

A point-by-point response to the reviews

Response to the first reviewer's comments

General comments:

This manuscript, AMT-2020-94, reports the evaluation of new O₃ xsec data sets (labeled as “BW”) measured in the Hartley and Huggins bands for the use of O₃ profile retrieval from OMI observations. The BW data sets were modeled by using a polynomial in a function of temperature in order to facilitate direct comparison with the current reference data set (“BDM”) and their application to the O₃ profile retrieval. They have found that the new data set, BW, shows a better performance in the retrieval of O₃ profile in terms of less oscillatory features in the retrieved profile and better agreement with the ozonesonde data. We found the manuscript written in a nice and compact manner; the presentation looks consistent. However, we are not convinced that we can agree with the authors' the interpretation of what is described in Sec. 2, which will be detailed below.

This manuscript has shown well that the new dataset, BW, is better than the BDM in the O₃ profile retrievals primarily because of their wider temperature coverage, esp. going down to 194 K critical to the retrievals in the transition layers (UTLS), which was not covered by the BDM dataset in temperature. Therefore, the conclusion of this work has been supported by the results presented in the manuscript. The topics of this paper highly relevant to the scope of AMT, so that we recommend a publication of this manuscript to AMT with a revision or a further clarification
Sec. 2. Specific comments and suggestions follow.

Responses to general comments

We would like to thank this reviewer for the constructive comments. We did our best to sincerely reply to 4 comments made by this reviewer.

Specific comments

C1. The authors wrote “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”. Does this mean that the BW xsec was normalized to that of SER. Clarify what the correction factors were and how (and what wavelengths) they were determined. Was this offset considered in the error budgets?

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, 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 offset uncertainty was determined from the standard deviation of the fit multiplied with chi since the residuals were not purely noise. The offset uncertainty was $1e-24$ cm²/molec, which is negligible. We think that this discussion is beyond the scope of this paper, which is not intended, for developing/introducing this spectroscopic data, but for applying this dataset on our retrievals. The related discussion will be addressed in a separate paper lead by the author of this dataset, Manfred Birk.

45 **C2.** Author wrote, “After offset correction polynomials of 1st order (<270.27 nm) and 2nd order (>270.27
46 nm) in temperature were fitted for each spectral point to improve the statistical uncertainty” and followed
47 by “Measured cross-sections are typically parameterized quadratically to be applied conveniently at any
48 atmospheric temperatures” using the following equation: $C = C_0 + C_1(T - 273.15) - C_2(T - 273.15)^2$.
49

50 **C2-1.** The agreement between the original data and the fitted data should be inspected or discussed for each
51 of the two data sets, BW and BDM, and discussed. Besides, direct comparison of their original data sets
52 between BW and BDM (prior to having them fitted to the polynomial), which may be done at T = 273 and
53 295 K provided that their temperature differences, $\Delta = 0.5$ and 0.7K, respectively, is insignificant, which
54 seems true because the authors argued the dominant coefficient C0 is almost independent of temperature.
55

56 **R2-1.** As mentioned in Section 2, the temperature correction has already been applied in the BW dataset
57 available to the public. This paper is devoted to atmospheric validation of the BW dataset, rather than
58 presenting the data det itself. We think that it is out of scope to give a detailed evaluation for the original
59 BW dataset where either offset and temperature correction is turn off because it is not officially published.
60 The detailed views on the original/corrected BW dataset will be provided in another paper written by Birk
61 and Wagner. In the ozone profile algorithm the cross sections parameterized using this quadratic equation
62 are typically used to represent the dependence of cross-section on the atmospheric temperature vertically
63 rather than the interpolated spectrum from original measurements. Therefore, this paper focused on
64 comparing coefficients and the parameterized cross-sections between BDM and BW datasets.
65

66 **C2-2.** We are not sure how well the Eq. (1) could have captured the temperature dependence of the xsec.
67 The xsec can be represented by integrated (line) intensities for the given frequency (wavelength) grid, and
68 the temperature dependence of the line intensities can be modeled by two
69 parameters, i.e., partition function (which we know well for O3) and the lower state energies (which we do
70 not know for the features of this work). Thus, one can simulate the intensity ratio to that at 296 K at various
71 temperature for a few representative cases of the lower state energies, as shown in Fig. X below. As we see,
72 Fig. X is similar to the right panel of Fig. 1, except for one thing that each curve in Fig. X represents
73 different values of the lower state energies, not the wavelength presented in Fig. 1. There is a possibility of
74 having the sampled wavelengths (such as 280, 290,..., in nm) possessing progressively higher value of their
75 (effective) lower state energies more appropriate to assume that each curve in Fig. 1 corresponds to a
76 different of multiple transitions falling into the particular wavelength data point grid (for instance,
77 280nm±resolution element). This point should be addressed properly to keep naive readers from being
78 misled to think the temperature dependences in Fig. 1 is attributed to the wavelengths.
79

80 **R2-2.** The quadratic equation was first found to represent well the temperature dependence of ozone cross
81 sections in the UV [Paur and Bass, 1985] and has now become the standard approach [Liu et al., 2007;2013;
82 Chehade et al., 2013a,b; Serdyuchenko et al., 2014]. In addition, Fig. X (this reviewer plotted) and Fig. 1
83 in this paper commonly imply that the dependence of the cross-section on the temperature tends to be linear
84 at shorter wavelengths and slightly non-linear at longer UV wavelengths. Therefore, the quadratic (2nd)
85 polynomials seem to be adequately fit the cross-section measurements. In revised manuscript, this
86 discussion has been better specified by adding “This quadratic equation was first found to represent well
87 the temperature dependence of ozone cross section in the UV (Paur and Bass, 1985) and has now become
88 the standard approach (Liu et al., 2007; 2013; Chehade et al., 2013a;2013b; Serdyuchenko et al., 2014)”
89 after the equation 1.

90 The approach suggested by the reviewers is somewhat similar to pseudolines that is sometimes employed
91 in the parametrizing the IR cross-sections, where temperature and pressure-dependent cross-sections are fit
92 to a HITRAN-like line list where “transitions” do not have quantum mechanical meaning but do reproduce
93 cross-sections. However, this approach is a lot more sophisticated than suggested by the reviewers because

94 there are more than one transitions (with different intensities and lower state energies) that underlie
 95 absorption at selected wavelength. This very non-trivial and intense task has never been applied to the
 96 electronic spectra yet.

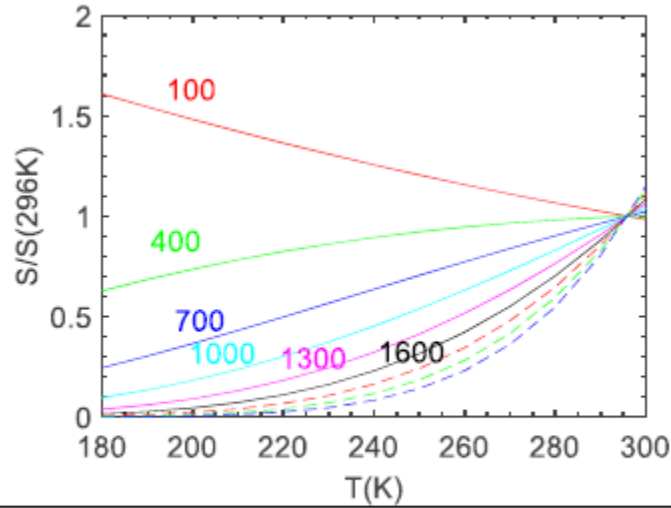


Fig. X $S/S(296K)$ vs. T at a given $E''(\text{cm}^{-1})$
 $= [100, 400, 700, 1000, 1300, \text{etc.}]$

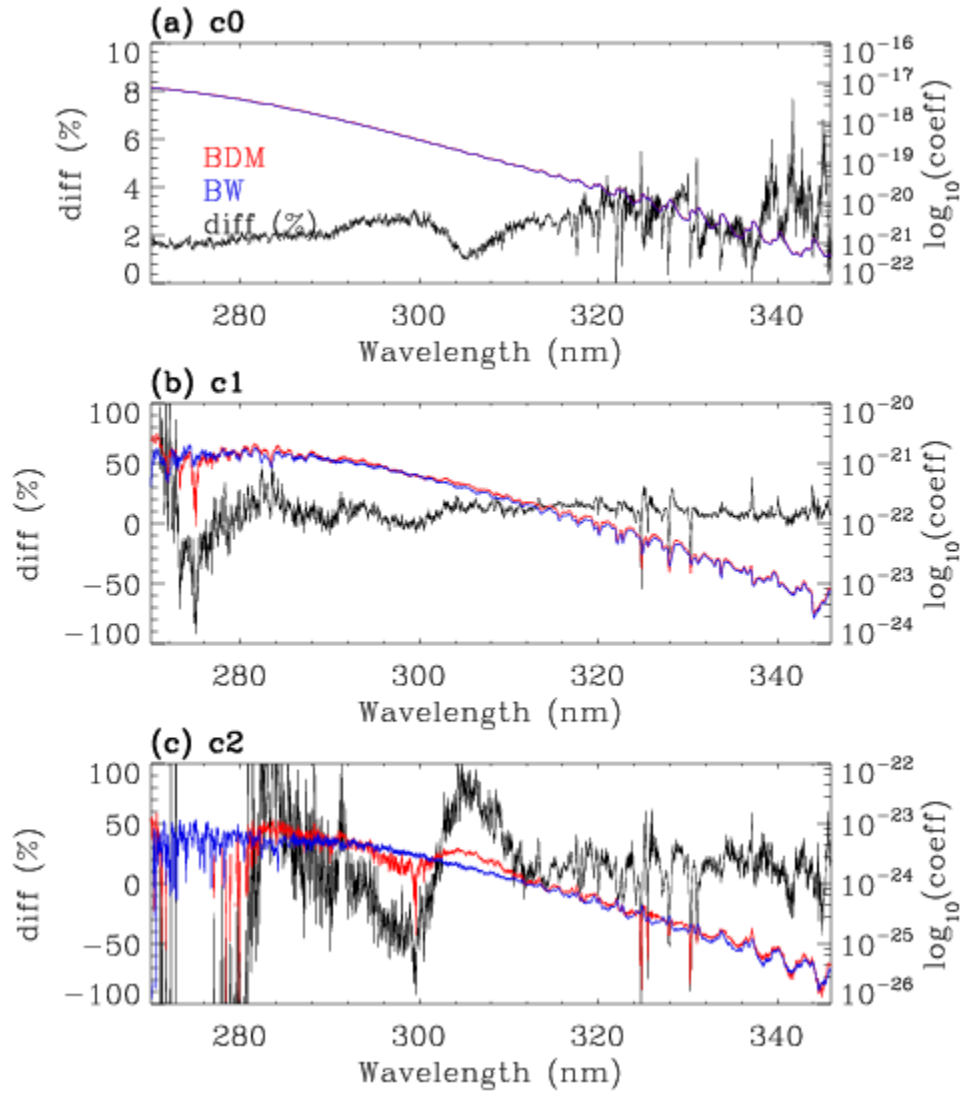
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 98

99 **C2-3** For the same reason, Fig. 2 is hard to interpret. The respective comparison of the C1 and C2 for two
 100 different data set as a function of nm could be legitimate only when the two data sets are measured at the
 101 same resolution because the effective lower state energies mentioned above would be the same. Therefore,
 102 the non-wavy feature of C2 for the BW data set would have more to do with the outcome of the resolution
 103 choice in the representation by Eq.(1), rather than it is telling the BW data set is superior to the BDM dataset
 104 in the temperature consistency. In other words, Fig. 2 shows which data set is better represented by Eq. 1
 105 rather than which data is closer to the truth. This section may stay, but with a specific statement, being
 106 provided for the readers on the point made above. The bottom line is that the BW data set is better than the
 107 BDM set because of the broader coverage of the measurement temperature, especially covering the
 108 temperature critical to UTLS layers, as was properly concluded by the authors in the manuscript.

