Retrieval of Carbon Monoxide Vertical Column Densities from SCIAMACHY Infrared Nadir Observations

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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. BIRRA (Beer InfraRed Retrieval Algorithm) is a least squares fit of the measured radiance with respect to molecular column densities and auxiliary parameters, nb. surface albedo, baseline and slit function width. Here special features of the code are shown along with results of carbon monoxide retrievals from SCIAMACHY near infrared nadir observations. In particular intercomparisons with other SCIAMACHY Infrared Nadir retrievals and with AIRS (Atmospheric Infrared Sounder onboard NASA-EOS-Aqua) will be presented.

1 Introduction

Nadir sounding of molecular column densities 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 methodology. This approach has also been successfully applied to SCIAMACHY's near infrared channels [Buchwitz et al., 2007, Frankenberg et al., 2005]. To gain greater flexibility and an efficient and robust inversion for the operational level 2 data processing, "BIRRA" has been developed at DLR.

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, and MIPAS and SCIAMACHY on ESA's Envisat.

In the framework of the ongoing algorithm verification, a careful intercomparison of BIRRA with independently developed algorithms, i.e., WFM-DOAS (developed by the University of Bremen) and IMLM (SRON — Netherlands Institute for Space Research, Gloudemans et al., 2005) has been performed. Moreover, molecular column densities retrieved from infrared atmospheric soundings are compared. Results of carbon monoxide retrievals for 2004 are presented here.

2 Retrieval Methodology

The objective of SCIAMACHY nadir NIR measurements is to retrieve information on gases such as N_2O, CH_4, or CO; e.g., volume mixing ratio $q_X(z)$ or density $n_X(z) = q_X(z) \cdot n_{air}(z)$ of molecule X. Unfortunately analysis of the NIR channels of SCIAMACHY is challenging because of

- Tiny signal on huge background (low signal-to-noise ratio)
- Channel 8: ice layer on the detector
- CO and N_2O retrieval: very weak absorbers

