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Discussions

Interactive comment on "Explorative study on GOME-2 total column ozone retrievals and the validation with ground-based and balloon measurements" *by* A. Wassmann et al.

Anonymous Referee #3

Received and published: 21 July 2015

Review of the manuscript entitled

Explorative study on GOME-2 total column ozone retrievals and the validation with ground-based and balloon measurements (doi:10.5194/amtd-8-4917-2015)

by A. Wassmann et al.

Recommendation:
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The manuscript is recommended for publication in AMT after performing a major revision, see the major comments below.

The authors describe a very interesting study for total column ozone retrievals based on a retrieval algorithm employing the scaling of a reference ozone profile. One of the advantages of the proposed method is that it allows one to analytically calculate total column averaging kernels. Furthermore, the explorative study treats the effect of the scan-angle dependence of GOME-2's instrument performance by discussing the efficiency of the proposed radiometric correction. Further items discussed in the manuscript are the relevance of the pseudo-spherical approximation in radiative transfer and for treating polarization effects in the forward model.

Despite the fact that manuscript is written rather well, there appear to be some scientific and algorithmic details which need further attention for preparing the revised version of the manuscript, see the discussion below.

Major comments:
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1) In the beginning of Section 2.2 the authors state on p. 4924 that the state vector of the retrieval comprises a total of six components (total ozone column c, the surface albedo A_s, spectrally linear dependence δA_s of the surface albedo, the amplitude a for the linear scaling of the ratio of Raman-scattering reflectance to the Rayleigh-scattering reflectance (using a pre-computed look-up table), a spectral shift $\Delta\lambda_s$ of the solar spectrum, and a spectral shift $\Delta\lambda_{ISRF}$ of the instrument spectral response function.

It is not clear to the reader how LINTRAN is used to compute the associated partial derivatives of the radiance (forward model) function with respect to the latter spectral shift parameters. Also, for the determination of the parameter a of the state vector, a look-up table is employed. How does this fit in the LINTRAN forward model?

The authors are asked to provide more detail about how these partial derivatives are evualated with LINTRAN.

2) p. 4925, equation (9): The meaning of the bold-face quantity K_i^{col} is not clear. Is it a matrix or a vector? Or is it the i-th component of a vector? From the middle part of equation (9) it seems that $\partial F_i / \partial c$ is a scalar quantity. Please clarify in the manuscript.

3) p. 4926, lines 9-11: "Consequently, when the correct relative profile is used for the scaling approach, the retrieved column can be interpreted as an estimate of the true column."

The reviewer has two questions to this sentence: How should one know about the correct relative ozone profile? Such a case only occurs in a "validation situation" for which measured ozonesonde or ozone lidar profiles are available for the satellite retrieval case (i.e. for both the actual time and geolocation for which satellite measurements and ground-based validation data are available). And even for such measurements there will be some observational error so that the knowledge of the "correct relative profile" refers to a hypothetical situation.

In the retrieval of the total ozone column for a particular geophysical location, one does not know in advance the vertical profile of the ozone concentration; also its column (resulting from vertical integration over the profile) is not known. Therefore, even if we take the relative profile shape as a priori, the outcome of the retrieval turns out to be an estimate for the total ozone column.

The authors are asked to clarify the above sentence on p. 4926 so that it reflects the real retrieval situation in which the correct relative profile shape is not known.

4) p. 4926, lines 14-16: Based on Borsdorff et al. (2014) it is stated that the regularization associated with profile scaling is identical with a Tikhonov regularization procedure of the first order employing an infinitely strong regularization strength.

What is the meaning of "first order" Tikhonov regularization? Is this associated with employing a first-order approximation for the first derivative in the smoothing operator

L_{n-p}?

