European  
46 Remote Sensing Satellite (ERS-2) in April 1995. Its successors continued the role of GOME for  
47 atmospheric ozone monitoring with Scanning Imaging Absorption SpectroMeter for Atmospheric  
48 ChartographY (SCIAMACHY) (Bovensmann et al., 1999) aboard the Environmental  
49 Satellite (ENVISAT), GOME-2s (EUMETSAT, 2006) aboard the MetOp-A and MetOp-B, and Ozone  
50 Monitoring Instrument (OMI) (Leveld et al, 2006) flown on the EOS Aura spacecraft. The good  
51 performance of OMI ozone profile retrievals in both stratosphere and troposphere has been  
52 demonstrated through extensive validation efforts using ozonesondes, aircraft, satellite data, and  
53 ground-based total ozone data (Pittman et al., 2009; Liu et al., 2010b; Bak et al., 2013b; 2015; Huang  
54 et al., 2017<sup>a,b</sup>). However, a portion of OMI radiance measurements has been affected by the partial  
55 blockage of the instrument's entrance slit, a problem termed the row anomaly, which started in 2007  
56 and grew serious in January 2009 (Schenkeveld, 2017). The Ozone Mapping and Profiler Suite (OMPS)  
57 aboard the Suomi National Polar-Orbiting Partnership (NPP) satellite launched in 2011 (Flynn, et al.,  
58 2014) represents the next generation of US instruments to continue the role of OMI in monitoring total  
59 ozone and ozone vertical profiles, together with the TROPOspheric Monitoring Instrument (TROPOMI)  
60 to be launched on board the Sentinel-5 Precursor satellite in 2017 (Veefkind et al., 2012). OMPS is a

61 sensor suite which consists of three instruments, the Nadir Mapper (OMPS-NM), the Nadir Profiler  
62 (OMPS-NP), and the Limb Profiler (OMPS-LP). The OMPS-NM is designed to measure the daily  
63 global distribution of total column ozone with an 110° cross-track field of view (FOV), similar to OMI  
64 and the Total Ozone Monitoring Spectrometer (TOMS) series (Bhartia and Wellemeyer, 2002). OMPS-  
65 NP is an ozone profiler sensor, measuring the vertical ozone profiles in the upper stratosphere, similar  
66 to the Solar Backscatter Ultraviolet (SBUV/2) series (Bhartia et al., 2013). The OMPS-LP is designed  
67 to measure ozone profiles in the stratosphere and upper troposphere at high vertical resolution, similar  
68 to the Microwave Limb Sounder (MLS). Both OMPS-NP and OMPS-LP are ozone profile sensors, but  
69 lack sensitivity to the troposphere due to the spectral coverage of 250-290 nm and the viewing geometry,  
70 respectively. Therefore, OMPS-NM is the only candidate for global monitoring of ozone profiles down  
71 to the troposphere even though its spectral resolution of 1.0 nm does not fully resolve the ozone  
72 absorption band features in the Huggins band and its spectral coverage of 300-380 nm is insufficient to  
73 retrieve stratospheric ozone profiles. The retrieving of ozone profiles including tropospheric ozone from  
74 OMPS-NM measurements has not yet been presented in the literature. The present effort fills the gap  
75 between OMI and upcoming satellite observations.

76 The final goal of this study is to demonstrate the successful performance of ozone profiles and  
77 tropospheric ozone retrievals from only OMPS-NM measurements. Thus, we refer to OMPS-NM  
78 simply as OMPS hereafter. The retrieval algorithm used in this study is based on the Smithsonian  
79 Astrophysical Observatory (SAO) ozone profile algorithm that was developed for GOME (Liu et al.,  
80 2005) and OMI (Liu et al., 2010a). The SAO OMI algorithm is based on an optimal estimation inversion  
81 (Rodgers, 2000) combined with accurate wavelength/radiometric calibration, forward model simulation,  
82 and good a priori knowledge. This algorithm has been implemented for ozone profile and SO<sub>2</sub> retrievals  
83 from GOME-2 instrument (Cai et al., 2011; Nowlan et al., 2011) and will be adapted to ozone profile  
84 retrievals from upcoming geostationary UV/VIS spectrometers including the Geostationary  
85 Environmental Monitoring Spectrometer (GEMS) (Bak et al 2013a) and Tropospheric Emissions:  
86 Monitoring of POllution (TEMPO) instrument (Chance et al., 2013, Zoogman et al., 2017) for  
87 monitoring air quality over North America and East Asia, respectively. OMPS has a similar instrument  
88 concept to OMI, GEMS, and TEMPO and hence the application of the similar retrieval algorithms to  
89 these measurements will provide an excellent opportunity for long-term trend analysis of ozone profiles,  
90 especially in the troposphere. The OMI algorithm is very similar to our OMPS algorithm, but it needs  
91 additional optimization for OMPS. In this paper we focus largely on characterizing OMPS  
92 measurements (1) through the cross-correlation between OMPS irradiances and a high-resolution solar  
93 reference to be used in the verification of OMPS slit function measurements and the characterization of

94 the wavelength registration and (2) through extracting the systematic and random components of fitting  
95 residuals between measured and calculated normalized radiances to be used in radiometric and  
96 measurement error calibrations, respectively. Several companion papers to follow will deal with the  
97 detailed error analysis, retrieval characteristics of the retrieved ozone profiles, and validation of  
98 retrievals.

99 The paper is divided into four sections: First, we give a description of OMPS-NM Level 1B (L1B)  
100 v2.0 data (Jaross, 2017) and the ozone profile algorithm in Sect. 2. Section 3 discusses the  
101 wavelength/slit function calibrations and measurement corrections for radiance and measurement error,  
102 respectively. Conclusions are in Sect. 4.

103

## 104 **2. Data and Method**

### 105 **2.1 OMPS measurements**

106 The Suomi NPP satellite is a NOAA/NASA scientific partnership, launched in 2011 into a 824 km sun-  
107 synchronous polar orbit with ascending node equator-crossing time at 13:30 local time. Routine  
108 operations began in 2012. Suomi NPP carries five instruments: The Visible/Infrared Imager Radiometer  
109 Suite (VIIRS), the Cross-track Infrared Sounder (CrIS), the Advanced Technology Microwave Sounder  
110 (ATMS), the Ozone Mapping and Profile Suite (OMPS), and the Clouds and the Earth Radiant Energy  
111 System (CERES). OMPS is a key instrument on Suomi NPP. The sensor suite has both nadir and limb  
112 modules. The nadir module combines two sensors: The Nadir Mapper for measuring total column ozone,  
113 and the Nadir Profiler for ozone vertical profile. The Limb Profiler module is designed to measure  
114 vertical ozone profiles with high vertical resolution from the upper troposphere/lower stratosphere to  
115 the mesosphere. The OMPS-NM employs a 2-D CCD that samples spectrally in one dimension and  
116 spatially in the other, similar to OMI. It has a 110 ° cross-track field of view, resulting in 2800 km  
117 instantaneous swath coverage at the earth's surface; this is sufficient to provide daily global coverage.  
118 It makes 400 swath lines per orbit with 36 cross-track measurements per swath line, resulting in a nadir  
119 footprint of 50 km × 50 km in its nominal configuration. Note that OMPS L1B data used in this  
120 investigation contain 36 cross-track pixels, because the L1B processing in the NASA Ozone SIPS  
121 retains the two central (near-nadir) instantaneous fields of views (IFOVs, 30 km × 50 km and 20 km ×  
122 50 km), without aggregating them into the nominal 50 km × 50 km pixel. The spectral coverage is from  
123 300 to 380 nm with a spectral resolution of ~ 1.0 nm and a sampling of 0.42 nm. The OMPS level 0 to  
124 1b processor was recently updated from version 1.0 to 2.0. The satellite measurements from the OMPS-

125 NM instrument used in this study are from version 2 of the NMEV-L1B data product (Jaross, 2017)  
126 available from the NASA Goddard Earth Sciences Data and Information Services Center (GES)  
127 DISC). The data consist of calibrated Earth-view radiance and solar irradiance data measured by the  
128 instrument between 300-380 nm. Seftor et al. (2014) documented many aspects of the previous version  
129 of the dataset that remain the same, but a number of changes for the V2 dataset do reflect advances in  
130 the characterization of the NM sensor (Seftor and Jaross, 2017) which are relevant to this study. These  
131 are summarized as follows: 1) recalculation of instrument band-pass functions in the 300-310 nm region  
132 affected by the dichroic element of the nadir instrument, 2) improved wavelength registration, 3) an  
133 update to the instrument radiance calibration, and 4) improvement to the stray light correction. The  
134 wavelengths below 302 nm are not used in this study, according to the recommendation of the OMPS  
135 science team.

