

Interactive comment on “Iterative maximum a posteriori (IMAP)-DOAS for retrieval of strongly absorbing trace gases: Model studies for CH₄ and CO₂ retrieval from near infrared spectra of SCIAMACHY onboard ENVISAT” by C. Frankenberg et al.

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General comments

The paper presents a method for the retrieval of atmospheric trace gases, which is especially applicable for trace gases strongly absorbing in the near-infrared spectral region as observed from space. The focus of the paper is the effect of pressure and tem-

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perature variations on the trace gas retrieval mainly via pressure-broadening, temperature sensitivity, and therefore related to climatology assumptions, which has been investigated through a theoretical model study. The need of fit parameters accounting for these variations (several atmospheric layers, climatological index) is clearly described. With the described method a new application of the optimal estimation methodology is introduced, taking into account height dependent temperature and pressure variations and, therefore, significantly reducing the corresponding errors as shown in the paper. Although a full IMAP-DOAS error analysis including a sensitivity study referring to relevant atmospheric parameters might be of scientific interest, with the presented focus the paper should be published in this journal.

Specific comments

Although the innovations of the presented method are described, these should be mentioned in a section explicitly describing and summarizing the specific properties and parameters of the new IMAP-DOAS retrieval algorithm. In section 2.4.1 ("Optimal Estimation"), which is part of section 2. "Basic Theory", a general introduction to the optimal estimation method is given. The following sentence "In the following, this method is referred to as IMAP-DOAS (iterative maximum a posteriori DOAS)" is inappropriate at this point, as no specific information on how the optimal estimation method had been applied within the IMAP-DOAS algorithm has been given up to then. It would be helpful to introduce at this point a section "Description of the algorithm" starting, e.g. "In the following, the IMAP-DOAS (iterative maximum a posteriori DOAS) method will be described in more detail" or similar.

As i understand the paper, it is mainly the consideration of different atmospheric height layers that better solves pressure and temperature induced variations, which otherwise lead to biases in the retrieval. This should be explicitly mentioned when describing the algorithm! How has the consideration of different height layers been implemented? For the construction of the state vector, you are using three retrieval layers: What is the reason for the chosen atmospheric height layering: Is it just an example, the result

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of an optimisation procedure,...? Have the derivatives been calculated using mean values according to these layers (especially referring to the Voigt-function) or rather for a vertically highly resolved atmosphere and then integrated according to the three retrieval layers?

It does not become clear what has been used as a priori information especially for the model study! E.g., it has been mentioned that biases arising from large differences between the a priori and the true state are taken into account by iteratively fitting. Has this been tested within the model study?

Abstract

1) Page 6068, "..expected total optical density..": It doesn't sound confiding if you iteratively change your expectations. Better: "model total optical density".

1 Introduction

2) Page 6069, "..first results from SCIAMACHY..": Please, incorporate Buchwitz et al., 2004!

2 Basic theory

3) Page 6070, "..directly proportional to the differential optical density:...": this refers to the correct equation (2), which, however, doesn't describe the differential optical density even for the case of no atmospheric scattering. This is only obtained after fitting a polynomial! Please, clarify!

4) Page 6071, "The total optical depths..": In the paper, "optical depth" and "optical density" are used having the same physical meaning (e.g. "optical depths" in the text (page 6087) and "optical density" in Fig. 3a,b,c). I suggest to stick to "optical density" throughout the paper!

2.1 Spectral line shape

5) Page 6073, "..for the model analysis of CO₂ and CH₄.": Except of the abstract, after

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the title this is the first time of "model analysis". Better: "..for the model analysis of CO2 and CH4 presented in this paper."

2.3 Sensitivity of the measurement

6) Page 6074, "Pressure broadening decreases the total values of...sensitivity of strong absorption lines" Strictly speaking, the total optical density decreases near the line center but increases in the spectral ranges of what is called the line wings. ".. decreases the maximum total optical density..." might fill this lack.

2.4 Linearisation points and derivatives

7) Page 6075, "..as will be shown in the following. If the actual atmospheric state...further iterations are necessary to yield unbiased results.": After mentioning the lack of Buchwitz et al. (2000) referring to height layer treatment, it is not clear if the suggestion of an iteration scheme is also part of criticism. It should be noted that the method introduced by Buchwitz et al. (2000) also, as others, uses an iteration scheme (see Buchwitz and Burrows, 2004) for the same reason as described in this paper. Furthermore, the impression that the authors claim to introduce the usage of an iterative scheme suggests itself. Please write: "..as will be shown in the following. <new paragraph> If the actual atmospheric state.....further iterations are necessary to yield unbiased results (see e.g. Buchwitz and Burrows, 2004)."

