Interactive comment on "Monte Carlo method for determining uncertainty of total ozone derived from direct solar irradiance spectra: Application to Izaña results" by Anna Vaskuri et al.

Anonymous Referee #2

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GENERAL COMMENTS

The paper by Anna Vaskuri aims at calculating the uncertainty of ozone retrievals from measurements of direct irradiance spectra taking into account correlations between spectral irradiance data. The unknown total ozone content is assumed to be retrieved by relative least squares fitting of the measuremed spectrum to a modeled spectrum (Eq. 8) and possible, spectrally-correlated systematic deviations are reproduced using three terms (full, unfavourable and random) of a cumulative Fourier series. This uncertainty model is applied to calculate the contribution of some components of the total uncertainty. The deviations of the retrieved ozone from the test instruments to

the ozone retrieved by a reference MkIII Brewer are briefly reported at the end of the manuscript.

In my opinion, the paper cannot be accepted in its current form and major revisions are required.

First, the paper was probably written very quickly and important information is missing, which makes the understanding quite difficult for the unexperienced reader:

- a complete introduction about the importance of ozone measurements and the assessment of their uncertainty should be included (it is only the first line, so far);

- it is not explained why spectral data should contain correlations (physical basis);

- the only characteristics of the instruments described in the manuscript are their spectral range. I believe that a study of the instrumental uncertainties should provide a thorough description of the instruments;

- a Montecarlo model was employed, but important details such as the number of samples that were used, the obtained statistical distribution, etc. are not mentioned;

- the uncertainty components written in the tables are not properly motivated in Sect. 5. Each number should be accompanied by a clear explanation;

- the discussion about the deviation of the three instruments is very superficial (e.g., "... the reason a the systematic deviation either in the linearity, stray light properties, or the calibration of the device") and inconclusive. How is it connected to the main topic of the paper?

I also found many inaccuracies:

- language inaccuracies are listed in the "Technical corrections" section. One for all: "Izaña results" in the title is very generic. At the Izaña atmospheric observatory (not simply "Izaña"), several activities are organised and the title should appropriately tell which campaign was taken into consideration;

- there is a persistent interchange of terms that should not be mixed: uncertainty, deviation, error, etc. (e.g., "uncertainty induced by deviation", p. 10 line 9);

- QASUME is not only a "high-quality reference instrument ... at PMOD/WRC": it is the World reference UV spectroradiometer! Anyway, it should be explained how a global irradiance instrument could measure direct solar irradiance spectra (p. 2 line 5: how was the field of view "limited"?);

- the retrieval method is NOT "consistent with the ozone measurements with Brewer" (cf. specific comment 1).

Secondly, and more seriously, I have several scientific concerns that are listed in the following section. Most of all, if a bold scientific basis of the uncertainty model is not provided (e.g. why the instrumental errors should behave like a full-period sinusoid), the manuscript only represents a theoretical exercise without any advantage for real-life users.

SPECIFIC COMMENTS

1/ Retrieval model

It should be explained why the retrieval method (Eq. 8) was chosen. An obvious drawback is that this method is not invariant for spectrally-constant factors ("full correlation" or systematic errors in the absolute calibration, as hypothesised for AVODOR). It should be stated what networks / instruments use this model. For example, it is false that "This approach is consistent with the ozone measurements with Brewer" (p. 7, line 17): the Brewer algorithm is invariant for "full spectral correlation" (therefore, the "full correlation" term would not make sense with a different retrieval method, e.g. for a method where the offset is also included in a DOAS-like fit). Also, since this method gives more weight to lower irradiances, the authors should carefully explain how the "wavelength region where the signal is above the noise floor" was determined (5E-3 and 1E-5 noise floors);

