Retrieval of atmospheric CO_2 from satellite near-infrared nadir spectra in a scattering atmosphere

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Abstract

An optimal estimation based retrieval scheme for satellite based measurements of XCO_2 (the column averaged mixing ratio of atmospheric CO_2) is presented enabling accurate retrievals also in the presence of optically thin clouds. The proposed method is designed to analyze near-infrared nadir measurements of the SCIAMACHY instrument in the CO_2 absorption band at 1580nm and in the O_2-A absorption band at around 760nm. The algorithm accounts for scattering in an optically thin cirrus cloud layer and at aerosols of a default profile. The scattering information is mainly obtained from the O_2-A band and a merged fit windows approach enables the transfer of information between the O_2-A and the CO_2 band. Via the optimal estimation technique, the algorithm is able to account for a priori information to further constrain the inversion. Test scenarios of simulated SCIAMACHY sun-normalized radiance measurements are analyzed in order to specify the quality of the proposed method. In contrast to existing algorithms, the systematic errors due to cirrus clouds with optical thicknesses up to 1.0 are reduced to values typically below 4ppm. This shows that the proposed method has the potential to reduce uncertainties of SCIAMACHY retrieved XCO_2 making this data product useful for inverse surface flux modeling. The work presented within this conference proceeding summarizes the results published by Reuter et al. (2009).

INTRODUCTION

Theoretical studies have shown that satellite measurements of XCO_2 (the column averaged dry air mole fraction of CO_2) have the potential to significantly reduce the CO_2 surface flux uncertainties (Rayner and O'Brien, 2001; Houweling et al., 2004). This requires an accuracy and precision of 1% or better (Rayner and O'Brien, 2001; Houweling et al., 2004; Miller et al., 2007; Chevallier et al., 2007).

Within the time period 2002-2009 SCIAMACHY was the only instrument measuring XCO_2 from space with significant sensitivity also to the lower troposphere. Therefore, the development of algorithms deriving XCO_2 from SCIAMACHY as accurate as possible with realistic error estimates is crucial to start a consistent long-term time series of XCO_2 observations from space.

In the literature one can find several somewhat different XCO_2 retrieval algorithms for SCIAMACHY data: The WFM-DOAS algorithm (weighting function modified differential absorption spectroscopy) was developed at the University of Bremen for the retrieval of trace gases from SCIAMACHY and has been described by Schneising et al. (2008); Buchwitz et al. (2005a,b), Buchwitz and Burrows (2004), and Buchwitz et al. (2000b). This algorithm is based on a fast look-up table (LUT) based forward model used to derive the number of CO_2 and O_2 molecules in the atmospheric column in order to derive XCO_2. Other groups have developed somewhat different approaches to retrieve XCO_2 or CO_2 columns from SCIAMACHY (e.g. Barkley et al., 2006a,c,b, 2007, Houweling et al., 2005). Bösch et al., 2006 and Schneising et al. 2008 showed that XCO_2 can be retrieved from SCIAMACHY with a single measurement precision of 1-2% assuming clear sky conditions. Additionally, Schneising et al. 2008 showed that a relative accuracy of about 1-2% for monthly averages at a spatial resolution of about 7°x7° can be achieved from SCIAMACHY measurements under clear sky conditions.

However, scattering at aerosol and/or cloud particles remains a major source of uncertainty for SCIAMACHY XCO_2 retrievals which easily exceeds the precisions and accuracy estimated for clear sky conditions. In this context, Schneising et al. 2008 showed that a thin scattering layer with an optical depth of 0.03 in the upper troposphere can introduce XCO_2 uncertainties of up to several percent.