109

110 **R2-3.** We agree with this comment; it could be not straightforward to compare the coefficients especially
 111 C1 and C2 derived from BDM and BW, respectively, due to different spectral resolutions and the strong
 112 correlation between C1 and C2 especially when the temperature dependence is weak. However, important
 113 insights are obtained from this figure; the comparison of C_0 indicates systematic biases between two
 114 datasets, by 2 % on average, with some spikes of up to 8 % at longer UV wavelengths above 315 nm mainly
 115 due to the different spectral resolution. The C_1/C_2 characterizes the linear/non-linear dependence of the
 116 cross-sections. As shown in Figure 3.c, the quadratic temperature dependence show different behaviors in
 117 290-310 nm, which is significantly correlated with the comparison of cross-section spectrum shown in
 118 Figure 4.

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120 Revised Figure 4.
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Response to the second reviewer's comments

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); Gorshchev et al. (2014)) was less suited for ozone retrievals using the OMI-spectrometer than the BDM data, despite a similar spectral resolution (0.01nm – 0.018nm for the 210 – 350nm 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.

177 **C2.** In the introduction, the authors give the impression that new cross sections should be measured at a
178 resolution of 0.01nm or better. This contradicts the use of new cross section data that have been obtained
179 at about 3 (> 285.7 nm) to 5 (< 285.7 nm) times lower resolution (see description of BW data set in section
180 2).

181 The spectral resolution requirement is from Orphal et al. (2016): ozone cross-sections should be measured
182 at high spectral resolutions (typically 0.01 nm in the ultraviolet-visible). So the citation of “a resolution of
183 0.01 nm or better” is not accurate and is probably confused with the wavelength calibration requirement
184 “the spectral wavelength) calibration must be very accurate, too (typically at least 0.01 nm). For the BW
185 dataset, measurements are performed at a coarser resolution to cover the broad spectral range as a tradeoff
186 or spectrally degraded in the post-processing to increase signal to noise ratio. Indeed, the spectral resolution
187 of 3.3 cm⁻¹ may have caused a very small deterioration of the highly resolved spectral features occurring
188 above 325 nm. The high resolution structures have only a very small contrast regarding the underlying
189 broad features. The impact is expected to be small, especially in view of the low resolution of the remote
190 sensing instruments.

191
192 **C3.** The authors use the terms Hartley and Huggins bands as well as OMI instrument windows to discuss
193 different spectral regions in the UV. While wavelength ranges for both of the OMI UV windows are
194 specified in the manuscript, no numbers are given for the Hartley and Huggins bands. Please indicate as
195 this would help readers to follow the discussion.

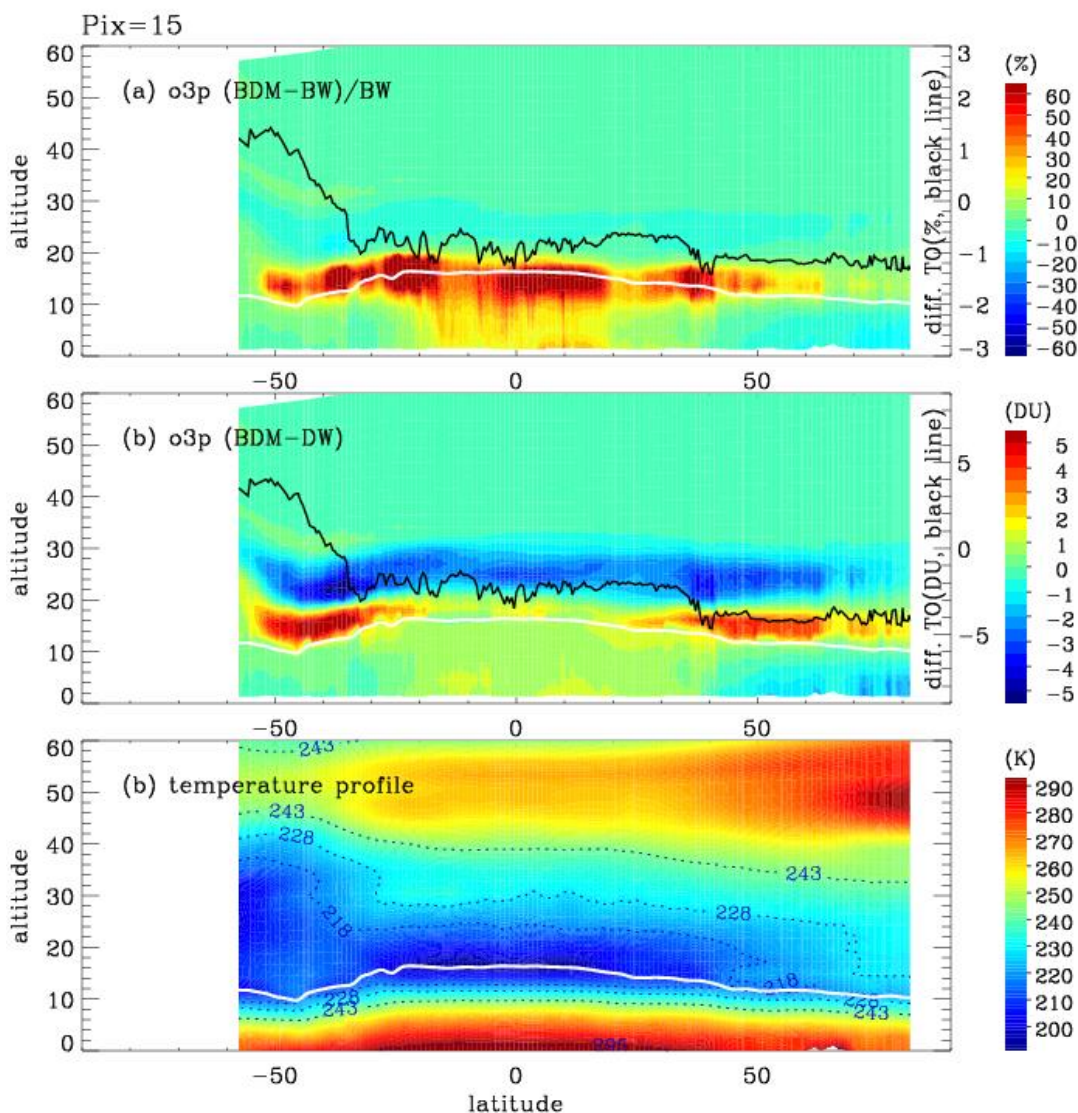
196 **R3.** We has specified the bands in the revised manuscript where these bands are first mentioned such as
197 “ C_0 values are similar to each other in the Hartley band (< 310 nm) with relative biases of 2-3%. However,
198 the Huggins band (> 310 nm) shows large spiky biases of up to 8%. C_1 and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

200
201 **C4.** There seem to be problems with the definitions of signs in some of the plots. For example, are the signs
202 in Figure 7 correct? I find that local negative spikes in the total ozone column difference (BDM-BW) also
203 correlate with cases where the tropospheric profile shows a tendency towards warmer colors (BDM > BW),
204 which would indicate that either of the two scales (total ozone (TOC) vs altitude dependent ozone) should
205 have a different sign. Another issue is the Antarctic +1%BDM-BW bias in the TOC. From Figure 4, one
206 would estimate that the cross section bias is positive when integrated all over the (270 – 346) nm wavelength
207 range (despite some few local negative spikes at low temperatures). This should result in a negative BDM-
208 BW bias of TOC. Anyway, the antarctic positive TOC bias needs to be discussed as compared to the lower
209 latitude value around -1% on the basis of the cross section data. In similar veins, the definition of the y-
210 axis of Figure 4 shows that the room temperature BW cross-section is negatively biased with respect to
211 BDM at low wavelengths. This is opposite to what is stated in line 254 of the manuscript (Relative to the
212 BDM data set, the BW data show systematic biases of 2–3% in C_0 at shorter wavelengths below 300 nm).

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

223 Figure 7 shows both relative and absolute differences of the retrieved ozone profiles with the corresponding
224 temperature profiles taken from the National Centers for Environmental Protection (NCEP) final (FNL)
225 operational global analysis data. Large differences of 20-50% commonly exist along the tropopause, where

226 the original BDM measurements could not cover atmospheric temperatures below 218 K (Fig. 7a). Some
 227 larger differences occur throughout the troposphere in the tropics likely due to the relative smaller retrieved
 228 partial ozone columns. The individual differences of retrieved ozone in the lower troposphere are $\sim 20\%$.
 229 However, the corresponding impact on the total column ozone, from integrating retrieved ozone profiles
 230 are overwhelmed by the stratospheric layers (20-30 km), as shown in Fig. 7b, where the ozone amount is
 231 relatively large and the dependence of ozone-cross sections on the temperature is still important. As a result,
 232 applying BDM causes an underestimation of total ozone except at the South Pole due to the biggest
 233 inconsistency of two cross-sections at the coldest temperature just above the tropopause in spite of smaller
 234 amount of ozone compared to upper stratospheric layers. The magnitude of this
 235 underestimation/overestimation is $\sim 1\%$, which is comparable to the overall accuracy ($\sim 1.5\%$) of the OMI
 236 operational total ozone product against ground-based measurements (McPeters et al., 2015).
 237