## 136 **2.2 OMPS simulations**

137 We use the Vector LInearized Discrete Ordinate Radiative Transfer (VLIDORT) model (Spurr, 2006;  
138 2008) to simulate OMPS radiances. VLIDORT is also able to simulate the analytic derivatives of  
139 radiance with respect to any atmospheric or surface parameter due to its full linearization capability.  
140 The polarization of light is taken into account in VLIDORT calculation, but the Ring spectrum is  
141 modeled using a single scattering RRS model (Sioris and Evans, 2000). We consider only Rayleigh  
142 scattering (no aerosol) and ozone absorption (no other trace gases), with Lambertian reflectance  
143 assumed for the surface and for clouds. Clouds are treated as a Lambertian reflector at cloud top, with  
144 a fixed albedo of 0.8 unless it is fully cloudy so that the cloud albedo ( $>0.80$ ) can be derived. Cloud  
145 fraction is required to simulate partial clouds as the weighted average between clear and cloudy scenes  
146 using the Independent Pixel Approximation (IPA). The forward model inputs used in VLIDORT are  
147 listed in Table 1.

## 148 **2.3 OMPS ozone profile retrievals**

149 The inversion from Backscattered UV measurements to the state of the atmosphere is performed  
150 using the well-known optimal estimation method (Rodgers, 2000). It calculates the a posteriori solution  
151 by iteratively and simultaneously minimizing the cost function consisting of the sum of the squared  
152 differences between measured and simulated radiances and between retrieved and a priori state vectors,

153 constrained by measurement error covariance matrix and a priori error covariance matrix. The a  
154 posteriori solution and cost function can be written:

155 
$$X_{i+1} = X_i + (K_i^T S_y^{-1} K_i + S_a^{-1})^{-1} [K_i^T S_y^{-1} (Y - R(X_i)) - S_a^{-1} (X_i - X_a)] \quad (1)$$

156 
$$\chi^2 = \left\| S_y^{-\frac{1}{2}} \{ K_i (X_{i+1} - X_i) - [Y - R(X_i)] \} \right\|_2^2 + \left\| S_a^{-\frac{1}{2}} (X_{i+1} - X_a) \right\|_2^2. \quad (2)$$

157 The inputs to the optimal estimation are defined as follows.  $\mathbf{X}$  is the state vector to be retrieved,  
158 consisting of ozone profiles as well as other geophysical parameters and spectroscopic parameters  
159 affecting the observed radiances and hence the retrieval of ozone profile. The 24 partial columns of  
160 ozone in DU are retrieved at 25 pressure levels that are initially set to be  $P_i = 2^{-i/2}$  atm for  $i =$   
161  $0, 1, \dots, 23$  (1 atm = 1013.25 hPa) with the top of the atmosphere at 0.087 hPa for  $P_{24}$ . The geophysical  
162 parameters include effective surface albedo and cloud fraction. The calibration parameters consists of  
163 two wavelength shift parameters between radiances and irradiances and between radiances and ozone  
164 cross sections and two scaling parameters for the Ring effect that account for filling-in of Fraunhofer  
165 lines in the solar spectrum due to rotational Raman scattering and mean fitting residuals that may not  
166 be accounted for properly in radiometric calibration. The a priori data for ozone is one of the key optimal  
167 estimation inputs because the retrieval solution comes mainly from a priori information rather than  
168 measurement information where the instrument sensitivity to the true ozone profile is insufficient. The  
169 a priori value ( $X_a$ ) and a priori error covariance ( $S_a$ ) of ozone is taken from the tropopause-based ozone  
170 profile climatology that is optimized to represent the dynamical ozone variability in the upper  
171 troposphere and lower stratosphere (Bak et al., 2013b). The measurement vector  $Y$  is defined as the  
172 logarithm of the earthshine radiances normalized to the daily solar irradiance.  $S_y$  is a measurement  
173 error covariance matrix that is assumed to be a diagonal matrix with diagonal elements being the squares  
174 of the assumed measurement errors. We use OMI ~~floor~~-noise ~~floor~~ errors (0.4 % below 310 nm, 0.2 %  
175 above, Huang et al., 2017a) as our preliminary measurement constraint and then derive OMPS ~~floor~~  
176 noise ~~floor~~ errors specified in Section 3.4.  $R(X)$  is the calculated radiances corresponding to  $X$ .  $K$  is  
177 a weighting function matrix representing partial derivatives of the forward model with respect to the  
178 atmospheric parameters,  $K_{ij} = \partial R_i(X) / \partial X_j$ . More detailed descriptions can be detailed in Liu et al.  
179 (2010a).

180

181 **3. Results**

182 **3.1 Slit Function and Wavelength Calibration`**

183 It is essential to investigate the best knowledge of the instrument slit function to convolve a high-  
184 resolution solar reference spectrum for wavelength calibration as well as to convolve high-resolution  
185 trace gas cross sections for simulation of earthshine spectra. A triangular bandpass with a fixed  
186 bandwidth of 1.1 nm has been typically used for Total Ozone Monitoring Instrument (TOMS), SBUV,  
187 and SBUV/2 monochromators. Slit functions of spectrometers such as OMI and GOME1/2 have been  
188 measured prior to launch using a tunable laser or analytically derived assuming a Gaussian-type shape  
189 if measured slit functions are unavailable or inaccurate. The OMPS preflight slit functions were  
190 measured-characterized for each CCD pixels (196 band centers and 36 cross-track positions), which has  
191 been adopted and modified for OMPS trace-gas retrievals such as in Yang et al. (2013; 2014) and  
192 Gonzalez Abad et al. (2016). The slit function modification is accomplished in the previous works  
193 (Yang et al., 2013, 2014) by stretching and shrinking the slit widths, i.e., by applying a wavelength-  
194 dependent scaling factor to the OMPS measured slit functions. According to Yang et al. (2013; 2014),  
195 we fit the scaling factor as a slit parameter so that variations in measured slit functions before and after  
196 launch could be taken into account.

197 Figure 1a shows an example of measured OMPS slit functions at 320 nm, illustrating that their  
198 shapes seem to be Gaussian and vary considerably over cross-track pixels, especially near the wings.  
199 Note that the 36 cross-track positions are denoted from 1 at the left edge and 36 at the right edge. The  
200 slit function shapes at 17<sup>th</sup> cross-track position are nearly consistent over wavelengths that we are  
201 focusing on for ozone retrievals (Fig. 1.b). Figure 1c displays the full width at half maximum (FWHM)  
202 including dependencies in both dimensions of the detector arrays. The spectral variation of the slit  
203 widths is insignificant (FWHMs vary by less than 0.01 nm), whereas average slit widths vary  
204 significantly across track by over 0.1 nm. This characteristic of measurement slit functions confirms  
205 that we should consider their cross-track dependence for OMPS slit functions, but their wavelength  
206 dependence is ignorable so that we can avoid the time-consuming convolution process.

207 We evaluate the usefulness of these measured slit functions for fitting both OMPS radiance and  
208 irradiance against the analytical slit functions assusing both standard Gaussian and super Gaussian  
209 distributions. We note all the Gaussian shapes used in this analysis are assumed to be symmetric. The  
210 Gaussian slit function is expressed as

211

$$S(\lambda) = \frac{k}{2w\Gamma\left(\frac{1}{k}\right)} \exp\left[-\left|\frac{\Delta\lambda}{w}\right|^k\right], \quad (3)$$

212 where  $k$  is the shape factor and  $w$  is the slit width, with relative wavelength to band center wavelength,  
 213  $\Delta\lambda$ . This function can describe a wide variety of shapes just by varying  $k$ ; for  $k=2$  it becomes the  
 214 standard Gaussian and  $w$  represents the half width at 1/e intensity (FWHM =  $2\sqrt{\ln 2} w$ ). Compared  
 215 to the standard Gaussian, the super Gaussian has broader peaks at the top and thinner wings if  $k$  is larger  
 216 than 2 whereas it has sharper peaks and longer tails if  $k$  is smaller than 2.  $w$  of the super Gaussian  
 217 function represents the half-width at 1/e<sup>th</sup> intensity (FWHM =  $2\sqrt[k]{\ln 2} w$ ). The symmetric or asymmetric  
 218 standard Gaussian has been commonly assumed to derive OMI, GOME, and GOME-2 slit functions  
 219 (Liu et al., 2005;2010; Nowlan et al., 2011; Cai et al., 2012; Munro et al., 2016). Recently the hybrid  
 220 combination of standard and flat-top Gaussian functions has been implemented for characterizing OMI  
 221 laboratory measurements of slit functions (Dirksen et al., 2006) and deriving airborne instrument slit  
 222 functions (Liu et al., 2015a;2015b; Nowlan et al., 2016). The concept of this hybrid Gaussian function  
 223 is very similar to the super Gaussian, but is a rather complex with more slit parameters. The super  
 224 Gaussian function was introduced and tested as an analytical slit function by Beirle et al. (2017) and  
 225 Sun et al. (2017a;b).