The XCO_2 retrieval algorithms for SCIAMACHY mentioned above have one thing in common: they do not explicitly account for scattering effects. This means, they either do not account for scattering at all or in an indirect way as the WFM-DOAS algorithm does by assuming that photon path-length modifications are identical at 0.76µm and 1.6µm. In this approximation, scattering related errors of CO_2 and O_2 cancel out when calculating XCO_2. For this reason, new XCO_2 retrieval algorithms optimized for SCIAMACHY nadir data are currently under development, explicitly considering scattering in optically thin cloud and aerosol layers (Reuter et al. 2009, Buchwitz et al. 2009)

PHYSICAL BASIS

Many physical parameters influence the spectrum of reflected solar radiation measured at the satellite instrument. The partial derivatives of the measured radiation with respect to these parameters are called the weighting functions (or Jacobians) of the parameters. Of course, it is only possible to retrieve those parameters having a unique weighting function, sufficiently different from all other weighting functions in terms of the instrument's accuracy. Very similar weighting functions can result in ambiguities of the retrieved corresponding parameters.

Fig. 1 shows for exemplary atmospheric conditions with moderate aerosol load and one thin ice cloud layer the weighting functions of three different scattering related parameters under a typical observation geometry in SCIAMACHY's spectral resolution. Additionally, the figure shows the XCO_2 weighting function which gives the change of radiation when columnar increasing the CO_2 concentration by 1ppm. For this example, the magnitude of its spectral signature is comparable to a change of the cloud top height (CTH) by 1km, the cloud water/ice path (CWP) by 0.2g/m^2, or to a change of the aerosol load by 100%. It is immediately noticeable that there are high correlations between the curves. Especially between the aerosol profile scaling (APS) and the cloud water/ice path weighting function as well as between the cloud top height and the XCO_2 weighting function. XCO_2 changes of 1ppm are approximately the detection limit due to SCIAMACHY's signal to noise (SNR) characteristics. This means, with SCIAMACHY it is actually not possible to discriminate XCO_2 values of a few ppm from significant changes of the given scattering parameters. Therefore, it is most likely not possible to retrieve scattering parameters simultaneously with the number of CO_2 molecules from measurements in this spectral band, only.

Analog to Fig. 1, Fig. 2 shows for identical atmospheric conditions the weighting functions of the same scattering parameters but for the O_2 fit window. Additionally, it shows the weighting function in respect to surface pressure p_s which can be used to derive the total number of air molecules within the atmospheric column by applying the hydrostatic assumption. The similarities between the weighting functions are less pronounced in this fit window. This applies especially when comparing the surface pressure weighting function to the weighting functions of the given scattering parameters. This originates by much stronger absorption lines in this fit window. As width and depth of absorption lines depend on the ambient pressure, saturation effects differ much stronger with height within this spectral region. Additionally, SCIAMACHY's resolution resolves the spectral structures of the gaseous absorption better within this fit window. Nevertheless, there are still similarities that are not negligible e.g. between the cloud top height and aerosol profile scaling weighting function. Differences of 1hPa are in the order of the detection limit according to SCIAMACHY's SNR characteristics. Therefore, it can be expected that independent information on the given scattering parameters can be extracted from this fit window simultaneously with information about the surface pressure.

In the following section we will describe, how the information on scattering parameters, which can be derived from the O_2 fit window, can be transported to the CO_2 fit window.

