INTERCOMPARISON OF VERTICAL COLUMN DENSITIES DERIVED FROM SCIAMACHY INFRARED NADIR OBSERVATIONS

Franz Schreier[(1)], **Sebastian Gimeno–Garcia**[(1)], **Michael Hess**[(1)], **Adrian Doicu**[(1)], **Albrecht von Bargen**[(1)], **Michael Buchwitz**[(2)], **Iryna Khlystova**[(2)], **Heinrich Bovensmann**[(2)], **and John P. Burrows**[(2)].

[(1)] *DLR — German Aerospace Center, Remote Sensing Technology Institute, Oberpfaffenhofen, 82234 Wessling, Germany;* `franz.schreier@dlr.de`

[(2)] *Institute of Environmental Physics (IUP), University of Bremen FB1, Bremen, Germany;* `Michael.Buchwitz@iup.physik.uni-bremen.de`

ABSTRACT

Nadir observations in the shortwave infrared channels of SCIAMACHY onboard the ENVISAT satellite can be used to derive information on CO, CH_4, N_2O, CO_2, and H_2O. Several scientific data analysis tools have been developed for retrieval of vertical column densities, and a significant upgrade of the operational level 2 data processor has been prototyped recently. WFM-DOAS, developed by University of Bremen, is a modified DOAS algorithm: A linearized radiative transfer model plus a low order polynomial is linear least squares fitted to the logarithm of the measured sun-normalized radiance. On the other hand, BIRRA (implemented at DLR) is a nonlinear least squares fit of the measured radiance. Trace gas vertical profiles are scaled in both cases to fit the observed data, further auxiliary parameters are code dependant. In this contribution we present results of an intercomparison of vertical column densities, nb. carbon monoxide, retrieved from SCIAMACHY infrared nadir observations.

Key words: SCIAMACHY, Infrared, Retrieval, Carbon Monoxide.

1. INTRODUCTION

Nadir sounding of vertical column densities of atmospheric gases is well established in atmospheric remote sensing. For UV instruments such as SCIAMACHY [Bovensmann et al., 1999] the analysis is traditionally based on a DOAS–type methodology. This approach has also been successfully applied for analysis of SCIAMACHY's near infrared channels [Buchwitz et al., 2007; Frankenberg et al., 2005; Gloudemans et al., 2005] and was the basis of the BIAS (Basic Infrared Absorption Spectroscopy) nonlinear least squares algorithm, a core element of the current operational level 2 data processor [Spurr, 1998]. In order to gain greater flexibility in the forward modelling and a more efficient and robust least squares inversion, a "Better InfraRed Retrieval Algorithm" (BIRRA) has been implemented recently [Schreier et al., 2006].

In the framework of the ongoing code verification, a careful intercomparison of BIRRA with the WFM-DOAS (Weighting Function Modified — Differential Optical Absorption Spectroscopy) code developed by the University of Bremen [Buchwitz et al., 2007] has been performed. After a short review of the theoretical background, common aspects as well as differences in the methodology and implementation of BIRRA and WFM-DOAS are presented in section 3. Setup and results of the intercomparison are discussed in section 4.

2. THEORY

2.1. Near Infrared Radiative Transfer

The intensity (radiance) I at wavenumber ν received by an instrument at $s = 0$ can be described by the integral form of the equation of radiative transfer [Liou, 1980]

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

where I_b is a background contribution and J is the source function comprising thermal emission, single and multiple scattering. In the near infrared, contributions from reflected sunlight become important, whereas thermal emission is negligible, Neglecting scattering for clear sky observations, the radiative transfer equation simplifies to

$$I(\nu) \;=\; r\, I_\mathrm{sun}(\nu)\, \mathcal{T}_\uparrow(\nu)\, \mathcal{T}_\downarrow(\nu) \quad (2)$$

where r is the reflection factor and $\mathcal{T}_\uparrow$ and $\mathcal{T}_\downarrow$ denote the transmission between reflection point (e.g. Earth surface) and observer and between sun and reflection point. The monochromatic transmission $\mathcal{T}$ (relative to the observer) is given according to Beer's law by

$$\mathcal{T}(\nu;s) \;=\; \exp\left[-\int_0^s \alpha(\nu,s')\,\mathrm{d}s'\right], \quad (3)$$

$$\alpha(\nu;s) \;=\; \sum_m k_m(\nu,s)\,n_m(s) + \alpha^{(c)}(\nu,s)\;, \qquad (4)$$

where α is the volume absorption coefficient, k_m and n_m are the absorption cross section and density of molecule m, respectively, and $\alpha^{(c)}$ the continuum absorption. Note that the absorption cross section is a function of altitude dependant pressure and temperature, i.e., $k(\nu,z) = k\big(\nu,p(z),T(z)\big)$.

