INTERCOMPARISON OF CARBON MONOXIDE RETRIEVALS FROM SCIAMACHY AND AIRS NADIR OBSERVATIONS

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ABSTRACT

Nadir observations in the near or thermal infrared channels of spaceborne spectrometers can be used to derive information on trace gases relevant for climate and air quality. In the course of the ongoing validation of the Beer InfraRed Retrieval Algorithm (BIRRA) developed for operational retrievals of carbon monoxide, methane, etc. vertical column densities from SCIAMACHY near infrared nadir observations, a new retrieval code CERVISA (Column EstimatoR Vertical Infrared Sounding of the Atmosphere) has been implemented for analysis of thermal infrared nadir observations of AIRS, TES, or IASI. Both codes share a large portion of routines, e.g., for line-by-line molecular 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 infrared with sun irradiance as source versus Schwarzschild's equation for the thermal infrared.

In this contribution, we present first results of the intercomparison of CO vertical column densities retrieved from AIRS and SCIAMACHY, including comparisons with the "official" AIRS carbon monoxide product.

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 instruments. For the operational level 2 data processing of SCIAMACHY near IR observations, a new code "BIRRA" (Beer InfraRed Retrieval Algorithm) has been developed at DLR [4]. 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 $\rightarrow$ 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 for three orbits over Africa in late 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 [5], a line-by-line code for arbitrary observation geometry (up, down, limb) and instrumental field-of-view and line shape that provides Jacobians by means of automatic differentation [6] and has been verified in extensive intercomparisons [e.g. 2, 7].

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 [8]

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

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 $\mathcal{S}$,

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

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

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

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,

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

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 [9] 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 the baseline correction(s) b enter the forward model $\boldsymbol{F} \equiv \widehat{I(\nu;\dots)}$, Eq. (1), linearly and the least squares problem (5) can be reduced to a separable nonlinear least squares problem [10].

3. INTERCOMPARISON OF SCIAMACHY AND AIRS CARBON MONOXIDE

Nadir observations in the shortwave infrared channels of SCIAMACHY [11] 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

- tiny signal on huge background, i.e. low signal-to-noise;
- ice layer on channel 8 detector;
- an increasing number of dead and bad pixels;
- 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 [12] the situation is much better, in particular absorption of CO in the $4\,\mu$m band is stronger.

3.1. Data and assumptions

This intercomparison is based on SCIAMACHY and AIRS Level 1 data of October 2003 covering Eastern Africa. 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 the Bremen bad/dead pixel mask have been used; hence a single spectrum comprises 51 data points in the interval 4282.686 to $4302.131\,{\rm cm}^{-1}$. Surface reflectivity was modelled with a second order polynomial, baseline was ignored. Scaling factors for CO, CH_4, and

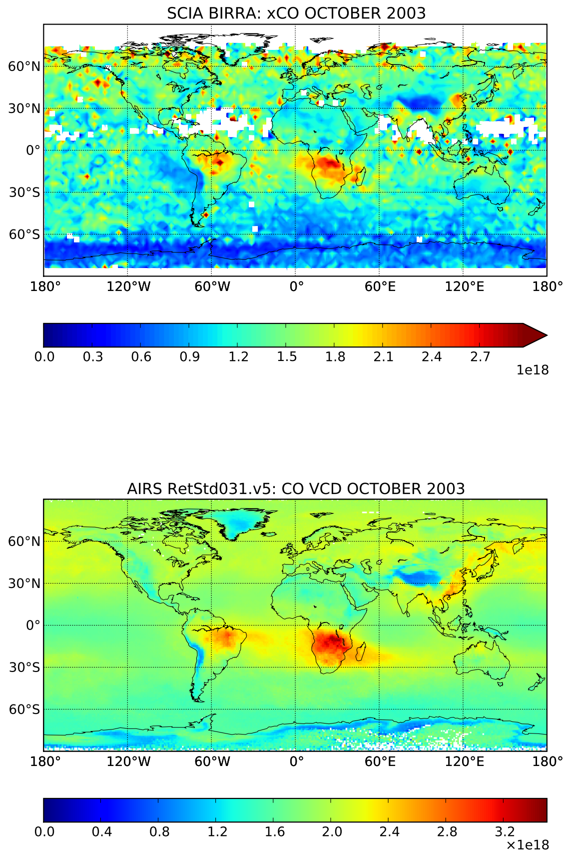

Figure 1. Comparison of October 2003 CO vertical column densities. (Single observations have been regridded and averaged into a $2.5^\circ \times 2.5^\circ$ global grid. AIRS CO VCD represent the field "`CO_total_column_A`" of the official level 3 product version v.5.)