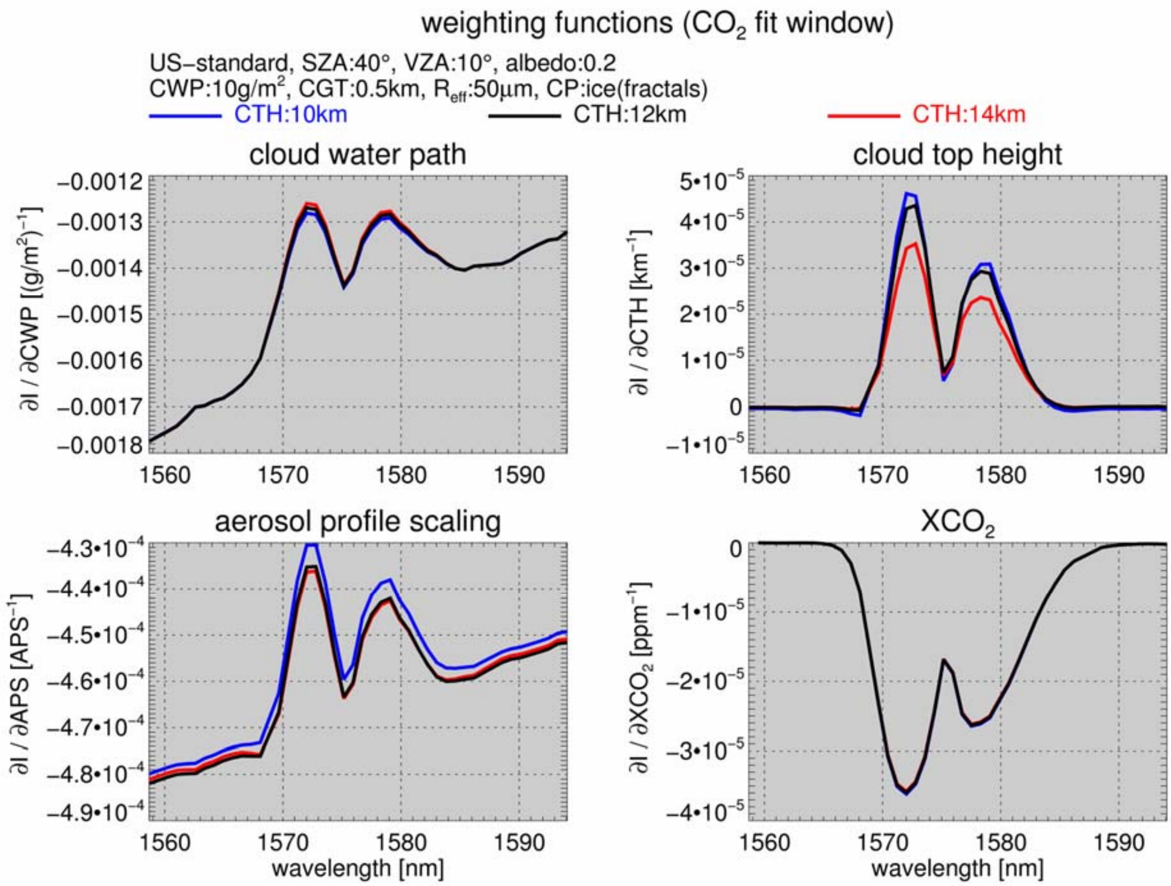

Figure 1: Weighting functions in the CO_2 fit window for three cloud scenarios based on a US-standard atmosphere including an optically thin ice cloud with a cloud top height of 10km (**blue**), 12km (**black**), and 14km (**red**): cloud water/ice path (**top/left**), cloud top height (**top/right**), scaling of the aerosol profile (**bottom/left**), and XCO_2 (**bottom/right**). The weighting functions are calculated with the SCIATRAN 3.0 radiative transfer code and are folded with SCIAMACHY's slit function.

INVERSION TECHNIQUE

We use an optimal estimation based inversion technique to find the most probable atmospheric state given a SCIAMACHY measurement and some prior knowledge. Nearly all mathematical expressions given in this publication as well as their derivation and notation can be found in the text book of Rodgers (2000).

The forward model $\boldsymbol{F}$ is a vector function which calculates for a given (atmospheric) state simulated measurements i.e. simulated SCIAMACHY spectra. Here, we use the SCIATRAN 3.0 radiative transfer code (Rozanov et al., 2005) in discrete ordinate mode and the correlated-k approach of Buchwitz et al. (2000a) to increase the computational efficiency. The input for the forward model are the state vector $\boldsymbol{x}$ and the parameter vector $\boldsymbol{b}$. The state vector consists of all unknown variables that shall be retrieved from the measurement (e.g. CO_2). Parameters which are assumed to be exactly known but affecting the radiative transfer (e.g. viewing geometry) are the elements of the parameter vector. The measurement vector $\boldsymbol{y}$ consists of SCIAMACHY sun-normalized radiances of two merged fit windows concatenating the measurements in the CO_2 and O_2 fit window. The difference of measurement and corresponding simulation by the forward model is given by the error vector $\boldsymbol{\varepsilon}$ comprising inaccuracies of the instrument and of the forward model:

$$\boldsymbol{y} = \boldsymbol{F}(\boldsymbol{x},\boldsymbol{b}) + \boldsymbol{\varepsilon} \tag{1}$$

