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Comment

Interactive comment on “Application of the Spectral Structure Parameterization technique: retrieval of total water vapor columns from GOME” by R. Lang et al.

R. Lang et al.

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Firstly, we wish to thank referee #2 for taking the time to perform such a rigorous and comprehensive review of our work. We feel that we have benefited by this and it has led to an overall improvement in the clarity and, in certain sections, the content of the paper. With the following response we want to address both the general and specific comments made regarding our submitted manuscript.

Full Screen / Esc

Print Version

Interactive Discussion

Original Paper

1. General Responses to Reviewer 2

1.1. Error analysis

The reviewer suggests to add a more detailed discussion related to the errors associated with the retrieved WVC values by SSP, and also the quality of the retrieved data compared with other sources of validation. We agree with the reviewer on both points and feel such improvements will help give a more complete picture regarding the precision and accuracy of the SSP method. It is important to point out that, to the best of our knowledge, there does not exist a complete error analysis of the ECMWF water vapor product. What is available in the literature are validations of ECMWF data which are made by comparing total WVC values with other sources (e.g. *Vesperini*, 1998). Therefore, a comparison of SSP and ECMWF data has to rely on the accuracy of the ECMWF data. We have included a short discussion concerning the quality of ECMWF data in the revised version of the paper (see conclusions section). A detailed discussion of the impact of systematic errors on the retrieved column by the 'dominant-layer approach', and the impact of multiple scattering in clear sky and aerosol-loading situations, is already included in the ACPD version of the paper. Regarding the model bias we provide the user with an empirical correction term (Eq. 12). The impact of multiple-scattering in various scenarios is demonstrated by a number of case studies modeled by a full scalar treatment of the equation of radiative transfer using a doubling adding method (DAM). In the revised version of the paper we improve on this error analysis, as suggested by the referee. This is done by

- (I) adding an appropriate error to the empirical quantities of the "dominant-layer" correction term,
- (II) by including (I) and the impact of multiple-scattering in the error analysis for the individual fit results and

Full Screen / Esc

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Original Paper

(III) by adding the shot noise contribution of the instrument to the total error on the retrieved column.

Such an error analysis of the individual fit results also implicitly includes the correlation impact of additional fit parameters like the surface albedo and the multiple-scattering correction term (for details see below).

1.2. Validation issues

In the ACPD version of the paper we compared the SSP retrieved WVC values with co-located ECMWF values. In the revised version we expand on this analysis by performing a full regression analysis of the scatter plots, calculating Pearson's r number and the 95% confidence interval limits as requested by referee #2. In addition we include a scatter plot and regression analysis comparison between the SSP and the OACS method. Even though OACS is conceptually different to SSP it uses a similar radiative transfer approach for an identical GOME data set. It should be kept in mind that, in contrast, for the global comparisons of the results to ECMWF data, there are temporal differences between the ECMWF and SSP retrieved data of up to 24 hours. This means that only significantly different features of both data sets over wider areas (covered by preferably more than one GOME track) can be identified as systematically different. This has already been included in the conclusions of the ACPD version of the paper.

1.3. Clouds

Here we would like to make a general statement about our treatment of clouds and the effect it has on the WVC retrievals discussed in this paper. We use a 10% cloud fraction

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limit to separate clear-sky (i.e. cloudless) GOME pixels from those contaminated by cloud. Cloud fractions below this limit we consider to be cloud free due to the magnitude of the errors associated with the GOME cloud-fraction product, which can differ from other products by more than 15% in some instances. We discuss this problem as a possible source of error (c.f. discussion section in the ACPD version of the paper). We do not state in the ACPD version that we can retrieve any meaningful WVC values when the GOME ground pixel contains significant cloud cover. The accurate treatment and modeling of clouds for retrievals of tropospheric trace gases in the visible and near infrared is currently under intensive discussion and, to the best of our knowledge, there is currently no comprehensive solution to the problem of cloud effects. It would go way beyond the scope of this paper to perform a quantitative analysis of the way in which clouds effect the retrieval when using the SSP method. Our purpose is simply to show that the use of SSP is realistic using moderate computing power. However, we can state that the 'intuitive' first-order effect of clouds on such retrievals, namely the blocking of the light from traversing through the lower layers of the atmosphere causing a drop in the total retrieved WVC, does not always occur. Sometimes the retrievals result in much higher WVC than those obtained for the surrounding cloud-free pixels, and usually do not look specifically different. One interpretation of this maybe that a potential decrease in the photon path-length by the blocking of the light is compensated for by an increase in the path-length due to multiple scattering events inside the cloud. The magnitude of this compensating effect is dependant on a number of cloud parameters (e.g. optical depth, droplet size distribution), which are usually not readily available for a given cloud. Moreover, a quantitative analysis of this effect is out of the scope of this paper.