2.4.1 Optimal estimation

8) Page 6080, "Since these variations...shows a different value.": For the generation of the measurement correlation matrix, it would be of interest if cross-correlations due to the transfer function spreading over a number of spectral pixels are relevant for the NIR-retrieval?

3.1.1 Retrieval results

9) Page 6085, "This effect could be only partly obviated...", "This is prevented by sup-
plying...": Please, describe the implementation of surface elevation information in more

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detail! Is the original layering maintained by reducing the boundary retrieval layer according to clouds/mountains? Or does the same layering just begin at a higher surface elevation? E.g. for the first case, at elevations above 3km the retrieved state should be near the a priori state according to the chosen regularisation. Btw., within the ground-pixel size of real SCIAMACHY measurements the surface elevation can be highly variable, in which cases effective surface elevations have to be assumed, which leads to additional errors.

4.1.1 Effect of atmospheric scattering

10) Page 6087, "Depending on their optical properties, surface reflectance and other parameters, aerosols can shorten as well as enhance the light path by up to a few percent.": The effects of aerosols on the near-infrared retrieval of greenhouse gases have been quantitatively investigated by Dufour and Breon (2003) and Buchwitz and Burrows (2004), which have to be referenced!

Technical corrections

Abstract

1) Page 6068: Preferably write "atmospheric trace gas retrieval" in the first sentence in order to put the paper into context at the beginning of the abstract.

2.1 Spectral line shape

2) Page 6072ff: Use a consistent set of variables: e.g. x appears in equations (4), (7), (8), (9), for each having a different meaning.

2.3 Sensitivity of the measurements

3) Page 6075, "Furthermore the nonlinearity increases...": "Furthermore the nonlinearity decreases with decreasing FWHM of the slit function being still present even for..."

2.4 Linearisation points and derivatives

4) Page 6075, "..derived from climatological profiles meteorological parameters...":
"..derived using climatological profiles of meteorological parameters..."

5) Page 6077, equation (14): It is the derivation of the transmission function at X_0
($d\ln\langle T(X)\rangle/dX|_{X_0}$, instead of $..T|_{X_0}..$ Outside the derivation $T|_{X_0}$ has to be replaced
by $T(X_0)$!

6) Figure 3 too small, 3c is not referred to in the text.

2.4.2 Temperature derivatives

7) Page 6082, "..a change in climatatology,...": "..a change in climatology,...".

3.1 Standard profiles

8) Page 6083, "These simulated measurements then were fed into different versions of
the retrieval algorithm.": Better: "These simulated measurements then were used for
different retrieval schemes."

3.1.1 Retrieval results

9) Page 6083, "Figure 6 shows the theoretical errors of a methane fit in a typical SCIA-
MACHY fit window...": Which fit window, those from Table 1?

10) Page 6086: No section 3.1.2! Avoid unnecessary sub-numbering!

3.2 Simulating enhanced CO₂ in the boundary layer

11) Page 6086, "..close to the sources and sinks...": Better: " where the sources and
sinks are...", to refer to the vertical distance. Otherwise, the next sentence could be
misunderstood.

4.1.2 Effect of surface elevation and albedo

12) Page 6087, "..the systematic error would be about 1.5% in the total column" ..of
which gas?

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13) Page 6088, "SCIAMACHY provides polarization measurement devices that can be used to derive this information.": Confusing, better: "...provides broadband detectors having higher spatial resolution...".

4.2.2 Effect of the uncertainty of broadening parameters

14) Page 6089, "Figure 11 shows the effect..." ..on the CH₄ retrieval...

15) Page 6089, Figure 11 is too small, the short cut DSOD in the figure caption is needless!

5 Conclusions

16) Page 6090, "...DOAS approach ius resolved...": "...DOAS approach is resolved..."

Figures

Use dots instead of commas for float numbers in the figures.

References to be added:

1) E. Dufour and F.-M. Breon, Spaceborne estimate of atmospheric CO₂ column by use of the differential absorption method: error analysis, Applied Optics, Vol. 42, No. 18, pages 3595-3609, 2003.

2) Buchwitz, M., and John P. Burrows, Retrieval of CH₄, CO, and CO₂ total column amounts from SCIAMACHY near-infrared nadir spectra: Retrieval algorithm and first results, Proceedings of SPIE 5235, Remote Sensing of Clouds and the Atmosphere VIII, K. P. Schäfer and A. Comeron and M. R. Carleer and R. H. Picard (Editors), 375-388, 2004.

3) Buchwitz, M., R. de Beek, J. P. Burrows, H. Bovensmann, T. Warneke, J. Notholt, J. F. Meirink, A. P. H. Goede, P. Bergamaschi, S. Körner, M. Heimann, J.-F. Müller, and A. Schulz, Atmospheric methane and carbon dioxide from SCIAMACHY satellite data: Initial comparison with chemistry and transport models, Atmos. Chem. Phys. Discuss.,

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2004.

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