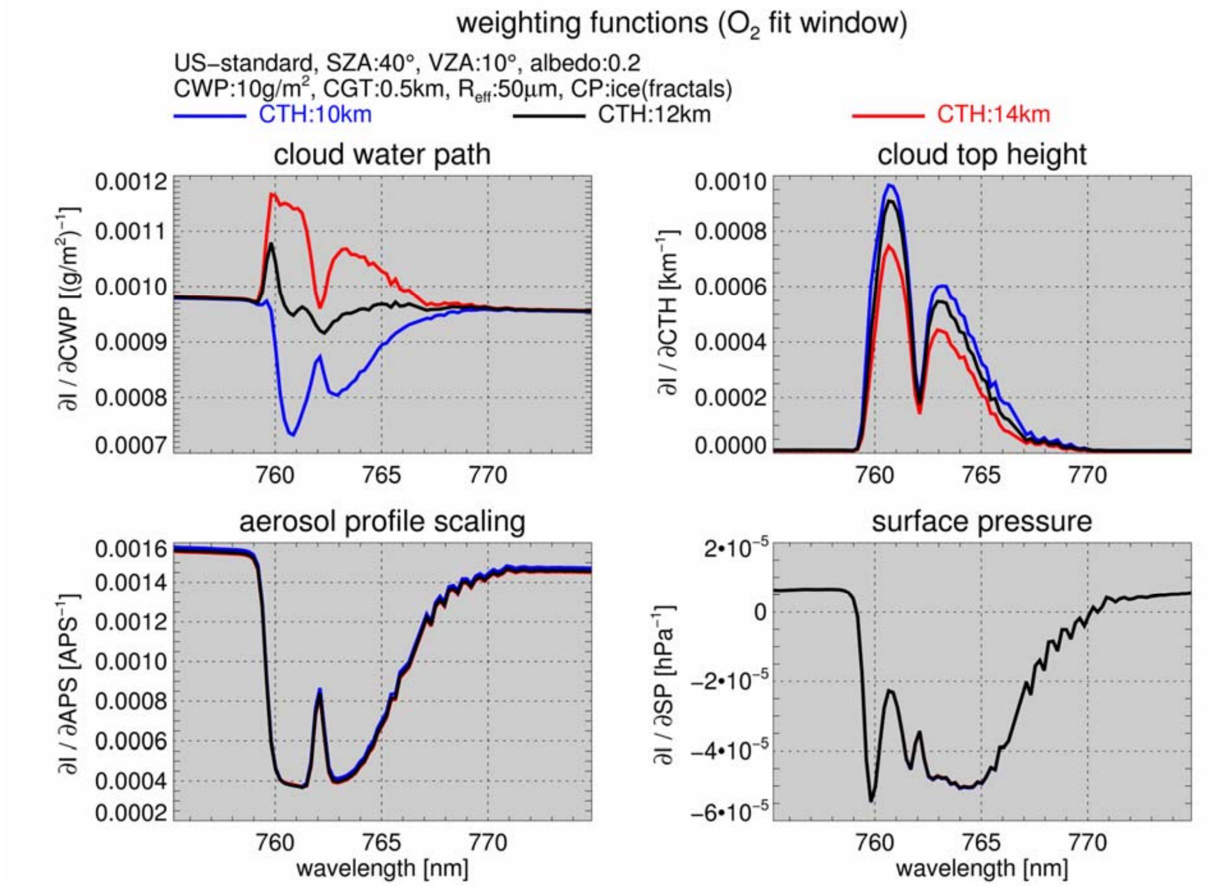

Figure 2: Weighting functions in the CO_2 fit window for three cloud scenarios based on a US-standard atmosphere including an optically thin ice cloud with a cloud top height of 10km (**blue**), 12km (**black**), and 14km (**red**): cloud water/ice path (**top/left**), cloud top height (**top/right**), scaling of the aerosol profile (**bottom/left**), and surface pressure (**bottom/right**). The weighting functions are calculated with the SCIATRAN 3.0 radiative transfer code and are folded with SCIAMACHY's slit function.