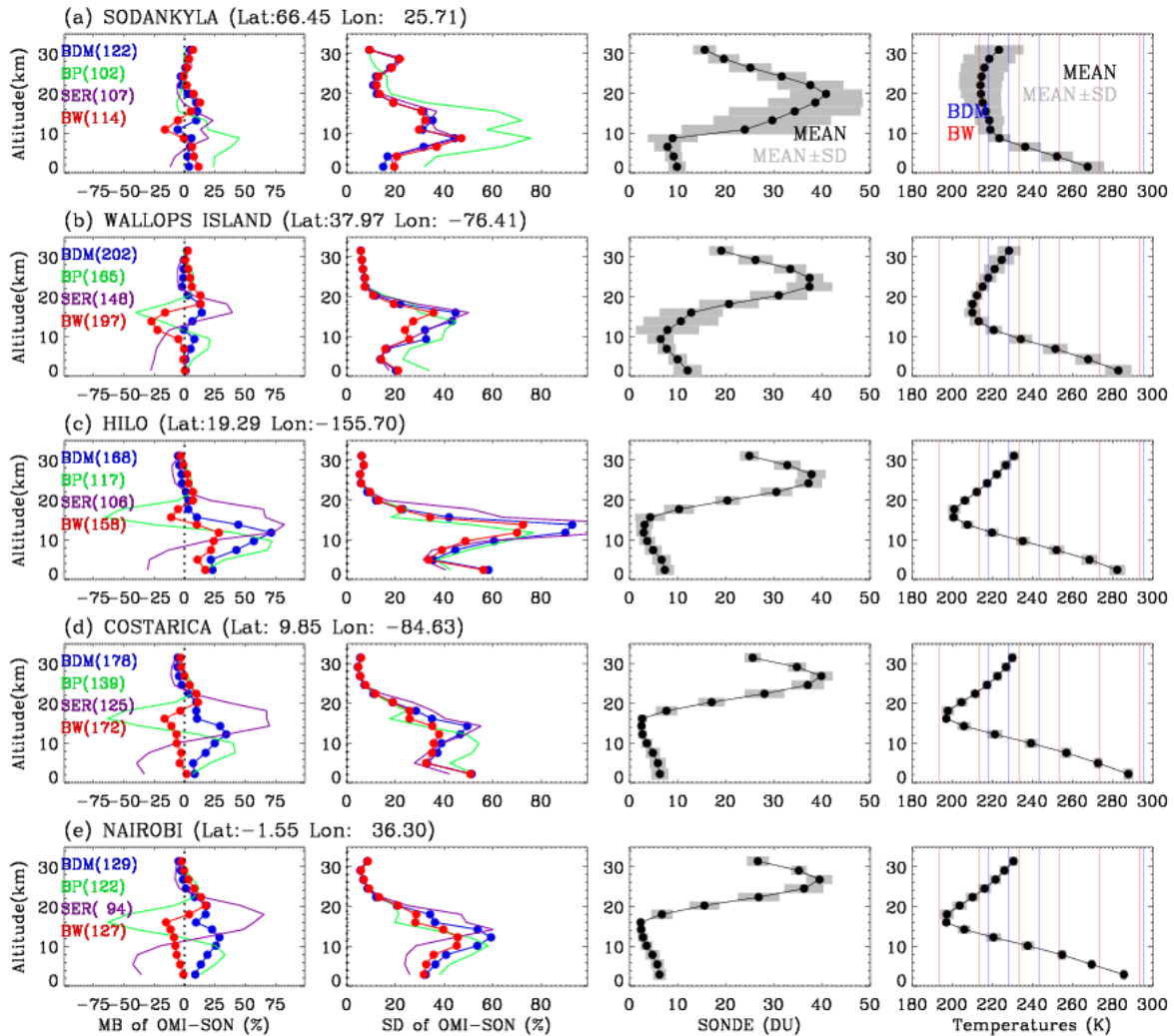
238
 239 **Figure 7 in the revised manuscript.**

240
 241

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

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

248
 249 **C6.** Fig. 9 shows the OMI mean biases with respect to a common reference (ozonesonde). It would be nice
 250 to plot the reference profiles (or mean profiles with their sdev) along with the bias percentages.
 251 **R6.** We have revised Figure 9, according to this comment. The revised figure is following:



252
 253 **Figure 9.**

254
 255
 256 **C7.** TEMPO is not the only mission that will critically depend on refined ozone spectral data. IASING and
 257 UVNS are another example of combining retrievals in different domains. In the discussion, the authors
 258 need to mention/cite other ongoing or future activities on the synergistic use of different spectral regions
 259 that rely on the 9.6 μm region and the Chappuis band, eg. Costantino et al. (2017) and/or others.

260 **R7.** Yes, there are many on-going projects requiring the advanced ozone spectral data. However, the ozone
261 profile algorithm used in this paper is optimized to retrieve ozone profiles from OMI BUV measurements
262 with the capability of processing GOME, OMPS, and GOME/2 measurements, commonly focusing on the
263 Hartley and Huggins bands. Furthermore, the TEMPO ozone profile algorithm has been under development
264 by extending this OMI algorithm from UV only to UV+Visible. There have been several studies including
265 this paper to recommend the reference ozone spectral data for UV spectral fitting, but nothing for the
266 Chappuis band. Therefore, in the last section of this paper we addressed the importance about evaluating
267 the visible ozone cross-section datasets, focusing on the SER and BDM datasets, which is one of priorities
268 in the development of the TEMPO ozone profile algorithm. In this context, we think that it is out of scope
269 to address other missions employing the thermal IR.

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271

272 **2. Technical**

273

274 **C1.** (L32) th → the

275 **R1.** It has been revised.

276

277 **C2.** (L95) indicate whether offset was assumed to be constant or wavelength dependent

278 (for wavelength dependent offset specify dependence and range)

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

282

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

284 **C3.** (L106) temperatures → temperature

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

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

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

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

291 **C8.** (L268) 200K → 200 K

292 **C9.** (L355) list all author names

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

294 **R2-R10.** We accepted all these suggestions.

295

296 **C11** (p. 15) Panels (a) - (c) should use logarithmic scales for the coefficients as BDM and

297 BW curves are indistinguishable from 0 at wavelengths ≥ 325 nm.

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

299

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

302 **R12.** In caption, it was detailed like “In the legend, the temperatures not covered by each dataset are
303 indicated with gray and black, for values beyond lower and upper boundaries, respectively”, but we added

304 “ $T > T_{\max}^{\text{BDM}}$ $T < T_{\min}^{\text{BDM}}$ ” in Fig. 3 a and “ $T > T_{\max}^{\text{BW}}$ $T < T_{\min}^{\text{BW}}$ ” in Fig. 3. b according to this comment.

305

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

307 **R13.** For clarification, the caption has been revised like “The impact of parameterizing the cross-sections
308 shown in Figure 3 on ozone profile retrievals, for (a) BDM and (b) BW, as a function of solar zenith angle

309 (SZA). The differences of retrieved ozone profiles are assessed in absolute (left panels) and relative (right
310 panels) units, respectively.”

311

312 **C14** (p. 19) & 22 Degree symbol ° before K in x-axis legend of Figure 9 needs to be deleted.

313 The same holds for the lower colour legend in Figure 7.

314 **R14.** °K has been corrected to K in indicated figures.

315

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

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

320

321

322 ● List of the revised figures : 2, 3, 7, 9, 10

323

324

325 **Impact of using a new ultraviolet ozone absorption cross-section** 326 **dataset on OMI ozone profile retrievals**

327

328 *Juseon Bak¹, Xiong Liu¹, Manfred Birk², Georg Wagner², Iouli E. Gordon¹, and Kelly Chance¹*

329 ¹*Harvard-Smithsonian Center for Astrophysics, Cambridge, MA, USA*

330 ²*Deutsches Zentrum für Luft- und Raumfahrt e.V. (DLR), Remote Sensing Technology Institute, Oberpfaffenhofen, D-*
331 *82234 Wessling, Germany*

332

Abstract

333 We evaluate different sets of high-resolution ozone absorption cross-section data for use in atmospheric
334 ozone profile measurements in the Hartley and Huggins bands with a particular focus on Brion-Daumont-
335 Malicet et al. (1995) (BDM), currently used in our retrievals, and a new laboratory dataset by Birk and
336 Wagner (BW) (2018). The BDM cross-section data have been recommended to use for retrieval of ozone
337 profiles using spaceborne nadir viewing Backscattered UltraViolet (BUV) measurements since its improved
338 performance was demonstrated against other cross-sections including Bass and Paur (1985) (BP) and those
339 of Serdyuchenko et al (2014) and Gorshelev et al. (2014) (SER) by the “Absorption Cross-Sections of
340 Ozone” (ACSO) activity. The BW laboratory data were recently measured within the framework of
341 the _ESA project SEOM-IAS (Scientific Exploitation of Operational Missions - Improved Atmospheric

342 Spectroscopy Databases) to provide an advanced absorption cross-section database. The BW cross-sections
343 are made from measurements at more temperatures and in a wider temperature range than BDM, especially
344 for low temperatures. ~~Compared to~~ Relative differences of cross-sections between –BW, and BDM cross-
345 sections are positively biased range from ~2 % at shorter UV wavelengths to ~5 % at longer UV wavelengths
346 at warm temperatures. Furthermore, these biases-differences dynamically increase by up to ± 40 % at cold
347 temperatures due to no BDM measurements having been made below 218 K. We evaluate the impact of
348 using different cross-sections on ozone profile retrievals from Ozone Monitoring Instrument (OMI)
349 measurements. Correspondingly, this impact leads to significant differences in individual ozone retrievals,
350 by up to 50 % in the tropopause where the coldest atmospheric temperatures are observed. Bottom
351 atmospheric layers illustrate the significant change of the retrieved ozone values, with biases-differences of
352 20 % in low latitudes, which is not the case in high latitudes because the ozone retrievals are mainly
353 controlled by a priori ozone information in high latitudes due to less photon penetration down to the lower
354 troposphere. Validation with ozonesonde observations demonstrates that BW and BDM retrievals show
355 altitude-dependent bias oscillations of similar magnitude relative to ozonesonde measurements, much
356 smaller than those of both BP and SER retrievals. However, compared to BDM, BW retrievals show
357 significant reduction in standard deviation, by up to 15 %, especially at the coldest atmospheric
358 temperatures. Such improvement is achieved mainly by the better characterization of the temperature
359 dependence of ozone absorption.

360 1. Introduction

361 Accurate knowledge of the absorption cross-sections of ozone and their temperature dependence is
362 essential for highly accurate measurements of atmospheric ozone (Orphal et al., 2016) as well as other trace
363 gases affected by the strong ozone absorption such as BrO, NO₂, SO₂, and CH₂O (e.g., Seo et al., 2019;
364 Theys et al., 2017). In the laboratory, measuring ozone cross-sections which can meet the high requirements
365 for accurate ozone profile measurements covering a wide spectral range (at least 270-340 nm) at high-
366 resolution (typically 0.01 nm) at a wide range of atmospheric temperatures (180-300 K) –is still
367 challenging ~~in covering a wide spectral range (at least 270-340 nm) at high resolution (at least typically 0.01~~
368 ~~nm) at a wide range of atmospheric temperatures (180-300 K)~~. The difficulties range from reactivity of
369 ozone to calibration standards. For instance, as discussed in the recent review by Hodges et al. (2019) the
370 accepted calibration of ozone cross-sections at the 254 nm mercury line (Hearn, 1961) was in need of
371 revision. In addition, simultaneous measurements of ozone in the microwave, infrared and ultraviolet
372 regions are subject to uncertainties due to systematic differences in the respective regions (~~cf. see discussion~~
373 ~~in~~ Birk et al. (2019) ~~and~~ Tyuterev et al. (2019) ~~for instance~~). The need to evaluate existing cross-sections

374 used for all atmospheric measurements of ozone and to make its recommendations initiated the “Absorption
375 Cross-Section of Ozone (ACSO) activity” that was established in 2008 and conducted in two phases (2009-
376 2011, 2013) (Orphal et al., 2016). The ACSO activity shows the need to continue laboratory ozone cross-
377 section measurements of highest quality.