2/ Uncertainty model

The uncertainty model (Eq. 9-10) is very complex. However, for the most part of the paper, only three terms of the Fourier series are used. Thus, I wonder why such a complex initial framework must be described. Also, it should be explained why deviations in measurements should follow this model. Coming to the "unfavourable correlation", "The obtained TOC value is affected most by spectral distortion that mimics the spectral shape of the ozone absorption... The first combination of constant offset and one sinusoidal function ... is closest to this extreme". However, from Eq. 10, this term varies with lambda1 and lambda2, so the width of the sinusoid is different for the three instruments and comparison of the results is difficult. Also, why should this term be a full sinusoid cycle? Why should the period of the oscillation be the same for all uncertainty components (calibration, measurement, cross sections, etc.)? Finally, it is obvious that phi has an enormous role for the "unfavourable correlation" term: depending on phi's value (i.e. similarity with ozone spectral cross section), the induced error could be huge or negligible. The role of phi should be explained better. Physically, what does phi represent? It is expected to randomly change in one instrument or not?

TECHNICAL CORRECTIONS

- p. 1 line 2, "directional irradiance": do you mean "direct irradiance"?

- p. 1 line 2, "correlations in the spectral irradiance data" is too generic: do you mean correlation of data within the same spectrum and measured at different wavelengths?

- p. 1 line 20, "analyse uncertainties": uncertainty of what? I guess in ozone retrievals...;

- p. 2 line 1-2: is the order in which the instruments are described (QASUME, AVODOR and BTS) the same as in the abstract (high-end scanning spectroradiometer, high-end array spectroradiometer and roughly adopted instrument)? If not, please avoid confusing the reader;

- p. 2 line 11: "total ozone content" is mentioned since the beginning of the paper, but formally defined only in page 6 (Eq. 4). Can you move Eq. 4 a bit earlier?

- p. 3 line 1, "vertical profiles were not implemented": what do you mean?

- p. 3 line 2, "shift the absolute values": values of what? "but should not have an effect": can you justify this hypothesis?

- p. 3 line 10, "the uncertainties ...are standard deviations": standard deviation of what series/samples? Can you mention which kind of measurements were employed?

- p. 3 line 11, "One of the instruments was the QASUME...": already said;

- p. 3 line 14, "every 15 minutes": explain that use of a scanning radiometer involves slower measurements, and why;

- p. 3 line 15: what is the spectral range of AVODOR? It is legitimate to say that an instrument "has been corrected"?

- p. 4 Table 1: is this table useful? The same numbers are repeated in Table 4. Also, provide bibliographic references about how each term in the "Standard uncertainty" column was calculated;

- p. 5 line 2, "fitting the ozone retrieval": can a single quantity be fitted?

- p. 5 line 5, "affects uncertainties with a factor of sqrt(N)": do you mean 1/sqrt(N)? If so, why the Brewer - which measures the irradiance for the ozone retrieval at only 4 wavelengths - is considered a reference in the paper?

- p. 6 line 1-2: give credit to Bouguer, Lambert and Beer (not Huber et al. 1995);

- p. 6 Eq. 3: a reference to the used extraterrestrial spectrum (QASUME-FTS) should be mentioned just after the equation;

- p. 6 line 12: theta is the angle at the observing site, not the angle betwen vacuum-to-air interface;

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- p. 7 line 10: the extinction coefficient is defined as dTau/dz, thus it has nothing to do with beta;

- p. 7 line 11: avoid the expression "terrestrial spectrum", the radiation is from the sun, not from the Earth. Use "solar spectrum at the Earth surface";

- p. 7 line 22, "As can be seen, the signal-to-noise ratios ... differ": how can I see it from the figure, without any explanation?

- p. 9 line 3: "noise" usually defines a random variable, while stray light is a systematic effect. Don't put them together in the same sentence;

- p. 10, Eq. 11: define "u";

- p. 10 line 20, "does not have any internal limitation to the shape of the error function": what do you mean?

- p. 11 line 3, "components stating fractions": what do you mean?

- p. 12 Table 4: why is "X" used instead of "TOC"?

- p. 12 line 2: was "r" defined?

- p. 13 line 20, "a wavelength shift will introduce unfavourable correlations": why? The ozone cross section has a complex shape;

- p. 13 lines 24-25, "the wavelength shift... should be corrected for the extraterrestrial spectrum": or vice-versa?