

Overall Comments:

In this work, Bak et al. provide a thorough description of “An improved OMI ozone profile research product version 2.0 with collection 4 L1b data and algorithm updates”. Although it is of significant scientific value to the space-borne atmospheric monitoring community, its presentation can be substantially improved, both in terms of research results and general phrasing.

.→ We appreciate the useful comments, and tried to improve the manuscript, in accordance with reviewer’s suggestion.

Specific Comments:

C1 Line 59: A degradation is provided in %, but the time range is not specified. Is this per decade, or 'now' with respect to beginning of mission? Idem for the wavelength stability in nm (also in line 155).

R1. The magnitudes of degradation and wavelength shift were taken from Schenkeveld et al. (2017) where OMI long-term stability is assessed over the period of 2005 to 2014. In this revised manuscript, Kleipool et al. (2022) has been referenced to indicate the long-term stability of OMI instrument over the period of 2005 to 2021. Accordingly, the related sentence has been revised as “the OMI instrument show progressively low optical degradation over the mission, with a change of ~ 3 % in the radiance over roughly 1.5 decades (Kleipool et al., 2022)” in introduction (Line 59 in the original manuscript). The corresponding statement in line 155 was removed in the revised manuscript for assuring the conciseness and consistency of the context.

C2 Line 62: “satellite ozone profile products have not been reliable for long-term analysis” sounds too strong. This should be rephrased.

R2. We agreed with this comment. It was rephrased as “OMI instrument show progressively low optical degradation over the mission, with a change of ~ 3 % in the radiance over roughly 1.5 decades (Kleipool et al., 2022). However, the long-term reliability of the OMPROFOZ product, particularly concerning tropospheric ozone measurements, remains susceptible to optical instrument degradation (Gaudel et al., 2018; Huang et al., 2018, 2017)..”

C3 Line 68: “latitude/season/viewing geometries” can be combinedly referred to with an optical path dependence? Please discuss appropriately.

R3. According to these comments, “and the dependence of retrieval quality on the latitude/season/viewing geometries” has been revised as “and suggested the need to address the spatiotemporal variations of the retrieval performance and the related cross-track dependency”.

C4 Lines 84-85: “Note that OMI measurements have been reprocessed to deliver the new collection 4 dataset” Does this apply to the entire time series, or a limited period only?

R4 OMI collection 4 L1b data is available for entire time series
(https://disc.gsfc.nasa.gov/datasets/OML1BRUG_004/).

C5 Lines 109-110: It is not clear where the codes between brackets refer to.

R5 The code in bracket indicates the DOI for the given dataset, which has been deleted in the manuscript, but provided as a part of the reference (e.g., Kleipool, Q. (2021a), OMI/Aura Level 1B Averaged Solar

Irradiances V004, Greenbelt, MD, USA, Goddard Earth Sciences Data and Information Services Center (GES DISC), Accessed: [2023-07-21], 10.5067/Aura/OMI/DATA1401, 2021a)

C6 Lines 126-127: Does the “KNMI flag” name apply in general, or in this work only?

R6 Most of the information regarding the OMI row anomaly is sourced from Schenkeveld et al (2017). The referenced paper also uses “KNMI/NASA (row-anomaly) flag”, NASA and KNMI flagging results to refer to the row-anomaly flag derived with each detection method.

C7 Lines 135-136: “In addition, OMI total column ozone product (OMTO3d) is used in deriving empirical correction spectra.” This sounds too vague. A reference or more detailed explanation is needed.

R7. According to this comment, we provided more details in the revised manuscript, as like “We applied OMI total column ozone product (OMTO3d) to adjust the ozone profile shape used as an input for deriving empirical correction spectra (Sect. 3.8).”

C8 Line 149: “48 x 26” instead of “38 x 26”?

R8 Thanks. It is corrected.

C9 Figure 1 may be too detailed or might need an explanation of the variables used.

R9. The most of the variables have been described in the text after Figure 1. In the revised manuscript, we have mentioned more variables and described it in more detail.

C10 Line 175: “assuming that measurement errors are uncorrelated among wavelengths” Is this a valid / common approach then? Please specify or provide referencing.

R10. It is very common to construct S_y as a diagonal matrix, where measurement errors are assumed to be uncorrelated among wavelengths, as suggested by Rodgers (2000) who introduced an inverse theory based on an optimal estimation.

C11 Lines 186-187: Explain with reference(s) how the correlation length is applied in the covariance matrix.

R11. We have specified how to apply the correlation length in the revised manuscript as “They are assumed to be uncorrelated between fitting parameters, except for atmospheric profiles with a correlation length of 6 km, which gives $S_y(i, j) = \sigma_i^a \sigma_j^a \exp(-|i - j|/6)$, where σ^a is a priori error, with i and j being layer numbers”

C12 Lines 207-209: What happens to levels below the effective surface pressure?