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

$$N_X \equiv \int_0^\infty n_x(z)\,dz\ .\tag{1}$$
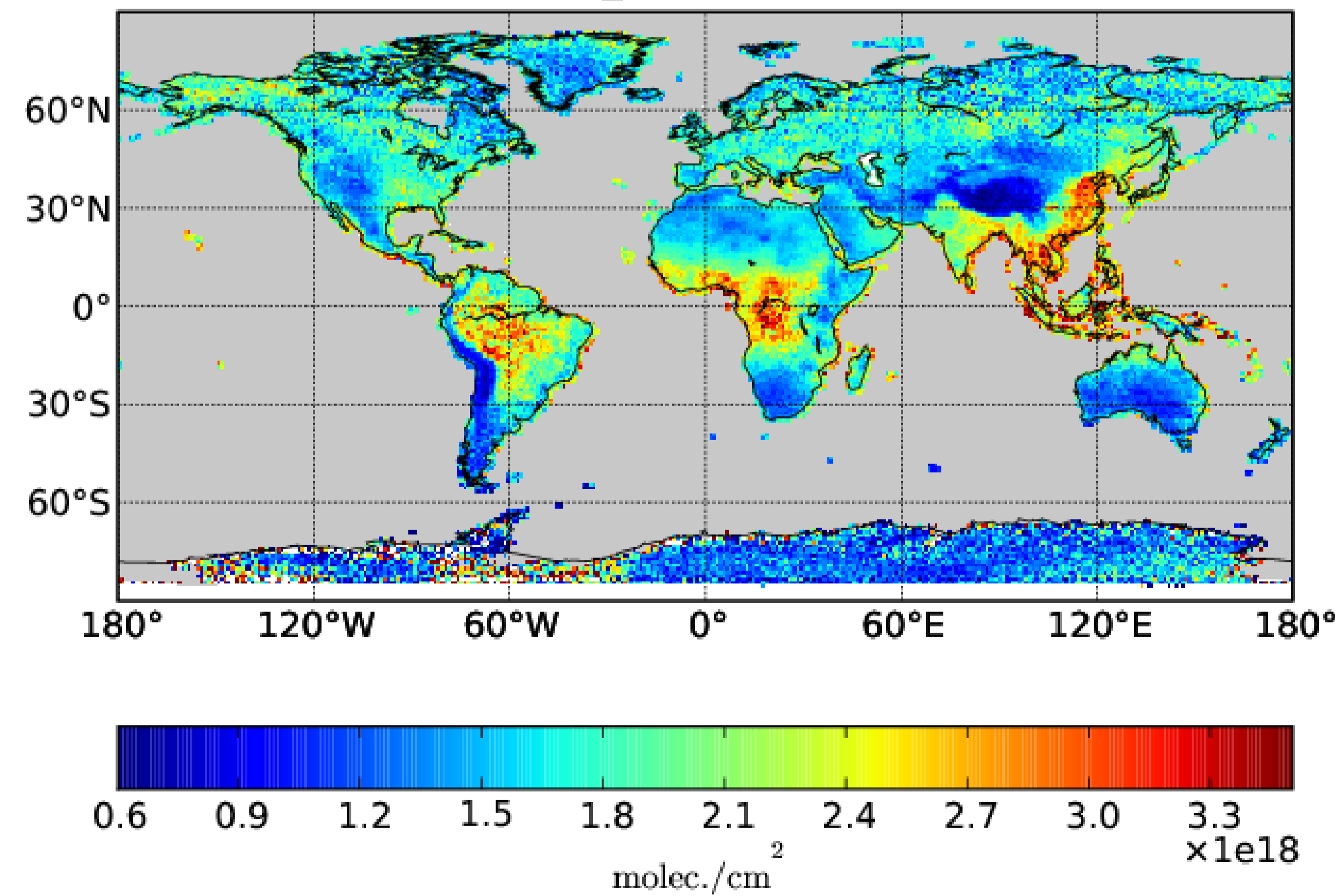
Figure 1: 2004 annual average of CO column densities retrieved with the BIRRA.

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2.1 The Forward Model: Near Infrared Radiative Transfer

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

$$I(\nu) \;=\; I_{\rm b}(\nu) \;-\; \int_0^\infty ds'\, J(\nu)\, \frac{\partial \mathcal{T}(\nu; s')}{\partial s'}\ ,\tag{2}$$

where $I_{\rm b}$ is a background contribution and J is the source function. In the near infrared, reflected sunlight turns out to be important, whereas thermal emission is negligible; For clear sky observations scattering can be neglected, and Eq. (2) simplifies to

$$I(\nu) \;=\; r(\nu)\, I_{\rm sun}(\nu)\, \mathcal{T}_\downarrow(\nu)\, \mathcal{T}_\uparrow(\nu)\tag{3}$$

$$= r(\nu) I_{\rm sun}(\nu) \exp\left[-\int_{z_{\rm b}}^{z_{\rm sat}}\frac{dz'}{\mu}\sum_m \alpha_m \bar{n}_m(z')\, k_m(\nu,z')\right] \exp\left[-\int_{z_{\rm b}}^{\infty}\frac{dz''}{\mu_\odot}\sum_m \alpha_m \bar{n}_m(z'')\, k_m(\nu,z'')\right]$$

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, 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.)