226 In general, when accurate measurements of slit functions are not available, the instrument line shape  
 227 of satellite observation is typically assumed to be the same for both radiance and irradiance  
 228 measurements, and then can be better determined from irradiances due to lack of atmospheric  
 229 interference. In general, the instrument line shape is assumed to be the same for both radiance and  
 230 irradiance measurements from satellite observation and determined from irradiances due to lack of  
 231 atmospheric interference. We simultaneously and iteratively determine the wavelength and slit  
 232 calibration parameters through cross-correlation of the measured OMPS irradiances to simulated solar  
 233 irradiances from a well calibrated, high-resolution solar irradiance reference spectrum (Chance and  
 234 Kurucz, 2010). The simulation of solar irradiance,  $I_s$  is described as

235

$$I_s(\lambda) = A I_o(\lambda + \Delta\lambda) \times \sum_{i=0}^2 P_i (\lambda - \lambda_{avg})^i, \quad (4)$$

236 where  $I_o$  is the convolved high-resolution solar reference spectrum with assumed slit functions,  $A$  is  
 237 the scaling parameter for  $I_o$ .  $\lambda + \Delta\lambda$  Indicates the process of wavelength calibration (e.g. shift and  
 238 squeeze); only the wavelength shift is considered in this study.  $P_i$  represents the coefficients of a scaling  
 239 polynomial (third order in this study). This approach was firstly introduced by Caspar and Chance

240 (1997), and is widely used for wavelength and slit function calibrations in trace gas retrievals from  
241 UV/visible measurements.

242 In this experiment, the slit parameters,  $w$  and  $k$  or slit scaling are fitted from daily measured  
243 OMPS irradiances over the wavelength range 302-340 nm at each cross-track position. Note that this  
244 slit calibration ignores the wavelength dependence for deriving analytic slit functions and slit scaling to  
245 the measured slit functions; this is a good approximation based on Fig. 1b as the wavelength dependence  
246 of the slit functions is small. But the variation of the slit shape with wavelength could be considered  
247 with OMPS preflight measured slit functions given for every CCD dimension if it becomes necessary.  
248 The left panels of Fig. 2 compare the derived slit parameters from OMPS irradiances using different  
249 functions. The red line of Fig. 2.a.1 shows that a slight change of the preflight-measured slit functions  
250 is required to model the OMPS irradiance measurements, by up to 4% at both edges. Therefore the  
251 benefit of fitting measured slit functions over fixing them is found to be trivial (~ 0.001 %) at nadir  
252 cross-track pixels (12-30<sup>th</sup>); for edge pixels, the improvement in fitting residuals is more noticeable, up  
253 to 0.18%. The shape factor ( $k$ ) of the derived super Gaussian functions is found to be ~ 2.3 for left swath  
254 and ~ 2.5 for right swath (Fig. 2.b.1), implying that they have broader peaks and thinner wings compared  
255 to the standard Gaussian if slit widths are equal. The slit widths of three different slit functions show  
256 similar variations with respect to cross-track positions. The FWHMs vary from widest at ~12<sup>th</sup> cross-  
257 track position to narrowest at the edges, but they are significantly narrower at the rightmost cross-track  
258 positions than at the leftmost ones. Compared to the standard Gaussian slit widths, the super Gaussian  
259 slit widths show a much better agreement with measured slit widths; the average difference of slit widths  
260 between measured and super (standard) Gaussian functions is ~ 0.01 (0.05) nm. In Fig. 3, an example  
261 of the derived slit functions and fitted preflight slit functions shows that the shapes are very similar.

262 The wavelength calibrations using different slit functions are characterized for the ozone fitting  
263 window and are shown in Fig. 4b. The shift parameter is determined from irradiance and radiance at  
264 second cross-correlation step after slit parameters are determined from irradiances at first cross-  
265 correlation step. Note that the wavelength shifts fitted between first and second steps are very similar,  
266 indicating little correlation between slit and wavelength calibration parameters. [This analysis indicates](#)  
267 [that the accuracy of wavelength registration in ozone fitting wavelengths is 0.03-0.06 nm for earthshine](#)  
268 [measurements and < 0.02 nm for solar measurements with consistent variation over all cross-track](#)  
269 [pixels. These wavelength errors are larger than those reported by Seftor et al. \(2014\), due to different](#)  
270 [fitting windows. They use 350-380 nm where prominent solar Fraunhofer absorption lines exist and the](#)  
271 [interference with ozone absorption lines are negligible. This analysis indicates that the accuracy of](#)  
272 [wavelength registration in level 1b data is on average 0.05 nm for earthshine measurements and within](#)

273 ~~0.02 nm for solar measurements with consistent variation over all cross track pixels.~~  
274 ~~However~~Furthermore, the wavelength calibration results using OMPS measured slit functions show  
275 different characteristics from those using both Gaussian-type slit functions, especially over left cross-  
276 track pixels. The different wavelength shifts are likely because the original OMPS slit functions show  
277 slight asymmetry and are used in the wavelength calibration of L1B data. There exists a  $\sim 0.07$  nm shift  
278 between irradiances and radiance. In ozone retrieval algorithm we shift neither radiance nor irradiance  
279 to a reference spectra before retrievals, but the shift between irradiance and radiance is adjusted during  
280 ozone retrievals to account for the on-orbit variations of wavelength shifts as mentioned in Sect. 2.3.

281 The right columns of Fig. 2 compare the impact of different slit functions on spectral fitting residuals  
282 of solar irradiances, together with the average fitting residuals as a function of cross-track position in  
283 Fig.4.a. Measured solar spectra are mostly within an average of  $\sim 1$  % of modeled solar spectra, except  
284 for the first few wavelengths. Based on these fitting results, we revise the fitting window to 302.5-340  
285 nm. The fitting residuals using a derived standard Gaussian function are the worst for all cross-track  
286 positions. On the other hand, the super Gaussian slit function similarly represents the measured slit  
287 function, but slightly improves the fitting accuracy at the 6~18 cross-track positions (Fig. 4.a). However,  
288 the benefit of using the super Gaussian function for fitting OMPS radiances over the standard Gaussian  
289 function is insignificant within 0.02 % (not shown here). These results agree well with Beirle et al.  
290 (2017), who demonstrated the similar benefit of using Standard and Super Gaussian slit functions on  
291 OMI and GOME-2 measurements. Moreover, the impact of using different slit functions could be less  
292 important for OMPS than OMI and GOME-2 due to its coarser spectral resolution.

293 In summary, super Gaussian functions are recommended for the OMPS instrument slit functions  
294 than the standard Gaussian functions if the on-orbit instrument slit functions largely deviate from the  
295 preflight-measured slit functions due to instrument degradation or thermal-induced variation. In the rest  
296 of this paper, the measured slit function is used for the analysis of OMPS measurements.

297

## 298 **3.2 Soft Calibration**

299 The OMPS instrument 2-D CCD detector array could be susceptible to artificial cross-track  
300 dependent errors that are commonly seen in OMI trace gas retrievals. To eliminate this impact on the  
301 OMI L2 product, soft calibration and post-processing cross-track smoothing have been typically  
302 implemented: the first correction removes the systematic wavelength and cross-track dependent  
303 component in measured radiances (Liu et al., 2010; Cai et al., 2012), whereas the second correction