R12 As mentioned, the bottommost level is the surface pressure.

C13. Line 276: Where is this tropopause pressure obtained from (also in Figure 2)?

R13. In this figure, the meteorological variables including the tropopause pressure are commonly taken from the NCEP reanalysis data, only to see the impact of applying different a priori ozone profile information on the retrieval. For clarification, we have inserted “It is noted that the meteorological variables are commonly taken from the NCEP reanalysis data to see the impact of applying different A priori ozone data on the retrieval.” in the caption of Figure 2.

C14 Lines 303-305: “However, the data transmission has been accidentally halted since June 2011 and hence climatological monthly mean data have been used as a back-up in the data processing.” Not clear whether this applies to v1 or v2.

R14 As mentioned, this happened to the v1 data processing. To avoid this risk, the meteorological input is switched to the internal meteorological products (OMUFPSLV, OMUFPMET)

C15 Lines 327-329: “BW measurements were better parameterized as quadratic temperature-dependent coefficients with uncertainties of 0.25-2 % whereas for BDM measurements fitting residuals of 2-20 % remains.” Also, lines 346-347 “radiometric uncertainties of the new reference spectrum are below ~ 1 % whereas for SAO2010 those range from 5% in the longer UV part to 15 %” That’s two times a factor of ten improvement, and might be the most impactful changes. This might be stressed in the conclusions and/or better explained and referenced?

R15. Note that the factor of 10 improvement for cross section occurs in the cross section fitting residuals after the temperature-dependent parameterization. It can also have a large impact on ozone profile retrievals when soft calibration is turned off (Bak et al., 2020). With soft calibration derived using consistent cross sections, some of the systematic differences due to cross sections can be greatly reduced; using BW can still improve the retrievals due to its better temperature dependence, but it does not cause the most impactful changes. The high-resolution solar reference is used mostly for wavelength and slit function calibration. Despite the much better agreement of TSIS HSRS with TSIS SIM observation than the SAO2010 reference, the improvement on the ozone profile retrieval is also relatively smaller, changing the tropospheric layer ozone columns by 5-7% (Bak et al., 2022).

C16 Why are different temperatures chosen for plots (a) and (b) in Figure 4?

R16 We plotted each cross-section data at all temperatures available from the original database (“not chosen”). In the original manuscript, it has been noted as “the BW dataset provides improved temperature coverage from 193 K to 293 K, every 20 K over the BDM dataset given only at five temperatures above 218 K”

C17 Line 401: Explain cross-product and I_h in the equation.

R17 Each represents “spectral convolution” and high-resolution radiance spectrum. In revised manuscript, the equation has been simply expressed as $\frac{\partial I}{\partial p}$ ($p = w \text{ or } k$) for conciseness and clarify. The implementation details to get $\frac{\partial I}{\partial p} (\frac{\partial S}{\partial p} \otimes I_h)$ through the slit function linearization can be found in Bak et al. (2019b), as indicated in the end of the corresponding section 3.6.

C18 Lines 411-412: A factor f_c seems to be missing the second term of the formula (while on the other hand f_c is not explained).

R18 We have specified the indicated equation as “ $I = I(R_{sfc}, P_{sfc})(1 - f_c) + I(R_{cloud}, P_{cloud}) f_c$ where R and P represent reflectivity and pressure at bottom level (surface or cloud) with f_c as an effective cloud fraction”

C19 Lines 412-413: “finer grids than at least 4 pixels per FWHM so that the spectral convolution is applied to account for OMI spectral resolution” This is too brief to be clear.

R19 To address this comment, we have revised this sentence as “According to the Nyquist criterion (Goldman, 1953), individual spectra need to be simulated at grid spacings finer than a minimum of two pixels (four pixels in practice) per spectral resolution”

C20 Table 4 and Table 5 seem to be missing?!

R20 We are very sorry to make this big mistake. Tables 4 and 5 have been inserted in Section 3.7 and Section 4, respectively.

C21 Lines 428-431: this is unclear if half-streams are not explained.

R21 The half-streams are just discrete ordinate streams in the half-space. For clarification, the definition of the half streams has been specified in the revised manuscript.

C22 Line 433: “(2 vs. 6) and number of layers (24 vs. 72)” which versions are compared here?

R22. As mentioned in the original manuscript (a look-up table (LUT)-based correction is performed, which enables to adjust the differences in RT variables due to different number of streams (2 vs. 6) and number of layers (24 vs. 72) as well as neglecting polarization effect), a LUT based correction is applied to improve the approximation errors in radiative transfer calculations, arising from low number of streams and coarse vertical layering as well as neglecting polarization effect. That is, the operational algorithm runs on-line RT model in scalar mode with the atmospheric layers of 24 and two streams. This approximation error is compensated with the look-up table correction in which the RT variables are pre-calculated in vector with the atmosphere layers of 72 and six streams.