378 Prior to ACSO activities, the available ultraviolet (UV) ozone-cross sections were thoroughly
379 reviewed by Orphal (2002, 2003) and as a result three datasets of ozone cross-sections were found to be in
380 agreement of 1-2 % with each other, including BP 1985 (Bass and Paur, 1985), BDM 1995 (Daumont et al.
381 1992; Brion et al., 1993; Malicet et al., 1995), and Global Ozone Monitoring Spectrometer (GOME) flight
382 model (Burrows et al., 1999) (GMFM). The BP dataset is no longer recommended for any atmospheric
383 ozone measurements (Orphal et al., 2016), but still used to keep the long-term consistency of ground-based
384 Dobson/Brewer total ozone records and spaceborne TOMS/OMI total ozone records (McPeters et al. 2015).
385 These cross-sections were also included in the 2004 edition of the HITRAN database (Rothman et al., 2005)
386 and remained unchanged in subsequent editions including HITRAN2016 (Gordon et al., 2017). Using
387 GMFM is restricted to GOME measurements because these cross-sections were measured at GOME
388 resolution (~0.2 nm). On the other hand, the high-resolution cross-sections of BDM were first applied by
389 Liu et al. (2005) for GOME ozone profile retrievals in the literature. In Liu et al. (2007), these three datasets
390 were thoroughly assessed to find the most suitable cross-sections for GOME ozone profile retrievals (290-
391 307 nm and 325-340 nm). As a result, they recommended using the BDM for ozone profile retrievals due
392 to much smaller fitting residuals and better agreement with ozonesonde measurements. Such improvement
393 is likely due to better spectral resolution and wavelength calibration of BDM than BP and GMFM. After
394 that, the recommendation of BDM for satellite ozone profile retrievals has been officially made by the
395 ACSO activities during the first phase (2009-2011) and the second phase (2013), respectively. The first
396 activity was focused on the intercomparison between BDM and BP, while the second activity was
397 additionally organized in response to the new publication of a high-resolution laboratory dataset covering
398 the temperature range of 193 to 293 K in 10 degree step by Serdyuchenko et al. (2014) and Gorshelev et al.
399 (2014) (abbreviated as SER). In the framework of the ACSO activity, Liu et al. (2013) evaluated the impact
400 of changing from BDM to SER on Ozone Monitoring Instrument (OMI) ozone profile retrievals (270-330
401 nm). The recommendation of the BDM was made again for use in ozone profile retrievals. Recently, a new
402 laboratory dataset was measured at the German Aerospace Center (DLR) within the framework of the ESA
403 project SEOM-IAS (Scientific Exploitation of Operational Missions - Improved Atmospheric Spectroscopy
404 Databases) in order to improve the atmospheric BUV retrievals from the TROPospheric Monitoring
405 Instrument (TROPOMI) on board the Sentinel 5-Precursor satellite (Birk and Wagner, 2018) (abbreviated
406 as BW). A publication with more details on [the](#) experiment and analysis is in preparation. [Here, we](#)~~This~~

407 ~~motivates us to~~ investigate if the current recommendation ~~could-should~~ be replaced with the BW dataset.
408 This work will also help making the decision on ~~what-which~~ cross-sections should replace BP measurements
409 in the HITRAN database.

410 This paper is organized as follows: Section 2 compares ~~the~~ quadratic coefficients in the parameterization
411 of temperature dependence and evaluates the parameterized cross-sections against interpolated ones.
412 Section 3 analyzes the differences in individual OMI retrievals due to different cross-sections, which are
413 evaluated against ozonesonde observations in Section 4. ~~Theis~~ paper is ~~finally~~ summarized and discussed
414 in Section 5.

415 2. Comparison of BDM and BW

416 The BW dataset is publicly available at <https://zenodo.org/record/1485588>, along with ~~some~~
417 experimental descriptions. A detailed publication is planned to describe the details of the experimental setup
418 and procedure so only a brief overview is given here. ~~The~~se cross-sections are given at six temperatures
419 (193, 203, 233, 253, 273, and 293 K) and at vacuum wavelengths in the spectral range 244 to 346 nm,
420 measured by means of Fourier-Transform Spectroscopy (FTS) at DLR at a spectral resolution of 3.3 cm⁻¹
421 (0.02-0.04 nm). A total of 191 measurements were recorded in two spectral ranges. Absorption cross-
422 sections were obtained at each temperature by means of a global least squares fit. Below 285.71 nm,
423 absorption cross-sections were smoothed to 7.7 cm⁻¹ (0.04-0.06 nm) resolution by convolving with a
424 Gaussian to reduce the noise. Offset corrections were made for each of the 6 temperatures by fitting to the
425 SER dataset ([constant for all wavelengths](#)) since it was measured at higher ozone column density and thus
426 considered more reliable regarding offset. After offset correction polynomials of 1st order (<270.27 nm)->
427 and 2nd order (>270.27 nm) in temperature were fitted for each spectral point to improve the statistical
428 uncertainty. The offset corrections have a minor effect on the cross-sections except for wavelengths above
429 ~330 nm. Figure 1.a illustrates BW measurements without polynomial fit in temperatures to be fairly
430 compared with BDM measurements (Fig. 1.b) with respect to the dependence of cross-sections on
431 wavelength and temperature. The BDM measurements are given at five temperatures (218, 228, 243, 273,
432 and 295 K) and at air wavelengths over the spectral range 195-519 nm with spectral resolution of 0.01-0.02
433 nm. Note that the wavelengths of these measurements are converted to vacuum wavelengths in Figure 1.b.
434 Measured cross-sections are typically parameterized quadratically to be applied conveniently at any
435 atmospheric temperatures using the following equation:

$$436 \quad C = C_0 + C_1(T - 273.15\text{K}) + C_2(T - 273.15\text{K})^2 \quad (1)$$

437 [This quadratic equation was first found to represent well the temperature dependence of ozone cross](#)

438 [section in the UV \(Paur and Bass, 1985\) and has now become the standard approach \(Liu et al., 2007; 2013;](#)
439 [Chehade et al., 2013a;2013b; Serdyuchenko et al., 2014\).](#) The non-linear least squares fitting [between](#)
440 [measured and parameterized spectrum used in this paper](#) converges typically within 3 iterations for both
441 BDM and BW. Measurements at 273 K are excluded for the BDM quadratic temperature fitting, according
442 to Liu et al. (2007). In Figure 2, the derived temperature dependent coefficients are illustrated, with their
443 relative differences. C_0 values are similar to each other in the Hartley band ([<310 nm](#)) with relative biases
444 of 2-3%. However, the Huggins band ([>310 nm](#)) shows large spiky biases of up to 8%. C_1 and C_2
445 represent linear and quadratic temperature dependences of absorption cross-sections, respectively. The
446 cross-sections in the Hartley band are almost independent of the temperature variation and thereby large
447 differences of these coefficients between two datasets are due the large correlation between C_1 and C_2
448 and are of minor importance to the parameterized cross-sections. However, the Huggins band shows the
449 distinctly different temperature dependence between [the](#) two cross-section datasets, especially for the
450 quadratic terms. For C_2 , the BW data show more monotonic wavelength dependence in the range 290-310
451 nm. Note that we determined that the parameterization schemes used in this work and Birk and Wagner
452 (2018) are very similar by the fact that no residuals remain when comparing BW cross-sections with these
453 two schemes (not shown here). Figure 3 compares the residuals of the fitted cross-sections relative to the
454 original measurements interpolated to many atmospheric temperatures using a spline scheme. The BDM
455 quadratic approximation has large positive residuals of up to 15 % for the temperatures ranging from 243
456 and 295 K due to insufficient sampling to account for the non-linearity of the temperature dependence,
457 especially for the longer UV wavelength range. Moreover, approximating the BDM cross-sections at
458 temperatures below 218 K results in errors of $\pm 5\%$ below 315 nm and up to $\pm 40\%$ above. Compared to
459 the BDM dataset, the parameterization of BW cross-sections results into significantly reduced residuals, of
460 0.25% below 320 nm and typically less than 2% at longer wavelengths if the temperature is within the
461 boundaries of the measurements. Residuals are within 5% even if the temperatures are out of the boundaries.
462 This demonstrates that the temperatures of BW measurements are well selected to characterize the
463 temperature dependence of ozone cross-sections, whereas [there are](#) cross-section errors due to the BDM
464 parameterization ~~exist~~. Figure 4 shows the direct comparison of parameterized cross-sections between
465 BDM and BW. The difference of cross-sections between BDM and BW are generally consistent with the
466 corresponding comparison of C_0 around 270 K. The differences at different temperatures are typically
467 within 2% for wavelengths below 310 nm except for several spikes around 276, 297, and 306 nm that are
468 correlated with the differences of C_2 . At wavelengths larger than 315 nm, the [inconsistency between BDM](#)
469 [and BW biases](#) shows large temperature dependence, with the [bias-differences range](#) increasing from $\sim 5\%$
470 at 315 nm to $\sim 20\%$ at 340 nm.

3. Impact of using different cross sections on ozone profile retrievals

OMI ozone profiles are retrieved at 24 layers from BUUV spectra for 270-309 nm in UV1 and 312-330 nm in UV2 using an optimal estimation technique (Liu et al. 2010). The ~~implemented~~ configurations ~~implemented~~ in this work are similar to those in Liu et al. (2013). One orbit of measurements on 1th July 2006 is used to see how our retrievals are changed due to using different cross-sections. Figure 5 shows the response of our retrievals to the parameterization errors shown in Figure 3 as functions of solar zenith angle (SZA). Compared to the BDM, the ozone retrievals are almost independent of the BW parameterization errors, with individual differences of 2-3% below 20 km and ~0% above. The differences of the BDM cross-sections with and without the parameterization are -5 to 15% in the lower troposphere at smaller SZAs and up to $\pm 20\%$ around 10 km at higher SZAs. The UV photon penetration down to the lower atmosphere decreases with SZAs increasing and thereby tropospheric ozone retrievals become insensitive due to cross-section errors at high SZAs, while a priori ozone information becomes more important to the retrieval. Figures 6-8 show the retrieval differences when parameterized BW and BDM cross-sections are implemented, respectively. To evaluate the different implementations, both fitting and retrieval accuracies are assessed. However, it is very hard to see large differences in fitting residuals at ~~the~~ final iteration compared to differences ~~on~~ of the retrieved elements of the state vector because the algorithm iteratively updates the state vector toward minimizing the differences in the spectral residuals. The fitting residuals are comparable at final iteration when applying BW and BDM dataset as shown in Figure 6.a except for noticeable smaller residuals ~~in~~ for 310-320 nm. However, we can find ~~the~~ distinct changes in the mean residuals of measured radiance to simulated radiance at ~~the~~ initial iteration, mainly over the wavelength range ~~of~~ 290 to 315 nm, up to 5 % as shown in Figure 6.b. On the other hand, Liu et al. (2007, 2013) demonstrated the distinct change of final fitting residuals when changing BDM to BP and GMFM, implying that using BW dataset improves fitting accuracies over using BP and GMFM, but produces similar fitting accuracies to using BDM and SER. ~~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-D~~ 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 relatively smaller retrieved partial ozone columns. The individual differences of retrieved ozone in the lower troposphere are ~ 20%. However, the corresponding impact on the total column ozone, from integrating retrieved ozone profiles areis 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. Corresponding differences of total column ozone, from

504 ~~integrating retrieved ozone profiles, are also presented by the black line in Fig. 7a. As a result, Applying~~
505 ~~applying~~ BDM causes an underestimation of total ozone except at the South Pole due to the biggest
506 inconsistency of two cross-sections at the coldest temperature just above the tropopause in spite of smaller
507 amount of ozone compared to upper stratospheric layers, despite the overestimation being prominent for
508 the individual layer columns in the troposphere. The magnitude of this underestimation/overestimation is
509 $\sim 1\%$, which is comparable to the overall accuracy ($\sim 1.5\%$) of the OMI operational total ozone product
510 against ground-based measurements (McPeters et al., 2015). The wavelength shifts between ozone cross-
511 sections and radiances are iteratively and simultaneously fitted with ozone for their respective UV1 and
512 UV2 channels. Figure 8 compares how the wavelengths of different cross-sections are adjusted in each
513 fitting window at nadir view. According to Schenkeveld et al. (2017), wavelength errors of OMI radiances
514 are expected to be ~ 0.002 nm in UV2 and ~ 0.015 nm in UV1. The fitted wavelength shifts fall in the ranges
515 of the OMI wavelength accuracy. Compared to the BDM, the BW dataset has the relative shifts of ~ 0.002
516 nm in the UV2. The mean shifts in the UV1 are comparable, 0.0087 nm and 0.0081 nm for BDM and BW,
517 respectively, whereas the variance of the fitted shifts over the latitude is reduced with the use of BW dataset
518 as the shifts are more stable south of 30°S . On the other hand, Liu et al. (2013) shows that the relative shifts
519 between SER and BDM are ~ 0.007 nm in both UV1 and UV2, and BP shifts vary largely with latitude by
520 up to 0.01 nm. These results indirectly demonstrate the similarity of the wavelength calibration quality
521 between BDM and BW measurements.

