INTERCOMPARISON OF NEAR INFRARED SCIAMACHY AND THERMAL INFRARED NADIR VERTICAL COLUMN DENSITIES

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ABSTRACT

Nadir infrared (IR) sounding can be used to derive information on trace gases relevant for climate and air quality. For vertical column density retrievals using SCIAMACHY near IR nadir observations, the BIRRA (Beer InfraRed Retrieval Algorithm) code has recently been implemented in the operational level 1 – 2 processor. For analysis of thermal IR nadir observations of AIRS, GOSAT, IASI, or TES, a closely related code CERVISA (Column EstimatoR Vertical Infrared Sounding of the Atmosphere) has been developed. Both codes share a large portion of modules, e.g., for line-by-line absorption and the nonlinear least squares solver. The essential difference is the part of the forward model devoted to radiative transfer through the atmosphere, i.e., Beer's law for the near IR versus Schwarzschild's equation for the thermal IR. For the ongoing validation of the BIRRA carbon monoxide CO and methane CH_4 products intercomparisons with thermal IR sounding data are performed. CERVISA retrieval results are compared both to the operational products of the IR sounder considered and to SCIAMACHY products retrieved with BIRRA.

Key words: Atmosphere, Remote Sensing, Carbon monoxide,ENVISAT-SCIAMACHY, AQUA-AIRS.

1. INTRODUCTION

Verification and validation is mandatory in computational science [1] and has been established as an integral part of (the assessment of) all atmospheric sounding missions. Whereas verification ("Is the code correct?") is frequently performed by means of code intercomparisons [e.g., 2, 3], a comparison of retrieval results with independent characterizations of the atmospheric state is essential for validation ("Is it the correct code?"). Clearly the true state of the atmosphere is difficult to obtain, so comparisons with retrievals using other remote sensing instruments are frequently used.

Nadir sounding of molecular column densities is well established in atmospheric remote sensing. Concentration profiles and/or vertical column densities (VCD's) are successfully retrieved from data recorded by infrared (IR) as well as ultraviolet–visible instruments. For the operational level 2 data processing of SCIAMACHY near IR observations, the "BIRRA" (Beer InfraRed Retrieval Algorithm) code has been developed at DLR [4] and recently been implemented as part of the official level 1b – 2 operational processor [5]. In view of the similarities between column density retrievals in the near and mid IR, a modified version of BIRRA called CERVISA (Column EstimatoR Vertical Infrared Sounding of the Atmosphere) has been implemented recently for level 1 – 2 processing of nadir thermal IR sounding data.

Carbon monoxide is an important trace gas affecting air quality and climate that is highly variable in space and time. About half of the CO comes from anthropogenic sources (e.g., fuel combustion), and further significant contributions are due to biomass burning. CO is a target species of several spaceborne instruments, nb. AIRS, MOPITT, and TES from NASA's EOS satellite series, IASI on MetOp, and MIPAS and SCIAMACHY on ESA's Envisat. Results of CO retrievals from AIRS and SCIAMACHY observations for several orbits along the eastern Africa coast line in October 2003 are presented here.

2. RETRIEVAL METHODOLOGY

2.1. Near vs Mid Infrared Radiative Transfer

The BIRRA and CERVISA forward models are based on MIRART/GARLIC [6], a line-by-line code for arbitrary observation geometry (up, down, limb) instrumental field-of-view and line shape that provides Jacobians by means of automatic differentation [7] and has been verified in extensive intercomparisons [e.g. 2, 8].