304 removes cross-track dependent biases in retrievals (Kurosu et al., 2004; Hormann et al., 2016). Figure  
305 5 compares our preliminary tropospheric and stratospheric ozone column retrievals with ~~collocated~~  
306 OMI retrievals on 14 March 2013. OMPS stratospheric retrievals show an excellent consistency with  
307 OMI even though OMPS measurements does not cover much of the Hartley ozone absorption  
308 wavelengths where most of the vertical information of stratospheric ozone comes from. This is because  
309 the separation of stratospheric ozone columns from tropospheric ozone columns is still mainly  
310 determined from wavelengths longer than 300 nm (Bak et al., 2013a). On the other hand, tropospheric  
311 ozone retrievals are positively biased with respect to OMI, by amounts largely dependent on the OMI  
312 cross-track position. Therefore, we decide to include a soft-calibration correction in our retrievals to  
313 eliminate wavelength and cross-track dependent errors in OMPS radiances. A general approach to the  
314 soft calibration is to characterize systematic differences between measured and computed radiances for  
315 scenes where we could assume that all parameters are known; the tropics were typically selected since  
316 ozone variability is relatively small (Liu et al., 2010). OMPS normalized radiances are simulated with  
317 collocated OMI ozone profiles averaged and interpolated onto  $5^\circ \times 5^\circ$  grid cells to fill in bad pixels  
318 mostly caused by the row anomaly. Other forward model inputs are described in Sect. 2. We use 25 days  
319 of data between 1 March 2013 and 25 March 2013 under the following conditions: latitude  $< 15^\circ\text{N/S}$ ,  
320 solar zenith angle (SZA)  $< 40^\circ$ , cloud fraction  $< 0.1$ , and surface reflectivity  $< 0.1$ . The systematic and  
321 random components of measured-to-simulated radiance ratios are displayed in Fig. 6. Agreement is  
322 mostly at the  $\pm 2\%$  level below 310 nm, except at wavelengths shorter than  $\sim 302.5$  nm where the  
323 systematic biases increase sharply due to the overcorrection of straylight in OMPS v2.0 data processing.  
324 For wavelengths longer than 310 nm, OMPS observations show negative biases with maximum of  $\sim 3\%$   
325 at 315 nm. The standard deviations of mean differences steadily increase from longer wavelengths to  
326 302.5 nm (2-2.5%) and then sharply rise up to  $\sim 4\%$ . The abnormal features of fitting residuals below  
327 302.5 nm shown in Figs. 2 and 6 provide a basis for why we select the lower boundary of the ozone  
328 fitting window as 302.5 nm. The soft calibration is applied before the fitting starts by dividing OMPS  
329 radiances by the derived correction spectrum just at the initial iteration with the assumption that the  
330 systematic biases consistently exist independent of space and time. Figure 7 shows how our  
331 tropospheric ozone retrievals are improved with our soft calibration in comparison with retrievals  
332 shown in Fig. 5.b. The usefulness of our soft calibration implementation is also evaluated through  
333 comparisons of the accuracies of the spectral fitting residuals with and without soft calibration as shown  
334 in Fig. 8. The mean fitting residuals without soft calibration are  $\sim \pm 1\%$  at shorter wavelengths  $< 320$   
335 nm for all latitudes and sky conditions, whereas for longer wavelengths they increase from 0.3 % to  
336 0.5 % with increasing latitudes. Our soft calibration dramatically improves the fitting accuracy for both

337 clear and cloudy pixels, especially over the tropics and mid-latitude regions; fitting residuals are mostly  
338 within 0.2 % at longer wavelengths  $> 310$  nm. In high latitudes, improvements can be identified, but  
339 large remaining systematic biases can still be found.

### 340 3.3 Common Mode Correction

341 In previous section, it is shown that our soft calibration effectively eliminates systematic biases of  
342 measurements relative to VLIDORT simulations for most cases, except for high latitudes/SZAs where  
343 there still exists a distinct wavelength-dependent pattern in fitting residuals because the soft calibration  
344 spectrum is derived only under small SZA conditions. In order to verify and correct such systematic  
345 biases remaining after soft calibration, we characterize spectral fitting residuals at the final iteration  
346 classified into 3 latitude/SZA regimes (southern polar region/SZA $>60^\circ$ , tropical region/ SZA $<40^\circ$ ,  
347 northern polar region/ SZA $>60^\circ$ ) for each cross-track position and for one day (14<sup>th</sup> or 15<sup>th</sup>) of each  
348 month. The remainder is called the common residual spectrum. Examples of derived common spectra  
349 are presented in Fig. 9 for March and August 2013. The main peak positions of residuals of all common  
350 residual spectra are well matched to each other. The amplitude of tropical residuals is very similar  
351 between two months, whereas the variation of the amplitude at high latitudes seems to be associated  
352 with snow/ice cover and SZA variations such that the amplitude is maximized during the polar winter  
353 season. Applying the common mode correction ([CMC](#)) means subtracting the common spectrum with  
354 amplitude determined iteratively along with the rest of state vector components from the measured  
355 spectrum. Fig. 10 compares the fitting residuals at high SZAs for one orbit of data on 02 March 2013  
356 with and without the common mode correction. It is evident that wavelength dependent fitting residuals  
357 are greatly reduced even for the first few wavelengths, with amplitude of spectral residuals reduced  
358 from  $\sim 1$  % to 0.5 %. Moreover, the common mode correction slightly reduces the standard deviations  
359 of residuals. The improvement is seen everywhere as shown in Fig. 11 where RMS of relative fitting  
360 residuals (ratio of fitting residuals to measurements error) is displayed for all individual pixels within  
361 one orbit.

### 362 3.4 Measurement Error Correction

363 The measurement error covariance matrix  $S_y$  is one of the essential inputs in an OE based algorithm,  
364 because it significantly affects the stability of retrievals and retrieval sensitivities. OMPS L1B v2.0 data  
365 contain the relative errors of radiance measurements, but these measurement errors ( $\sim 0.04$  % @ 320

366 nm) were too small to regularize our ozone fitting process so that many retrievals fail due to negative  
367 or large positive ozone values as a result of over fitting. Ideally, the measurement errors need to include  
368 not only photon shot noise but also other kinds of random noise errors caused by readout, straylight,  
369 dark current, geophysical pseudo-random noise errors due to sub-pixel variability and motion when  
370 taking a measurement, forward model parameter error (random part), and other unknown errors.  
371 However, OMPS measurement errors reported in the L1B only include photon shot noise and read-out  
372 errors, which underestimate the overall measurement error. For this reason, OMI ~~noise~~-noise floor (NF)  
373 errors instead of OMPS random-noise errors are imposed on our preliminary retrievals, as mentioned  
374 in Sect 2.3. However, better signal-to-noise ratios (SNRs) could be expected for OMPS than OMI due  
375 to OMPS's coarser spectral and spatial resolutions, as shown from the improved detection limit of  
376 OMPS H<sub>2</sub>CO retrievals compared to OMI as discussed in Gonzalez Abad et al. (2016). Fig. 11 also  
377 implies that there is room for increasing the Degrees of Freedom for Signals (DFS) to current ozone  
378 retrievals by regularizing them using the improved measurement error instead of using OMI ~~floor~~-noise  
379 ~~NF~~ errors; the ideal value of RMS is one, but our RMS is mostly within 0.4 at low and mid-latitudes. The  
380 random-noise component of measurements could be derived from standard deviations of spectral fitting  
381 residuals (Cai et al., 2012; Liu et al. 2015b). Fig. 12 shows how we derive the measurement errors to  
382 improve our retrievals. We first characterize the minimum measurement errors from fitting residuals  
383 under nearly clear-sky condition at SZAs < 40° and cross-track pixels between 4 and 33; note that no  
384 radiometric calibration is applied to these fitting residuals. The standard deviations of fitting residuals  
385 are nearly invariant at longer wavelengths > 310 nm and show a significant increase from ~ 0.1 % at  
386 310 nm to ~ 0.3 % at 302 nm as plotted with the red dashed line in Fig. 12.a. We eliminate the low-  
387 frequency portion of the noises with a 4<sup>th</sup> order polynomial fit to define the minimum OMPS ~~floor~~-noise  
388 ~~(FN)-NF~~ errors as plotted with the red solid line in Fig. 12.a. The derived ~~FN~~-NF errors are ~ 2 (1.5-  
389 4) times smaller than OMI ~~floor~~-noise ~~NF~~ errors above (below) 310 nm and thereby could increase the  
390 measurement information in our retrievals. We impose the minimum ~~FN~~-NF errors as a measurement  
391 constraint in our algorithm when SZAs are smaller than ~ 20°, whereas they are multiplied by a SNR  
392 scaling factor to increase measurement errors as a function of SZAs. Figure 12.b shows an example of  
393 how derived measurement errors increase with SZA at the boundary wavelengths of the ozone fitting  
394 window, with errors from 0.24 % to 0.45 % for 302.5 nm and from 0.097 % to 0.19 % for 340 nm.

395 Figure 13 shows the effect of using the derived ~~FN~~-NF errors on our retrievals. The RMS of fitting  
396 residuals increases from 0.2-0.4 to 0.4-0.8 in swath lines 50-350, where SZAs are within ~ 60°, due to  
397 SNR increases, whereas the average fitting residuals slightly improves by 0.015 %. Using the new ~~FN~~-  
398 ~~NF~~ errors slightly increases the number of iterations; one or more iterations are required for ~ 24 % of

399 the total retrieved pixels and hence our fitting process converges mostly within 3-4 times, except for  
400 thick clouds where the number of iterations increases to 6. Using the derived ~~FN-NF~~ errors significantly  
401 increases the retrieval information content. Both stratospheric and tropospheric DFSs are improved by  
402 0.2-0.4 under mild SZAs and by up to 0.2 under high SZAs as shown in Fig. 14, so that tropospheric  
403 ozone retrievals demonstrate  $\sim 1$  DFS in low/mid latitudes, which is similar to OMI retrievals (Liu et  
404 al., 2010a). Fig 15.a shows the retrieved tropospheric ozone column distribution with two radiometric  
405 calibrations (soft, CMC) and OMPS ~~NFFN~~ errors. Compared to Fig 7.b without CMC and OMI ~~FN-NF~~  
406 errors, the cross-track dependent noises over the polar region are smoothed due to CMC and the columns  
407 are enhanced in the tropics and the northern mid-latitudes due to OMPS ~~NFFN~~ errors. Successful  
408 tropospheric retrievals typically require better than 0.2-0.3 % fitting accuracy between measured and  
409 modeled radiances in the Huggins band (310-340 nm) (Munro et al., 1998). Our fitting algorithm meets  
410 this requirement after carefully applying empirical calibrations as shown in Fig 15.b; the average fitting  
411 residuals are within 0.1 % for moderate SZAs, with insignificant dependence on cross-track position.