C23 Lines 435-438: “Note that the Ring simulation remains unchanged from v1 algorithm; the spectral structure of the Ring signal is externally simulated with the iterative fitting of amplitude of the Ring spectrum and then subtracted from the measured spectral reflectance.” Please provide reference.

R23 This concept of accounting for ring effect has been adopted from the OMPROFOZ v1.0 algorithm so that Liu et al. (2010) is cited as a reference according to this comment.

C24 Lines 446-447: “along-track stripes that are commonly found in OMI trace gas products” Should this be clear from the plots? Please provide references.

R24 The cross-track dependent biases are clearly found in both fitting residuals (Figure 8.a) and tropospheric ozone retrievals (Fig 8. b and c) (along-track stripes in the global map). We thus derive the cross-track dependent soft calibration spectra (Fig. 9) to reduce stripes (see. Fig. 8 d-e-f). According to this comment, we have added several references (e.g. Wang et al. 2016; Kroon et al., 2011; LN Lamsal et al. 2021)

C25 Section 3.9: Please explain important “pseudo-absorber” concept for clarity of common mode correction.

R25 The common mode correction is implemented to address the remaining spectral residuals after soft calibration. The soft calibration is applied to the measured spectrum once before ozone spectral fitting. The common model spectrum is iteratively adjusted as a pseudo-absorber to absorb the remaining residuals. This common mode correction is intended for improving the fitting accuracy, but also helps to smooth out the cross-track dependent biases in the tropospheric ozone retrievals, in particular at the extreme nadir-off pixels (please take a look at Fig. 8 d-f vs Fig.12 a-c).

C26 Section 4: Why the severe limitation of having 3 sites above Central Europe only? To what extent are these results globally valid?

R26 The main objective of this paper is to describe the implementation changes for re-processing OMI collection 4 ozone profile product, with algorithmic updates including radiative transfer calculations,

slit function parameterization, soft calibration, new pseudo absorbers and input changes (a priori ozone data, high-resolution solar reference, ozone cross-sections). And we verified the improvements of the implementation changes by evaluating the spectral fitting quality and the geophysical structures of the retrieved ozone distribution. Ozone profile retrievals were also evaluated in terms of quality and short/long-term consistency against the ozonesonde measurements achieved from three stations in the Central Europe. We limited this comparison with ozonesondes at three stations due to the computation budget. However, we definitely have a plan to report the global and long-term validation results when the fully reprocessed product is available.

C27 Line 545: A 3 sigma for ‘extreme values’ seems quite low. Real outliers are typically beyond that.

R27 This comparison intended for changing the retrieval quality from v1 to v2. Therefore, we don’t necessarily apply the tight outliers for a fair comparison. However, we definitely have a plan to report the global and long-term validation results when the fully reprocessed product is available. According to this comment, we will apply the tight outliers in the upcoming validation activity.

C28 Line 611: What does “continued externally” mean?

R28. The OMPROFOZ product is officially released just for the initial version and has never been changed, while each algorithm detail has been improved without applying into the operational algorithm. For clarification, we have revised the related phrase as follows “~which has not been updated since its initial data release. In this paper, we introduce algorithmic updates for reprocessing the OMPROFOZ product to enhance the retrieval accuracy and to ensure long-term consistency. This second version will be released at GES-DISC while the first version will remain archived at AVDC.”

Technical corrections

C1 Line 51: “has been contributed”

R1 It has been edited as “has contributed”

C2 Line 113: “shorter” refers to “shorter-wavelength”?

R2 Yes. “the shorter spectra” has been edited to “the shorter wavelength”

C3 Line 132: “stricter and more reliable”

R3 Thanks. “stricter and reliable” has been edited to “stricter and more reliable”

C4 Line 133: “flags are raised” instead of “flags are flagged”

R4 Thanks. “flags are flagged” has been edited to “flags are raised”

C5 Please explain norm symbols (with lower and upper 2) in equation (2).

R5. “where $\| \cdot \|_2^2$ denote the sum of each element squared” has been inserted after the equation 2.

C6 Line 471: “stripes”

R6. Accepted.

C7 Line 549: “relatively not serious” is unscientific phrasing.

R7 The indicated phrase has been edited as “the row anomaly affects the data in a few rows”

C8 Figure 13: The legends for mean bias and standard deviation seem to be reversed.

R8. Thanks for finding this mis-print. The legends have been corrected.

C9 Lines 650: please put dates on “in progress” for future reference.

R9 We have expected that the PROFOZ v2.0 data will be released in 2024, probably before July for the entire mission, but the schedule is changeable with the simulation in the data processing center.