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TOWARDS AN IMPROVED CO_2 RETRIEVAL ALGORITHM FOR SCIAMACHY ON ENVISAT

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ABSTRACT

Global satellite observations of the column-averaged dry-air mixing ratio of CO_2, denoted XCO_2, in combination with inverse modeling has the potential to reduce currently large uncertainties of regional CO_2 surface fluxes. This requires very high accuracy and sensitivity to the lower troposphere. The only instrument with high surface sensitivity prior to the launch of GOSAT (launch 2009) is SCIAMACHY on ENVISAT. It has been shown that XCO_2 spatio-temporal variations of a few ppm can be detected with SCIAMACHY (after averaging) when using the WFM-DOAS version 1.0 (WFMDv1.0) retrieval algorithm. Detailed comparisons with state-of-the-art global CO_2 models show however significant differences, which are not well understood. In order to assess to what extent these differences can be explained by retrieval biases - and to generate an improved SCIAMACHY XCO_2 data product in the future - we started to develop an advanced retrieval algorithm called BESD (Bremen optimal EStimation DOAS). Here an initial implementation of BESD (version 0.1) is described and first retrieval results are presented based on simulations and real data. BESD aims at combining the advantages of DOAS and Optimal Estimation (OE) primarily to reduce scattering related errors caused by aerosols and residual clouds. BESD permits simultaneous multi fit-window retrievals using the relevant absorption bands of CO_2 (1.58 µm) and O_2 (0.76 µm). BESD will be further developed in the future. This will comprise the use of *a-priori* information on aerosols and clouds from various information sources. The ultimate goal of this activity is to produce an XCO_2 data set covering the entire lifetime of SCIAMACHY (2003 to about 2013) with a quality high enough for regional CO_2 surface flux inverse modeling on the global scale as needed by projects such as the GMES atmosphere project MACC.

1. INTRODUCTION

Carbon dioxide (CO_2) is the most important anthropogenic greenhouse gas causing global warming [11]. Despite its importance our knowledge about CO_2 sources and sinks has significant gaps [10]. Appropriate knowledge about the CO_2 sources and sinks is needed for reliable prediction of the future climate of our planet [10].

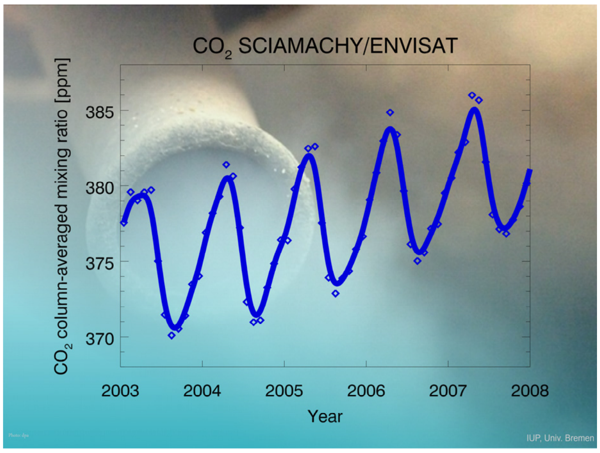


Fig. 1: Time series of atmospheric CO_2 as retrieved from SCIAMACHY using WFMDv1.2 (see Schneising et al., this issue). Each symbol shows a monthly average of the northern hemispheric XCO_2 in ppm. The solid line is based on smoothing the monthly averages. Clearly visible is the annual CO_2 increase primarily caused by burning of fossil fuels (as indicated by the photo in the background showing an automobile exhaust plume; photo: dpa). The strong CO_2 seasonal cycle is mainly due to CO_2 uptake and release by the terrestrial biosphere.

It has been identified that satellite observations of CO_2 can add important information to better constrain regional CO_2 surface fluxes than currently possible with the very accurate and precise but sparse network of surface stations [14]. This requires high accuracy of the satellite retrievals because even very small regional biases would lead to significant errors of the inferred surface fluxes [10].

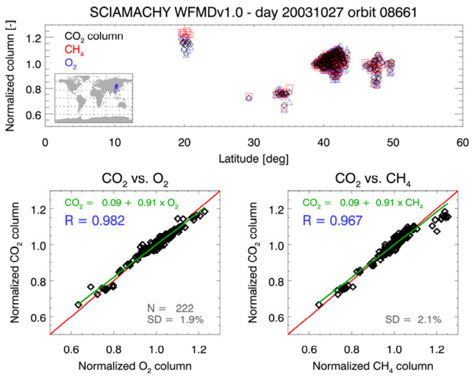
It has been shown that SCIAMACHY [1] has the potential to contribute to a significant uncertainty reduction of the terrestrial CO_2 surface fluxes [9]. At the Institute of Environmental Physics (iup) of the University of Bremen, Germany, the WFM-DOAS (WFMD) retrieval algorithm has been developed and is continuously being improved to retrieve information about CO_2 [8,16] (Fig. 1) and other important atmospheric gases from the SCIAMACHY nadir spectra such as methane (CH_4) [17] and carbon monoxide (CO) [7].