The instrument is taken into account by convolution of the monochromatic intensity spectrum (3) with an spectral response function $\mathcal{S}$ (e.g., Gaussian or hyperbolic with width γ)

$$\widehat{I(\nu)} \;\equiv\; (I \otimes \mathcal{S})(\nu) \;=\; \int_{-\infty}^{\infty} I(\nu) \times \mathcal{S}(\nu - \nu')\,d\nu'\ .\tag{4}$$

Introducing the total optical depth τ_m of molecule m, the forward model is written as

$$\vec{F}(\vec{x}) \equiv \widehat{I(\nu)} \;=\; r\, I_{\rm sun}(\nu) \exp\left[-\sum_m \alpha_m \tau_m(\nu)\right] \otimes \mathcal{S}(\nu,\gamma) + b\ .\tag{5}$$

The BIRRA forward model is based on MIRART (Modular IR Atmospheric Radiative Transfer), a general purpose line-by-line code [Schreier and Schimpf, 2001]:

- Molecular spectroscopic parameters from HITRAN, GEISA, or JPL databases. Continuum (e.g., CKD).
- Derivatives of transmission or radiance spectra by means of automatic differentiation [Griewank, 2000].
- Arbitrary observation geometry (up/downlooking, limb) and instrumental field-of-view and line shape.
- Verification by intercomparisons, nb. von Clarmann et al. [2002], Melsheimer et al. [2005].

2.2 The Inverse Problem — Nonlinear Least Squares

The standard approach to estimate the desired quantities $\vec{x}$ from a measurement vector $\vec{y}$ relies on (nonlinear) least squares fit

$$\min_x \left\|\vec{y} - \vec{F}(\vec{x})\right\|^2\ .\tag{6}$$

Here $\vec{F}$ denotes the forward model (5), and the unknown state vector $\vec{x}$ is comprised of the geophysical and instrumental parameters $\vec{\alpha}, \gamma, r$ and an optional additive baseline correction b (more generally r and b are polynomials in wavenumber). For the nonlinear least squares problem (6), BIRRA uses solvers of the PORT Optimization Library [Dennis, Jr. et al., 1981] based on a scaled trust region strategy. Optionally, a least squares with simple bounds (to prevent, e.g., negative values for physical quantitites such as column densities) or a separable nonlinear least squares solver [Golub and Pereyra, 2003] can be used.

To compensate for variations of the meteorological conditions (e.g., pressure) and for instrumental artefacts (e.g., calibration, slit function), the vertical column density of CO is derived as

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

Furthermore, column densities are averaged in 1dg latitude/longitude bins with doubtful values rejected:

- PORT least squares converged with $\|\mathrm{Residual}\|$ decreased
- No "forbidden" x values
- Scaling factors: $0 \leq \alpha_{\rm CO} \leq 2$ and $0.7 \leq \alpha'_{\rm CH4} \leq 1.3$ ($\alpha'_{\rm CH4}$ throughput corrected)
- Latitudes in interval [80S,80N], only overland

3 Results

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 4282.68615 to $4302.13102\,\mathrm{cm}^{-1}$. An US standard atmosphere was assumed. Surface reflectivity was modelled wih a second order polynomial, baseline was ignored.