The reviewer has some difficulties with the concept of the "infinite regularization strength". What does this really mean? Generally speaking, with the λ parameter in the cost function one may enforce weak or strong regularization. But what happens for infinitely strong regularization in the expression for the cost function (i. e. the norm which needs to be minimized)? How can it be minimized if λ goes to infinity? Isn't there the risk of over-smoothing the problem at hand? - Please discuss in more detail in the revised manuscript.

5) Regarding the profile scaling approach to finally retrieve total ozone columns, the reviewer has the following questions:

Generally speaking, a difficuly exists to find the derivative of the simulated radiance with respect to the total columnar ozone, since the radiative transfer model (it is presumed that this is also the case for LINTRAN) requires partial ozone columns for each of its model layers. Therefore, in order to find the Jacobian matrix of the radiance at the TOA (top of the atmosphere) for total column retrieval, one has to define a suitable map between the partial columns in each model layer and the total ozone column. With the forward model, one can always compute the full Jacobian matrix of the TOA radiance with respect to all possible changes of the partial ozone columns (i. e. in all model layers). What is not known is, in which manner each of these partial derivatives will contribute to the Jacobian of the radiance for the total column. Consequently, there are infinitely many ways to force a change, say, by 1 DU ozone, of the total ozone column. The simplest way to treat this situation is to "force" a scaling of the initial profile. The authors call this initial profile there the "reference ozone profile".

Questions: How does LINTRAN calculate the full Jacobian matrix of the TOA radiance with respect to the total ozone column? Does LINTRAN compute new full Jacobian matrices for each iteration step (Gauss-Newton iteration for solving the minimization problem)?

6) Question related to the use of the ozone climatology to define a reference ozone profile:

On p. 4927, the authors write that, for a particular geo-location, the Fortuin and Kelder (1998) climatology for ozone is used for finding the appropriate reference ozone profile with which the iterative retrieval (Gauss-newton iteration) is initialized. The Fortuin and Kelder (1998) ozone climatology provides on a monthly basis a single ozone profile for each 10 degree latitude band.

And further on the same page it is stated that "Retrievals are performed for three different reference ozone profiles, the US standard ozone profile (NOAA, 1976), the corresponding profile extracted from the climatology by Fortuin and Kelder (1998), which provides ..."

The reviewer's questions are connected with the wording "corresponding ozone profile" in the above sentence.

- How does the condition number of the Jacobian matrix K change if one takes either i) the US standard atmosphere ozone profile, or ii) the corresponding Fortuin Kelder climatological ozone profile, or iii) the measured ozonesonde profile as the respective reference profile?

- How does the dimension of the null-space of K change in either of these situations i), ii) and iii)?

The reason for the above questions is that, with more realistic initial ozone profiles, both the condition number of$K$ as well as the null-space of the associated linear operator can be modified in favor of a more reliable retrieval result for the total ozone column.

The authors are asked to discuss this point in the revised version of the manuscript.

7) A question related to the global mean bias and standard deviation of the suggested total column profile scaling retrieval:

How does the suggested profile scaling approach compare globally with the GOME-2 results reported by Loyola et al. (2011) who refer to a global mean bias and standard deviation of -0.28 +/- 0.7

If one considers the results of dataset 2 in Table 1, the mean bias of the authors' results may turn out to be similar to the Loyola et al. (2011) case.

For Brewer spectrometers Loyola et al. (2011) find a larger global bias of -1.22. How is the global performance of the suggested algorithm when considering the Brewer stations? Is there any solar zenith dependence of the presented results, and is the solar zenith angle dependence similar for all ground-based spectrometers used in the comparison?

8) Total number of figures:

A total number of 19 figures in this manuscript is considered to be too high. The authors are asked the reduce the total number to, say, 15, either by leaving out certain figures, or by suitably combining the information of some figures into a single one.

Minor comments:
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p. 4918, line 15: Typo, "Futhermore"

p. 4920, line 2: Typo "measurments"

p. 4966, Figure 14, caption: Typo "(Right panel) Same as right panel ..."

p. 4967, Figure 15, caption: "... and the Lambertian surface albeo 0.1

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