According to Eq. 5.3 of Rodgers (2000), we aim to find the state vector $\boldsymbol{x}$ which minimizes the cost function $\chi 2$:

$$\chi^2 = \left(\boldsymbol{y} - \boldsymbol{F}(\boldsymbol{x},\boldsymbol{b})\right)^T \mathbf{S}_\varepsilon^{-1} \left(\boldsymbol{y} - \boldsymbol{F}(\boldsymbol{x},\boldsymbol{b})\right) + \left(\boldsymbol{x} - \boldsymbol{x_a}\right)^T \mathbf{S}_a^{-1} \left(\boldsymbol{x} - \boldsymbol{x_a}\right) \tag{2}$$

Here, $\mathbf{S}_\varepsilon$ is the error covariance matrix corresponding to the measurement vector, $\boldsymbol{x}_a$ is the a priori state vector which holds the prior knowledge about the state vector elements and $\mathbf{S}_a$ is the corresponding a priori error covariance matrix which specifies the uncertainties of the a priori state vector elements as well as their cross correlations. Even though the number of state vector elements (26) is smaller than the number of measurement vector elements (134), the inversion problem is under-determined. The weighting functions of some state vector elements show quite large correlations under certain conditions. This especially applies to the weighting functions corresponding to the ten-layered CO_2 profile but also to some of the weighting functions shown in Fig. 1 and Fig. 2. For this reason we use a priori knowledge further constraining the problem and making it well-posed. However, for most of the state vector elements the used a priori knowledge gives only a weak constraint and is therefore not dominating the retrieval results. Furthermore, we use only static a priori knowledge of XCO_2.

According to Eq. 5.8 of Rodgers (2000), we use a Gauss-Newton method to iteratively find the state vector $\hat{\boldsymbol{x}}$ which minimizes the cost function.

$$\begin{aligned} \boldsymbol{x}_{i+1} &= \boldsymbol{x}_i + \hat{\mathbf{S}} \left[\mathbf{K}_i^T \, \mathbf{S}_\varepsilon^{-1} \left(\boldsymbol{y} - \boldsymbol{F}(\boldsymbol{x}_i, \boldsymbol{b})\right) - \mathbf{S}_a^{-1} \left(\boldsymbol{x} - \boldsymbol{x}_a\right)\right] \\ \hat{\mathbf{S}} &= \left(\mathbf{K}_i^T \, \mathbf{S}_\varepsilon^{-1} \, \mathbf{K}_i + \mathbf{S}_a^{-1}\right)^{-1} \end{aligned} \tag{3}$$

Within this equation, $\mathbf{K}$ is the Jacobian or weighting function matrix consisting of the derivatives of the forward model in respect to the state vector elements $\mathbf{K} = \partial \boldsymbol{F}(\boldsymbol{x},\boldsymbol{b}) / \partial \boldsymbol{x}$. In the case of convergence, $\boldsymbol{x}_{i+1}$ is the most probable solution given the measurement and the prior knowledge and is then denoted as maximum a posteriori solution $\hat{\boldsymbol{x}}$ of the inverse problem. $\hat{\mathbf{S}}$ is the corresponding covariance matrix consisting of the variances of the retried state vector elements and their correlations.

Our state vector consist of the following 26 elements: wavelength shift, full width half maximum of the slit function, 2nd order albedo polynomial, scaling of the H_2O profile, shift of the temperature profile, effective cloud top height (CTH), effective cloud water/ice path (CWP), scaling of a default aerosol profile (APS), ten-layered CO_2 mixing ratio profile, and surface pressure.