The intensity (radiance) I at wavenumber ν received by an instrument at $s = 0$ is described by the equation of

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radiative transfer [9]

$$I(\nu) \;=\; I_{\rm b}(\nu)\,\mathcal{T}(\nu) \;-\; \int_0^\infty {\rm d}s'\, J(\nu,s)\, \frac{\partial \mathcal{T}(\nu;s')}{\partial s'}, \quad (1)$$

where $\mathcal{T}$ is transmission, $I_{\rm b}$ is a background contribution, and J is the source function. The instrument is taken into account by convolution of the monochromatic intensity spectrum (1) with a spectral response function $\mathcal{S}$,

$$\widehat{I(\nu)} \equiv (I \otimes \mathcal{S})(\nu) = \int_{-\infty}^{\infty} I(\nu) \times \mathcal{S}(\nu-\nu')\, {\rm d}\nu' \,. \quad (2)$$

In the near infrared, reflected (and scattered) sunlight becomes important, whereas thermal emission is neglegible. For clear sky observations scattering can be neglected, hence

$$\begin{aligned} I(\nu) \;&=\; r(\nu)\, I_{\rm sun}(\nu)\, \mathcal{T}_\uparrow(\nu)\, \mathcal{T}_\downarrow(\nu) \qquad (3)\\ &=\; r I_{\rm sun} \times \exp\left[-\int_0^\infty \frac{{\rm d}z'}{\mu} \sum_m \alpha_m \bar{n}_m(z')\, k_m(\nu,z')\right] \\ &\qquad \times \exp\left[-\int_0^\infty \frac{{\rm d}z''}{\mu_\odot} \sum_m \alpha_m \bar{n}_m(z'')\, k_m(\nu,z'')\right] \end{aligned}$$

where r is reflection (albedo) and $\mathcal{T}_\uparrow$ and $\mathcal{T}_\downarrow$ denote transmission between reflection point (e.g. Earth surface at altitude $z_{\rm b}$) and observer and between sun and reflection point, respectively. k_m and $\bar{n}_m(z)$ are the (pressure and temperature dependent) absorption cross section and reference (e.g., climatological) density of molecule m, and α_m are the scale factors to be estimated. (Note that for simplicity we have used a plane–parallel approximation with $\mu \equiv \cos\theta$ for an observer zenith angle θ and $\mu_\odot$ for the solar zenith angle $\theta_\odot$; moreover continuum is neglected here.)

In the mid (thermal) infrared solar irradiance can be neglected, and the signal is a combination of attenuated surface emission and thermal emission of the atmosphere,

$$\begin{aligned} I(\nu) \;&=\; \epsilon(\nu)\, I_{\rm surf}(\nu)\, \mathcal{T}_\uparrow(\nu) \;+\; I_{\rm atm}(\nu) \qquad (4)\\ &=\; \epsilon(\nu)\, B(\nu, T_{\rm surf})\, \mathcal{T}_\uparrow(\nu) \\ &\qquad +\; \int_0^\tau B(\nu, T(\tau))\, \exp\left(-\tau'(\nu)\right) {\rm d}\tau' \end{aligned}$$

where τ denotes optical depth ($\mathcal{T} = {\rm e}^{-\tau}$) and $\epsilon = 1 - r$ denotes surface emissivity.

2.2. The inverse problem — nonlinear least squares

The standard approach to estimate the unknown $\boldsymbol{x}$ from a measurement vector $\boldsymbol{y}$ relies on (nonlinear) least squares

$$\min_x \|\boldsymbol{y} - \boldsymbol{F}(\boldsymbol{x})\|^2 \quad (5)$$

Here $\boldsymbol{F}$ denotes the forward model, and the unknown state vector $\boldsymbol{x}$ is comprised of the geophysical and auxiliary (e.g., instrumental) parameters.

For the nonlinear least squares problem (5) BIRRA and CERVISA use solvers of the PORT Optimization Library [10] based on a scaled trust region strategy. BIRRA and CERVISA provides the option to use a nonlinear least squares with simple bounds (e.g., nonnegativity) to avoid unphysical results. Note that the surface reflectivity r (and an optional baseline correction(s) b) enter the forward model $\boldsymbol{F} \equiv \widehat{I(\nu;\dots)}$ linearly and the least squares problem (5) can be reduced to a separable nonlinear least squares problem [11].