522

523 **4. Validation with ozonesonde observations**

524 Ozonesonde measurements at five stations during the period 2005 to 2008 are used to evaluate the
525 retrieval accuracy of ozone profile retrievals using different cross-sections. In addition to the currently used
526 BDM and the new BW datasets, BP and SER previously assessed in Liu et al. (2013) are included in this
527 evaluation. Typically, high-resolution vertical structures of ozonesonde profiles (~ 100 m) are degraded to
528 OMI resolution (6-10 km in the stratosphere, 10-15 km in the troposphere) using retrieval averaging kernels
529 to eliminate the effect of OMI smoothing errors (80% of total retrieval errors in the lower stratosphere and
530 troposphere) in comparison with ozonesondes; as a result, the standard deviations of comparisons are
531 typically reduced by a factor of 2 in the troposphere and lower stratosphere while the comparisons of mean
532 biases are less impacted by using OMI smoothing errors or not. In this paper, the conclusion on which cross-
533 section data should be used stays the same no matter whether ozonesonde profiles are vertically smoothed
534 or not, so we present validation results only using original ozonesonde measurements. In Figure 9, mean
535 biases of the retrieved ozone profiles relative to ozonesondes and the corresponding standard deviations are
536 presented at each station, arranged by-in latitude from north to south, together with corresponding

537 [ozonesonde ozone profiles and](#) temperature profiles.

538 In layers above ~20 km, a negligible impact of using different cross-sections is found because the
539 measurement information comes mainly from the Hartley ozone absorption band with little dependence on
540 temperature variation. Both BP and SER measurements provide a wider temperature range and more
541 samplings than BDM, but switching from BDM to BP / SER results in large altitude-dependent oscillations
542 of mean biases below ~20 km and noticeably fewer successful retrievals, consistent with Liu et al. (2013).
543 These oscillations tend to be wider with the minimum atmospheric temperatures decreasing such that the
544 mean biases increase $\pm 50\%$ at mid/high latitudes (210-215 K) to $\pm 70\%$ at low latitudes (200-205 K), which
545 is partly due to smaller ozone concentration in the tropics and hence the larger relative differences. This
546 result implies a defect in accounting for the temperature dependence in both the BP/SER cross-section
547 datasets, especially in the lower temperature range. Using BDM and BW cross-sections generally show
548 much smaller altitude-dependent oscillations of mean biases. The magnitudes of the biases are smaller for
549 BDM for the two middle/high latitude stations, but smaller for BW at the other, lower latitude stations. The
550 BW retrievals typically show negative biases of up to 30% relative to BDM retrievals. The number of
551 successful BW retrievals is slightly smaller than that of BDM retrievals because the negative biases cause
552 more occurrences of negative ozone so that the retrieval convergence is more difficult. It is difficult to
553 determine which one is better for ozone profile retrievals from the mean biases as OMI radiances contain
554 systematic radiometric calibration errors (Liu et al., 2010) and ozonesonde observations can also contain
555 systematic measurement errors (Liu et al., 2006).

556 As seen from the comparison of standard deviations in the middle panels, the use of BW consistently
557 gives significantly smaller standard deviations, by 5-20% in the lower stratosphere and upper troposphere
558 except for the high latitude station, Sodankyla. BW, BDM, and SER retrievals show similar standard
559 deviations at this station probably due to relatively warmer temperature, ~210-220 K in this altitude range.
560 In Figure 10, individual differences of layer column ozone between OMI retrievals and ozonesondes using
561 BDM and BW datasets are plotted as a function of temperatures for 8 layers below ~20 km. In this
562 comparison, the noticeable reduction of the scatter between OMI and ozonesonde, by 5-15% at layers from
563 17 to 8.5 km as well as by a few % below or above them, after applying BW cross-sections is further evident.
564 Improvements of the retrieval precision corresponding to standard deviations have been less often
565 achieved than those of the retrieval accuracy corresponding to mean biases; for examples, systematic errors
566 in ozone profile retrievals could be reduced by accounting for polar mesospheric clouds (Bak et al. 2016)
567 and slit function errors (Bak et al. 2019) as well as applying empirical calibration (Bak et al. 2017) whereas
568 the reduction of the standard deviations was achieved only in Bak et al. (2013) by better representing

569 dynamically induced ozone variability in the a priori ozone. This significant improvement in standard
570 deviations indicates that temperature dependence is better characterized at the lower temperatures near
571 ~200K by the BW dataset.

572

573 **5. Summary and discussion**

574 This paper evaluates the recently measured laboratory high-resolution BW (2018) ozone cross-section
575 data within the framework of the ESA project SEOM-IAS to see whether or not the current recommendation
576 ~~could~~should be changed for improving ozone profile retrievals from UV measurements. The BDM (1993)
577 dataset has been regarded as the standard ozone absorption cross-section in space-based ozone profile
578 retrievals from BUUV measurements: thereby we focused on comparing BW and BDM datasets and their
579 impact on our ozone profile retrievals from OMI BUUV measurements. Compared to BDM, given at 5
580 temperatures ranging from 218 to 295 K, the BW dataset provides improved temperature coverage of 193
581 to 293 K, every 20 K. To conveniently apply the cross-section measurements at any temperature, we
582 quadratically parameterized its temperature dependence using iterative non-linear least squares fitting. The
583 273 K measurements are excluded in the BDM parameterization to improve the fitting residuals at other
584 temperatures. However, the BDM parameterization causes increasing biases-fitting residuals in approximate
585 cross-sections at lower temperatures using their 243 and 218 K measurements, especially at longer
586 wavelengths in the Huggins band (up to 20%). It reveals serious errors of up to $\pm 40\%$ in representing the
587 values at lower temperatures out of the BDM measurements. In comparison, the BW approximation is very
588 closely parameterized to the original data, typically within 2%, while most of the atmospheric temperatures
589 are covered by the BW dataset; the biases-residuals increase to $\pm 5\%$ at temperatures below 195 K.
590 Correspondingly, individual ozone profile retrievals show less sensitivity ~~due to~~to the BW parameterization
591 errors, with biases-differences of $\sim 2\%$ or less over the altitude range. On the other hand, using the
592 parameterized BDM causes biases-an overestimation of 5-10% at bottom layers in the low latitudes and 10-
593 20% at the tropopause. Relative to the BDM dataset, the BW data show systematic biases-differences of 2-
594 3% in the cross section at $\theta \approx 273\text{K}$ (C_o) at shorter wavelengths below 300 nm, but larger spikey biases
595 differences of up to 8% at wavelengths longer than 315 nm. The differences in C_1 and C_2 ~~implies-imply~~
596 a distinctly different temperature dependence especially in non-linearity in the Huggins bands. We then
597 compared ozone profile retrievals from one orbit of OMI measurements with BW and BDM cross-section
598 datasets. Using different datasets gives comparable results in the wavelength shifts of cross-sections relative
599 to OMI radiance wavelengths and fitting residuals at the final iteration, respectively. However, the initial

600 iteration gives ~5% differences in fitting residuals near 290-315 nm, which results in significant differences
601 of the adjusted ozone profiles at the final iteration, ~50% at the tropopause across most latitudes and ~20%
602 at the bottom layers in the low-latitudes. To evaluate the quality of ozone retrievals, ozonesonde
603 measurements are compared at five stations. In this validation, we include other cross-section datasets, BP
604 (1985) and SER (2014). Compared to the large vertical oscillation of mean biases for OMI ozone profiles
605 using BP and SER, the BW retrievals show mean biases comparable to or sometimes improved over the
606 BDM retrievals. The most important improvement due to switching from BDM to BW is the significant
607 reduction of the standard deviations, by up to 15% in the lower stratosphere and upper troposphere where
608 atmospheric temperatures are lower than ~200_K.

609 Based on this evaluation, switching our ozone absorption cross-section reference from BDM to BW is
610 very promising for OMI ozone profile retrievals. However, in this evaluation soft calibration is turned off
611 and thereby the final decision on our algorithm will be made after further evaluating our retrievals with
612 BW-based soft calibration. In order to make a robust recommendation it might be useful for the ACSO
613 committee to organize another activity to assess the impact of applying this new dataset on other ozone
614 measurements on column ozone or profiles from various platforms. The results of this work in addition to
615 that of Orphal et al. (2016) will help the HITRAN committee to decide which cross-sections should be
616 included in HITRAN2020 edition.

617 Using different ozone cross-sections could also cause an important change in SO₂ retrievals fitted in the
618 Huggins band and therefore ~~the~~ the impact of applying both ozone and SO₂ cross-sections available from the
619 BW datasets (<https://zenodo.org/record/1492582>) should be evaluated. However, the spectral coverage of
620 the BW dataset is insufficient for the spectral fitting of other trace gases such as BrO and HCHO, both of
621 which have significant interference ~~with~~ ~~from~~ ozone. Ozone cross-sections in other wavelength ranges,
622 such as the mid-infrared region near 9.6 μm and the Chappuis band (400-650 nm), have not been thoroughly
623 evaluated in the literature. The ozone profile algorithm used in this work will be implemented for the
624 Tropospheric Emissions: Monitoring of Pollution (TEMPO) satellite combining the UV and visible
625 measurements to improve the detection of boundary layer ozone. Therefore we should extend this work to
626 find the most suitable ozone cross-sections in the TEMPO visible ozone channel (540-740 nm), focusing
627 on SER 2014 covering from 213 to 1100 nm (193-293 K in 10K steps) and that of Brion et al. (1998) which
628 provides measurements at 218 and 295 K from ~520 nm to ~650 nm. Moreover, the need to improve wide
629 spectral range laboratory cross-section measurements of ozone is still required to advance atmospheric
630 ozone and other trace gases measurements.

631 ***Author contributions.*** JB and XL designed the research; MB, GW, and IG contributed to oversight and guidance

632 for ozone cross-sections; JB conducted the research and wrote the paper; XL and KC contributed to analysis and
633 writing.

634 **Competing interests.** The authors declare that they have no conflicts of interest.