The instrumental response is taken into account by convolution of the monochromatic intensity spectrum (1) with a spectral response function $\mathcal{S}$ (e.g., Gaussian)

$$\widehat{I(\nu)} \;\equiv\; (I\otimes\mathcal{S})(\nu) \;=\; \int_{-\infty}^{\infty} I(\nu)\times\mathcal{S}(\nu-\nu')\,\mathrm{d}\nu'\;. \qquad (5)$$

2.2. The inverse problem — nonlinear least squares

The objective of SCIAMACHY near infrared measurements in nadir viewing geometry is to retrieve information on the vertical distribution of trace gases such as N_2O, CH_4, or CO, e.g., the volume mixing ratio $q_X(z)$ or number density $n_X(z) = q_X(z)\cdot n_{\mathrm{air}}(z)$ of molecule X. The standard approach to estimate the desired quantities $\boldsymbol{x}$ from a measurement $\boldsymbol{y}$ (a vector of m components) relies on (in general nonlinear) least squares fit

$$\min_{\boldsymbol{x}} \|\boldsymbol{y}-\boldsymbol{F}(\boldsymbol{x})\|^2\;. \qquad (6)$$

Here $\boldsymbol{F}$ denotes the forward model $\mathbb{R}^n \rightarrow \mathbb{R}^m$ essentially given by the radiative transfer and instrument model. Because of the ill-posed nature of vertical sounding inverse problems, it is customary to retrieve column densities

$$N_X \equiv \int_0^{\infty} n_x(z)\,\mathrm{d}z\;. \qquad (7)$$

3. CODES

3.1. BIRRA

The forward model is based on the MIRART (Modular InfraRed Atmospheric Radiative Transfer) line-by-line code, developed for arbitrary observation geometry, instrumental field-of-view and spectral response functions [Schreier and Schimpf, 2001]. Molecular spectroscopic parameters can be read from HITRAN [Rothman et al., 2005], GEISA [Jacquinet-Husson et al., 1999], or JPL [Pickett et al., 1998] databases. Continuum corrections to the absorption coefficient are supported [e.g., Clough et al., 1989]. Derivatives of transmission and/or radiance spectra are obtained by means of automatic differentation [Griewank, 2000]. MIRART has been extensively verified by intercomparisons with other codes, cf. von Clarmann et al. [2002]; Melsheimer et al. [2005].

Denoting by c_m the scale factors to be estimated and by $\bar{n}_m(z)$ the reference (e.g., climatological) densities of molecule m, the upwelling monochromatic radiance (2) can be written as

$$I(\nu) = rI_{\mathrm{sun}}(\nu)\exp\left[-\int_0^{\infty}\frac{\mathrm{d}z'}{\mu}\sum_m c_m\bar{n}_m(z')\,k_m(\nu,z')\right] \exp\left[-\int_0^{\infty}\frac{\mathrm{d}z''}{\mu_\odot}\sum_m c_m\bar{n}_m(z'')\,k_m(\nu,z'')\right] \qquad (8)$$

where we have used the plane–parallel approximation with $\mu \equiv \cos\theta$ for an observer zenith angle θ and $\mu_\odot$ for the solar zenith angle $\theta_\odot$ (for simplicity continuum is neglected here). Introducing the total optical depth of molecule m (for the reference profiles and the entire path),

$$\begin{aligned} \boldsymbol{F}(\boldsymbol{x}) \;&\equiv\; \widehat{I(\nu)} \qquad (9)\\ &=\; r\,I_{\mathrm{sun}}(\nu)\,\mathrm{e}^{-\sum_m c_m\tau_m(\nu)} \otimes \mathcal{S}(\nu,\gamma) \;+\; b\;, \end{aligned}$$

where the state vector $\boldsymbol{x}$ is comprised of geophysical and instrumental parameters $\boldsymbol{c},\gamma,r$ and an optional baseline correction b (generally a polynomial).