3. INTERCOMPARISON OF SCIAMACHY AND AIRS CARBON MONOXIDE

Nadir observations in the shortwave infrared channels of SCIAMACHY [12] onboard the ENVISAT satellite can be used to derive information on CO, CH_4, N_2O, CO_2, and H_2O, e.g., profiles of volume mixing ratio $q_X(z)$ or density $n_X(z) = q_X(z) \cdot n_{\rm air}(z)$ of molecule X. Unfortunately, the analysis of the NIR channels of SCIAMACHY is challenging because of

- — an increasing number of dead and bad pixels;
- — ice layer on channel 8 detector;
- — CO (and N_2O) are very weak absorbers (with $\mathcal{T}_{\rm CO} \approx 0.99$ for a vertical path)

Furthermore vertical sounding inversions are ill-posed, so it is customary to retrieve only column densities (VCD)

$$N_X \equiv \int_{z_{\rm ground}}^\infty n_X(z)\, {\rm d}z \;=\alpha_X \int_{z_{\rm ground}}^\infty n_X^{\rm (ref)}(z)\, {\rm d}z \,. \quad (6)$$

For CO retrieval from infrared nadir sounders such as AIRS [13] the situation is much better, in particular absorption of CO in the $4\,\mu{\rm m}$ band is stronger. Despite these drawbacks of SCIAMACHY it is nebertheles quite useful because of its greater sensitivity to the lower troposphere.

The BIRRA results retrieved from SCIAMACHY represent the "dry air column density", i.e., CO VCD corrected by the scaling factor of methane considered here as a proxy for cloud fraction and cloud top height, scattering, instrument issues, and climatology,

$${\rm xCO} \equiv N_{\rm CO} \times \frac{\alpha_{\rm CO}}{\alpha_{\rm CH4}} \,. \quad (7)$$

The data has been filtered according to the following criteria:

- Convergence of the fitting algorithm
- Solar zenith angle smaller than $80°$
- CO VCD positive and smaller than $1.5 \cdot 10^{19}\,{\rm cm}^{-2}$
- CH_4 scaling factor close to one, $0.7 \le \alpha'_{\rm CH4} \le 1.3$ (where $\alpha'_{\rm CH4}$ is throughput corrected)

Similar filtering is also used in case of CERVISA retrievals.

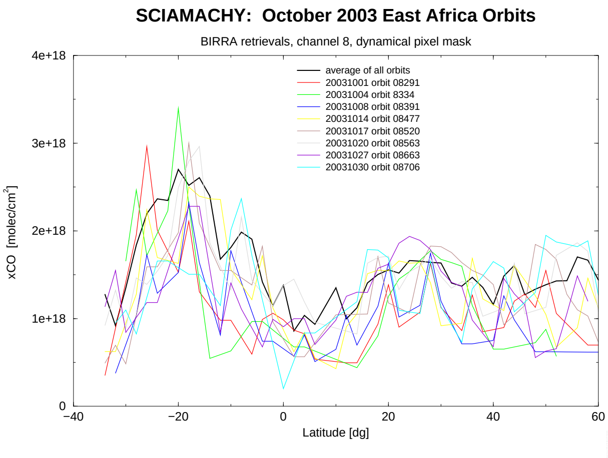

Figure 1. SCIAMACHY carbon monoxide vertical column densities retrieved from "East Africa orbits" and averaged over all longitudes within a 1 dg latitude bin (October 2003).

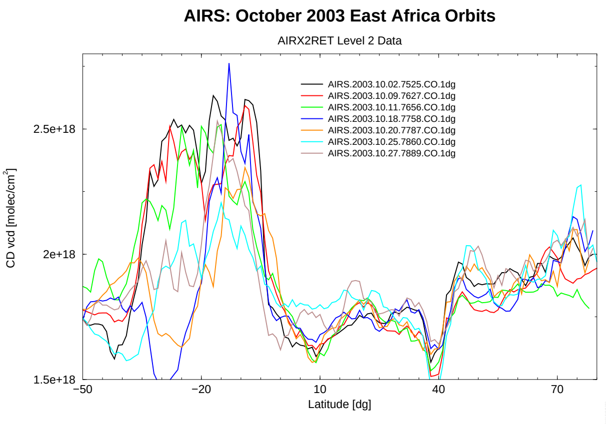

Figure 2. AIRS carbon monoxide vertical column densities averaged over all longitudes within a 1 dg altitude bin (AIRX2RET product). The labels refer to year, month, day, and orbit number.