#### 412 4. Conclusions

413 The OMI ozone profile algorithm has been adapted and modified to retrieve tropospheric ozone and  
414 ozone profiles from OMPS-NM L1B 2.0 product. To verify the best knowledge of OMPS instrument  
415 slit functions, we evaluate OMPS preflight measured slit functions and analytical slit functions  
416 assuming standard and super Gaussian distributions through cross-correlation using a high-resolution  
417 solar reference spectrum. We also adjust preflight measured slit functions to post-launch OMPS  
418 measurements by broadening/squeezing them by up to 4%, which slightly improves the fitting residuals  
419 at nadir cross-track pixels, but by up to 0.18% (e.g., from 0.75% to 0.6% at the first cross-track position)  
420 at edge pixels. The super Gaussian slit functions better represent OMPS irradiances than the standard  
421 Gaussian and even the preflight measured slit functions, but the fitting residuals of radiances with  
422 different slit functions show insignificant differences. OMPS measured slit functions are finally  
423 implemented in our OMPS ozone fitting retrievals because they take account of the slight dependence  
424 of slit functions on wavelengths.

425 We perform two kinds of radiometric calibrations to eliminate the systematic components of fitting  
426 residuals. First, we apply “soft calibration” to OMPS radiance before retrievals. This correction  
427 spectrum is derived as a function of wavelength and cross-track position by averaging the ratio of  
428 measured radiances to simulated radiances using collocated OMI ozone profile retrievals in the tropics  
429 under nearly clear-sky conditions for 25 days of May 2013. Applying soft calibration to OMPS radiance

430 dramatically improves the spectral fitting residuals, especially under low to moderate SZA. The  
431 amplitude of fitting residuals decreases from 1 % to 0.2 %. Therefore, the significant cross-track striping  
432 pattern shown in preliminary OMPS tropospheric ozone retrievals is mostly eliminated. Second, the  
433 CMC is implemented to compensate fitting residuals uncorrected by soft calibration, especially for high  
434 SZA retrievals. This correction spectrum is derived as functions of wavelength and cross-track position  
435 by averaging one day's fitting residuals over the tropics and northern/southern high latitude regions,  
436 respectively. The amplitude of the correction spectrum is iteratively and simultaneously adjusted with  
437 ozone. It is found that the amplitude of the fitting residuals decreases by a factor of 2 due to the CMC  
438 over high latitudes.

439 Our preliminary algorithm uses OMI ~~floor noise~~<sup>NF</sup> errors to represent measurement constraints  
440 because OMPS L1B random-noise errors are too tight to stabilize retrievals. However, we found that  
441 OMI ~~floor noise~~<sup>NF</sup> errors cannot sufficiently constrain our OMPS retrievals, indicating that there is  
442 room to increase the retrieval sensitivity to measurement information by improving measurement  
443 constraints. Therefore, we derive the minimum ~~floor noise~~<sup>(FN)</sup><sup>NF</sup> error corresponding to standard  
444 deviations of spectral fitting residuals over the tropics. The derived minimum ~~FN~~<sup>NF</sup> error is  $\sim 0.097\%$   
445 in 310-340 nm and increases to  $\sim 0.24\%$  at 302.5 nm, which is smaller than OMI error by a factor of  
446 1.5-4 below 310 nm and 2 above. We apply this OMPS ~~FN~~<sup>NF</sup> error at SZAs  $< \sim 20^\circ$  and those  
447 multiplied by a SNR scaling factor to take into account the decreasing SNR with increasing SZA at  
448 SZAs  $> \sim 20^\circ$ ; at SZA  $= 90^\circ$  errors becomes 0.45 % at 302.5 nm and 0.19 % at 340 nm. Using OMPS  
449 ~~NF~~<sup>N</sup> errors as a retrieval constraint slightly improves the fitting residuals, by 0.015 % on average, and  
450 both stratospheric and tropospheric ozone retrieval sensitivity (DFS increases by 0.2-0.4), but requires  
451 1 or more additional iterations for convergence. In this study, we meet the requirement to achieve  
452 successful tropospheric ozone retrievals in terms of DFS ( $> 1$ ) and fitting residuals ( $< 0.2\text{-}0.3\%$ ) with  
453 empirical calibrations optimized to OMPS L1B measurements. In future work, we will characterize  
454 OMPS ozone profile retrievals, present error analysis, and validate retrievals using a reference dataset,  
455 to verify that the quality of OMPS ozone retrievals is adequate for scientific use.

456

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617 **Table1. Surface and atmospheric input parameters and cross section data used in forward model**  
618 **calculations.**

Forward model Parameters	Data Source
O <sub>3</sub> cross sections	Brion et al. (1993)
Ozone Profile <sup>a</sup>	OMI ozone profiles from Liu et al. (2010)
Temperature profile, surface/tropopause pressure	Daily National Centers for Environmental Prediction (NCEP) final (FNL) operational global analysis data ( <a href="http://rda.ucar.edu/datasets/ds083.2/">http://rda.ucar.edu/datasets/ds083.2/</a> )
Surface albedo	OMI surface climatology (Kleipool et al., 2008)
Cloud fraction	Derived at 347 nm
Cloud-top pressure <sup>b</sup>	OMPS Cloud Optical Centroid Pressures (OCPs) (Vasilkov et al., 2014)

619 <sup>a</sup>OMI ozone profiles retrieved at 48×52 km<sup>2</sup> with spatial coadding and then interpolated to 5° × 5° to fill  
620 bad pixels.

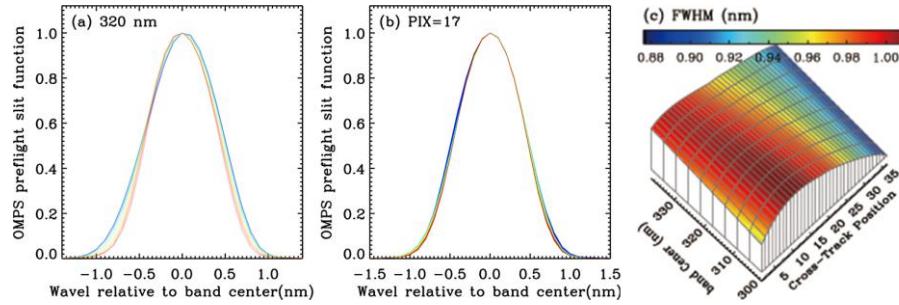
621 <sup>b</sup>OCPs retrieved from OMPS-NM L1B v1.0 measurements using a rotational Raman scattering cloud  
622 algorithm.

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631 Figure 1. (a) OMPS preflight slit function at 320 nm band center, with colors representing different cross-  
632 track positions from 1 (blue) to 36 (red). (b) Same as (a), but for the 17<sup>th</sup> cross-track position, with colors  
633 representing different wavelengths from 300 nm (blue) to 340 nm (red). (c) Full Width at Half Maximum  
634 (FWHM) in nm as functions of cross-track positions (x-axis) and band center wavelengths (y-axis) ranging  
635 from 300 to 340 nm.

