

General comments:

The manuscript AMT-2020-94 provides a comparison of UV ozone retrievals from the OMI instrument using a new cross section data set (BW, provided in the frame of the ESA SEOM-IAS project) with the standard data set from Reims (BDM). Overall, the manuscript is very well written, nicely structured and argued. Selected figures do well illustrate the discussion in the manuscript. The presentation is scientifically sound and clear. The topic fits nicely within the journal scope and, therefore, I can fully recommend publishing the manuscript. There are a few issues to the current paper that need to be addressed before publication, however.

Responses to general comments

We would like to thank this reviewer for the constructive comments. All the comments made by this reviewer were addressed in the revised manuscript.

C1. The analysis is based on a new cross section data set (BW data) that at this point of time is openly available, but has not yet been published in the scientific literature. It therefore lacks yet the scrutiny of the peer-review process. While this is a regrettable fact, it does not invalidate the present work. But the authors must carefully discuss what might possibly be an inherent contradiction. In a previous study (Liu et al., 2013), the authors have concluded that another recent UV cross-section data set (the SER data from Bremen, Serdyuchenko et al. (2014); Gorshelev et al. (2014)) was less suited for ozone retrievals using the OMI-spectrometer than the BDM data, despite a similar spectral resolution (0.01 nm – 0.018 nm for the 210 – 350 nm range) and a much better temperature coverage (data between 193 K and 293 K on a grid of 10 K; see Weber et al. (2016) for example). Surprisingly, the same data set (SER) is now used to 'calibrate' the new BW data (see lines 95-99 of the manuscript): Offset corrections were made for each of the 6 temperatures by fitting to the SER dataset since it was measured at higher ozone column density and thus considered more reliable regarding offset. The offset corrections have minor effect on the cross-sections except for wavelengths above 330 nm. The procedure of dismissing the SER data set for ozone retrieval, but using it for calibration is confusing and needs further explanation. The calibration procedure is even more surprising as the correction actually does not seem to impact the results of the present paper, because corrections are claimed to have minor effects within the OMI windows (>330 nm). The necessity of making an offset correction arises from the measurement technique/setup at DLR. It thus needs to be explained why there is the need to make an offset correction in the first place and why the SER data do not suffer from the same problem.

R1. Offset errors in the baseline of the measured spectra cause offset errors in the absorption cross section. Since the column amount of the ozone was limited by the relatively small absorption path of 22.1 cm the offset error in the ACS was relatively large, up to $2e-22$ cm²/molec. Around 344 nm this amounts to about 20% of the ACS. At 330 nm the offset is about 4%. At 270 nm the offset is about 0.0025%. In order to correct this error fits of the BW ACS to the SER ACS fitting a scalar and an offset were performed in the range 317-350 nm. The offset error in the SER ACS were much smaller due to the significantly longer absorption path (270 cm). The scalar was ignored. The offset was used to correct the entire wavelength range, but it would not have made a difference if we had limited it to the fit range since the offset error influence below 330 nm is negligible. The SER data used for the offset fit were at longer wavelength and measured with an FTS, too. The structure of the spectra in this region agreed well beside a scalar up to 1.03, depending on temperature. In the lower wavelength range the SER data were obtained using a grating spectrometer and there were distinct differences in the structure. The offset correction is only relevant when using ACS at longer wavelength (e.g. Brewer, Dobson). In the current paper, however, opaque regions at lower wavelength are of interest, where the impact of the offset is rather small. As addressed to the answer to comment 1 from the first review, this discussion is out of scope to be detailed in this paper.

C2. In the introduction, the authors give the impression that new cross sections should be measured at a resolution of 0.01 nm or better. This contradicts the use of new cross section data that have been obtained at about 3 (> 285.7 nm) to 5 (< 285.7 nm) times lower resolution (see description of BW data set in section 2).

R2. The spectral resolution requirement is from Orphal et al. (2016): ozone cross-sections should be measured at high spectral resolutions (typically 0.01 nm in the ultraviolet-visible). So the citation of “a resolution of 0.01 nm or better” is not accurate and is probably confused with the wavelength calibration requirement “the spectral wavelength) calibration must be very accurate, too (typically at least 0.01 nm).” So we change the text from “at least 0.01 nm” to “typically 0.01 nm.” For the BW dataset, measurements are performed at a coarser resolution to cover the broad spectral range as a tradeoff or spectrally degraded in the post-processing to increase signal to noise ratio. Indeed, the spectral resolution of 3.3 cm^{-1} may have caused a very small deterioration of the highly resolved spectral features occurring above 325 nm. The high resolution structures have only a very small contrast regarding the underlying broad features. The impact is expected to be small, especially in view of the low resolution of the remote sensing instruments.