3.1. Data and assumptions

This intercomparison is based on SCIAMACHY and AIRS Level 1 data of October 2003 covering Eastern Africa, see Fig. 1 and Fig. 2. In this observation period large biomass fire existed esp. in Mozambique, which should be clearly visible in CO column densities derived from nadir sounding instruments.

For the retrieval of carbon monoxide vertical column densities with BIRRA, level 1 data of SCIAMACHY channel 8 applying a dynamical bad/dead pixel mask [14] have been used; a single spectrum comprises about 50 data points in the interval 4282.7 to $4302.1\,\mathrm{cm}^{-1}$ $(2323 - 2335\,\mathrm{nm})$. Surface reflectivity was modelled with a second order polynomial, baseline was ignored. Scaling factors for CO, CH_4, and H_2O were fitted along with the Gaussian slit function half widths and the reflectivity coefficients.

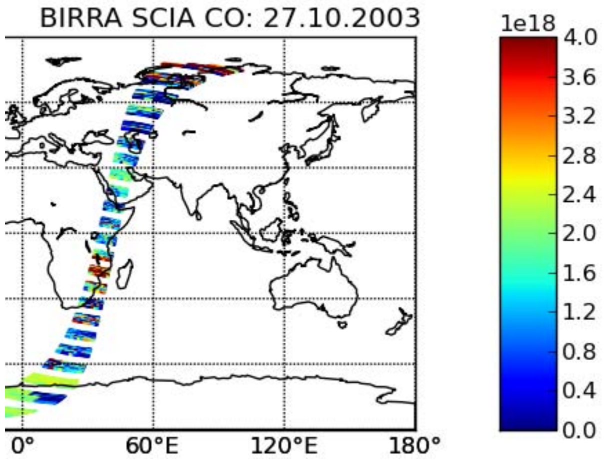

Figure 3. SCIAMACHY carbon monoxide vertical column densities from Orbit 8663, 27. October 2003. Single observations have been regridded and averaged into a $1^\circ \times 1^\circ$ global grid.

CO column density retrievals from AIRS were performed for several orbits in October 2003 passing over Mozambique. Note that all these orbits are night-time observations with a North-East to South-West flight direction ("parallel" to SCIAMACHY-Envisat, AIRS day-time observations originate from orbits with a North-West to South-East flight direction). According to McMillan et al. [15] the $2181 - 2220\ \mathrm{cm}^{-1}$ microwindow containing 42 spectral points is used for AIRS CO retrievals; to improve the quality of the CO_2 column fits, this window was extended to $2250\,\mathrm{cm}^{-1}$. In addition to the CO scaling factor, CO_2, H_2O, and N_2O are considered as unknowns, too.

For BIRRA SCIAMACHY retrievals pressure and temperature profiles were read from the CIRA dataset [16], providing monthly mean values for the altitude range $0 - 120\,\mathrm{km}$ with almost global coverage (80N – 80S in 5dg steps). Trace gas concentrations were taken from a coarse resolution version of the US standard atmosphere.

For CERVISA AIRS retrievals atmospheric temperature profiles were taken from the AIRS Level 2 data product and averaged for every scan line (across track). Likewise the surface temperature as given by AIRS L2 were used as input.

For BIRRA and CERVISA molecular absorption was modelled using the HITRAN2008 database [17]) along with the CKD continuum corrections [18]. The spectral response function was assumed to be Gaussian.

