SCIAMACHY/WFM-DOAS TROPOSPHERIC CO, CH_4, AND CO_2 SCIENTIFIC DATA PRODUCTS: VALIDATION AND RECENT DEVELOPMENTS

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ABSTRACT

The three "carbon gases" carbon monoxide (CO), methane (CH_4) and carbon dioxide (CO_2) are important atmospheric constituents affecting air quality and climate. The near-infrared nadir spectra of reflected solar radiation measured by SCIAMACHY on-board ENVISAT contain information on the vertical columns of these gases which we retrieve using the scientific algorithm WFM-DOAS. For CH_4 and CO_2 our main data products are dry air column averaged mixing ratios (XCH_4 in ppbv and XCO_2 in ppmv) determined by simultaneous measurements of the dry air mass obtained from oxygen (O_2) for CO_2 and CO_2 for methane. Our CO data product is the CO vertical column in molecules/cm^2. Our previous activities focussed on the year 2003. The year 2003 data set (WFM-DOAS version 0.5 CO and XCH_4; version 0.4 XCO_2) has been extensively validated by comparison with a network of ground-based FTIR stations. We shortly summarize the main results of this validation effort which also resulted in the identification of some problems, e.g., a solar zenith angle dependent bias of the version 0.5 XCH_4 of up to a few percent. Recently we have generated a new data set for all three gases covering the time period 2003-2005 (CO version 0.6; XCH_4 and XCO_2 version 1.0). We give an overview about the algorithm improvements and present selected results. We show that the new data set is significantly improved for all three gases in terms of quantity (more data even for 2003) and quality (e.g., no solar zenith angle dependent bias for methane; no need for (large) scaling factors for the CO_2 and O_2 columns). A first detailed comparison with ground-based FTIR measurements is presented elsewhere in this issue (Dils et al., 2006b).

1. INTRODUCTION

Carbon monoxide (CO) is an important air pollutant affecting local air quality and carbon dioxide (CO_2) and methane (CH_4) are the two most important anthropogenic greenhouse gases and contribute to global climate change. The near-infrared nadir spectra of reflected solar radiation measured by SCIAMACHY [2] on-board ENVISAT contain information on the vertical columns of these gases which we retrieve using the scientific algorithm WFM-DOAS [3-7, 9-10]. Here we present an overview of the current status of this activity. In Section 2 we shortly summarize the main results of the comparison of the previously generated year 2003 data set (CO v0.5, CH_4 v0.5, CO_2 v0.4) with ground-based FTIR measurements. For details we refer to [7] (retrieval method and comparison with global reference data) and [9] (validation using ground-based FTIR measurements). In Section 3 we present our recent activities which focus on generating a larger and qualitatively improved data sets for all three gases covering the time period 2003-2005 (CO v0.6, CH_4 v1.0, CO_2 v1.0).

2. PREVIOUS YEAR 2003 DATA SET: CO v0.5, CH_4 v0.5, AND CO_2 v0.4

Our previous activities focussed on the year 2003 mainly because this was the target year of the EU project EVERGREEN (see http://www.knmi.nl/evergreen). The resulting year 2003 data set data [7] set has been compared with corresponding measurements of a network of ground based FTIR stations [9]. The main results of this comparison are summarized in Tab. 1.

Despite the good agreement with the reference data the following major problems with this data set had been identified:

- Carbon monoxide: No major problems have been identified (possible exception: too high CO over Europe in summer 2003).
- Methane: The methane v0.5 year 2003 data set has a solar zenith angle (SZA) dependent bias of up to a few percent for large SZAs due to calibration problems [7]. This problem has been solved for the new v1.0 data set presented in the next section which has been retrieved using spectra with an improved calibration (Level 1 version 5 instead of version 4).
- Carbon dioxide: The CO_2 version 0.4 columns and the corresponding O_2 columns (used to compute the column averaged mixing ratio data product XCO_2) had to be scaled with constant factors (1.27 for CO_2 and 0.85 for O_2) to compensate for a systematic underestimation of the CO_2 columns and a systematic overestimation of the O_2 columns. These problems have been solved for the new version 1.0 data set presented in the next

section (by using Level 1 version 5 instead of version 4 spectra (solves CO_2 scaling factor problem) and by extending the WFM-DOAS reference spectra look-up table to better taking into account the albedo dependence of the nadir radiance and by excluding the albedo weighting function from the O_2 fit (solves O_2 scaling factor problem)).