Version 1.0 of WFM-DOAS (WFMDv1.0) has been used to retrieve column-averaged mixing ratios (mole fractions) of CO_2, denoted XCO_2, from all available SCIAMACHY nadir spectra during 2003-2005 [16]. It has been shown by comparison with ground-based FTS retrievals, global models such as NOAA's CarbonTracker, surface CO_2 observations and other data sets such as anthropogenic CO_2 emission inventories and population density, that SCIAMACHY can detect spatio-temporal CO_2 variations of a few ppm after spatio-temporal averaging (see [16] and references given therein). It has also been shown that significant differences exist when comparing the SCIAMACHY WFMDv1.0 XCO_2 retrievals with a state-of-the-art global CO_2 model such as CarbonTracker [12]. Both data sets - model and satellite - suffer from several error sources. CarbonTracker is based on assimilating sparse CO_2 surface observations and relies significantly on the quality of the underlying terrestrial biosphere model and the accuracy of the description of (vertical) transport. The satellite retrievals are also not perfect. Retrieval biases may be caused by unaccounted variability of aerosols and residual clouds which leads to scattering related light path errors. In [16] it is pointed out that a large fraction of the difference between SCIAMACHY and CarbonTracker over the southern hemisphere may be due to unaccounted scattering by thin cirrus clouds.

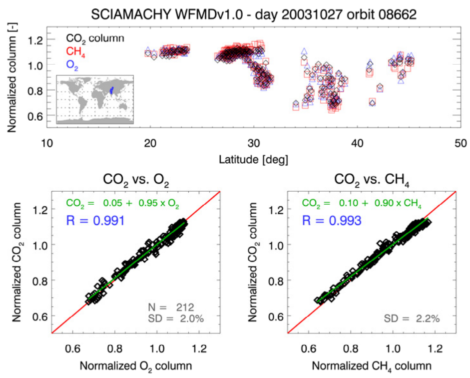
When comparing uncertain data sets it is difficult to identify what fraction of the observed difference is due to which data set. Therefore we are investigating if indications for shortcomings of the SCIAMACHY WFMDv1.0 XCO_2 data product can be identified by an analysis of the SCIAMACHY data product without relying on external data sets. One approach is to compare the retrieved CO_2, O_2 and CH_4 columns. As an example, Fig. 2 shows WFMDv1.0 results for three orbits from 27 Oct. 2003. WFMD is based on independent single fit-window retrievals. For the greenhouse gas data product, which comprises XCO_2 and XCH_4, three fitting windows are used [16,17]: one to determine the CO_2 vertical column, one to get the O_2 vertical column and one to get the CH_4 vertical column. In a second step the independently retrieved CO_2 and O_2 columns are used to compute XCO_2, and the CH_4 and CO_2 columns are used to compute XCH_4.

Fig. 2a shows an example of what one would expect from what is known about the relative (percentage) variability of the column-averaged mixing ratios of these gases due to their sources and sinks along an orbit (O_2: << 1%, CO_2: ~2%, CH_4: several percent), namely typically a higher correlation of CO_2 with O_2 (here R=0.982; standard deviation (SD) of the column ratios: 1.9%) compared to the correlation of CO_2 with CH_4 (R=0.967, SD=2.1%), mainly because of the relatively high variability of methane. Fig. 2a shows that at around 20°N the (normalized) methane column is a few percent higher compared to CO_2 and O_2 due to methane emissions from, e.g., rice paddies in south-east Asia. Far away from strong methane emission sources it is however typically observed that the agreement between CO_2 and CH_4 is similar or even significantly better compared to CO_2 and O_2. Figs. 2b and 2c show examples for this. This is most likely due to light path errors, which cancel better in the CO_2 to CH_4 ratio (because these to gases are retrieved from near-by spectral regions) compared to the CO_2 to O_2 column ratio (because these two gases are retrieved from spectrally distant spectral regions with quite different sensitivities to scattering processes).

