

Response letter to Referee #1 on the manuscript “Monte Carlo method for determining uncertainty of total ozone derived from direct solar irradiance spectra: Application to Izaña results”

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Article reference: amt-2017-403

Authors: We thank Anonymous Referee #1 for the valuable comments that helped us in improving the manuscript. We have included below our detailed responses to all comments.

Specific Comments

“P1 L14: “The reason often is that the correlations are not known”. It would be better to insert “unknown” into the previous sentence before “correlations” and remove this sentence entirely.”

Authors: We remove that sentence and move “unknown” to the sentence before. After this change, the sentence is: “One frequently overlooked problem with uncertainty evaluation is that the spectral data may hide systematic wavelength dependent errors due to unknown correlations (Kärhä *et al.* (2017b, 2018); Gardiner *et al.* (1993)).”

“P1 L17: This would be better phrased as a complete uncertainty budget being necessary to understand long term environmental trends, rather than increased uncertainties improving the reliability of long term trends.”

Authors: We revise the sentence as: “Complete uncertainty budgets for quantities measured are necessary to understand long term environmental trends, such as changes in the stratospheric ozone concentration (e.g. Molina and Rowland (1974)) and solar UV radiation (e.g. Kerr and McElroy (1993); McKenzie *et al.* (2007)).”

“P2 L5: Better as “...excluding the remainder of the sky”. Also should state field of view of each instrument here or a later point in the field campaign section.”

Authors: We revise the sentence as: “The field of view of the spectroradiometers has been limited so that they measure direct spectral irradiance of the Sun, excluding most of the indirect radiation from the remainder of the sky.”

We included the field of view of each spectroradiometer in Section 2: The field of view with a full opening angle is 2.5° for QASUME (Gröbner *et al.* (2017)), 2.8° for BTS (Zuber *et al.* (2017b)), and 1.5° for AVODOR according to the manual of the collimator tube used, J1004-SMA by CMS Ing.Dr.Schreder GmbH.

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“P2 L6: This section may be better called "The Izaña field measurement campaign and instrument description", and include some additional details on each instrument - e.g. the field of view and other pertinent details. Alternatively the uncertainty tables would be better moved to later in the manuscript where the individual contributions are discussed.”

Authors: We revise the title of Section 2 as: “ATMOZ field measurement campaign and instrument description” and move Tables 1, 2 and 3 to Section 4.

We include more details of the instruments after line 10 on page 3 as:

“The data sets measured by three different spectroradiometers were studied in this work. These spectroradiometers use different techniques to measure the spectral distribution of radiation. Monochromator-based spectroradiometers like QASUME, measure one nearly monochromatic wavelength band at a time, and thus measuring the full spectrum is relatively slow. On the other hand, they usually have significantly better stray light properties than array-based spectroradiometers like BTS and AVODOR, which image the full spectrum at once by dispersing the incoming radiation towards a photodiode array.

QASUME spectroradiometer collects and guides the incoming radiation with input optics and a quartz fiber bundle to the entrance slit of a Bentham DM150 double monochromator (Gröbner *et al.* (2005)). One wavelength at a time can be selected by rotating the two gratings of the double-monochromator. Then, the monochromatic signal is measured with a photomultiplier tube. QASUME is usually operated in global spectral irradiance mode (Gröbner *et al.* (2005); Hülsen *et al.* (2016)), but during the campaign it was equipped with a collimator tube with a full opening angle of 2.5° allowing the measurement of direct solar spectral irradiance (Gröbner *et al.* (2017)). The measurement range of QASUME during the campaign was limited to 250 nm – 500 nm with a step interval of 0.25 nm, so that one spectrum was measured every 15 minutes. To ensure stable outdoor measurements, the double-monochromator of QASUME was mounted inside a temperature-controlled weather-proofed box (Hülsen *et al.* (2016)).

BTS spectroradiometer utilizes a stationary grating and a back-thinned cooled CCD array detector, mounted in a Czerny-Turner configuration (Zuber *et al.* (2017a, b)). To measure direct solar spectrum, BTS was equipped with a collimator tube with a full opening angle of 2.8° designed by PTB, and it uses an internal filter wheel system with 8 filter positions together with a specific measurement routine to reduce stray light. BTS was mounted on a solar tracker, EKO STR-32G by EKO Instruments Co., Ltd., with pointing accuracy better than 0.01°. A weather-proof housing with temperature control allows BTS operation at the ambient temperatures from –25 °C to 50 °C. During the ATMOZ campaign, the housing temperature of BTS was measured to be stable within 0.1 °C (Zuber *et al.* (2017b)). The measurement range of BTS was 200 nm – 430 nm with a step size of 0.2 nm during the campaign. One spectrum was measured every 45 seconds.