635
636 **Data availability.** The BW cross-section dataset is available at <https://zenodo.org/record/1485588>. OMI
637 Level1b radiance datasets are available at https://aura.gesdisc.eosdis.nasa.gov/data/Aura_OMI_Level1/
638 (last access: 31 Nov 2019). The ozonesonde data used to validate our ozone profile retrievals were obtained
639 through the WOUDC and SHADOZ. The WOUDC dataset is available at
640 <https://woudc.org/data/products/ozonesonde/> (last access: 31 Nov 2019) and for the SHADOZ dataset at
641 <https://tropo.gsfc.nasa.gov/shadoz/Archive.html> (last access: 31 Nov 2019).

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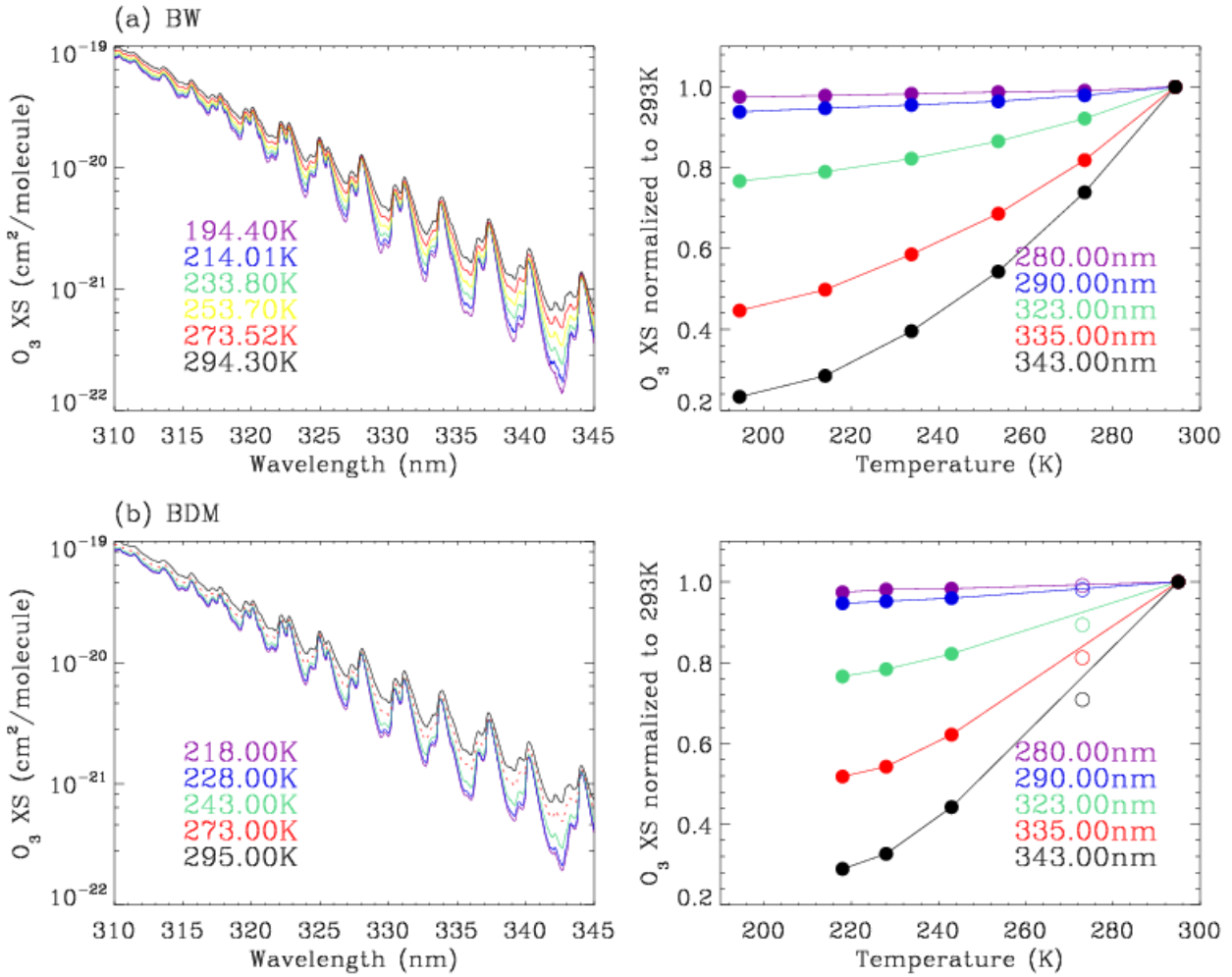
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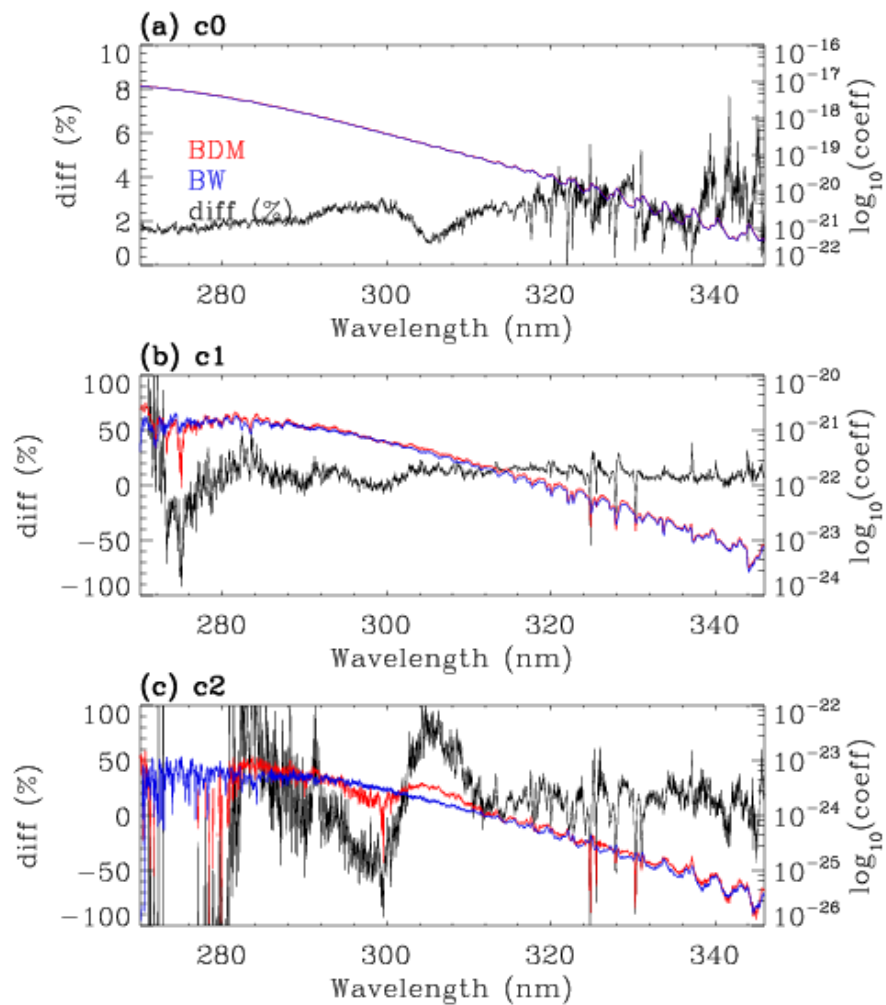


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 762 **Figure 1. (Left) Measurements of ozone absorption cross-sections at all selected temperatures in**
 763 **the Huggins bands taken from (a) BW (2018) and (b) BDM (1995), respectively. (Right) For BW,**
 764 **the experimental data are plotted without the quadratic parameterization for a fair comparison**
 765 **with BDM. BDM measurements at 273 K are plotted with a dotted line on the left and with open**
 766 **circles on the right, because the data at this temperature are not recommended for use, by Liu et**
 767 **al. (2007).**