(a)



(b)



(c)

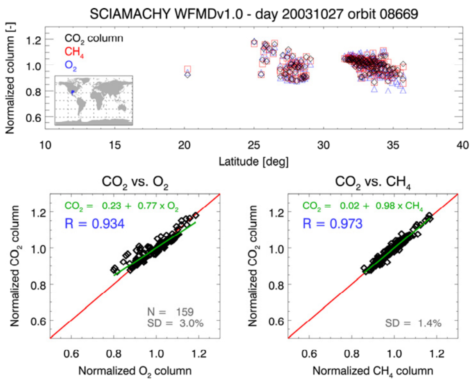


Fig. 2: SCIAMACHY/WFMDv1.0 CO_2, O_2, and CH_4 columns and their correlations for three orbits from 27. Oct. 2003 ((a): orbit 8661 covering parts of south-east Asia, (b): 8662 (Himalayas and India), (c): 8669 (north America)). The vertical columns are normalized by their mean value. The (single) top figures of each panel show the retrieved columns as a function of latitude. The (two) figures at the bottom of each panel show scatter plots of pairs of columns (N: number of retrievals classified "good" by WFMDv1.0, SD: standard deviation of the column ratios).

The WFMD algorithm [3-8,16,17], which is based on least-squares fitting a linearized radiative transfer model (RTM) to the SCIAMACHY sun-normalized radiance spectra, is a very fast algorithm based on a look-up-table (LUT) approach of pre-calculated radiances and their derivatives. Single (constant) vertical profiles of CO_2, aerosols, etc., are used for the retrieval to obtain the linearization point for the radiative transfer (RT) simulations. The retrieved columns are not constrained by *a-priori* information about their assumed variability. This has advantages and disadvantages. An important advantage is that the observed (retrieved) variability is free of any influence of the assumed variability of the parameter of interest. WFM-DOAS has no knowledge about spatio-temporal CO_2 variations (apart from variations of surface topography). For example, the annual CO_2 increase shown in Fig. 1 comes entirely from the SCIAMACHY spectra. The algorithm has no knowledge about increasing CO_2 levels or that CO_2 has a seasonal cycle. Another important advantage of using a single atmospheric scenario for the retrieval is that this limits the number of needed RT simulations and permits the use of a RTM LUT of manageable size and therefore permits fast retrievals – a very important aspect. A disadvantage is that for parameters, which influence the RT but are not retrieved using WFMD, such as aerosols and thin clouds, it would potentially be highly beneficial to better consider them in the retrieval. An important aspect in this context is the limited *a-priori* information on aerosols and thin clouds but also the limited information on these parameters in the SCIAMACHY spectra. The aim of the ongoing development of the new BESD algorithm, which will be described in the next section and in [13], is to make optimum use of the available information.

2. RETRIEVAL ALGORITHM "BESD"

The new Bremen optimal EStimation DOAS (BESD) algorithm will be based – as the name suggests - on Optimal Estimation (OE) [15] (see also [2]). BESD permits to consider uncertain *a-priori* information, e.g., on aerosols and cirrus clouds, to constrain the retrieval.

Databases with *a-priori* information on aerosols and clouds are currently under construction and are therefore not used for the results presented here. Information sources are satellite instruments on ENVISAT (e.g., AATSR, MERIS), instruments on other satellites (e.g., MODIS, CALIOP), either directly (individually or merged) or after assimilation into a model (e.g., the GEMS aerosol product). We are also assessing to what extent currently unexploited scattering information from SCIAMACHY can be used, e.g., from the saturated water band around 1.37 µm located in SCIAMACHY channel 6.

For the initial implementation and results presented here only the information contained in three spectral regions covered by SCIAMACHY has been used: the O_2 A-band spectral region around 760 nm, a weak CO_2 band around 1.58 µm and a weak methane band around 1.66 µm (see Fig. 3). The state vector elements and their assumed *a-priori* uncertainties are listed in Tab. 1. All parameters are assumed to be uncorrelated. For the retrieval a three layer atmosphere is used here (for the RT simulations a higher vertical resolution is used). The definition of the vertical layers is based on the surface pressure p_o: The lower troposphere (LT) is defined as the range from 0.4-1.0 (in units of p_o), the upper troposphere (UT) from 0.15-0.4, and the stratospheric (ST) layer from 0-0.15.

Note that here only one of the many possible settings for BESD is discussed. A detailed discussion concerning more sophisticated settings (e.g., using dedicated cloud parameter Jacobians) is given in [13].

How BESD works is illustrated in Fig. 3 using simulated SCIAMACHY nadir measurement. Shown are the most relevant BESD input and output data and parameters.