AVODOR spectroradiometer has a stationary grating and a back-thinned cooled CCD array detector in a Czerny-Turner configuration. AVODOR measures the spectrum from 200 nm to 540 nm with a step size of 0.14 nm in the UV region. During the ATMOZ campaign, the field of view of AVODOR was limited to 1.5° by a commercial collimator tube used, J1004-SMA by CMS Ing.Dr.Schreder GmbH. The spectral range of AVODOR was limited between 295 nm and 345 nm

by a combination of two solar blind filters to reduce stray light from the visible and infrared parts of the solar spectrum. The solar blind filters were mounted between the collimator tube and the fiber entrance of the spectroradiometer. One spectrum was measured every 30 seconds.”

“**P2 L15:** "mountain Teide" » "Mount Teide at *an* altitude..."”

Authors: Corrected according to reviewer’s suggestion. The revised sentence reads: “The measurements took place on the Mount Teide at an altitude of 2.36 km above the sea level (28.3090° N, 16.4990° W).”

“**P2 L16** "Station pressure of 772.8 hPa was monitored during the campaign with a standard uncertainty of 1.3 hPa" » "Station pressure was monitored during the campaign and determined to be 772.8 hPa with a standard uncertainty of 1.3 hPa"”

Authors: Corrected according to reviewer’s suggestion.

“**P4 L4:** "The tables also give division of the uncertainty components to different correlation types as described in Section 4." » "The tables also attribute uncertainty contributions to different correlation types as described in Section 4." I think this is what you mean, either way needs a rephrasing to clarify.”

Authors: We admit this sentence is not clear so we remove it. We move Tables 1, 2 and 3 to Section 4.

“**P10 L2:** "equal *to* unity"”

Authors: Corrected according to reviewer’s suggestion. The revised sentence is: “The weights γ_i for the base functions are selected in an N -dimensional spherical coordinate system (Hicks and Wheeling (1959)) in such a way that the variance of the final deviation function equals to unity.”

“**P10:** This section on the MC description is clearly the core of the study and where the error estimates are derived, but needs more work and clarification. The details and reasoning behind the approach may be in Karha et al 2017, but it would assist reader of this manuscript to relate MC model and, for example, its sinusoidal terms to physical sources of uncertainty, and how these are calculated for random, unfavourable, and full correlations. At present this isn’t clear.”

Authors: We agree that the core of the paper needs more attention, and we clarify many parts in the text. The text about spectral correlations in the introduction is modified as:

“TOC can be determined from spectral measurements of direct solar UV irradiance (Huber *et al.* (1995)). We have developed a Monte Carlo (MC) based model to estimate the uncertainties of the derived TOC values. One frequently overlooked problem with uncertainty evaluation is that the spectral data may hide systematic wavelength dependent errors due to unknown correlations (Kärhä *et al.* (2017b, 2018); Gardiner *et al.* (1993)). Omitting possible correlations may lead into underestimated uncertainties for derived quantities, since spectrally varying systematic errors typically produce larger deviations than uncorrelated noise-like variations that traditional uncertainty estimations predict. Complete uncertainty budgets for quantities measured are necessary to understand long term environmental trends, such as changes in the stratospheric

ozone concentration (e.g. Molina and Rowland (1974)) and solar UV radiation (e.g. Kerr and McElroy (1993); McKenzie *et al.* (2007)).

Physically, correlations may originate, e.g., from lamps or other light sources used in calibrations. If their temperatures change e.g. due to ageing or current setting, a spectral change in the form of Planck's radiation law is introduced. Non-linearity in the responsivity of a detector causes systematic differences between high and low measured values. The introduced spectrally systematic but unknown changes in irradiance may change the derived TOC values significantly, exceeding the uncertainties calculated assuming that the uncertainty in irradiance behaves like noise. The presence of correlations in measurements can be seen in many ways. For example, problems have occurred when new ozone absorption cross-sections have been taken into use (Redondas *et al.* (2014); Fragkos *et al.* (2015)). Derived ozone values may change significantly because different systematic errors are included in the different cross-sections. Also, TOC estimated from a measured spectrum often depends on the wavelength region chosen, although the measurement region should not affect the result much."