[Full Screen / Esc](#)[Print Version](#)[Interactive Discussion](#)[Original Paper](#)

2. Response to Specific Comments

2.1. Fitting uncertainties

In the revised version of the paper we use the Jacobian of the large-scale trust region optimization method from the last iteration step, in order to derive the required fitting uncertainties, as suggested by the reviewer. The problem with using standard packages, which readily generate such covariance matrices, is that they often implicitly assume that the errors provided are normally distributed, which is usually not the case, except for the contribution due to shot noise of the instrument. In the ACPD version of the paper we focus more on the impact of the systematic errors on the retrieved columns rather than the impact of the shot noise, which is, for the GOME instrument, very small. For the revised version we now combine fitting uncertainties of both the shot noise and systematic errors (see above) in order to attach a specific error estimate to each retrieved WVC value. To achieve this we adopt the approach of *Rodgers, 2000*. From the Jacobian we evaluate the distribution matrix of the linearized problem, which is then multiplied by the specific error vector, to get either the retrieval noise error or the forward model error [*Rodgers, 2000*]. The distribution matrix is evaluated from a singular value decomposition of the Jacobian. For the revised version of the paper we attach a total error to each retrieved WVC for the single GOME track (Fig. 6, ACPD version) in order to show the dependence on measurement geometry, presence of clouds and geolocation. The systematic error estimates are taken from

- (I) the error on the bias derived from the fit results to the line-by-line modeled spectra (section 6, ACPD version) and
- (II) the fits to the results of the DAM model in section 7 of the ACPD paper (multiple scattering and aerosol contribution).

Full Screen / Esc

Print Version

Interactive Discussion

Original Paper

In addition, the shot noise error is taken from GOME level 1b data for each individual fit and added to the systematic error contribution using the distribution matrix. Errorbars have been added to both scatter plots with which we compare cloud-free SSP results with values given by ECMWF and OACS for two GOME tracks. Both tracks (one of which is shown in Fig. 6, APCD version) are collocated with ECMWF data with a temporal overlap of one hour.

The derived total error estimates maybe correlated with (apart from those contaminated by clouds) the retrieved surface albedo and the retrieved WVC. In an additional figure, which has been included in the revised version of the paper, the total error on the WVC and the error on the retrieved albedo (estimated in the same way as explained in this section) have both been plotted versus the retrieved WVC. These results are also compared to the differences between the DAM model inputs and the SSP retrieval results as already presented in Table 1 and 2 in APCD (Section 7).

2.2. Bias correction

Forward-lbl-modeled spectra are used to evaluate the bias correction by means of SSP fits to these spectra and by comparing the WVC fit results with the WVC used for the forward modeled spectra. The parameters A to D, representing surface albedo and multiple-scattering contribution, which must be included in these forward-lbl calculation, are obtained from fits of forward-lbl results to real GOME measurements by keeping the WV-profile fixed. For the 25 forward-modeled spectra, significantly different measurement geometries and geolocations have been chosen in order to cover most possible scenarios for the parameters A to D. The fixed WV-profiles were taken from ECMWF and assumed to be close to the real profile for the sake of evaluating realistic values for A to D. In the revised version of the paper we add clarity regarding this point in the text.

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2.3. SSP-OACS comparison

We added a scatter plot in the revised version which compares the WVC values retrieved using the SSP and OACS method to aid the reader in comparing the performance of both methods.

2.4. Dimension of w parameter

As noted by the referee, the w parameter is unitless. By using the units $\delta\lambda^{-1}$ we simply wished to illustrate that w is a fraction of the detector pixel spectral width. We agree that this can lead to some confusion and have subsequently removed the units from both the figure and the text.

2.5. Path-length factor

We restricted our theoretical discussion to strict nadir viewing, meaning that the cosine μ of the angle between the zenith and the satellite is 1. For the global retrieval we use east, center and west pixels of GOME, where the geographical co-ordinates of the center position of each pixel determines the angle with respect to the satellite. In this case μ is not equal to 1, and the geometrical path-length factor changes to $\frac{\mu_o + \mu}{\mu_o \mu}$, which we use for the global retrievals in the ACPD version of the paper, although we did not explicitly state this. We now specify this point in more detail during the description of the global retrievals, and use the general form of the path-length factor in the theoretical discussion, including the μ -scaling of the single-scattering part.

[Full Screen / Esc](#)[Print Version](#)[Interactive Discussion](#)[Original Paper](#)

2.6. Surface reflectivity

In the revised version of the paper the surface albedo Λ has been included as a multiplicative factor in R_{surf} assuming a Lambertian reflecting surface [Lang et al., 2002a] in order to prevent confusion. Now, R_{surf} represents the contribution of photons traversing the direct light path and are only reflected at the surface. This term includes a description of the removal of light on its way through the atmosphere by absorption, as well as Rayleigh scattering out of the light path.

2.7. Use of HITRAN'96

The water-vapor line-parameter data for our band region given in HITRAN-2000 is very similar to that in HITRAN'96. No additional lines are added but line intensities differ slightly due to corrections described by Giver, 2000. The most recent update, HITRAN-2001, does not differ from HITRAN-2000 concerning the water-vapor absorption within our band. A recent study by Veihelmann, 2002, has shown that the differences between HITRAN'96 and HITRAN-2000 are negligible when compared to high-resolution fourier-transform sun-spectrometer measurements within our absorption band. We used HITRAN'96 instead of HITRAN-2000 for efficiency reasons because the cross-section calculations for construction of the look-up tables were already available from the OACS retrievals (where the computation of a typical look up table takes approximately 1 week of processor time on an 800MHz PC).

This author response is followed by a second part dealing with the more specific and technical comments of referee #2.

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