Atmos. Chem. Phys. Discuss., 5, S4512–S4518, 2005
www.atmos-chem-phys.org/acpd/5/S4512/
European Geosciences Union

Atmospheric Chemistry and Physics Discussions

Interactive comment on "Water vapour profiles by ground-based FTIR spectroscopy: study for an optimised retrieval and its validation" *by* M. Schneider et al.

M. Schneider et al.

Received and published: 16 December 2005

The authors appreciate all the comments made by the referees, and below they first answer the comments of each referee in detail and subsequently describe the changes of the manuscript resulting from these comments.

Response to referee R. Lang:

Generally we would like to state that the information about the vertical distribution of

the absorber is mainly obtained from the shape of the absorption line. This is possible since the applied spectra are highly-resolved and a single absorption line is described by several spectral pixels. In the infrared the line shape is determined by pressure broadening. Different temperature dependencies of different lines contain some but much less information. Hence the simultaneous fit of temperature is only introduced to avoid a misinterpretation of spectral signatures as described in detail in subsection 3.3 and not to benefit from its information content. This clarification may already contest some of the doubts formulated by the referee in his comment #I.

The referee states that the logarithmic retrieval does improve the sensitivity and that there are indications for an improved accuracy. He further states, that the reasons for these improvements are so far unknown. This needs further clarification of how we calculated the errors. The random error was calculated as the variability of the difference between retrieved and real amount relative to the variability of the retrieved amount ($\epsilon_{ran} = \frac{\sigma_{(\hat{\mathbf{x}}-\mathbf{x})}}{\sigma_{\hat{\mathbf{x}}}}$ (noise to signal error)), i.e. it is the proportion of the retrieved variability that is due to errors. The systematic error was calculated as the mean of the real amount and the mean of the retrieved amount relative to the mean of the retrieved amount ($\epsilon_{sys} = \frac{\overline{\mathbf{x}}-\overline{\hat{\mathbf{x}}}}{\overline{\hat{\mathbf{x}}}}$). This kind of error definition has some important drawbacks: (a) it attributes too low retrieval sensitivity, which is a systematic error component, to the random error, and (b) for a log-normal distribution an error characterisation in the form of a mean and variance is inappropriate. To overcome these drawbacks we changed the error classification made in Section 3. In the revised manuscript we use a least squares fit between the real amounts and the retrieved amounts. The systematic error, or mean behavior of the retrieval is then represented by the regression curve, while the scattering around the curve represents the random error. This new and more correct error representation demonstrates that the retrieval on a logarithmic scale reduces mainly the systematic error if compared to the linear retrieval. The logarithmic retrieval leads to a self-consistent result. It is linearly correlated to the real data, i.e. it has the same sensitivity for low and high mixing ratios. It correctly maps the real atmospheric evolution. On the other hand, the correlation of linearly retrieved data with the real data

ACPD

5, S4512–S4518, 2005

is non-linear. The linear retrieval is more sensitive around low mixing ratios than around high mixing ratios. This deficiency makes it nearly impossible to correctly detect upper tropospheric water vapour variabilities. For further details of the relevant changes in the manuscript see point C) below.

I) The referee state that we do not consider errors due to incorrect modelling of pressure broadening. This is not correct. The random as well as the systematic errors caused by a systematic error in the pressure broadening coefficient is examined in detail. The results are given in Table 2-5 and Fig. 7. The referee mentioned that the applied pressure profile might be incorrect. We calculated our pressure profiles from the surface pressure measured at the observatory and from the ptu-sonde's temperature profile assuming a hydrostatic atmosphere. These uncertainties should lie at least one order of magnitude below the uncertainties of the pressure broadening coefficient: an uncertainty of surface pressure of 0.1 % versus an uncertainty of pressure broadening of 1 %.

The referee further states that the Gauss contribution to the spectral line shape and the temperature dependence of the line intensity is dominant to the overall line shape in the UT/LS region. This is incorrect. As aforementioned in the infrared the line shape is dominated by the pressure broadening. Here the Doppler broadening, which causes a Gaussian line shape, only becomes equal to the pressure broadening above 30-35 km. We obtain the information about the vertical distribution of the absorber nearly exclusively from pressure broadening. Hence our whole retrieval bases on an accurate modelling of pressure broadening.