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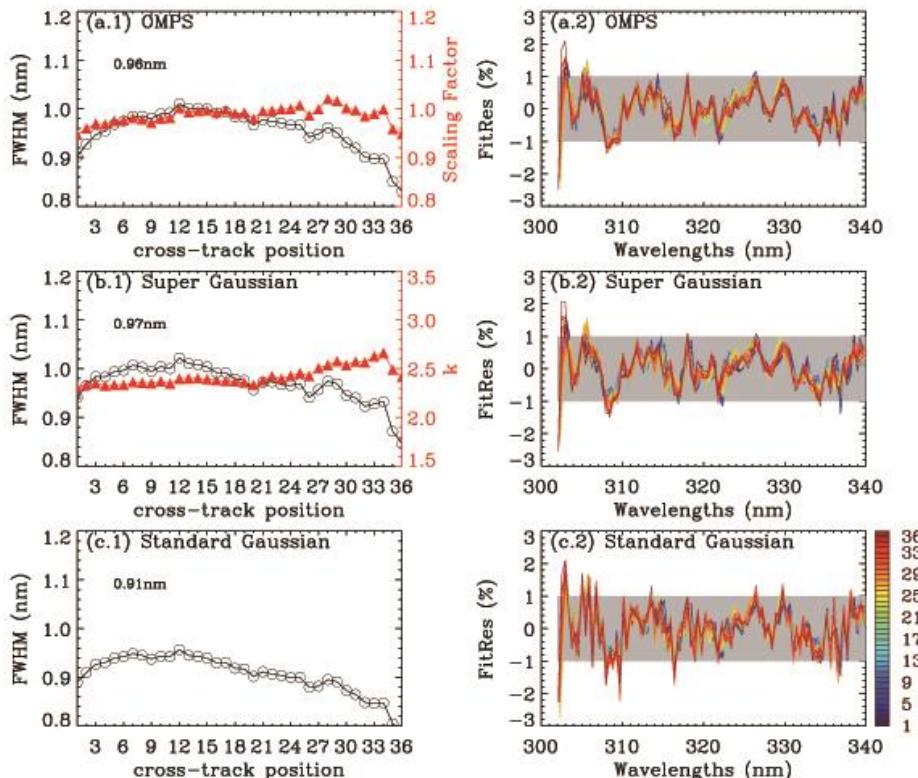
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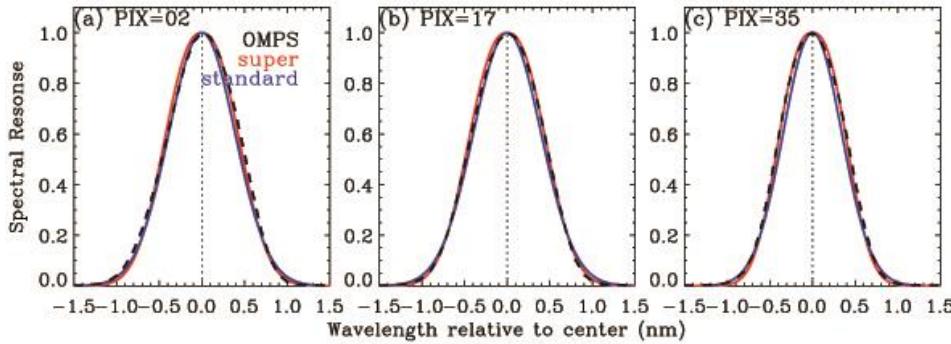


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Figure 2. (Left) Slit function parameters as a function of cross-track position (1<sup>th</sup>-36<sup>th</sup>) for three different slit functions from OMPS irradiance measurements (302-340 nm) for orbit 7132 on 14 March 2013. The legends represent the FWHM averaged over all spectral pixels. (Right) The corresponding relative fitting residuals between measured and simulated irradiance spectra.

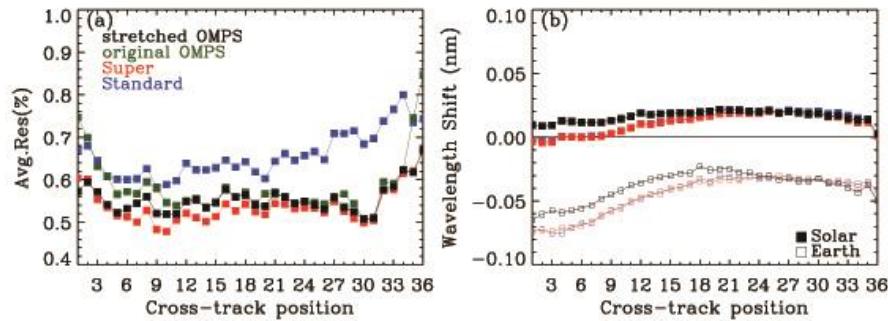
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669 **Figure 3.** Comparison of OMPS measured slit measurements (black)  
670 and derived slit functions assuming a standard Gaussian (red) and super Gaussian (blue) for orbit 7132.

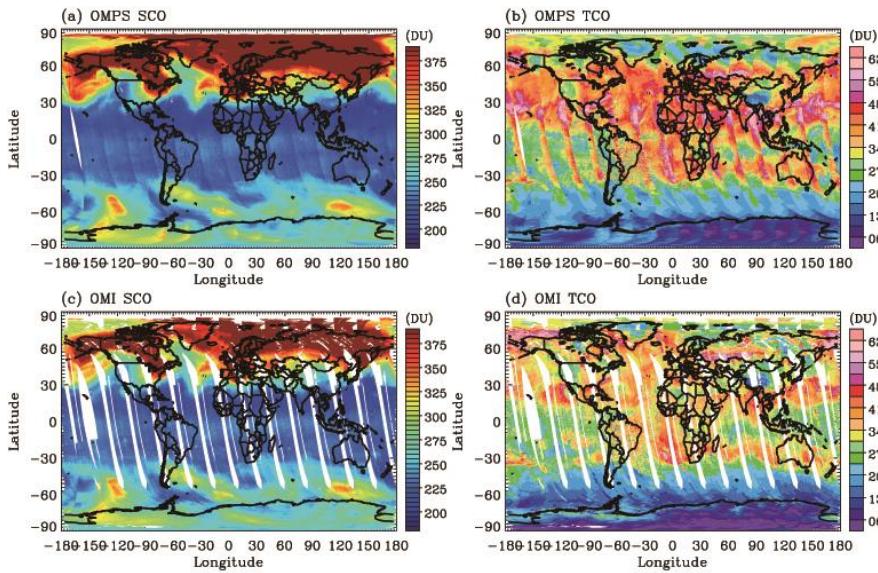
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673 **Figure 4.** Same as Fig. 2, but for (a) average fitting residuals (%) as a function of cross-track positions. The  
674 green line represents the fitting residuals with measured OMPS slit functions without fitting a scaling factor.  
675 (b) Wavelength shifts between OMPS irradiance and reference spectrum (filled symbols) and between  
676 OMPS radiance at the middle swath line and reference spectrum (opened symbols).

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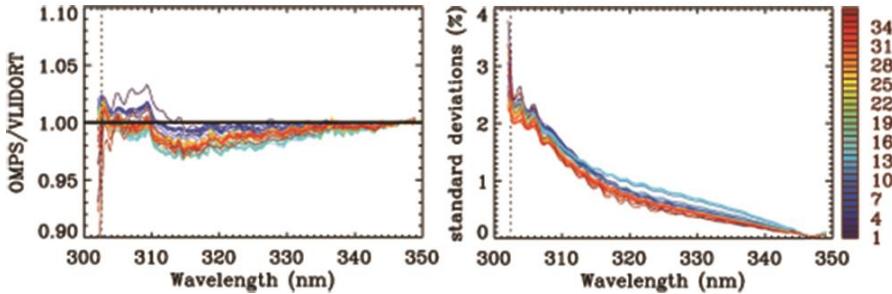
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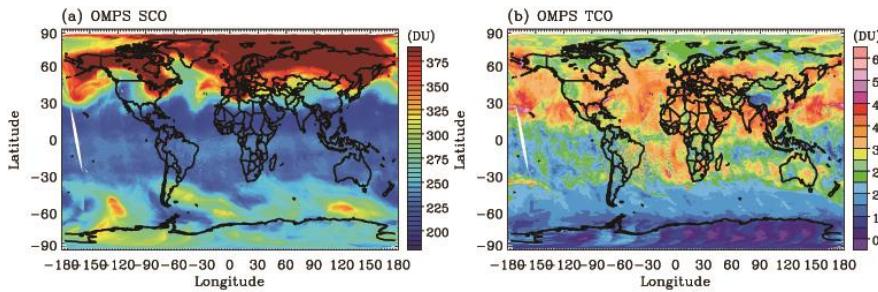
685 **Figure 5. Maps of stratospheric and tropospheric ozone column on 14 March 2013, retrieved from OMPS**  
686 **(top) without any correction and OMI (bottom) measurements, respectively.**

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Figure 6. (a) Soft calibration spectrum derived from OMPS measured to simulated radiance ratio at initial iteration, as a function of wavelength ranging from 302 nm to 350 nm. The vertical dotted line indicates 302.5 nm. OMPS data used in this calculation is limited to tropical clear-sky conditions (latitude <  $\pm 15^\circ$ , cloud fraction < 0.1, surface reflectivity < 0.1) for 25 days between 1 March 2013 and 25 March 2013. Forward model inputs listed in Table 1 are used for OMPS simulations. (b) Standard deviations of fitting residuals. Different colors represent various cross-track positions.