The annual average of 2004 CO columns are shown in Fig. 1. Intercomparisons of monthly means with other SCIAMACHY retrievals and with AIRS are shown in the subsequent figures. These months indicate local sources of CO associated with highly populated areas and biomass burning as well as seasonal variability.
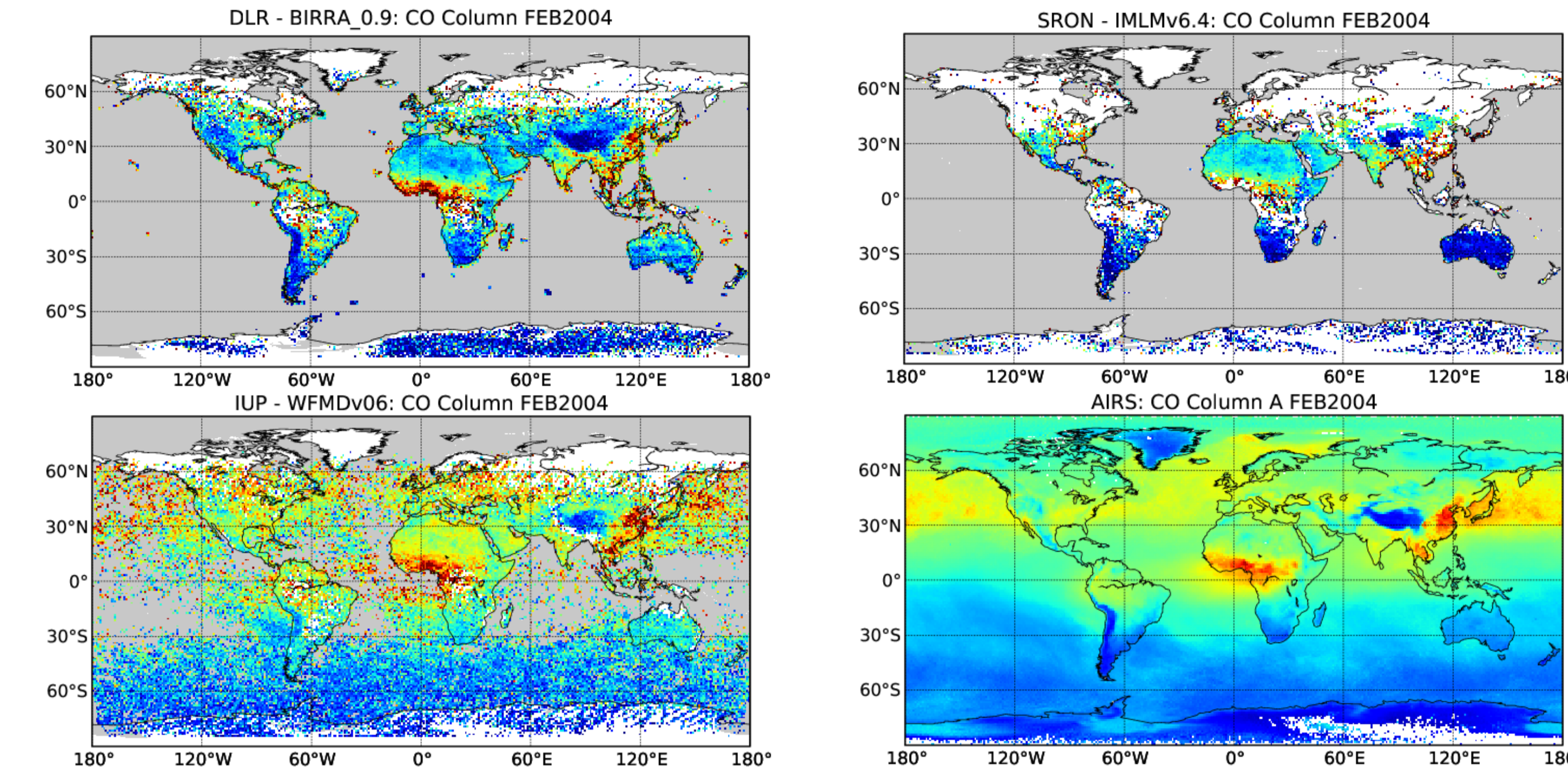
Figure 2: Comparison of February 2004 CO column densities. (Same color bar as in Fig. 1.)