SCIAMACHY Data Product	N	BIAS [%]	SCATTER [%]	R [-]
CO column: WFM-DOAS v0.5	**22362**	**-0.01**	**25.1**	**0.86**
Methane column averaged mixing ratio XCH_4: WFM-DOAS v0.5 (SZA bias corrected)	**42072**	**-3.28**	**1.93**	**0.80**
WFM-DOAS v0.5 (not corrected)	*42072*	*-4.09*	3.36	*0.72*
CO_2 column averaged mixing ratio XCO_2: WFM-DOAS v0.4 (limited comparison with three non-ideal stations)	**7704**	**-6.95**	**3.78**	**0.42**

Tab. 1: Summary of the comparison of the SCIAMACHY WFM-DOAS v0.5 CO, v0.5 methane and v0.4 CO_2 year 2003 data set with ground based FTIR measurements. N is the number of SCIAMACHY measurements which have been compared with the FTIR measurements, BIAS is the relative difference SCIA-FTIR in percent, SCATTER is the standard deviation of the difference in percent, and R is the correlation coefficient (more details are given in [9]).

2. IMPROVED NEW YEARS 2003-2005 DATA SET: CO v0.6, CH_4 v1.0, AND CO_2 v1.0

2.1 General retrieval algorithm improvements

The new year 2003-2005 data set has been generated by implementing the following improvements/changes:

- Use of an extended look up table of reference spectra mainly w.r.t. surface albedo.
- Use of Level 1 version 5 spectra (with nominal calibration) instead of (dark signal "patched") version 4 spectra.
- Use of improved spectroscopy: HITRAN 2004 [13] instead of HITRAN 2000/2001 [12].
- Implementation of several minor modifications, e.g., surface altitude interpolation of reference spectra for CH_4 and CO_2 instead of next neighbour approach, optimization of the definition of the quality flag which defines a "successful" CO and CH_4 measurement; definition of a quality flag for the CO_2 product.
- For CO retrieval from channel 8 a new static detector dead/bad pixels mask has been generated - optimised for 2003-2005 - by analysing fit residuals.

2.2 Carbon monoxide (CO) version 0.6

Carbon monoxide columns are retrieved from a small spectral fitting window located in SCIAMACHY channel 8 (2324.4-2335.0 nm). Apart from the retrieval algorithm changes as listed in Section 2.1 the WFM-DOAS version 0.6 CO retrieval algorithm is essentially identical with the WFM-DOAS version 0.5 algorithm described in [7].

Figure 1 shows as an example a global CO column map for the year 2004. Maps for all three years and for all 36 months of the time period 2003-2005 can be found on the WFM-DOAS web site: http://www.iup.uni-bremen.de/sciamachy/NIR_NADIR_WFM_DOAS/index.html.
Note that the color scale is a slightly modified version of the color scale used for MOPITT (see NCAR MOPITT web page http://www.eos.ucar.edu/mopitt) [8]. As the SCIAMACHY CO columns are typically somewhat higher than MOPITT we have extended the MOPITT color scale by adding two additional colors for columns above $3x10^{18}$ molecules/cm^2. We display the SCIAMACHY CO columns using the MOPITT color scale to enable an easy direct visual comparison of the monthly mean values of both sensors using the monthly mean data plots of both sensors available in the internet (MOPITT/NCAR and SCIAMACHY/WFM-DOAS web pages).

Figure 2 shows a quantitative comparison with MOPITT for six regions for the years 2003 and 2004. For 2003 the results are nearly identical as shown in [9]

for the version 0.5 product (except for Europe in summer where the quality of the new v0.6 CO data product appears to be higher).

2.3 Methane (CH_4) version 1.0

Methane columns are retrieved from a small spectral fitting window (1629-1671 nm) located in SCIAMACHY channel 6. CO_2 from channel 6 is used as a proxy for the light path and the simultaneously retrieved CO_2 column is used to estimate the air column necessary to compute a methane column averaged mixing ratio (CO_2 retrieval is described in the next section). Apart from the retrieval algorithm changes as listed in Section 2.1 the WFM-DOAS version 1.0 methane retrieval algorithm is essentially identical with the WFM-DOAS version 0.5 algorithm described in [7]. Figure 3 shows SCIAMACHY v1.0 methane for the year 2003 compared to TM5 model simulations. The largest regional differences are over northern South America in qualitative agreement with the findings of Frankenberg et al., 2005 [11].