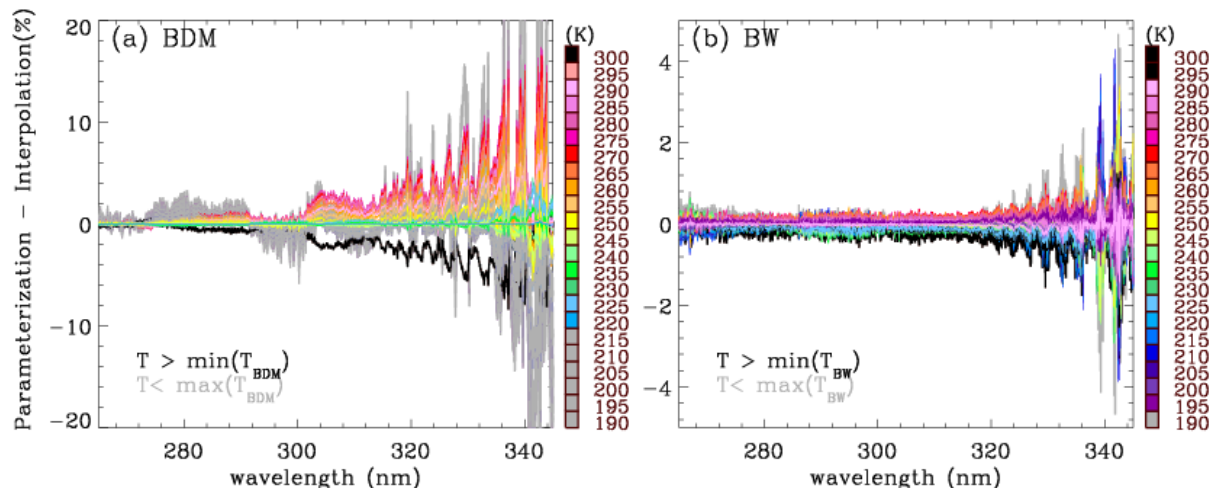
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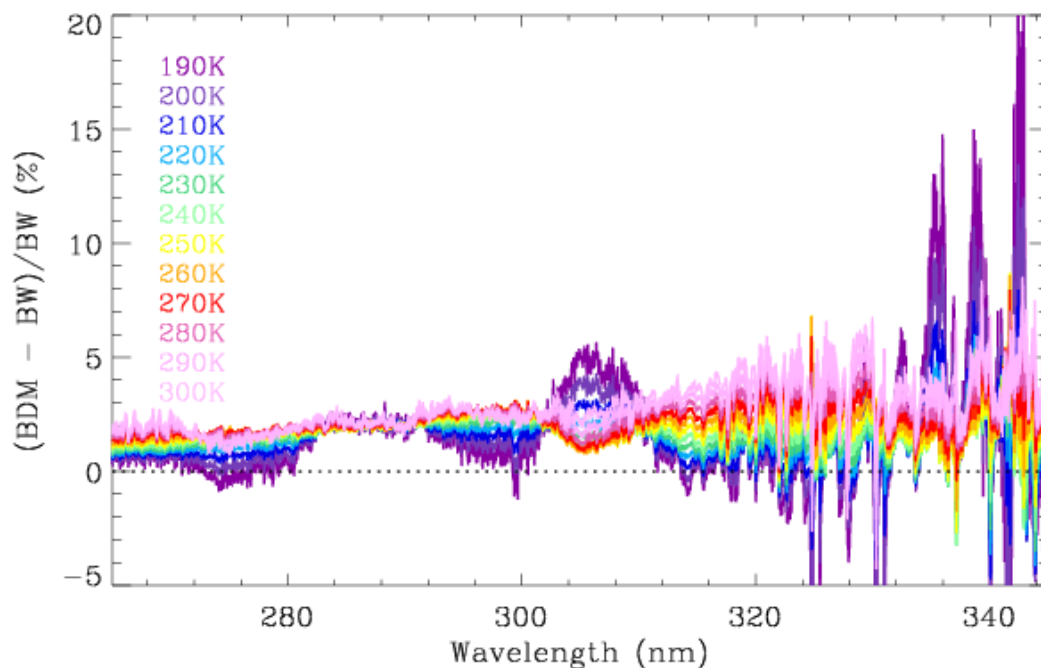
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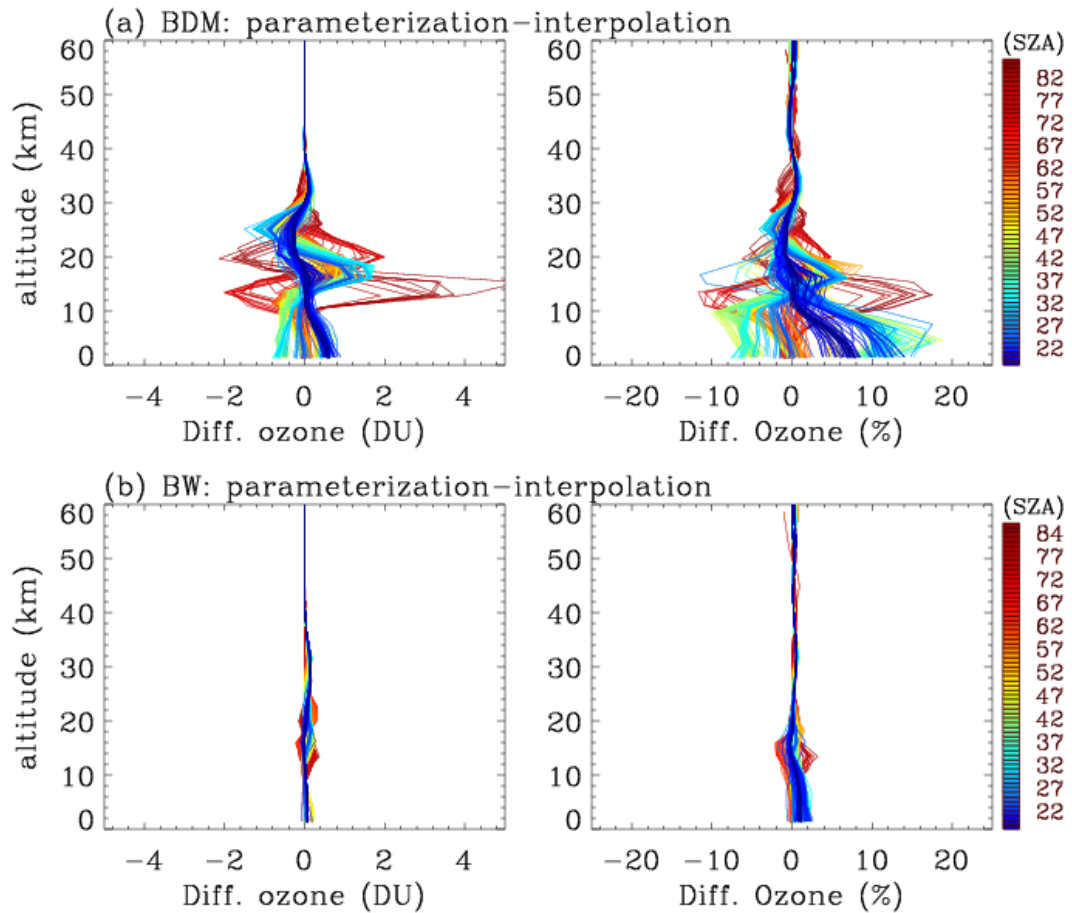
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 772 **Figure 2. Quadratic coefficients ($\text{cm}^2/\text{molecule}$) to parameterize the temperature dependence of**
 773 **ozone cross-sections for BDM (red) and BW (blue), respectively, with their relative differences**
 774 **$(\text{BDM}-\text{BW})/\text{BW}$ in black.**



775
 776 **Figure 3. Relative differences of ozone cross-sections parameterized and spline interpolated at**
 777 **temperatures between 190 and 300 K, for (a) BDM and (b) BW, respectively. In the legend, the**
 778 **temperatures not covered by each dataset are indicated with gray and black, for values beyond**
 779 **lower and upper boundaries, respectively; so slightly different color scales are actually used in**
 780 **these two panels for those outside the measured temperature range.**



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 782 **Figure 4. Same as Figure 3, but for relative differences (%) of parameterized ozone cross-sections**
 783 **between-of BDM and BW.**



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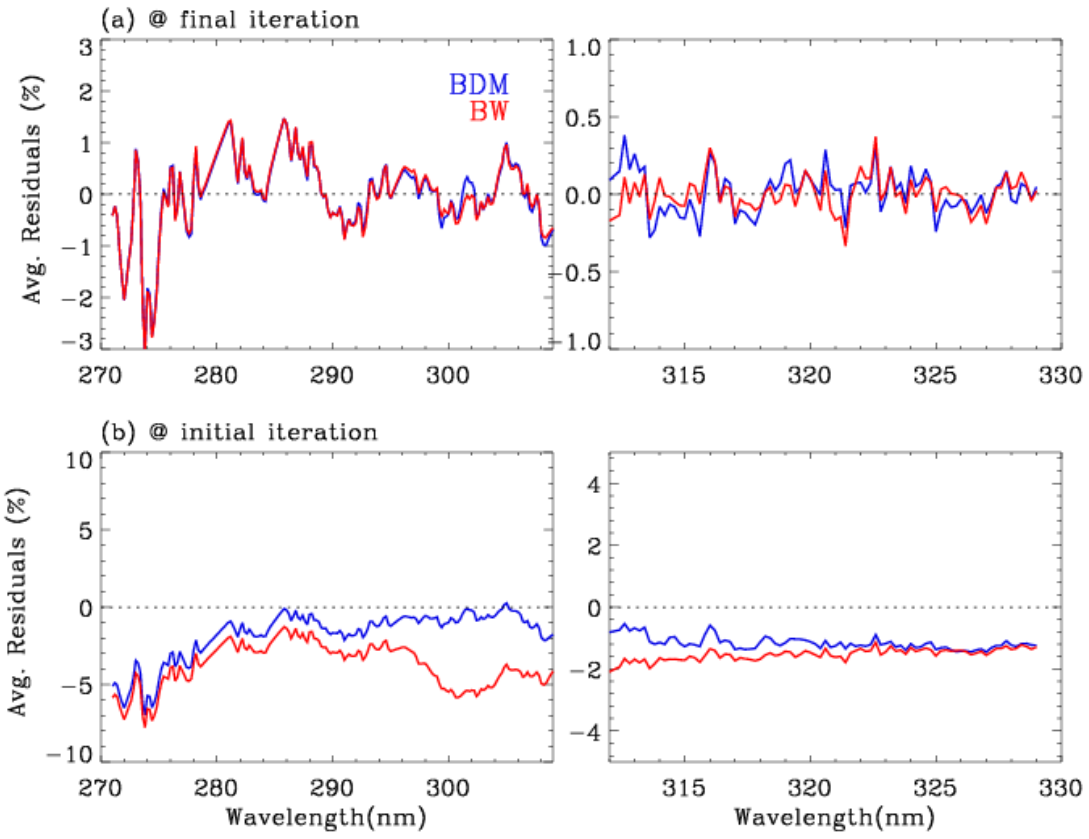
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Figure 5. The impact of parameterizing the cross-sections shown in Figure 3 on ozone profile retrievals, for (a) BDM and (b) BW, as a function of solar zenith angle (SZA). The differences of retrieved ozone profiles are assessed in absolute (left panels) and relative (right panels) units, respectively.

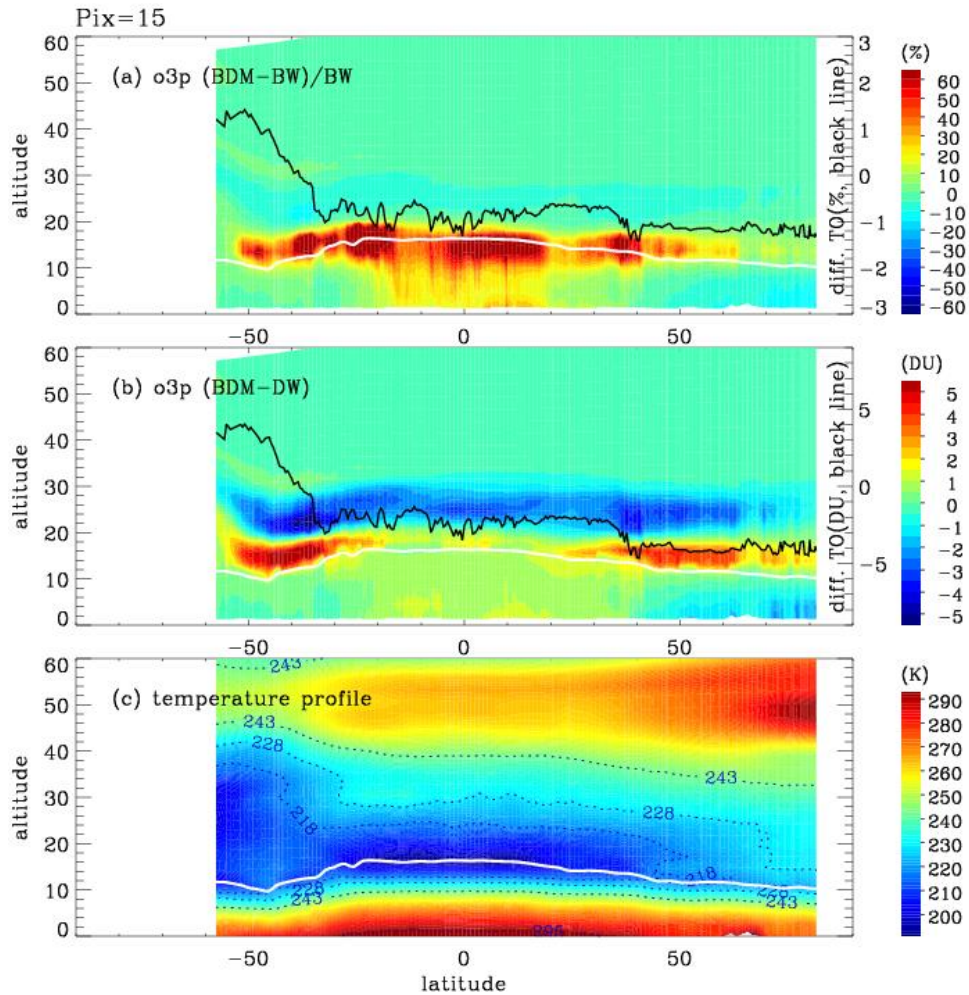


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793 **Figure 6. Comparison of mean fitting residuals at latitudes of 15° S to 15° N at (a) final iteration**
 794 **and (b) initial iteration, respectively, when using BDM (blue) and BW (red).**