For the solution of the nonlinear least squares problem (6) BIRRA uses solvers provided in the PORT Optimization Library [Dennis, Jr. et al., 1981] based on a scaled trust region strategy. BIRRA 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 $\boldsymbol{F} \equiv \widehat{I(\nu;\ldots)}$, Eq. (9), linearly and the least squares problem (6) can be reduced to a separable nonlinear least squares problem [Golub and Pereyra, 2003].

3.2. WFM-DOAS

The forward model is the radiative transfer model SCIATRAN version 1.2 [Buchwitz et al., 2000]. SCIATRAN takes multiple scattering fully into account. SCIATRAN solves the radiative transfer equation for pseudo-spherical geometry and is valid for nadir observations (for the full range of SCIAMACHY scan angles) up to a solar zenith angle of about 92 degrees. To enable a fast retrieval, a look up table scheme for the radiances and their derivatives has been implemented.

The inversion procedure in WFM-DOAS is a modified DOAS algorithm. A linearized radiative transfer model plus a low order polynomial P is linear least squares fitted to the logarithm of the measured sun-normalized radiance,

$$\ln I_i^{\mathrm{mod}}(\boldsymbol{N}) \;=\; \ln I_i^{\mathrm{mod}}(\boldsymbol{N}^{\mathrm{ref}}) \;+\; P(\lambda_i,\boldsymbol{a}) \;+\; \sum_m \frac{\partial \ln I_i^{\mathrm{mod}}}{\partial N_m}\times\left(N_m - N_m^{\mathrm{ref}}\right)\;. \qquad (10)$$

Here $\boldsymbol{N}$ denotes the vector of column densities N_m, Eq. (7), comprising all relevant molecules. The trace gas vertical profiles are scaled for the fit (i.e., the profile shape is not varied).

Fit parameters comprising the state vector $\boldsymbol{x}$ in Eq. (6):
• Scaling factor for CO, CH_4, and H_2O columns
• Shift parameter for temperature profile
• Parameters for low order polynomial.

3.3. Common Aspects, Auxiliary Data

In order to minimize systematic biases (due to the channel 8 ice layer, clouds and aerosols, albedo variability, etc.) the CO column is scaled with a dimensionless factor. This factor is the a-priori methane column ($3.6 \cdot 10^{19}\,\mathrm{molecules/cm^2}$ for sea level) divided by the methane column retrieved simultaneously from the same fitting window.

- Use of a newly generated static dead/bad detector pixel mask optimized for the time period 2003 – 2005;
- Fitting window: 2324.4 – 2335.0 nm in channel 8;
- Molecular spectroscopic data from HITRAN 2004 [Rothman et al., 2005];
- Atmospheric profiles: US Standard atmosphere;

4. THE INTERCOMPARISON

For this intercomparison we concentrate on carbon monoxide, an important atmospheric trace gas highly variable in space and time that affects air quality and climate. About half of the CO emissions come from anthropogenic sources (e.g., fossil 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, and SCIAMACHY.

This study is based on SCIAMACHY Level 1c data of orbit 8663 (27. October 2003) covering Russia, the Arabic peninsula, and 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.

In Fig. 1 we compare the "xCO" data products, i.e, the retrieved CO column densities corrected by CH_4. Enhanced CO emissions over Southern Africa are found in both retrievals. These findings are confirmed in the following plots showing CO column densities averaged in 1° latitude bins. In Fig. 2 problems of both codes over the ocean due to the low signal lead to a large scatter of the retrieval results. These outliers are obviously removed when the averaging includes only data passing the quality checks (e.g., "physical" lower and upper bounds, "good" residuals, . . .), see Fig. 3. As BIRRA currently neglects scattering, the comparison in Fig. 4 only includes cloud free scenes. Finally, Fig. 5 shows "'good" data over cloud free scenes, also illustrating the MOPITT operational CO product [Deeter et al., 2003]. All 2D plots show a good correlation over the African continent, and — albeit different absolute numbers — similar trends over the northern (mostly cloudy) hemisphere.

5. SUMMARY AND OUTLOOK

A significant upgrade of the operational SCIAMACHY near infrared nadir level 2 algorithm BIRRA has been intercompared with the WFM-DOAS code of the University of Bremen. Despite significant conceptual differences in forward modelling and inversion (linear vs. nonliner least squares) a good overall agreement has been found esp. over Africa. Reasons for discrepancies are subject to further investigations.