II) The sondes used for the construction of a-priori profiles and for the comparison are all launched at 12 km southeast or 35 km northeast of the observatory, where the official ptu-sonde stations are located. Ptu-sonde data, in particular for the UT/LS region have some deficiencies. Maybe Lidar measurements would allow a validation of higher quality.

ACPD

5, S4512–S4518, 2005

The objective of this paper was to demonstrate that the ground-based FTIR technique enables to detect UT water vapour. This is only possible when the measurements are of high quality and the slant column amounts for the lower troposphere are low. Hence in mid-latitudes only mountain observatories would have this capability. A discussion of operational use of the data is far beyond the context of this paper.

Response to referee #2:

1) We will change from a nomenclature of layers to grid points. The in-situ instrument operating at the observatory is a Rotronic MP100H.

2) As correctly mentioned by the referee $\mathbf{S_a}$ is generally singular. Performing an eigenvalue decomposition and neglecting the contributions from eigenvectors with small eigenvalues allows calculating a pseudo inverse. However this pseudo inverse does not span a fraction of the solution space large enough to stabilize the retrieval. Hence the pseudo inverse of $\mathbf{S_a}$ has to be slightly modified. The introduction of statistical perturbations at each level increases the rank of the pseudo inverse and finally allows a stable retrieval. For further details see section 6.2 in Hase et al. (2004).

3) The covariances are determined directly from the sonde data. We decided to focus on correlation matrices since they are easier to present. Their elements are all of the same order of magnitude (between -1 and 1), whereas in the case of water vapour the elements of the covariance matrices extend over 8 orders of magnitude.

4) Eq. (5) gives the χ^2 value for a vector with zero mean as mention just above the equation in the text. But we agree, it is better to formulate it for the more general case

ACPD

5, S4512–S4518, 2005

and in consistency to the rest of the paper, i.e. for a non-zero a-priori. So we will change the text and Eq. (5) to: $\chi^2 = (\mathbf{x} - \mathbf{x_a})^T \mathbf{S_a}^{-1} (\mathbf{x} - \mathbf{x_a})$

5) The section 3.5 of our paper characterizes the posterior ensembles for both retrievals on a linear and logarithmic scale. It demonstrates that the states obtained by the logarithmic retrieval maintain a principle characteristics of the a-priori states: the log-normal distribution. On the other hand, retrievals performed on a linear scale convert the prior log-normal distribution into a posterior quasi-normal distribution. These simple analyses show that the logarithmic retrieval keeps much closer to the real distribution, or in other words it correctly constrains the solution vectors. To support this conclusion we added a cross check of normal distribution of the logarithmic posterior ensemble to Figure 13. It now clearly shows that the linear posterior ensemble is much closer to a normal distribution than the logarithmic one and that the linear retrieval is incorrectly constrained. For these analyses the posterior covariance matrix is calculated by $\mathbf{S}_{\hat{\mathbf{x}}} = \epsilon\{\hat{\mathbf{x}}\hat{\mathbf{x}}^T\}$, with the whole ensemble of solution vectors $\hat{\mathbf{x}}$ corresponding to the real states $\mathbf{x}$, which are applied for the calculation of $\mathbf{S_a}$: the ensemble applied for the posterior characterizations is not smaller than the one applied for the prior characterizations (the contrary is erroneously commented by the referee). The matrix $\mathbf{S}_{\hat{\mathbf{x}}}$ is singular due to the similar a-priori contribution to all $\hat{\mathbf{x}}$. Therefore only can a pseudo inverse be calculated. This is done by considering the 3 largest eigenvalues (condition number of 50-100). A method suggested in Rodgers (2000) in chapter 12.2. The posterior χ^2 values are then given by $(\hat{\mathbf{x}} - \mathbf{x_a})^T \mathbf{S}_{\hat{\mathbf{x}}}^{-1} (\hat{\mathbf{x}} - \mathbf{x_a})$.

The referee suggests to overcome the singularity problem by not regarding posterior χ^2 values but by calculating a $\chi^2_{\mathbf{referee}}$ by: $(\hat{\mathbf{x}}-\mathbf{x_a})^T \mathbf{S_a}^{-1} (\hat{\mathbf{x}}-\mathbf{x_a}) + \epsilon^T \mathbf{S_\epsilon}^{-1} \epsilon + (\hat{\mathbf{x}}-\mathbf{x})^T \hat{\mathbf{S}}^{-1} (\hat{\mathbf{x}}-\mathbf{x})$ with $\hat{\mathbf{S}}$ being a typical covariance of the posterior pdf of a single ensemble's member state ($\hat{\mathbf{S}}^{-1} = \mathbf{K}^T \mathbf{S_\epsilon}^{-1} \mathbf{K} + \mathbf{S_a}^{-1}$).