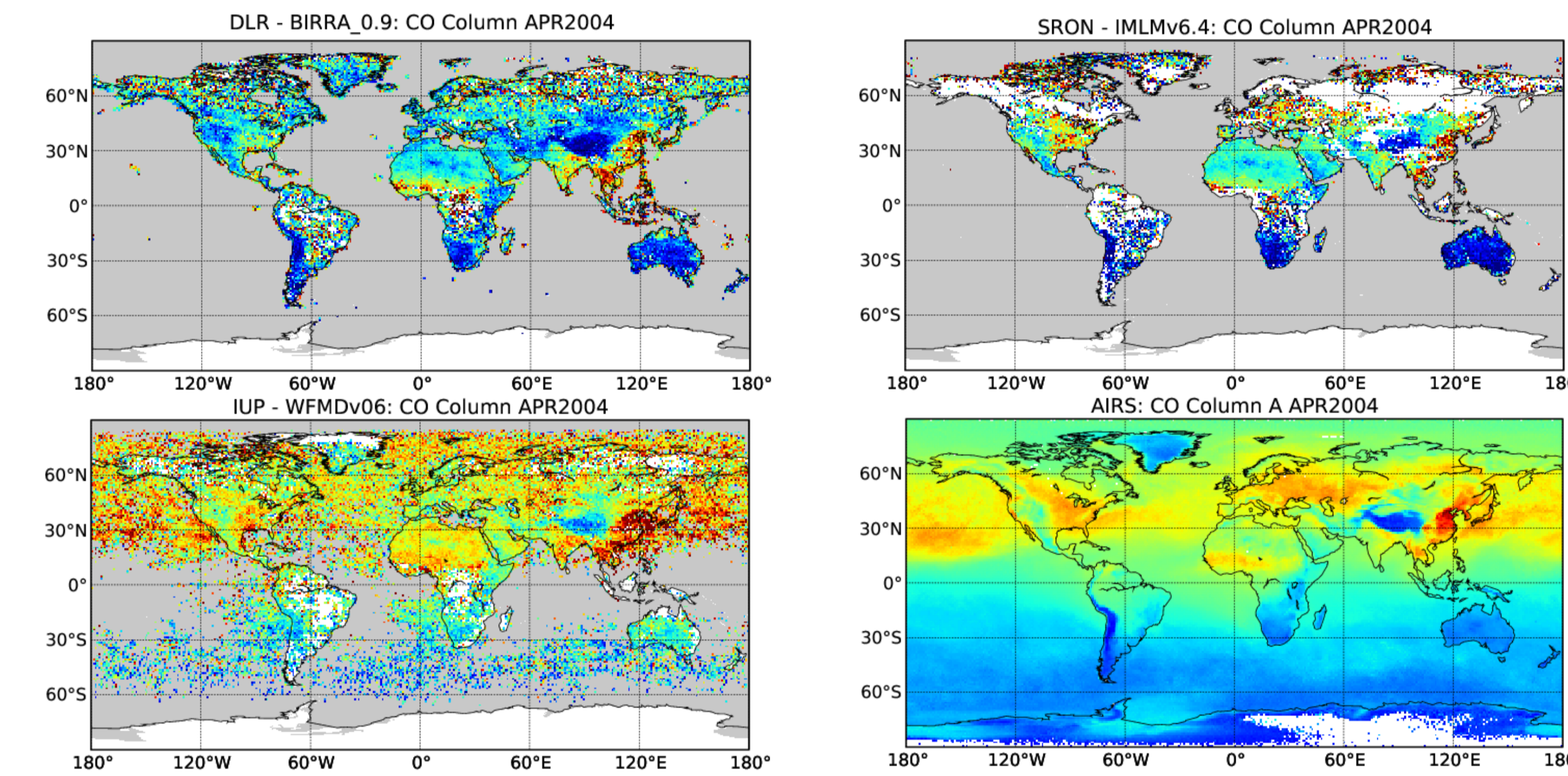
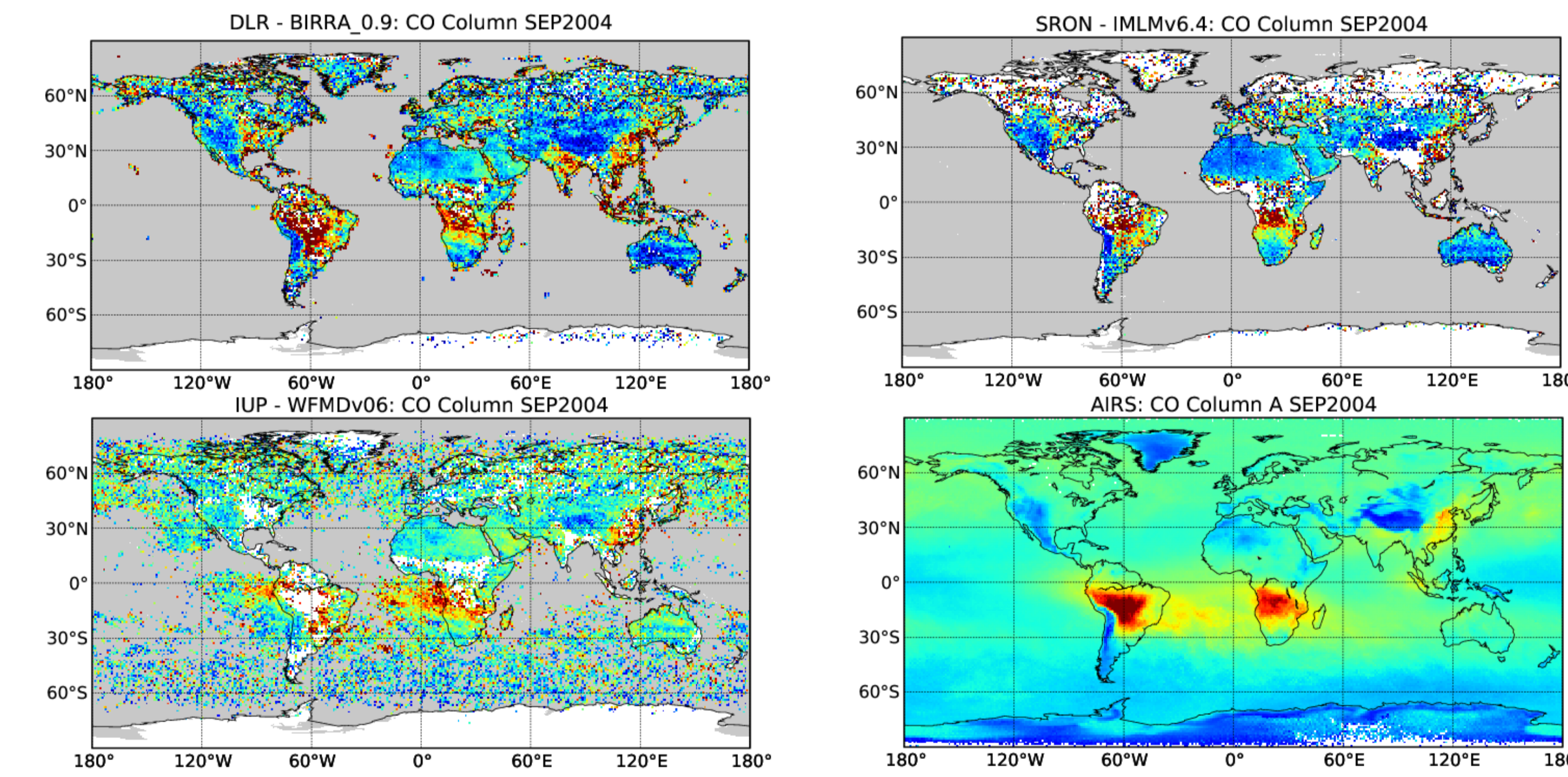**Figure 3:** Comparison of April 2004 CO column densities.

Figure 4: Comparison of September 2004 CO column densities.

4 Summary and Outlook

Carbon monoxide column densities retrieved with the "BIRRA" prototype of the operational SCIAMACHY near IR nadir level 2 processor have been compared with results obtained by the WFM-DOAS (University of Bremen) and IMLM (SRON) algorithms. Furthermore, intercomparisons with the CO product obtained with the Atmospheric Infrared Sounder (AIRS) have been shown. Results indicate high sensitivity to the bad/dead pixel mask and the crucial importance of correct filtering of dubious retrieval results. Despite significant conceptual differences of the three SCIAMACHY codes w.r.t. forward modelling and inversion a good overall agreement has been found.

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