ERROR ANALYSIS

Within the error analysis, the retrieval algorithm is applied to SCIAMACHY measurements simulated with SCIATRAN 3.0 using a modified US-standard atmosphere and a common viewing geometry (40° solar zenith angle, 10° viewing zenith angle). The corresponding measurement error covariance matrices are assumed to be diagonal. They are calculated for an exposure time of 0.25s using the instrument simulator that was also used for the calculations of Buchwitz and Burrows (2004).

Two strategies are followed within the error analysis. First, we concentrate on the retrieval's capability to reproduce the state vector elements. In this context, Fig. 3 illustrates the results of a set of test scenarios where only state vector elements are modified. However, radiative transfer through a scattering atmosphere can be very complex. Thinking about the almost infinite number of possible ensembles of scattering particles, all with different phase functions, extinction, and absorption coefficients, a set of three scattering related state vector elements is by far not enough to comprehensively describe all possible scattering effects. For this reason, we set up several different test scenarios in a second step to estimate the retrieval's sensitivity to aerosol and cloud micro and macro physical parameters which are not part of the state vector but of the parameter vector. Analogous to Fig. 3, Fig. 4 shows the results for those scenarios where parameter vector elements are differing from their default values.

CONCLUSIONS

An optimal estimation based XCO_2 retrieval scheme for measurements in the O_2-A band and in the weak CO_2 absorption band at 1580nm has been presented. Within the first part of our error analysis we proved that the retrieval is capable to reproduce modifications to the state vector elements. In this context, the precision of the retrieved XCO_2 was between 3 and 4ppm for most of the analyzed scenarios which is smaller but similar to the 1-2% precision range experimentally determined for the WFM-DOAS 1.0 retrieval scheme (Schneising et al., 2008). Slightly lower values were observed for scenarios with high albedo and therefore large signal to noise values. Much larger stochastic errors of up to 12.3ppm were observed for low albedos of snow or open ocean.

The accuracy for scenes with optically thin cirrus clouds was drastically enhanced compared to a WFM-DOAS like retrieval. At solar zenith angles of 40°, the presence of ice clouds with optical thicknesses in the range of 0.01 to 1.00 contributed with less than 0.5ppm to the systematic absolute XCO_2 error. This compares to systematic XCO_2 errors of a WFM-DOAS like retrieval scheme in the range of 3 to more than 400ppm. However, the WFM-DOAS 1.0 processing chain efficiently filters cloud contaminated scenes so that such large errors do not occur in the WFM-DOAS data product.