C3. The authors use the terms Hartley and Huggins bands as well as OMI instrument windows to discuss different spectral regions in the UV. While wavelength ranges for both of the OMI UV windows are specified in the manuscript, no numbers are given for the Hartley and Huggins bands. Please indicate as this would help readers to follow the discussion.

R3. We has specified the bands in the revised manuscript where these bands are first mentioned such as “ C_0 values are similar to each other in the Hartley band ($< 310 \text{ nm}$) with relative biases of 2-3%. However, the Huggins band ($> 310 \text{ nm}$) shows large spiky biases of up to 8%. C_1 and C_2 represent linear and quadratic temperature dependences of absorption cross-sections, respectively”

C4. There seem to be problems with the definitions of signs in some of the plots. For example, are the signs in Figure 7 correct? I find that local negative spikes in the total ozone column difference (BDM-BW) also correlate with cases where the tropospheric profile shows a tendency towards warmer colors (BDM $>$ BW), which would indicate that either of the two scales (total ozone (TOC) vs altitude dependent ozone) should have a different sign. Another issue is the Antarctic +1%BDM-BW bias in the TOC. From Figure 4, one would estimate that the cross section bias is positive when integrated all over the (270 – 346) nm wavelength range (despite some few local negative spikes at low temperatures). This should result in a negative BDM-BW bias of TOC. Anyway, the antarctic positive TOC bias needs to be discussed as compared to the lower latitude value around –1% on the basis of the cross section data. In similar veins, the definition of the y-axis of Figure 4 shows that the room temperature BW cross-section is negatively biased with respect to BDM at low wavelengths. This is opposite to what is stated in line 254 of the manuscript (Relative to the BDM data set, the BW data show systematic biases of 2–3% in C_0 at shorter wavelengths below 300 nm, . . .).

R4. The contour map gives an impression that applying BDM causes the overestimation, especially around the tropopause where the coldest temperature/the lowest ozone amount is found. The impact of applying different cross-section dataset on total ozone retrievals are overwhelmed mainly by the lower stratospheric layers where the ozone amount is relatively large and the dependence of ozone-cross sections on the temperature is relatively important. Please take a look at the revised Figure 7 also including the contour map for absolute differences in the unit of DU (Figure 7.b), which shows that applying BDM causes the significant negative biases in the lower stratosphere (20-30 km) and then total ozone columns are underestimated. On the other hand, the BDM based total ozone columns are overestimated in South Pole due to the biggest inconsistency of two cross-sections at the coldest temperatures just above the tropopause. In the revised manuscript, this part has been better specified in page 6 as following:

Figure 7 shows both relative and absolute differences of the retrieved ozone profiles with the corresponding temperature profiles taken from the National Centers for Environmental Protection (NCEP) final (FNL) operational global analysis data. Large differences of 20-50% commonly exist along the tropopause, where the original BDM measurements could not cover atmospheric temperatures below 218 K (Fig. 7a). Some larger differences occur throughout the troposphere in the tropics likely due to the relative smaller retrieved partial ozone columns. The individual differences of retrieved ozone in the lower troposphere are $\sim 20\%$. However, the corresponding impact on the total column ozone, from integrating retrieved ozone profiles are overwhelmed by the stratospheric layers (20-30 km), as shown in Fig. 7b, where the ozone amount is relatively large and the dependence of ozone-cross sections on the temperature is still important. As a result, applying BDM causes an underestimation of total

ozone except at the South Pole due to the biggest inconsistency of two cross-sections at the coldest temperature just above the tropopause in spite of smaller amount of ozone compared to upper stratospheric layers. The magnitude of this underestimation/overestimation is $\sim 1\%$, which is comparable to the overall accuracy ($\sim 1.5\%$) of the OMI operational total ozone product against ground-based measurements (McPeters et al., 2015).