Initial BESD state vector elements			
#	**ID**	**Comment**	**Uncertainty (relative) [-]**
		Polynom 757 – 772 nm	
22	POLa02	Quadratic term	1000
21	POLa01	Linear term	1000
20	POLa00	Constant term	1000
		Polynom 1558 – 1595 nm	
19	POLb02	Quadratic term	1000
18	POLb01	Linear term	1000
17	POLb00	Constant term	1000
		Polynom 1630 – 1669 nm	
16	POLc02	Quadratic term	1000
15	POLc01	Linear term	1000
14	POLc00	Constant term	1000
13	O2__02	O_2 ST	0.001
12	O2__01	O_2 UT	0.001
11	O2__00	O_2 LT	0.002
10	AES_02	Scattering ST	0.05
9	AES_01	Scattering UT	5.0
8	AES_00	Scattering LT	1.0
7	H2O_00	$H_2O(z)$ scaling	2.0
6	TEM_00	T(z) scaling	0.10
5	CH4_02	CH_4 ST	0.02
4	CH4_01	CH_4 UT	0.08
3	CH4_00	CH_4 LT	0.16
2	CO2_02	CO_2 ST	0.01
1	CO2_01	CO_2 UT	0.04
0	CO2_00	CO_2 LT	0.06

Tab. 1: Initial BESD state vector elements and their associated uncertainties. From top to bottom: polynomial coefficients (POL), O_2 layer columns (LT: lower troposphere, UT: upper troposphere, ST: stratosphere), aerosol and cloud layer scattering optical depth (AES), scaling factors for H_2O and temperature profile, CH_4 and CO_2 layer columns.

As can be seen from Fig. 3a, the low-resolution 3-layer CO_2, CH_4 and scattering profiles can be well retrieved and a large uncertainty reduction has been obtained especially in the lower troposphere. For O_2 the uncertainty reduction is small because O_2 is strongly constrained also in the troposphere. The assumption here is that O_2 (and surface pressure) is well enough known but CO_2, CH_4, aerosols and thin clouds not. The *a-priori* uncertainty of the CO_2 column is assumed to be 3.9%, which is reduced to 1.0% *a-posteriori*. The CH_4 column *a-priori* uncertainty is 9.8%, which is reduced to 2.1% *a-posteriori*. The true scattering vertical optical depth (in the following referred to as AOD, where AOD = sum of layer AES; the AES are the fit parameters for aerosol and cloud layer scattering optical depth listed in Tab. 1) of aerosols and clouds is 0.2 (at 1.6 µm; 0.4 at 760 nm). The retrieved AOD is 0.19 (the assumed *a-priori* AOD is 0.1). The results shown are valid for an albedo of 0.1 and a solar zenith angle of 50^o. The atmospheric condition roughly corresponds to northern mid-latitude summer conditions with lower tropospheric CO_2 compared to a yearly average and higher tropospheric CH_4. The difference between the true and the retrieved CO_2 column is –0.5% ("Bias" in green in the bottom row; includes the smoothing error), the CH_4 column bias is 1.8% and the O_2 column bias is –0.6%. The CO_2 column smoothing error is 0.35% and the CH_4 column smoothing error is 0.52%. As XCO_2 is essentially the ratio of the retrieved CO_2 and the O_2 column, the XCO_2 bias is +0.1% (0.4 ppm) due to nearly perfect cancellation of the CO_2 and O_2 column errors. This example indicates that XCO_2 can be well retrieved despite large uncertainties due to aerosols and clouds. This is promising but only a necessary (and not a sufficient) condition for an improved XCO_2 data product, as reality is more complex.

Fig. 3b shows the corresponding Jacobian or "K" matrix. This matrix consists of derivatives, one for each state vector element, which correspond to the percentage change of the sun-normalized radiance per percentage change of the corresponding parameter (exception: polynomial). As can be seen, the derivatives for O_2 and scattering (AES) are significantly correlated at SCIAMACHY spectral resolution. The derivatives therefore indicate that both parameters, O_2 and AES, cannot be fully independently retrieved. This is the main reason for the strong constrained used here for O_2 (or, essentially equivalent, surface pressure).

Fig. 3c shows details for all state vector elements. As can be seen, an uncertainty reduction larger than 50% has been achieved for CO_2 and CH_4 in the lower troposphere, the H_2O column, the tropospheric scattering parameters, and all polynomial coefficients.

Fig. 4 shows BESD results for the same model atmosphere except different scattering profiles (Fig. 4a-4d) and for less constrained O_2 in the lower troposphere. Fig. 4a shows that the XCO_2 bias (here essentially the CO_2 column smoothing error) is 0.23% if the true scattering profile is equal to the assumed *a-priori* profile. Figs. 4b-4d show retrievals for three cases where the true scattering profiles (shown in green) differ significantly from the assumed *a-priori* profile (black). In all cases the scattering profiles can be retrieved reasonably well with large uncertainty reduction in the troposphere (the retrieved profiles are shown in red). The same is true for CO_2 and CH_4. Fig. 4e however shows that a large response (significant error) of the retrieved O_2 column is observed, if the O_2 *a-priori* uncertainty in the lowest layer is relaxed to 3% (instead of 0.2%). This is due to the significant correlation of the O_2 and scattering (AES) Jacobians. Because of this we also investigate approaches using different settings for BESD than the one discussed here [13].