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Figure 7. Same as Figure 5 (a) and (b), but for OMPS ozone retrievals with soft calibration.

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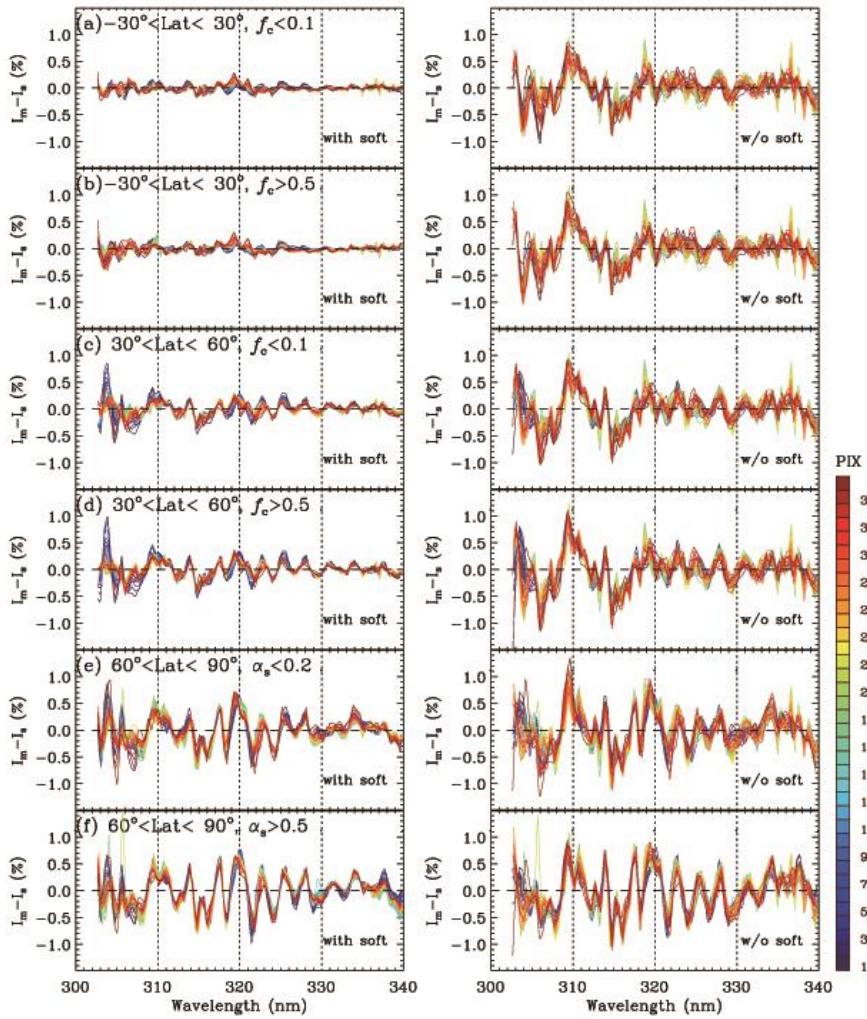
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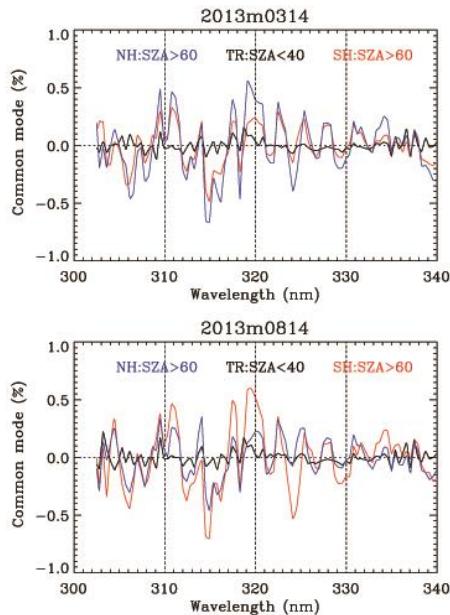
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709 **Figure 8. Comparison of fitting residuals on 14 March 2013 with (left) and without (right)**  
710 **soft calibration for 6 cases: (a-b) Tropics and (c-d) mid-latitudes each for clear sky**  
711 **(effective cloud fraction,  $f_c < 0.1$ ) and cloudy ( $f_c > 0.5$ ) conditions and (e-f)**  
712 **high-latitudes for snow-free and snow-covered surface conditions.**  
712 **Different colors represent different cross-track positions.**



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714 **Figure 9. Common mode spectra derived from final fitting residuals at the 17<sup>th</sup> cross-track position using**  
 715 **one day of measurements in March (upper) and August (lower), respectively. Note that tropical residuals**  
 716 **are derived from nearly clear-sky conditions where SZA < 40°, cloud fraction < 0.1, and surface albedo <**  
 717 **0.1. No special data screening is applied for polar residual spectra, except for SZA > 60°.**

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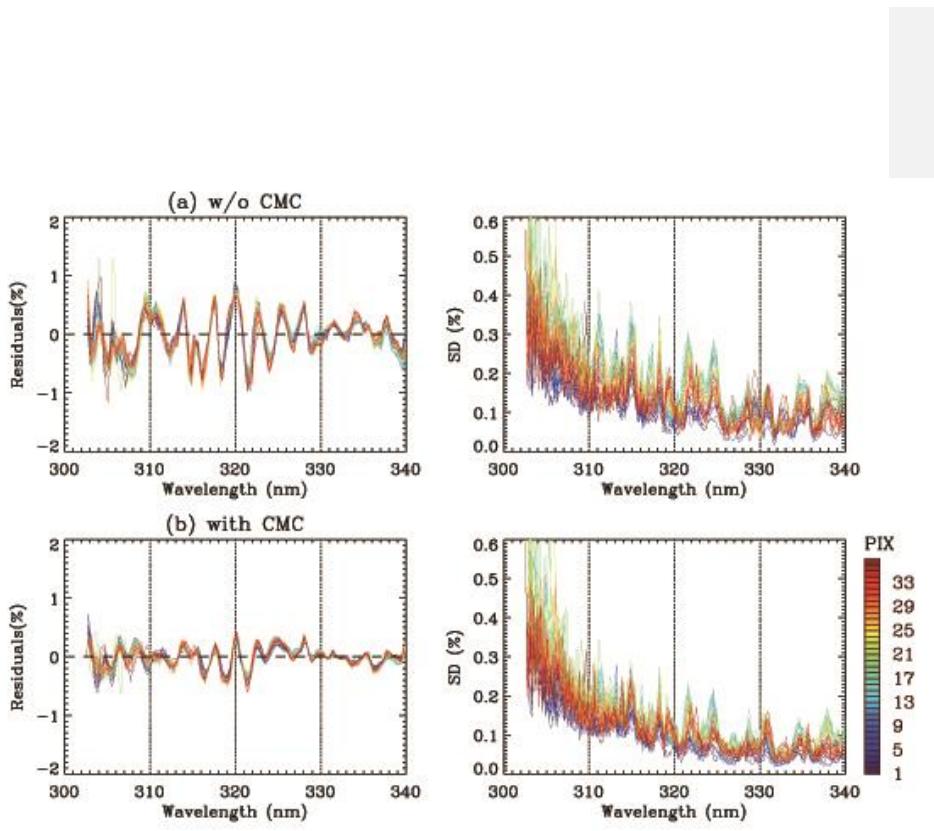
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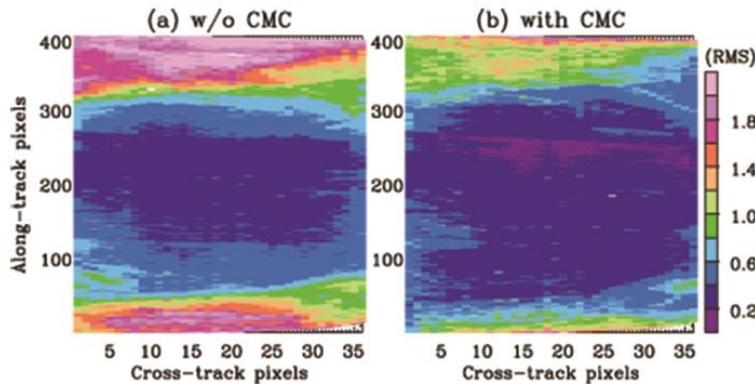


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 728 Figure 10. Comparisons of mean fitting residuals (%) and its standard deviations (%) for latitude  $> 60^\circ$ ,  
 729 with different cross-track positions in different colors for one orbit data (6962) on 02 March 2013, without  
 730 (a) and with (b) common residual-mode correction.