H_2O were fitted along with the Gaussian slit function half widths and the reflectivity coefficients.

CO column density retrievals from AIRS were performed for three orbits (7868, 7889, and 7996 at October 26, 27, and 28) passing over Mozambique. Note that the October 26 and 28 data originate from dayside observations with a South-East to North-West flight direction, whereas orbit 07889 is nighttime with North-East to South-West ("parallel" to SCIAMACHY-Envisat). In accordance with McMillan et al. [13] the $2181 - 2220\ \mathrm{cm}^{-1}$ microwindow containing 42 spectral points was used. In addition to scaling factors for CO, CO_2, H_2O, and N_2O surface temperature was considered as unknown.

For BIRRA SCIAMACHY retrievals pressure and temperature profiles were read from the CIRA dataset [14], 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 HITRAN2004 database [16] (with updates for H_2O) along with the CKD continuum corrections [17]. The spectral response function was assumed to be Gaussian.

3.2. Results

In Fig. 1 a comparison of SCIAMACHY and AIRS monthly mean carbon monoxide vertical column densities for October 2003 are shown. Note that a single AIRS L1 granule has 9×1350 spectra, so an AIRS orbit 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.

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,

$$\mathrm{xCO} \equiv N_{\mathrm{CO}} \times \frac{\alpha_{\mathrm{CO}}}{\alpha_{\mathrm{CH4}}} . \tag{7}$$

Single observations have been regridded and averaged into a $2.5^\circ \times 2.5^\circ$ global grid. 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 $1.5 \cdot 10^{19}\ \mathrm{cm}^{-2}$
- CH_4 scaling factor close to one, $0.7 \leq \alpha'_{\mathrm{CH4}} \leq 1.3$ (where α'_{CH4} is throughput corrected)

No cloud filtering has been used. Along with the weak signal this is the main reason for the noisy data over the ocean. The noise at high latitudes is mainly due to the low signal in that regions.

Both products show enhanced CO densities over Southern Africa, the Amazonian region, and populated areas in East Asia. Moreover the SCIAMACHY—BIRRA results indicate high CO concentrations over Mumbay and the Ganges river valley.

In Fig. 2 results of CERVISA retrievals using AIRS L1 data (AIRIBRAD) from three orbits overpassing southeast Africa are compared with the "official" AIRS L2 data distributed by NASA (AIRX2RET). CO column densities (given as a function of latitude and longitude) have been averaged in 1dg latitude bins, with "bad" retrieval results (least squares return code indicating failure, $\mathrm{VCD_{CO}} > 10^{19}\ \mathrm{cm}^{-2}, \ldots$) filtered out. A series of CERVISA retrievals with slightly different settings had been performed (e.g., number of gases included, continuum on/off, baseline, …), and including a baseline