3. INITIAL BESD RETRIEVALS

To apply the BESD algorithm to real SCIAMACHY data, a simple initial RTM LUT scheme has been developed, which will also be further improved in the future. This LUT consists of radiances and their derivatives for different scenarios. Parameters covered are the solar zenith angle (SZA), surface albedo, and the surface elevation (pressure). The LUT consists of 450 scenarios covering all relevant wavelengths and layer altitudes. The size is approx. 2 gigabytes. A simple next neighbor scheme is used to select an appropriate scenario for a given SCIAMACHY measurement. The SZA is obtained from the Level 1 files. The surface elevation is determined using a surface elevation data base and the geo-location information given in the Level 1 files. For the surface albedo a simple LUT scheme has been developed using the transparent spectral regions in each spectral fitting window.

The first BESD retrievals obtained using the newly implemented algorithm using real SCIAMACHY data are shown in Figs. 5 and 6. Two sites have been selected for initial tests, Sahara and Park Falls, Wisconsin, USA. The Sahara site has been chosen to see how BESD performs under extreme desert dust storm conditions. Under these conditions most of the WFMDv1.0 XCO_2 results are significantly overestimated and need to be filtered using an absorbing aerosol index (AAI) satellite data product as described in [16]. The results shown in Fig. 5 suggest that BESD seems to be less sensitive to desert dust storm aerosol compared to WFMDv1.0. The retrieved AOD correlates to some extent with the AAI. The AODs are shown as anomalies (i.e., the corresponding mean value has been subtracted; note that the mean value of the AOD as retrieved by BESD is negative). Park Falls has been selected because it represents northern mid-latitude conditions. The results shown in Fig. 6 indicate that BESD performs quite similar as WFMDv1.0. The retrieved AOD shows a reasonable correlation with the AOD from MODIS (R=0.58). The absolute values are however often unphysical (negative) - an important finding that needs further study.