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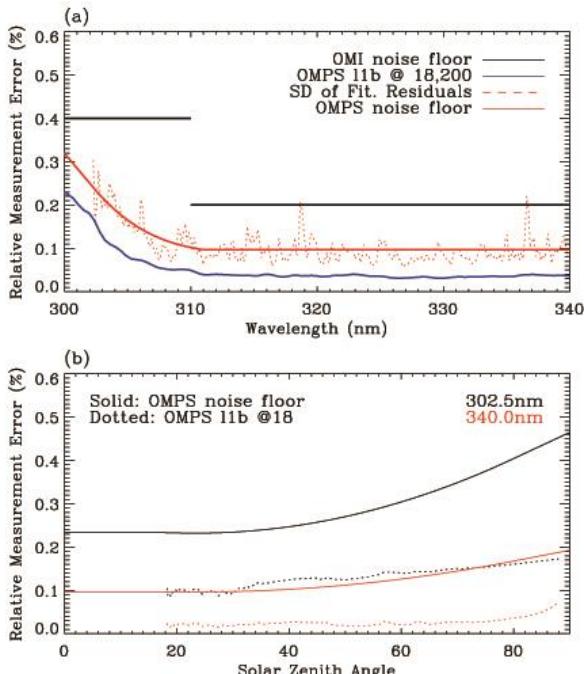
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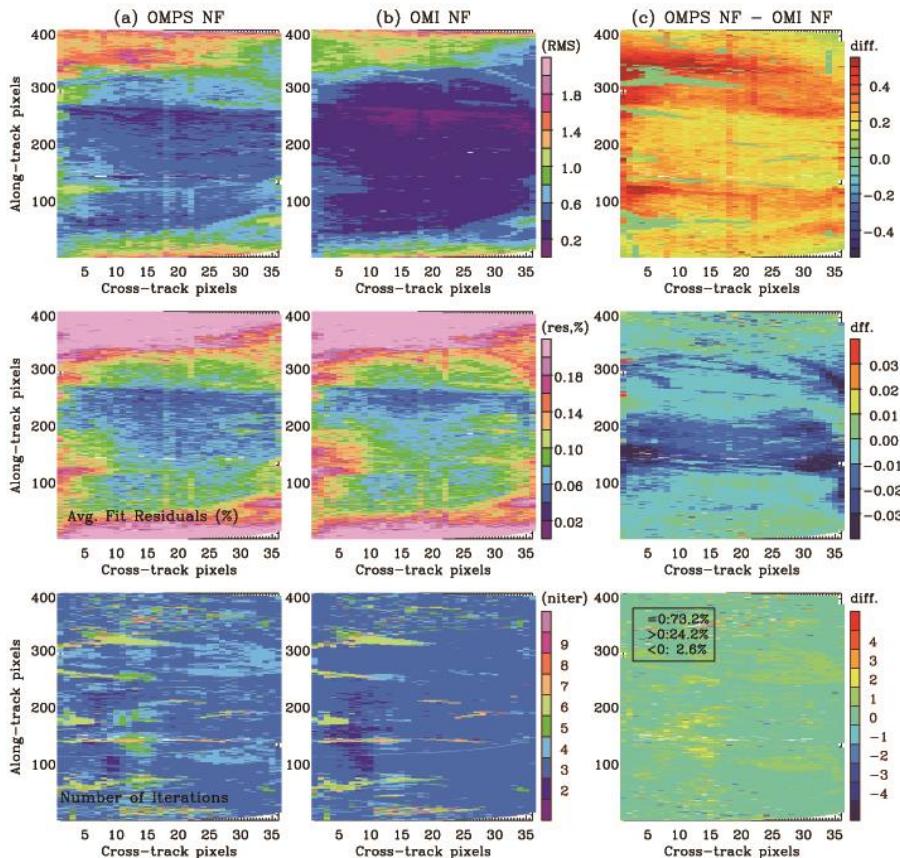
735 Figure 11. Same as Figure 10, but for Root Mean Square (RMS) of fitting residuals relative to the  
 736 measurement errors as functions of along- and cross-track pixels. The RMS is defined as  $\sqrt{\frac{1}{n} \sum_i^n \left( \frac{Y_i - R_i}{S_y^{1/2}} \right)^2}$ .  
 737 Note that OMI floor-noise floor errors (0.4% at wavelengths < 310 nm, and 0.2% at wavelengths > 310 nm)  
 738 are used to define RMS.



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740 Figure 12. (a) Standard deviations of spectral fitting residuals for 14 March 2013 under clear-sky conditions  
 741 and for small SZAs  $< 40^\circ$  (red dotted line), with the 4<sup>th</sup> order polynomial fitting of them (red solid line)  
 742 called “OMPS ~~noise~~ noise floor (FNF) error”. This FNF error represents the minimum measurement  
 743 constraint implemented in OMPS ozone fitting process. OMI floor noise error (black line) and OMPS L1B  
 744 v2.0 random-noise error (blue line) (orbit: 7132, cross-track: 18, along-track: 200) are also shown for  
 745 comparison in the same panel. (b) OMPS ~~noise~~ noise floor at 302.5 nm and 340 nm as a function of SZAs (solid line),  
 746 with the corresponding OMPS L1B v2.0 measurement error (dotted line).

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749 Figure 13. Top: Comparison of RMS of fitting residuals relative to the assumed measurement errors as  
 750 functions of cross-track and along-track pixels for orbit 7132 with (a) OMPS NFFN (first column) and (b)  
 751 OMI NFFN (second column), respectively, with (c) their absolute differences (third column). The definition  
 752 of RMS is given in Fig. 11. Middle: Comparison of average fitting residuals relative to the simulated  
 753 radiances (%), which are similar to RMS, except that radiance differences are normalized to measured  
 754 radiances instead of measurement errors. Bottom: Comparison of the number of the retrieval iterations.

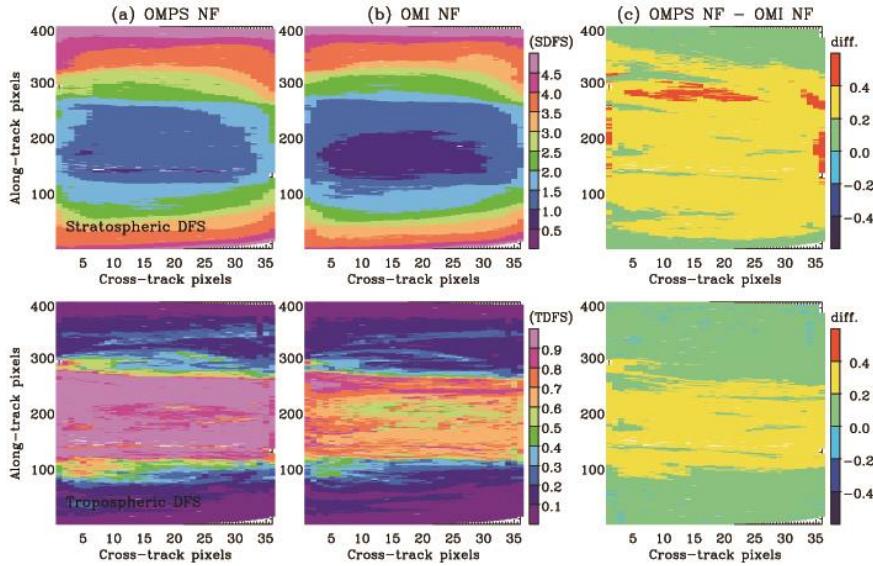
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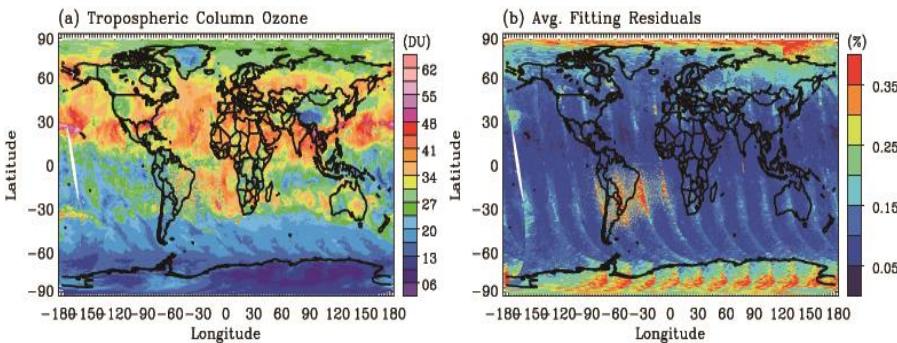


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761 Figure 14. Same as Fig. 13, but for the integrated Degrees of Freedom for Signal (DFS) in the stratosphere  
762 and troposphere (bottom), respectively.

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765 Figure 15. (a) Same as Fig 7.b, but for improved retrievals with common mode correction and OMPS floor  
766 noise floor error, (b) corresponding average fitting residuals (%).