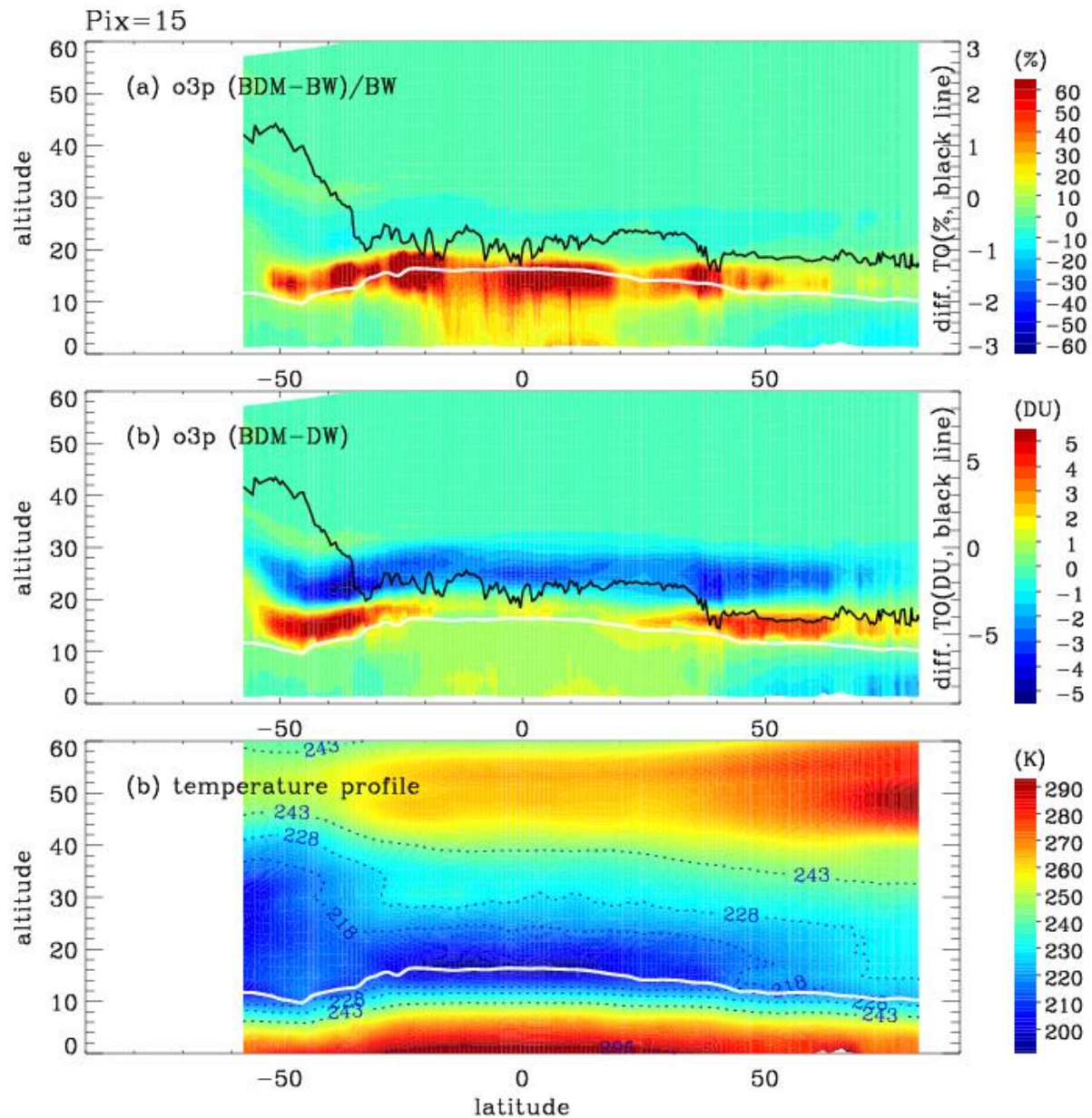


Figure 7 in the revised manuscript.

C5. In the comparison between BDM and BW in section 3, the BW data set is taken as the baseline scenario. Because section 3 only provides a relative comparison and not an accuracy assessment, the authors should avoid the impression that BW is the truth (even though it compares more favorably with ozonesonde data presented in the next section 4). Instead of saying that BDM causes an underestimation or overestimation, it should just be stated that BDM estimates are lower or higher than estimates from BW.