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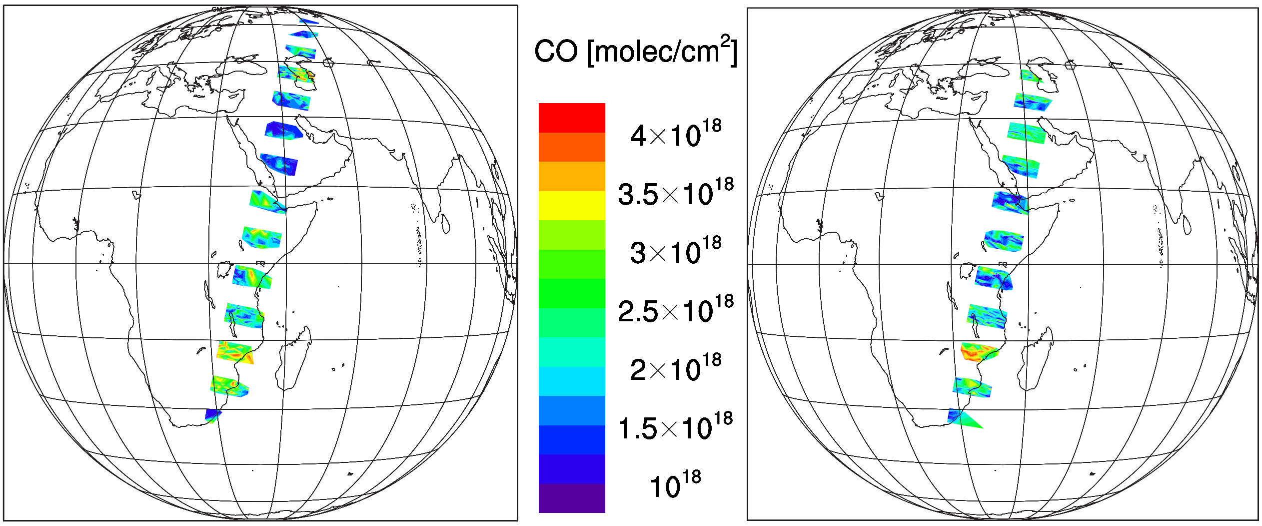

Figure 1. Comparison of CO column densities retrieved with the BIRRA (left) and WFM–DOAS (right) codes. Only results passing the quality check are shown. The enhanced CO emissions over Mozambique are clearly visible in both retrievals.

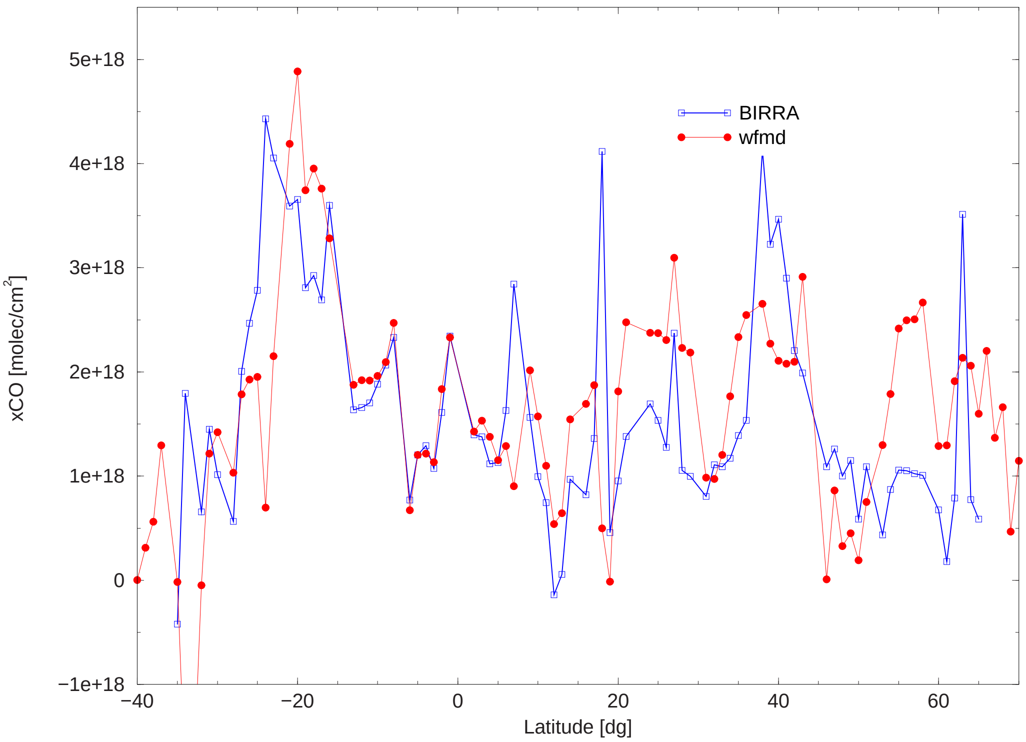

Figure 2. Comparison of CO column densities retrieved with the BIRRA and WFM–DOAS codes. (Column densities have been averaged in 1dg latitude bins.)