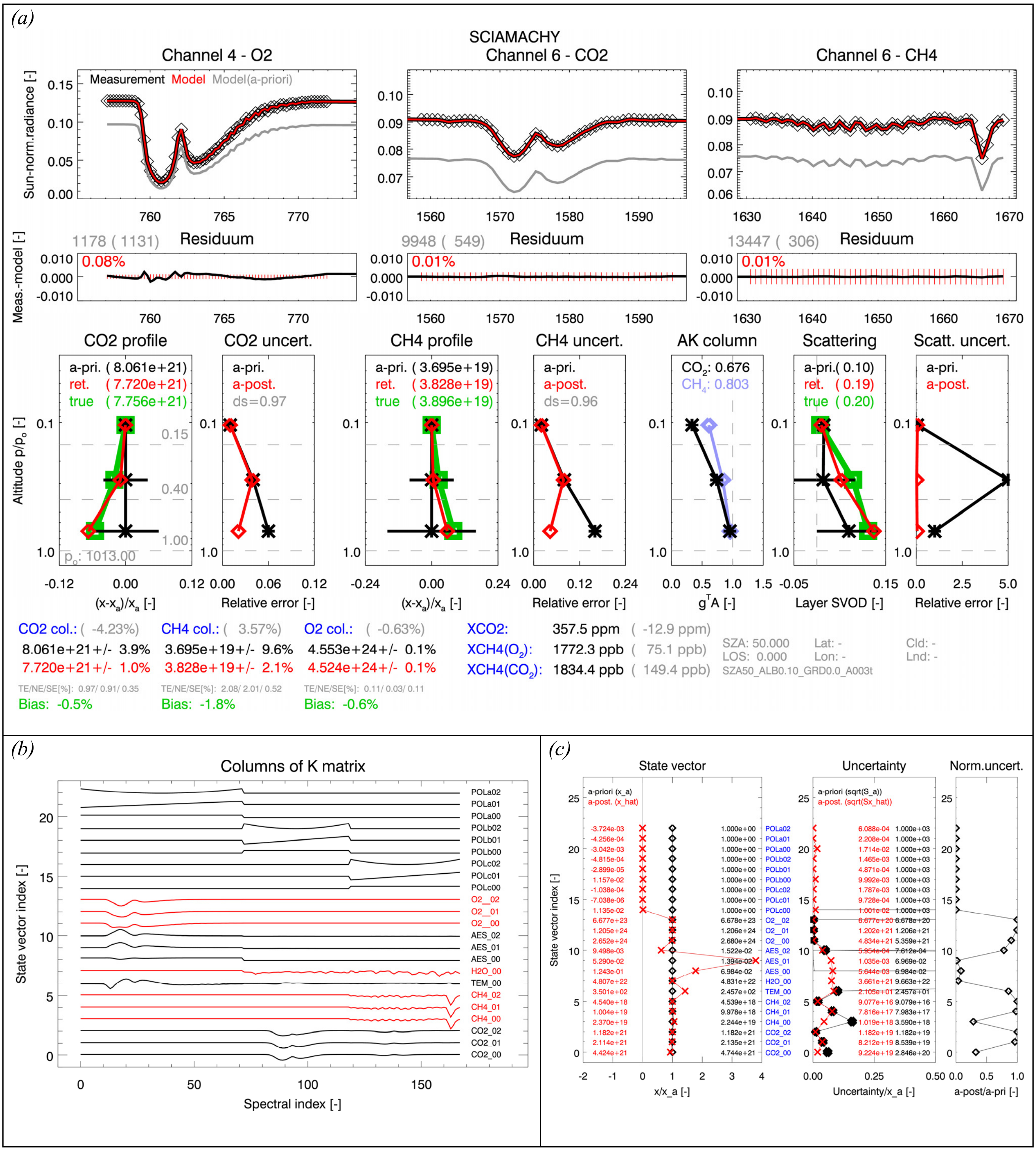


Fig. 3: (a) Shown in the top row are simulated SCIAMACHY nadir measurements (black symbols) for the three spectral regions covering O_2 (left), CO_2 (middle) and CH_4 (right) absorption bands. The a-priori spectrum is shown in grey. It has been simulated using a model atmosphere, which differs from the model atmosphere used for the simulated measurements. The differences are: (i) the CO_2 profile (the true profile – normalized to the a-priori profile (black) - is shown in green in the bottom left panel), (ii) the CH_4 profile (bottom middle panels), and (iii) the scattering coefficient profile (bottom right). The retrieved profiles are shown in red. All profiles are shown with their uncertainties. Also shown in the bottom row are the CO_2 and CH_4 vertical column averaging kernels. The panels in the second row show the fit residuum, i.e., the relative difference between the measurement and the fitted RTM after the BESD fit. The root-mean-square (RMS) of the fit residuals in the three fitting windows are also listed (the values are very small, e.g., 0.01% for CO_2, as no noise has been added to the spectra). The assumed signal-to-noise ratios of the spectra are given in grey in brackets. (b) Corresponding Jacobian ("K") matrix. (c) Detailed information about the state vector elements and their a-priori and a-posteriori uncertainties (see also Tab. 1).