R5. We agree with this comment. The manuscript has been revised to reflect this suggestion.

C6. Fig. 9 shows the OMI mean biases with respect to a common reference (ozonesonde). It would be

nice to plot the reference profiles (or mean profiles with their sdev) along with the bias percentages.
R6. We have revised Figure 9, according to this comment. The revised figure is following:

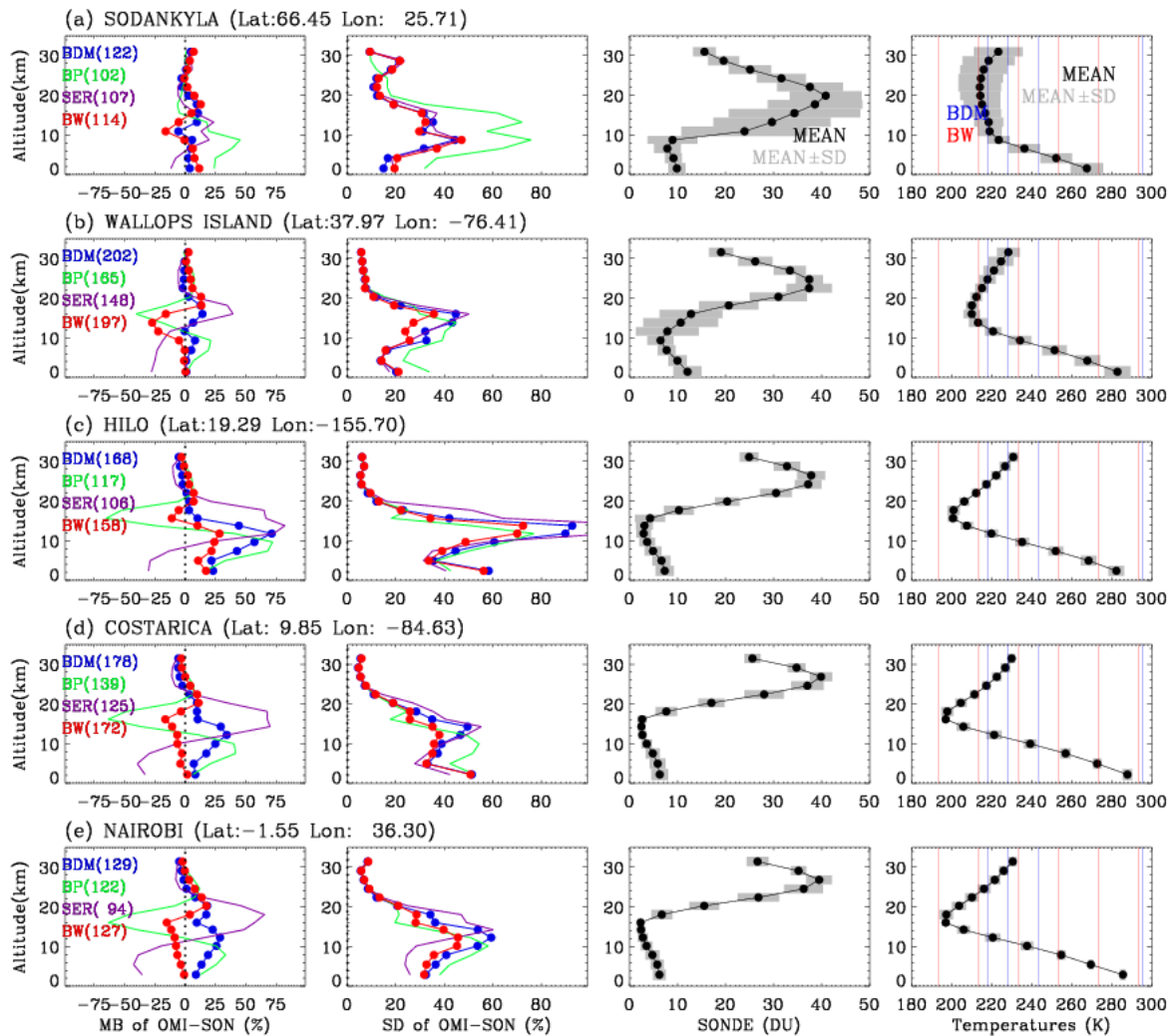


Figure 9.