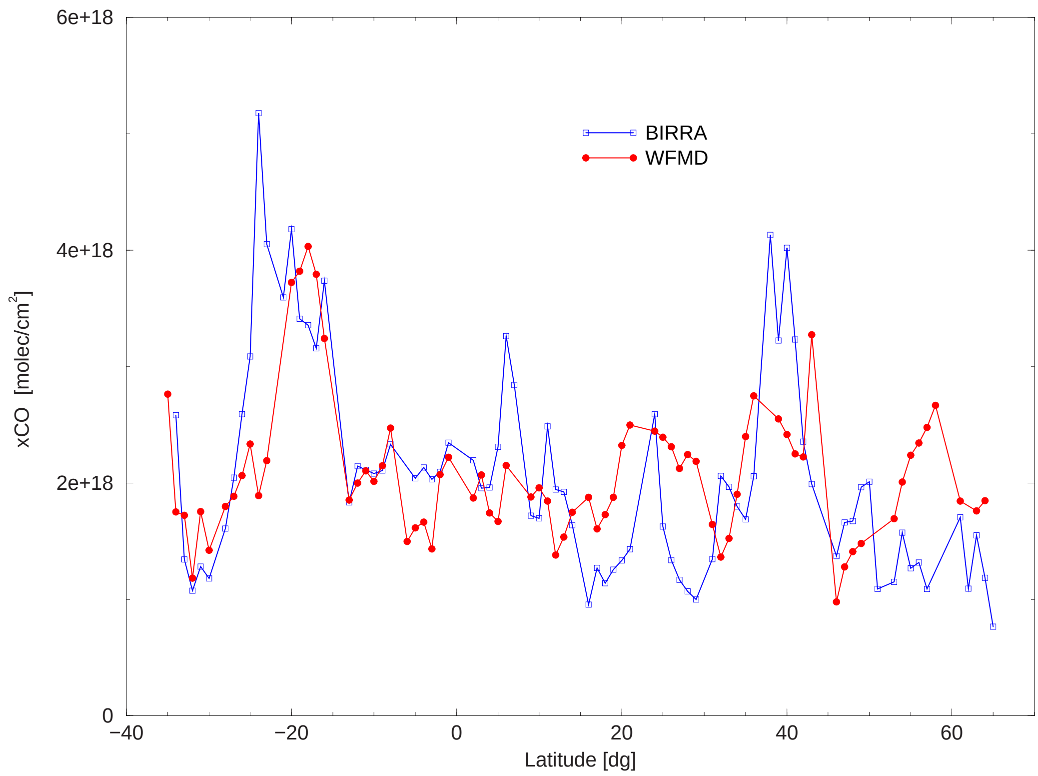

Figure 3. Comparison of CO column densities (averaged in 1dg) retrieved with the BIRRA and WFM–DOAS codes. Only data passing the quality check have been included in the averaging.