2.4 Carbon dioxide (CO_2) version 1.0

Carbon dioxide (CO_2) columns are retrieved from a small spectral fitting window (1558-1594 nm) located in SCIAMACHY channel 6. Oxygen (O_2) columns from channel 4 (755-775 nm) are retrieved to compute a CO_2 column averaged mixing ratio XCO_2. Figure 4 shows a comparison with TM3 model simulations over North America for 2003. A similar comparison is shown in [1] using a modified version of WFM-DOAS based on computationally much more expensive on-line radiative transfer simulations.

5. SUMMARY

We have presented an overview about the current (December 2006) status of the retrieval of carbon monoxide, methane and carbon dioxide columns from SCIAMACHY near-infrared nadir spectra using the WFM-DOAS algorithm. The new methane and CO_2 version 1.0 data products will be released soon. The new CO version 0.6 data product for 2003-2005 presented here has been released and is available from the authors on request (for details see SCIAMACHY/WFM-DOAS web page : http://www.iup.uni-bremen.de/sciamachy/NIR_NADIR_WFM_DOAS/index.html).

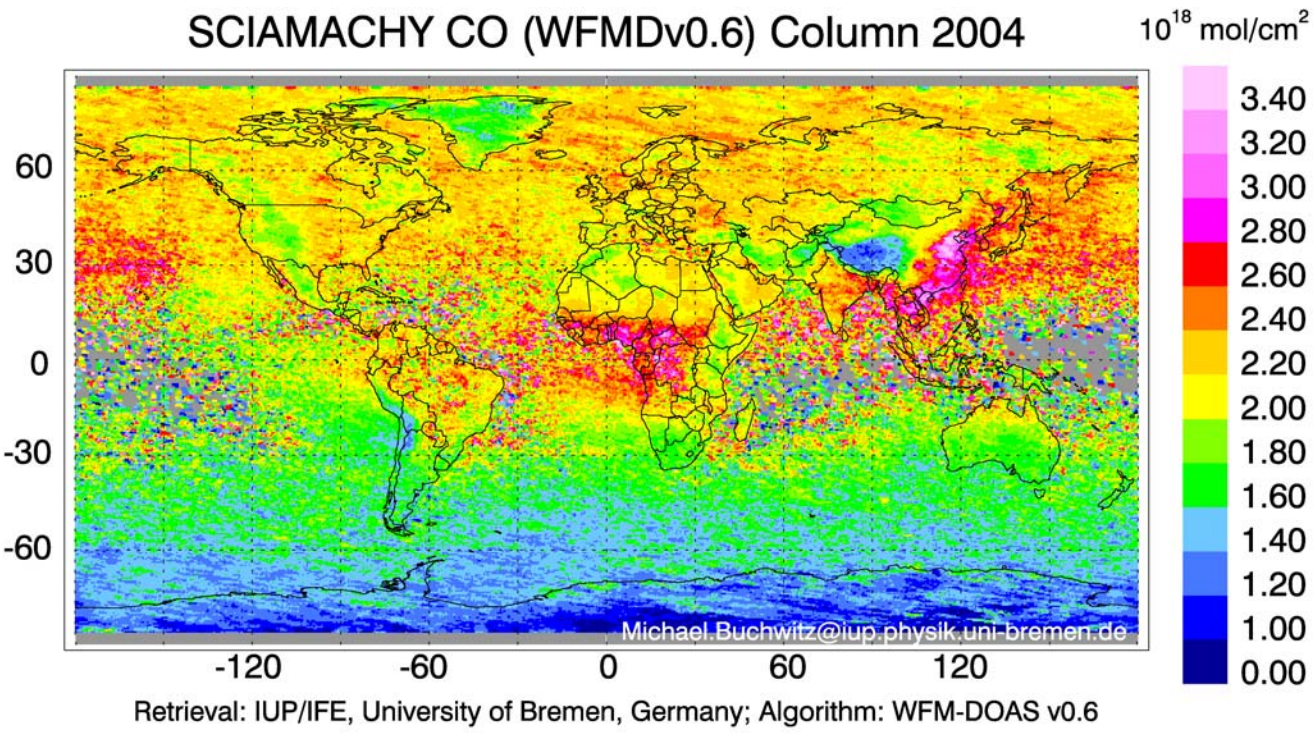

Fig. 1: Year 2004 average of SCIAMACHY/WFM-DOAS version 0.6 CO columns.