C7. TEMPO is not the only mission that will critically depend on refined ozone spectral data. IASING and UVNS are another example of combining retrievals in different domains. In the discussion, the authors need to mention/cite other ongoing or future activities on the synergistic use of different spectral regions that rely on the 9.6 μm region and the Chappuis band, eg. Costantino et al. (2017) and/or others.
R7. Yes, there are many on-going projects requiring the advanced ozone spectral data. However, the ozone profile algorithm used in this paper is optimized to retrieve ozone profiles from OMI BUV measurements with the capability of processing GOME, OMPS, and GOME/2 measurements, commonly focusing on the Hartley and Huggins bands. Furthermore, the TEMPO ozone profile algorithm has been under development by extending this OMI algorithm from UV only to UV+Visible. There have been several studies including this paper to recommend the reference ozone spectral data for UV spectral fitting, but nothing for the Chappuis band. Therefore, in the last section of this paper we addressed the importance about evaluating the visible ozone cross-section datasets, focusing on the SER and BDM datasets, which is one of priorities in the development of the TEMPO ozone profile algorithm. In this context, we think that it is out of scope to address other missions employing the thermal IR.

2. Technical

C1. (L32) th → the

R1. It has been revised.

C2. (L95) indicate whether offset was assumed to be constant or wavelength dependent (for wavelength dependent offset specify dependence and range)

R2. The associated sentence has been revised for clarification from “Offset corrections were made for each of the 6 temperatures by fitting to the SER dataset” to “Offset corrections were made for each of the 6 temperatures by fitting to the SER dataset (constant for all wavelengths)”

C2. (L97) (<270.27 nm) > and → (<270.27 nm) and

C3. (L106) temperatures → temperature

C4. (L107) Should use terms $(T - 273.15K)$ and $(T - 273.15K)^2$ including the unit of K in eq. (1).

C5. (L170) 0.015 in UV1 → 0.015nm in UV1

C6. (L254) BW data show systematic biases of 2-3% in C_0 → BW data show systematic biases of 2-3% in the cross section at 0°C (C_0)

C7. (L255) The difference in C1 and C2 implies distinctly different → The differences in C1 and C2 imply a distinctly different

C8. (L268) 200K → 200 K

C9. (L355) list all author names

C10. (L364) J. Quant. Spectrosc. Ra. → J. Quant. Spectrosc. Radiat. Transfer

R2-R10. We accepted all these suggestions.

C11 (p. 15) Panels (a) - (c) should use logarithmic scales for the coefficients as BDM and BW curves are indistinguishable from 0 at wavelengths ≥ 325 nm.

R12. We revised Figure 2 to use logarithmic scales in y-axis.

C12 (p. 16) Legend to Figure 3 should contain hint on the factor of five different scales used in panels (a) and (b).

R12. In caption, it was detailed like “In the legend, the temperatures not covered by each dataset are indicated with gray and black, for values beyond lower and upper boundaries, respectively”, but we added “ $T > T_{\max}^{\text{BDM}}$ $T < T_{\min}^{\text{BDM}}$ ” in Fig. 3 a and “ $T > T_{\max}^{\text{BW}}$ $T < T_{\min}^{\text{BW}}$ ” in Fig. 3. b according to this comment.

C13 (p. 17) Legend to Figure 5 should better describe what is on the plot.

R13. For clarification, the caption has been revised like “The impact of parameterizing the cross-sections shown in Figure 3 on ozone profile retrievals, for (a) BDM and (b) BW, as a function of solar zenith angle (SZA). The differences of retrieved ozone profiles are assessed in absolute (left panels) and relative (right panels) units, respectively.”

C14 (p. 19) & 22 Degree symbol $^\circ$ before K in x-axis legend of Figure 9 needs to be deleted. The same holds for the lower colour legend in Figure 7.

R14. $^\circ\text{K}$ has been corrected to K in indicated figures.

C15 (p. 21) Annotations MB and $MB \pm SD$ in upper right panel are misleading (there is no mean bias in the temperature plot). The 294 K temperature line for the BDM temperature point is drawn differently (thicker, other colour) than the other temperature lines.

R15. This figure has been replotted after correcting indicated annotations and line.