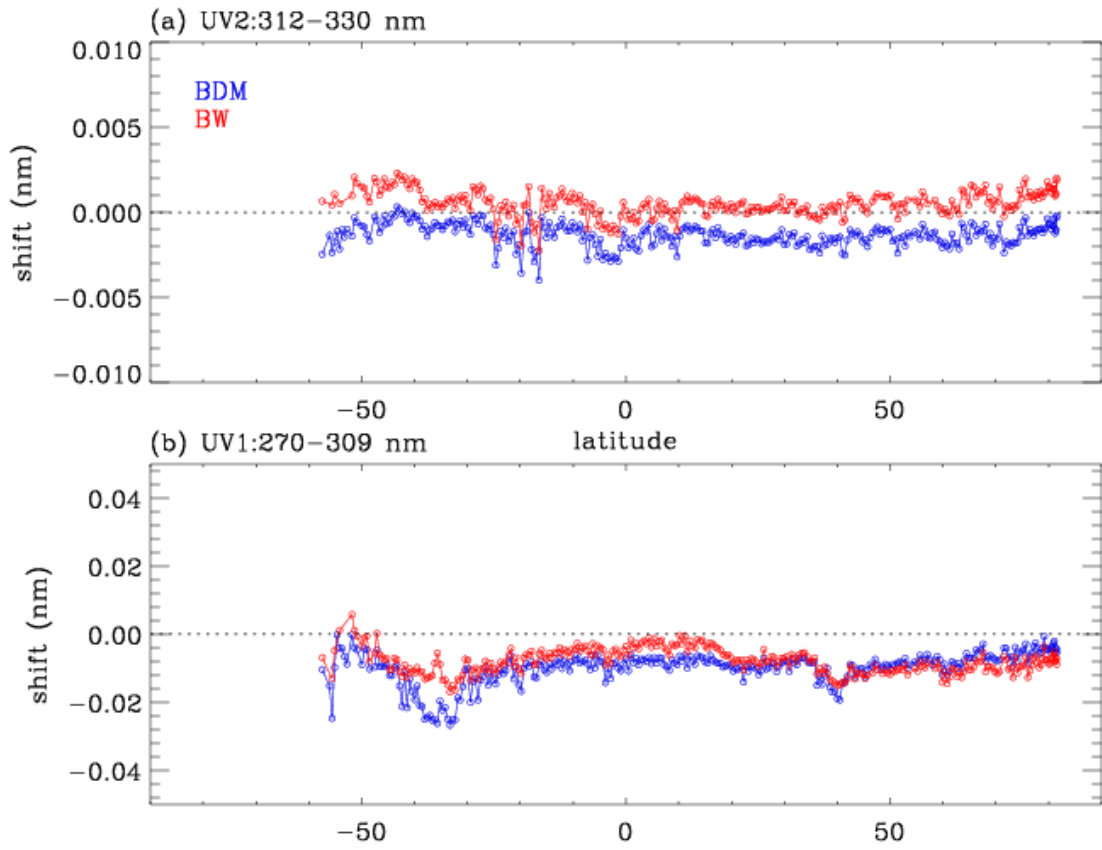
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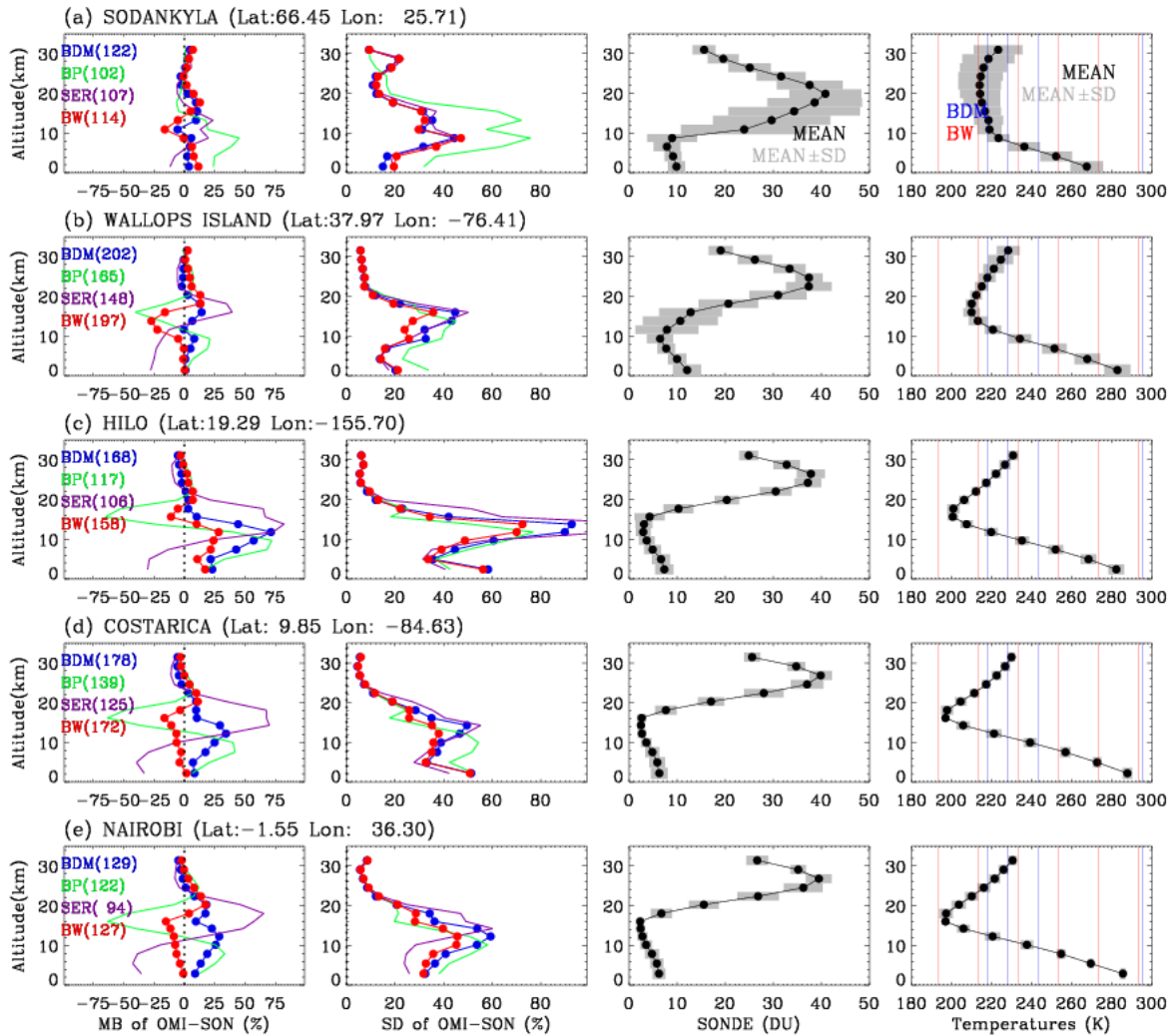
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798 Figure 7. (a) Percent Difference $((\text{BDM-BW})/\text{BW} \times 100\%)$ of retrieved ozone profiles using BDM
 799 and BW datasets at nadir view, (b) absolute differences in the unit of DU and (c) corresponding
 800 temperature profiles in the retrievals. In the upper panel (a) and (b), the black line represents the
 801 differences of integrated column ozone. The white line in both panels represents the tropopause
 802 height.



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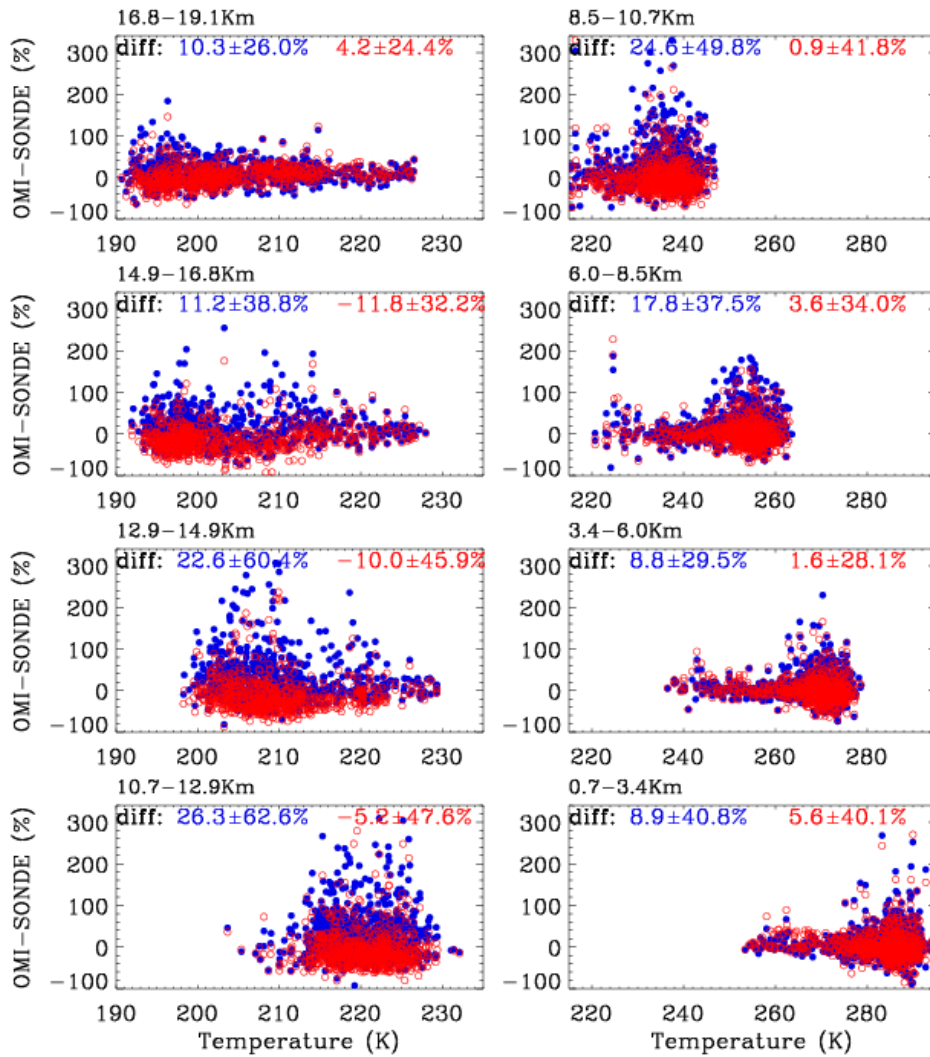
804 **Figure 8. Comparison of the wavelength shifts (nm) between ozone cross-sections and OMI**
 805 **radiances at the nadir view for using BDM (blue) and BW cross-sections, respectively.**



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807 **Figure 9. (1st Left column) Mean biases of relative differences between OMI and ozonesonde ozone**
 808 **profiles at five stations arranged with decreasing latitude when four different cross-sections are**
 809 **applied to OMI retrievals, with (Middle-2nd column) the corresponding standard deviations—and,**
 810 **(3th column) ozonesonde and –(Right-4th column) mean-temperatures (black circle) of-averaged**
 811 **from individual profiles (gray). The numbers after the four cross-sections in the legends show the**
 812 **number of successful retrievals. Blue and red vertical colors in the right-last panels represent the**
 813 **temperatures used to derive the quadratic coefficients from BDM and BW measurements,**
 814 **respectively.**

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817 **Figure 10. Scatter plots of individual differences between OMI retrievals using BDM (blue) and BW**
 818 **(red) cross-sections and ozonesonde measurements for each layer from the surface (bottom right)**
 819 **to 19.1 km (top left) as functions of layer temperature. Mean differences and standard deviations**
 820 **for both cross-sections are shown in the legends.**

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