From Eq. (10) in Mengitsu Tsidu (2005) and by applying $\hat{\mathbf{S}}^{-1} \approx \frac{1}{2}\mathbf{H}$ we conclude that $\chi^2_{\mathbf{referee}}$ is then the second-order Taylor series expansion of the cost function around

ACPD
5, S4512–S4518, 2005

the minimum obtained from the applied Gauss-Newton method. We further deduced that $\chi^2_{\mathbf{referee}}$ is then the minimum value of the cost function that would be achieved by the Hessian method, but we do not see how this value may help to assess whether the linear or the logarithmic retrieval works better. In our opinion the Hessian method improves the accuracy of involved error covariance matrices, but does not significantly improve the derived profiles (Mengitsu Tsidu, 2005). In the case of water vapour retrieved on a logarithmic scale nonlinearities of the inversion function become important (section 3 of our paper). This prohibits to use the gain matrix $\hat{\mathbf{G}}$ for error calculation, instead a full treatment (forward calculation and subsequent retrieval of a large ensemble of profiles) is the only method to accurately estimate the errors.

In neither case the Hessian method fits into the context of our paper. Our suggested transformation on a logarithmic scale allows to apply the a-priori information correctly. It allows to formulate a correct cost function, which as shown in our paper improves the sensitivity of the retrieval. In contrast the Hessian method is a more precise iteration method to achieve the minimum of a cost function.

Further changes and details of aforementioned changes in the revised manuscript:

A) Classification of days with especially good UT sensitivity: We changed from the retrieval based DOF-UT criterion to a criterion based more directly on the atmospheric situation: low lower tropospheric slant columns and not too low signal to noise ratio. This classification allows to select days with unsaturated lines und low aerosol loading nearly independently from the retrieval. Whereas the DOF-UT criterion depends strongly on the retrieval and thus the selected sub-ensemble differs if DOF values from the linear or logarithmic retrieval are used. In this context we made the estimations for two different sub-ensembles: One which allows to detect UT variability in nearly 30 % of all days and another one which even allows to detect variabilities in the tropopause region (only on 10 % of all days). These changes make former Figure 4 unnecessary,

ACPD

5, S4512–S4518, 2005

and the last paragraph before subsection 3.1 was replaced by explanations about the new criterions. This also implies changes in Fig. 4 (former 5), 5 (former 6), 6 (new), 7, 8, 9, 10, 11, 12, 15, 16, and 17, and in Tables 2-7.

B) Representative layers: We changed the layer representing the upper troposphere from 7.6-12.4 km to 7.6-10.0 km and introduced a layer representing the tropopause region 8.8-11.2 km. This is done in accordance to the results of the sensitivity analysis (Fig. 4, former Fig. 5). This also implies changes in Fig. 12, 16, and 17, and in Tables 2-7.

C) In the revised manuscript random and systematic errors are separated by means of a least squares fit. The method is explained in the second paragraph of section 3. And in more detail in the second paragraph of section 3.1. This changed error definition provokes major changes in section 3 and we introduced a new Figure (Figure 6). But now in the revised manuscript version attribution to random and systematic errors is made correctly. As a consequence the kind of improvement of the logarithmic retrieval becomes much clearer. Beside section 3 some phrases of subsection 4.4 need to be adjusted to this changed error definition. The better description of the improvements also affects the formulations of the conclusions (end of first paragraph of section 6). It implies changes in Fig. 4 (former 5), 5 (former 6), 6 (new), 7, 8, 9, 10, 11, 12, 15, 16, and 17, and in Tables 2-7.

D) Subtropical water vapor time series: We added a time series for the tropopause region (8.8-11.2 km). This amount can be retrieved for 10 % of all days. Furthermore we extended the results with data from our new instrument — a Bruker IFS 125HR — which is in operation since January 2005. These changes affect Fig. 17.

Interactive comment on Atmos. Chem. Phys. Discuss., 5, 9493, 2005.