Regarding the above paragraphs, a new reference was included in the AMT Discussion manuscript:

Redondas A., Evans R., Stuebi R., Köhler U., and Weber M.: Evaluation of the use of five laboratory-determined ozone absorption cross sections in Brewer and Dobson retrieval algorithms, *Atmos. Chem. Phys.*, 14, 1635–1648, 2014.

Near Tables 1 – 3 about the uncertainty budgets of the three spectroradiometers, which were moved to Section 4, we place text about how the uncertainties and correlations have been estimated:

"The uncertainties due to radiometric calibration include factors such as the uncertainty of the standard lamp used, and the additional uncertainty due to noise and alignment. QASUME has been validated using various methods, thus the uncertainty due to calibration is low (Hülsen *et al.* (2016)). For QASUME and BTS, we assume the correlations to be equally distributed between *full* correlation, *unfavourable* correlation, and *random* correlation (Kärhä *et al.* (2018)). Spectra measured with AVODOR are significantly noisier, thus half of the uncertainty is associated to the *random* component. Values for instability of the calibration lamp are based on long-term monitoring. The lamp irradiances have been noted to gradually drop with no significant wavelength dependent structure within the wavelength region concerned. Non-linearity values are estimations of the operators of the devices. Non-linearity is typically manifested so that the responsivity of the device changes gradually from high readings to low readings. This can cause significant change in the TOC values, thus we assume the correlation type to be *unfavourable*. Uncertainties due to device stability and temperature dependence are based on long-term monitoring. The changes have been found to be independent on wavelength in the region concerned, thus *full* correlation is assumed. Noise is the average standard deviation of typical measurements at noon over the wavelength region concerned. The wavelength scales of the devices have been checked using emission lines of gas discharge lamps. The uncertainty values

given are the estimated standard deviations of the possible remaining errors after corrections. Wavelength error can introduce a significant change in TOC, because it introduces an error in the form of the derivative of the spectral irradiance. Thus, *unfavourable* correlation is assumed. Most of the uncertainty components are slightly wavelength dependent but to simplify simulations, average uncertainty values are used over the wavelength range between 300 nm and 340 nm.”

Regarding the paragraph above, one reference was updated in the AMT Discussion manuscript:

Kärhä P., Vaskuri A., Pulli T., and Ikonen E.: Key comparison CCPR-K1.a as an interlaboratory comparison of correlated color temperature, J. Phys.: Conf. Ser., 972, 012012, 2018. doi:10.1088/1742-6596/972/1/012012

To clarify the uncertainty components in Table 4, we also include new sentences in the AMT Discussion manuscript before line 5 on page 14:

“For components (a) – (d) in Table 4, the mechanism of contributing to the uncertainty of TOC is known. We know the standard uncertainty of the O₃ layer altitude of 26 km to be $u = 0.5$ km, so we vary the altitude accordingly and note the variance of the resulting TOC.”

“P16 L3: If Brewer #183 is included as a reference instrument, then it would be useful to include a similar uncertainty budget for this instrument, even if only summarised. Also the community would find it useful to put these results into context and comparison with those observed at instrument intercomparisons, and often quoted as a measure of instrument or data quality. i.e. for Brewers is the actual uncertainty determined by the MC methodology much large than expected from the intercomparison error, and, what is the primary source (so efforts can be made to reduce it).”

Authors: We thank the referee for the suggestion to include an overall uncertainty budget of Brewer #183. However, this study focuses on MC uncertainty calculation from full spectrum ozone retrieval. An overall uncertainty budget of the double ratio technique ozone retrieval (e.g. for Brewers and Dobsons) is subject of another publication from the ATMOZ field measurement campaign, which is under preparation, but not citable yet. The Brewer data shown in this publication serve only for comparison of the retrieved ozone during the campaign.

Additional notes by the authors

As we modified the retrieval algorithm by including a new offset factor c to compensate for full spectral deviations, the results compared with the AMT Discussion paper will slightly change. Please, see separate response letter addressed to Referee #2 for full details.