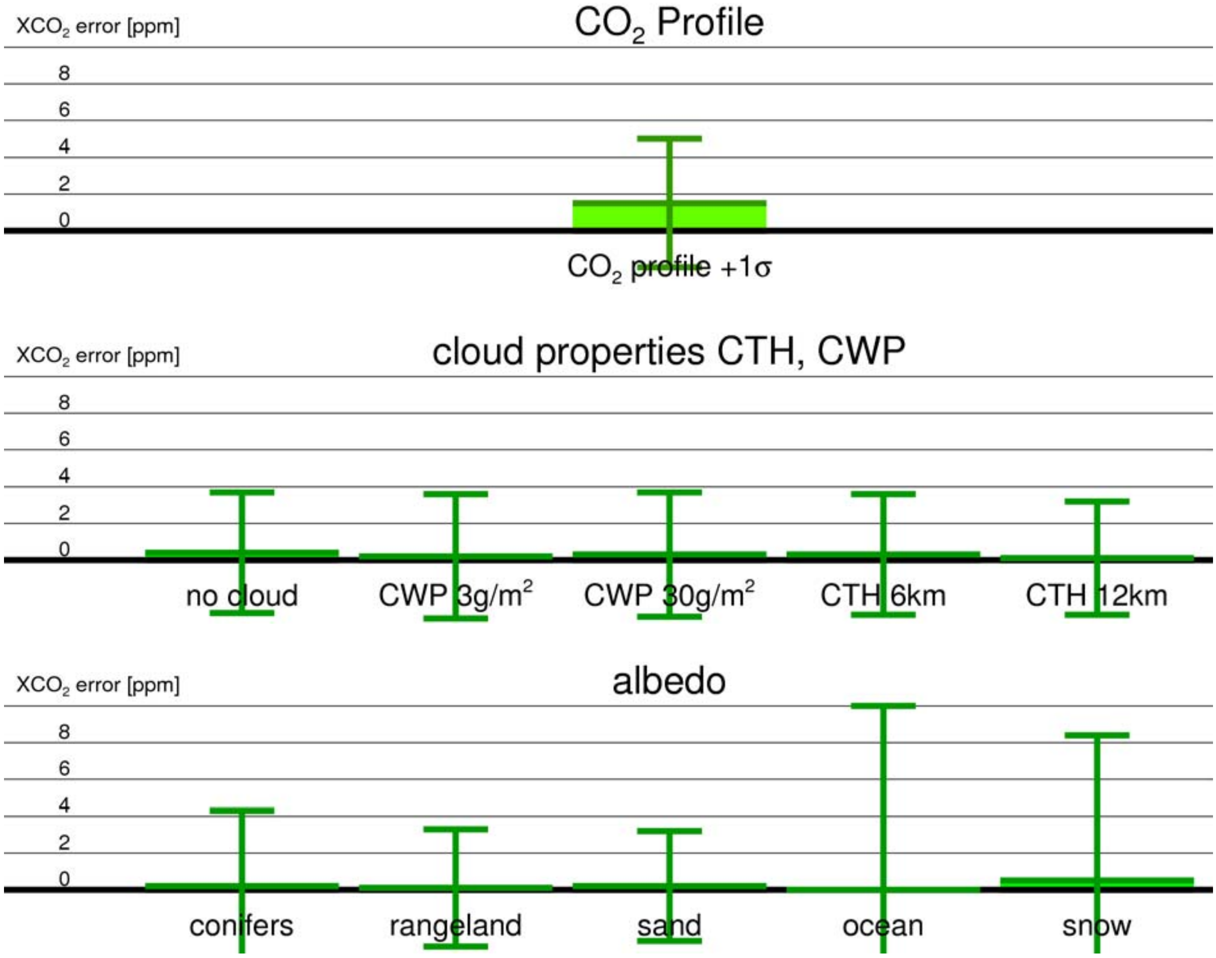

Figure 3: Absolute systematic and stochastic errors of the retrieved XCO_2 when modifying only individual state vector elements.

Scattering in clouds and aerosols was described by only three state vector elements. For this reason, the retrieval's sensitivity to other scattering relevant (not retrieved) parameter vector elements has been analyzed. These were the type of the aerosol scenario, micro physical cloud properties like particle size, shape, and state of aggregation and macro physical cloud properties like cloud geometrical thickness (CGT), multilayer clouds, and cloud fractional coverage (CFC).

Our results show that the aerosol scenario has only a weak impact on the retrieved XCO_2 resulting in systematic errors below ±0.5ppm except for one scenario with extreme aerosol load where the systematic error amounted to 6.5ppm. In respect to cloud micro physical properties, we found that the retrieval performed better and with smaller residuals for ice clouds than for water clouds although lower CWP values have been used for the water clouds. The reason for this is the default cloud which consists of ice particles. The systematic XCO_2 errors of the "micro physical cloud properties" scenarios with ice clouds were most times below ±4ppm. However, for water clouds larger systematic errors were observed. Not retrieved macro physical cloud properties contributed with -2.8 to 0.9ppm to the systematic XCO_2 error. In this context, the largest effect was observed for the cloud fractional coverage.

The results presented here indicate that it is theoretically possible to retrieve XCO_2 from SCIAMACHY nadir measurements meeting the 1% accuracy and precision requirement in many cases even in the presence of thin ice clouds. This represents an important step forward for the improvement of XCO_2 retrieval schemes for SCIAMACHY for the following reasons: i) Most cloud detection schemes are not able to detect sub visible cirrus clouds. ii) Rigorous masking of clouds with optical thicknesses as small as 0.1 or lower would drastically reduce the amount of available data. iii) Large satellite pixels with sizes of 30 times 60km have a high probability for being cloud contaminated.