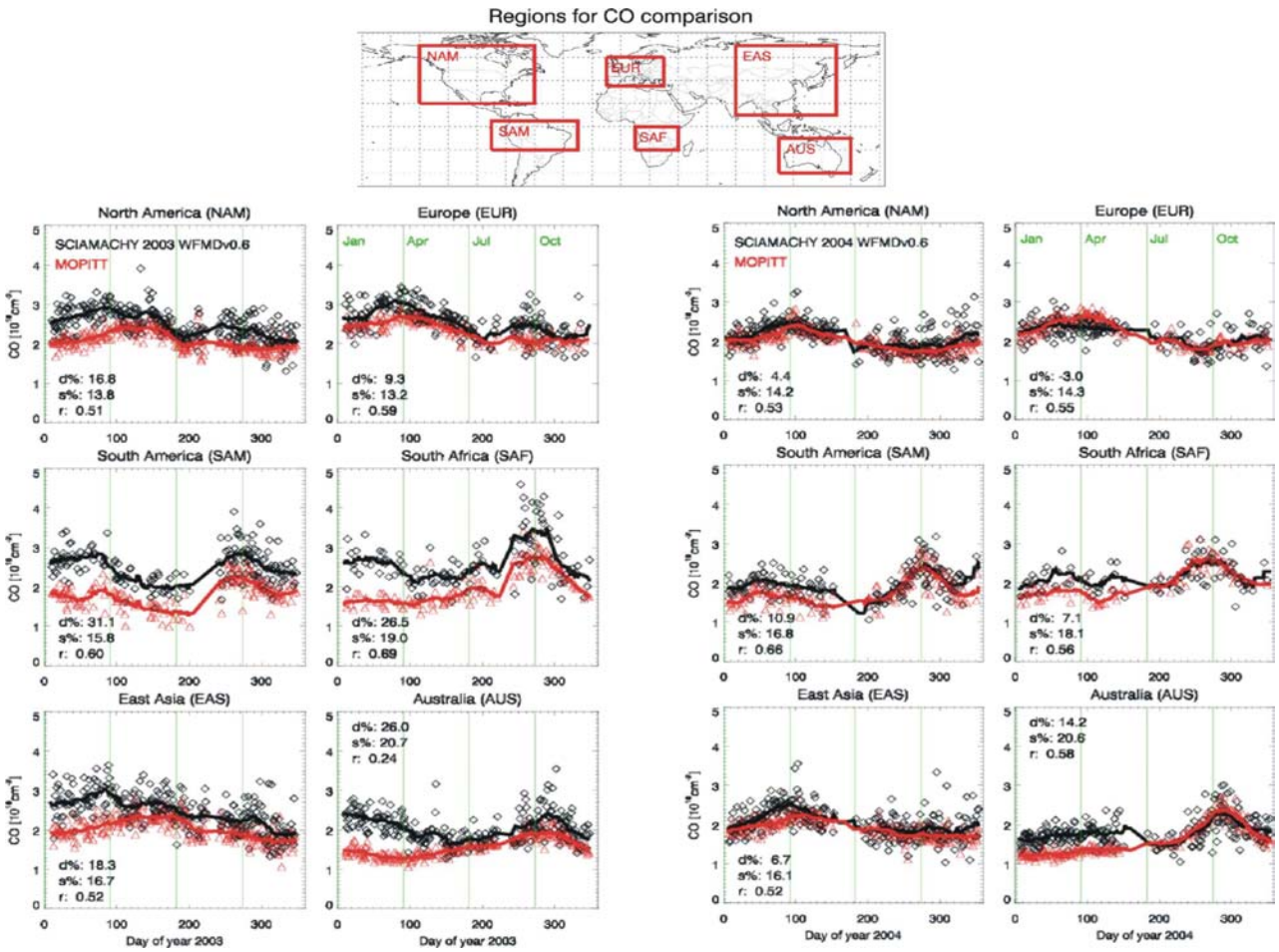

Fig. 2: Comparison of SCIAMACHY WFMDv0.6 CO columns (black) with MOPITT (red) for six regions for the years 2003 (left) and 2004 (right). The location of the six regions is shown in the top panel. The symbols show the averages of all coincident measurements within a region for a given day. For SCIAMACHY all measurement have been averaged for which the WFMDv0.6 quality flag indicates a (potentially) successful measurement. The solid lines represent a 30 days running average. For each region the following numbers have been computed based on the (not smoothed) daily averages: d% is the mean difference SCIA-MOPITT in percent, s% denotes the standard deviation of the difference in percent, and r is the linear correlation coefficient. The comparison method used here is exactly identical with the method used for WFMDv0.5 year 2003 data as described in [7].