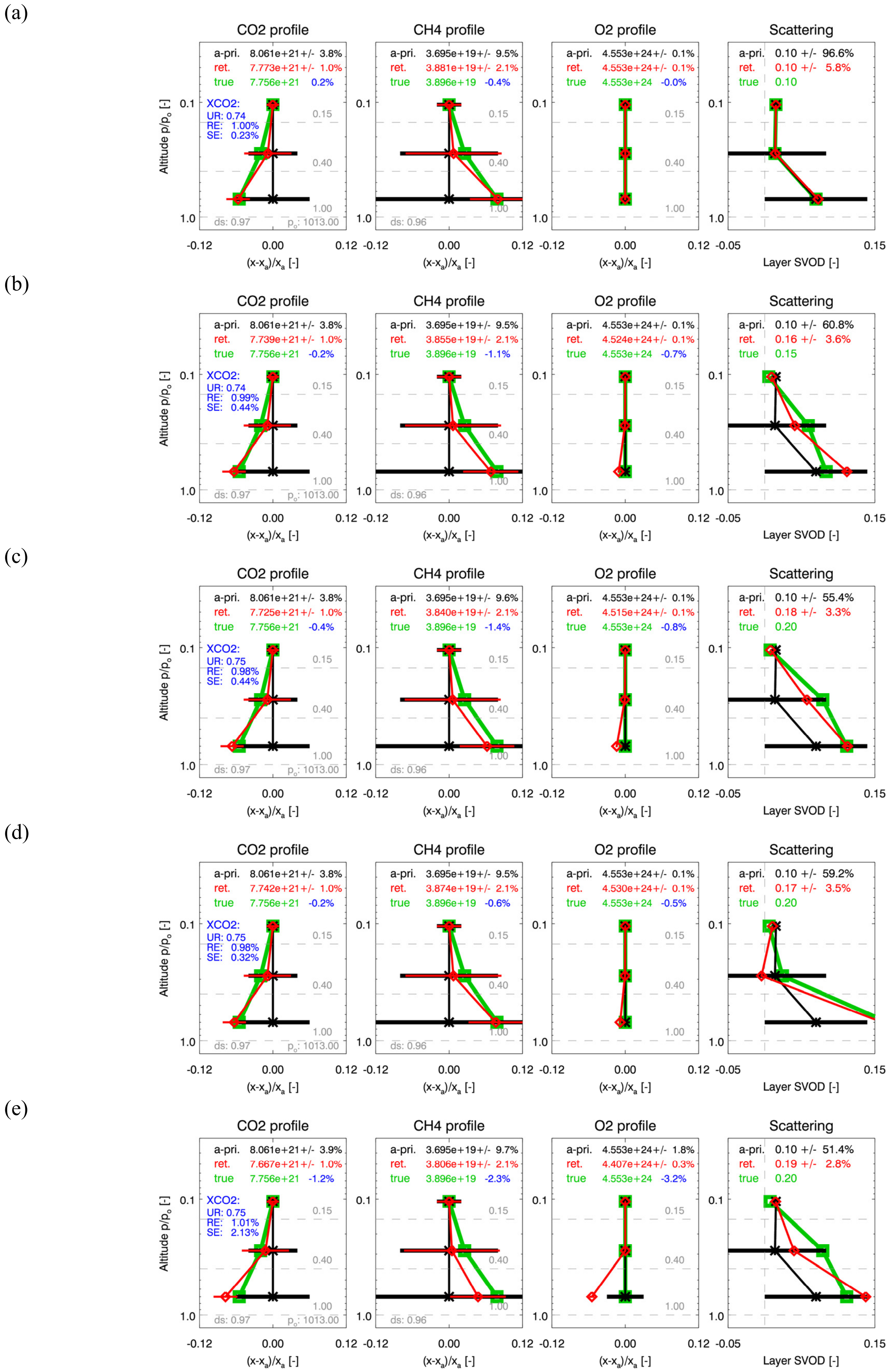


Fig. 4: Results of simulated BESD retrievals using different scattering profiles: (a) true scattering profile (green) equal to a-priori profile, (b-d) true scattering profiles significantly different from the a-priori profile. (e) as (c) but for relaxed O_2 a-priori uncertainty in the lowest layer (+/-3% instead of +/-0.2%). The following numbers are given for XCO_2: Uncertainty reduction (UR), retrieval random error (RE), and systematic error (SE; includes the smoothing error).