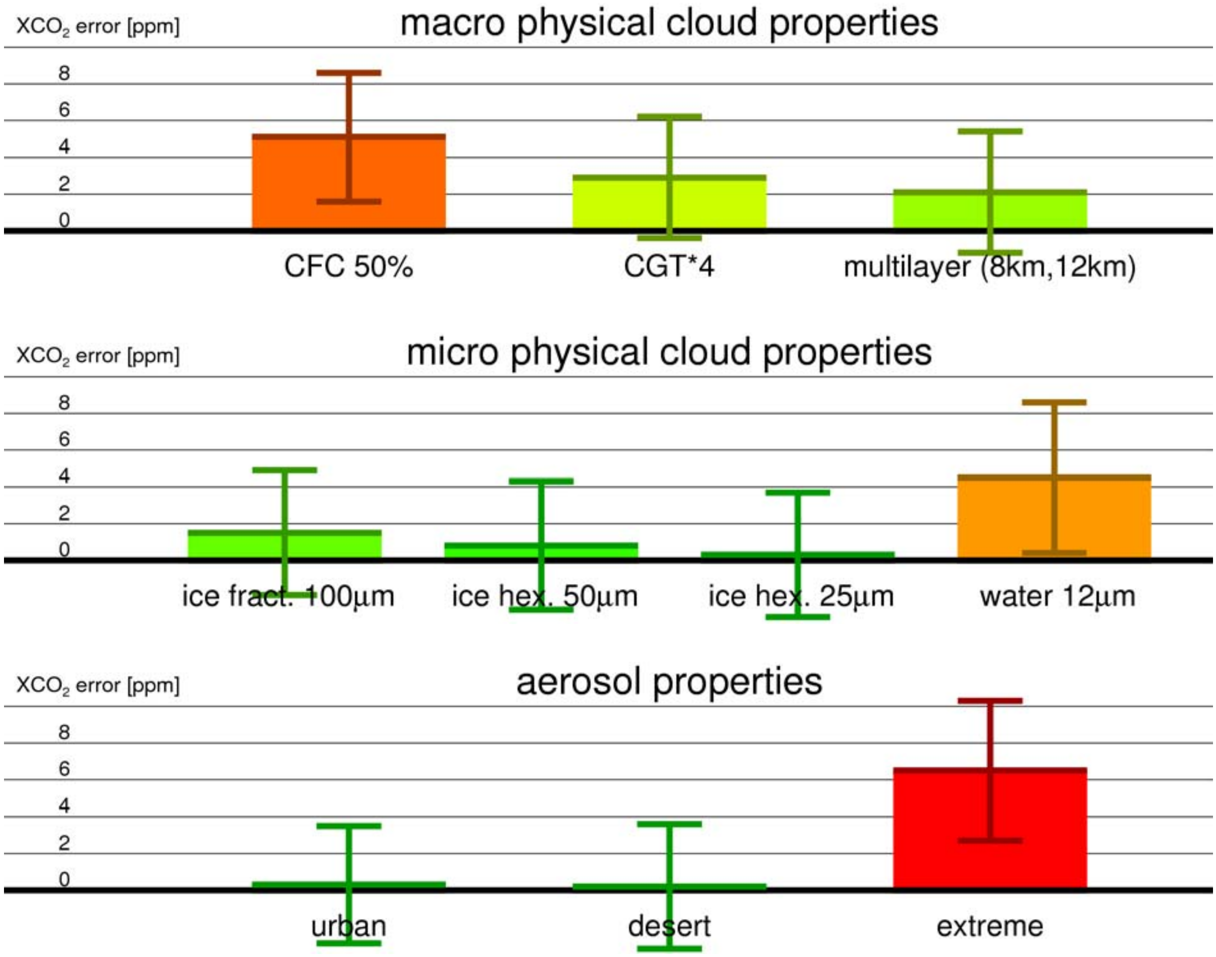

Figure 4: Absolute systematic and stochastic errors of the retrieved XCO_2 when modifying parameter vector elements.

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