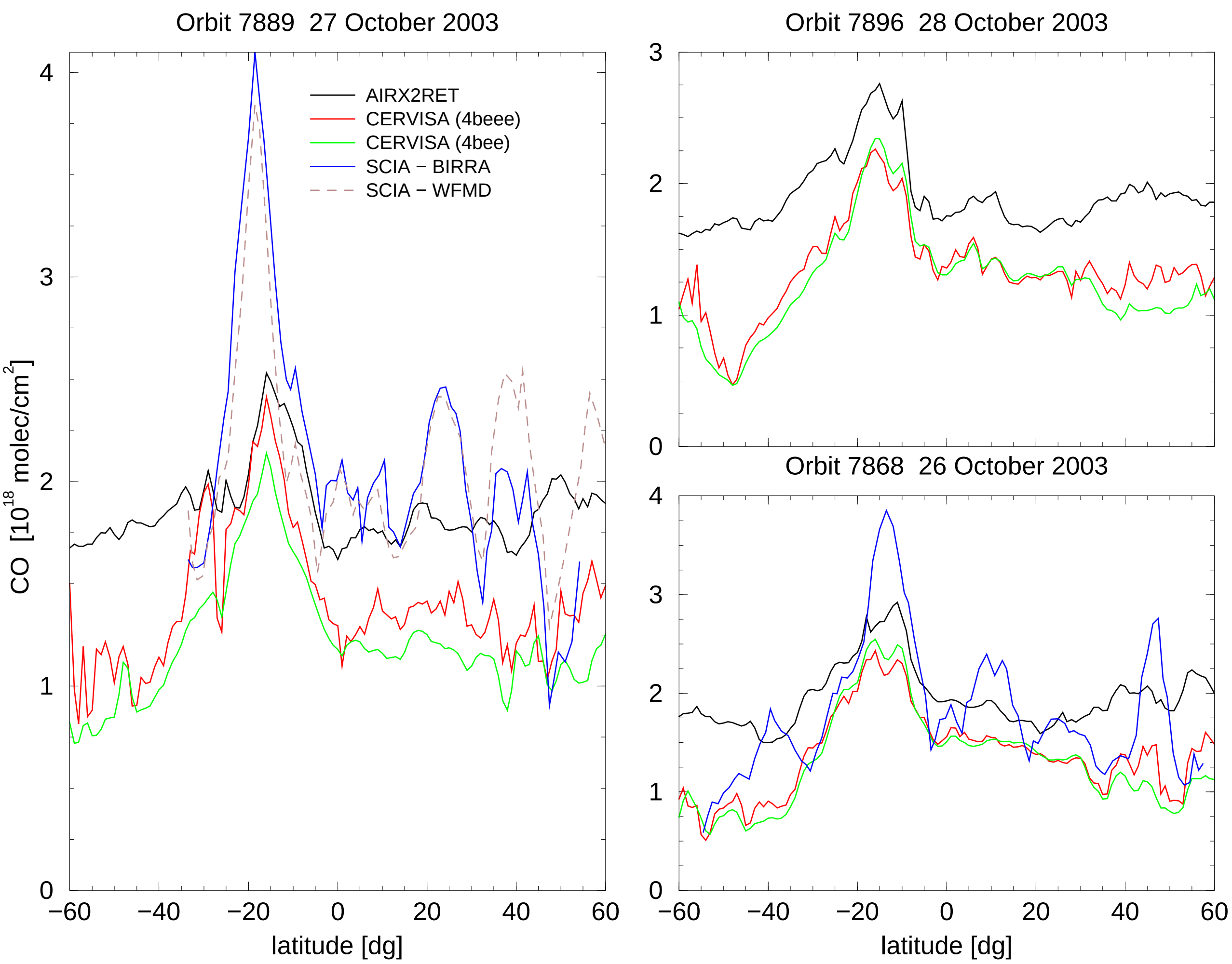

Figure 2. Comparison of CO vertical column densities as a function of latitude. For CERVISA 4 gases, a constant baseline correction, and surface emissivity as a linear or quadratic polynomial in wavenumber were fitted (labels "4bee" and "4beee").

and/or emissivity (modeled as polynomials in wavenumber) as further fit parameter turned out to be important. The enhanced CO emissions over Mozambique are clearly visible in all retrievals.

A reasonable good agreement (except for a vertical shift) between CERVISA and AIRX2RET is only found for low latitudes, whereas for high latitudes discrepancies become evident. Note that the AIRS L2 product indicates — on the average — increasing cloud coverage with increasing latitudes, however, CERVISA (and BIRRA) presently do not consider aerosols and clouds. Furthermore CERVISA retrievals were performed using an US standard profile for all trace gases, i.e., the H_2O and O_3 profiles available from the AIRS L2 products were not used.

For October 26 and 27 the corresponding results derived from SCIAMACHY orbit 8649 and 8663 are shown, too. The CO averaged over all longitudes within an 1dg latitude bin show larger scatter (see discussion above). The enhanced CO is significantly higher and slightly shifted to the south. Clearly a perfect match of AIRS and SCIAMACHY derived VCD's cannot be expected for several reasons, e.g., different altitude sensitivities of near and mid infrared spectra, SCIAMACHY daytime vs AIRS nighttime observation, different spatial coverage esp. "out of Africa", etc.

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, and retrievals using AIRS Level 2 water profiles.

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