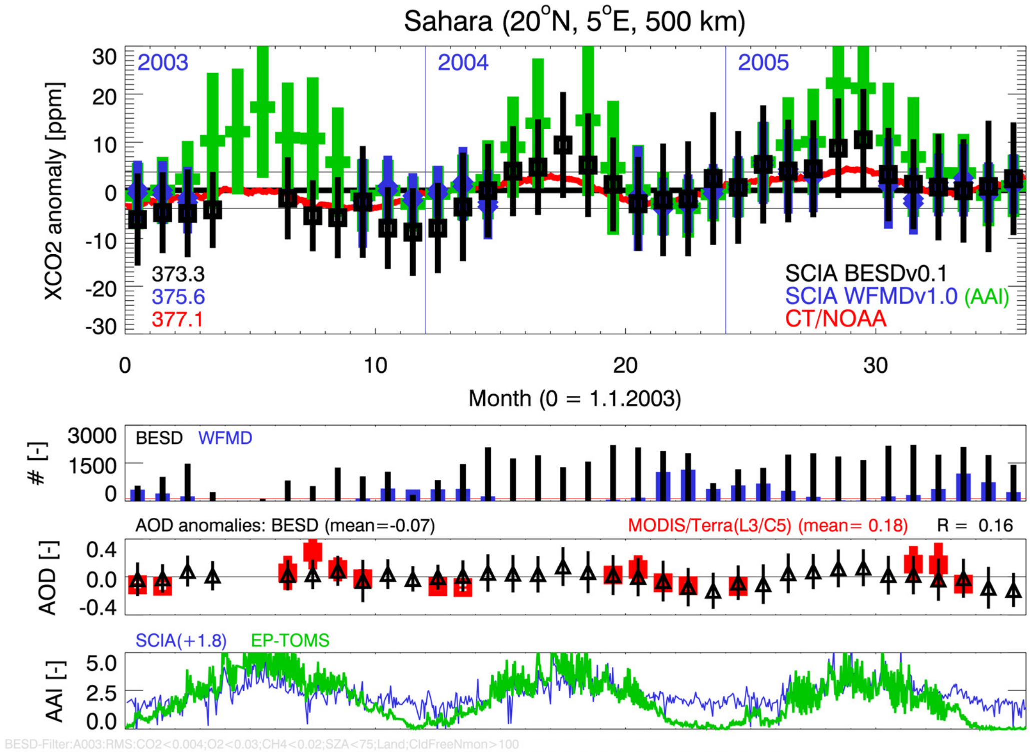


Fig. 5: First results of the BESD retrieval algorithm as applied to real SCIAMACHY data. Shown are 3 years of BESD XCO_2 retrievals over the Sahara. Top panel: BESD XCO_2 monthly averages and corresponding standard deviations are shown in black. Red: CarbonTracker XCO_2. Green: WFMDv1.0 XCO_2 without absorbing aerosol index (AAI) filtering (overestimated in case of strong desert dust storms, i.e., when AAI is high). In blue the final AAI filtered WFMDv1.0 XCO_2 data product is shown. The bottom panel shows EarthProbe TOMS AAI (green) and SCIAMACHY AAI (blue). 2^{nd} panel: Number of "good" BESD and AAI filtered WFMDv1.0 XCO_2 retrievals per month. 3^{rd} panel: BESD retrieved AOD (black, AOD = layer AES summed over all layer). For comparison the MODIS AOD at 550 nm is shown in red. The XCO_2 and the AODs are shown as anomalies, i.e., with corresponding mean values subtracted.

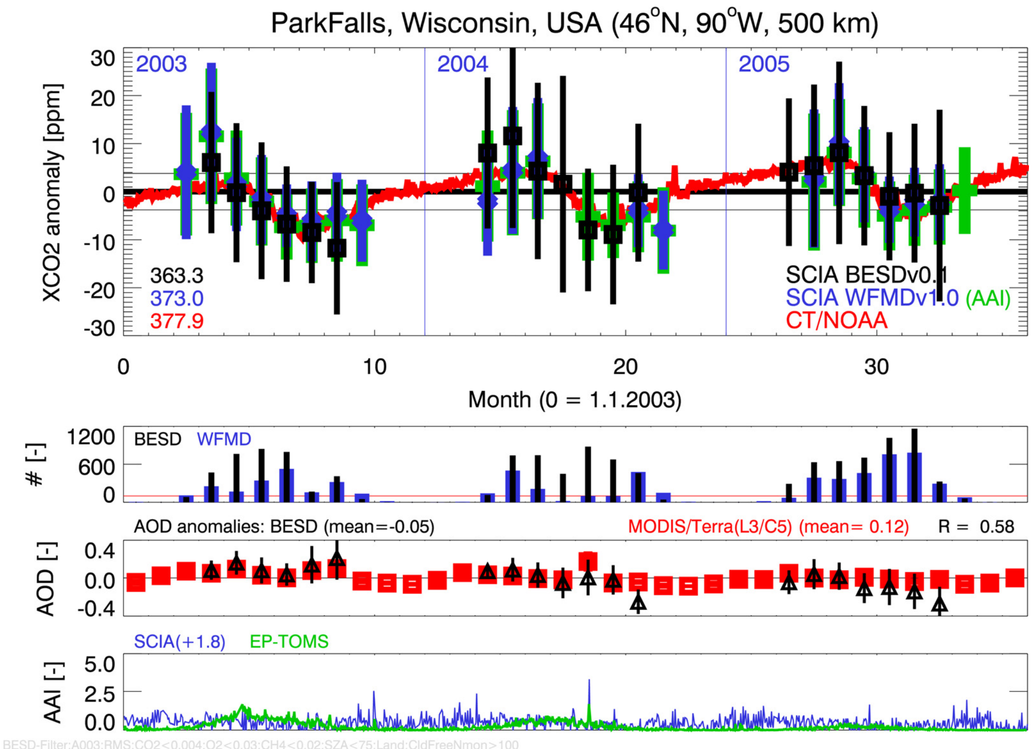


Fig. 6: As Fig. 5 but for Park Falls, Wisconsin, USA.

5. SUMMARY

First results from a new retrieval algorithm called BESD have been presented. BESD is under development to generate an improved SCIAMACHY XCO_2 data product in the future. BESD aims at combining the advantages of DOAS and Optimal Estimation and permits simultaneous multi spectral fit-window retrievals and the use of *a-priori* information on aerosols and clouds in order to reduce scattering related XCO_2 errors. The first results presented here are encouraging but also indicate that a significant amount of further study and development work is needed before an improved SCIAMACHY XCO_2 data product will be available generated with BESD.

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