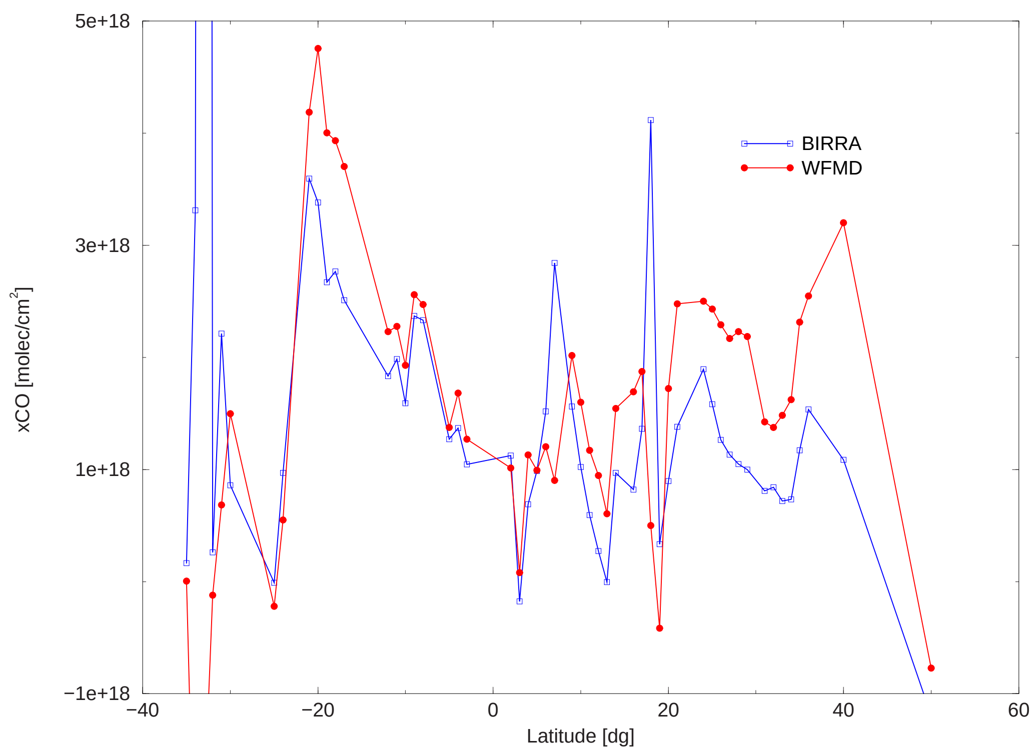

Figure 4. Comparison of CO column densities of cloud clear scenes retrieved with the BIRRA and WFM–DOAS codes. (1 dg latitude averages)

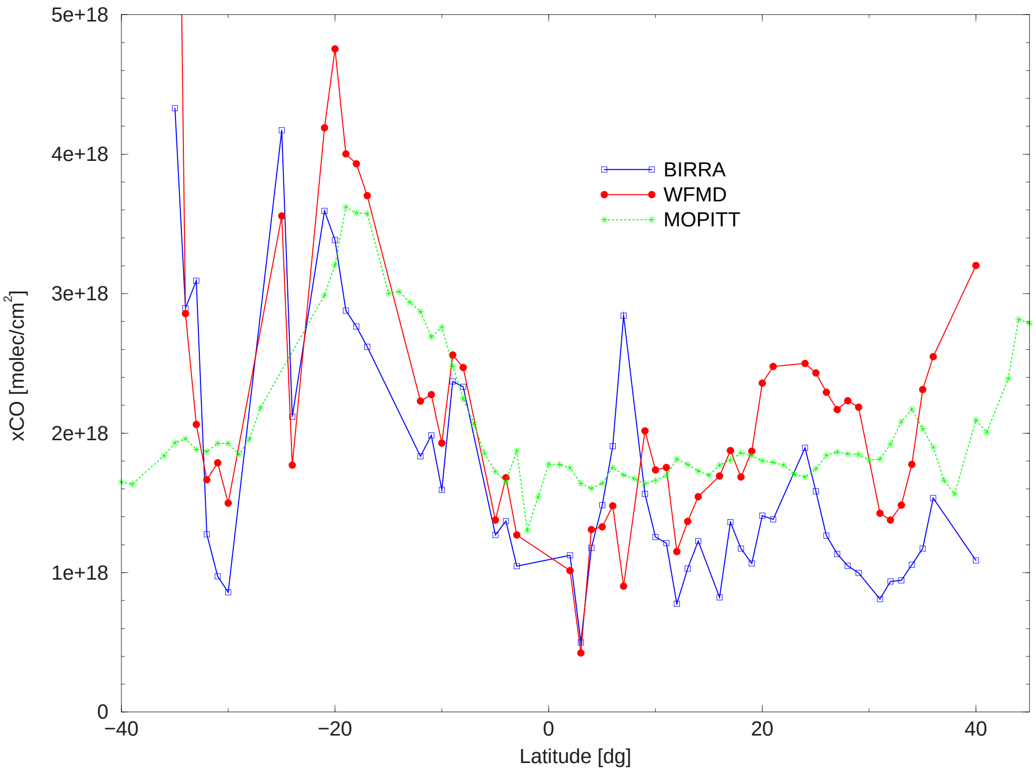

Figure 5. Comparison of CO column densities of cloud clear scenes retrieved with the BIRRA and WFM–DOAS codes. Only "good" data have been included in the averaging. As a reference MOPITT data are shown, too.

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