3.2. Results

Carbon monoxide vertical column densities as a function of latitude are shown for SCIAMACHY–BIRRA retrievals in Fig. 1; Corresponding AIRS Level 2 data extracted from the AIRX2RET product files are plotted in

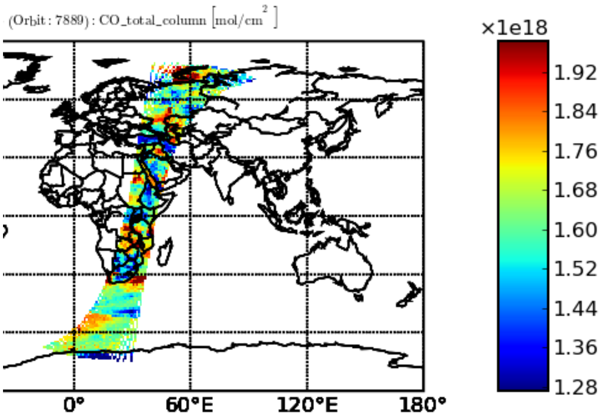

Figure 4. AIRS carbon monoxide vertical column densities from Orbit 7889, 27. October 2003 (AIRX2RET product).

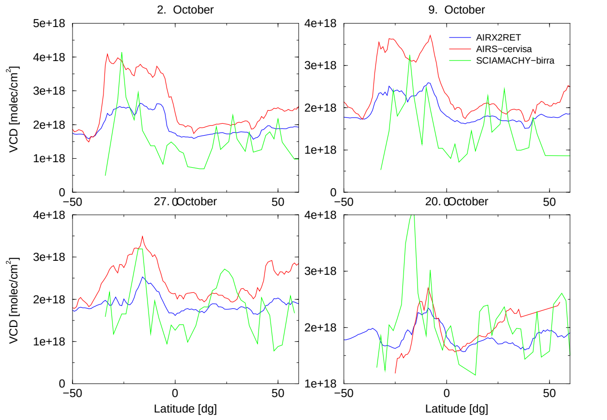

Figure 5. Carbon monoxide vertical column densities averaged over all longitudes within a 1 dg altitude bin: AIRS Level 2 product (AIRX2RET) vs. AIRS–Cervisa retrievals vs. SCIAMACHY–Birra retrievals.

Fig. 2. Enhanced CO columns over south–East Africa can be cleary seen in both plots; furthermore, both products show a minimum in the equatorial region and a slight increase towwards northern latitudes. However, absolute values are different, and the SCIAMACHY products is “noisier”.

When comparing AIRS and SCIAMACHY carbon monoxide retrievals one should note that a single AIRS L1 granule has 9×1350 spectra, so an AIRS orbit (about a dozen granules) gives more than 20 000 observations; On the other hand, a SCIAMACHY state typically consists of 260 spectra, resulting in about 2000 spectra per orbit. Furthermore, absorption due to CO in the thremal infrared is much stronger than in the near infrared. As a consequence, SCIAMACHY retrievals show much more scatter than AIRS retrievals.

A color contour map of CO columns seen by SCIAMACHY and AIRS on October 27. is given in Fig. 3 and Fig. 4. As in the 2D plots the enhanced carbon monoxide over Mozambique is clearly visible in both maps.

In Fig. 5 a comparison of AIRX2RET, AIRS–CERVISA, and SCIAMACHY–BIRRA longitude averaged carbon monoxide vertical column densities for four East Africa orbits in October 2003 is shown. The features showing up in the two AIRS retrievals are clearly similar, although the columns retrieved by CERVISA are higher, probably due to a different conversion scheme to translate the molecular density scaling factors actually fitted to the vertical column densities. Differences between AIRS and SCIAMACHY column densities have already been observed by other groups, and can be partly explained by a different altitude sensitivity of thermal and infrared sounders.

4. SUMMARY AND CONCLUSIONS

A modified version “CERVISA” of the “BIRRA” prototype of the operational SCIAMACHY near IR nadir level 2 processor has been implemented, and first results of carbon monoxide vertical column density retrievals from mid IR spectra have been shown. The CERVISA column densities were compared both with the official AIRS Level 2 product and with BIRRA results from SCIAMACHY observations. Ongoing work on CERVISA will focus on code improvement (e.g., aerosol/cloud and spectral response function modeling) and optimization.

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