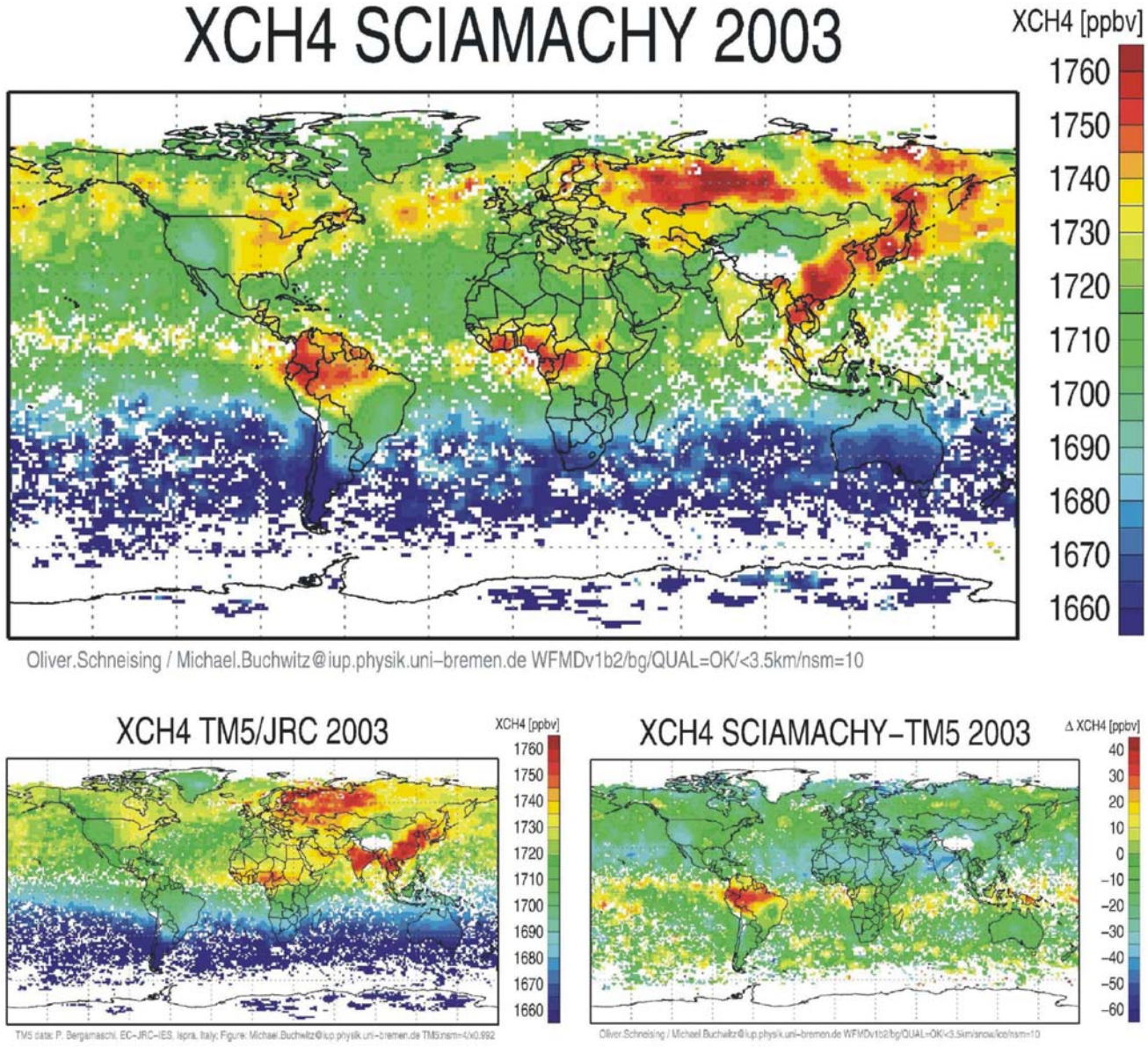

Fig. 3: *Top: Methane column averaged mixing ratios as retrieved from SCIAMACHY using WFM-DOAS version 1.0 for the year 2003. Bottom left: Corresponding TM5 model simulations (courtesy P. Bergamaschi, EC-JRC, IES, Ispra, Italy). Bottom right: Difference SCIAMACHY minus TM5. The SCIAMACHY averaging kernels have not been applied to TM5.*

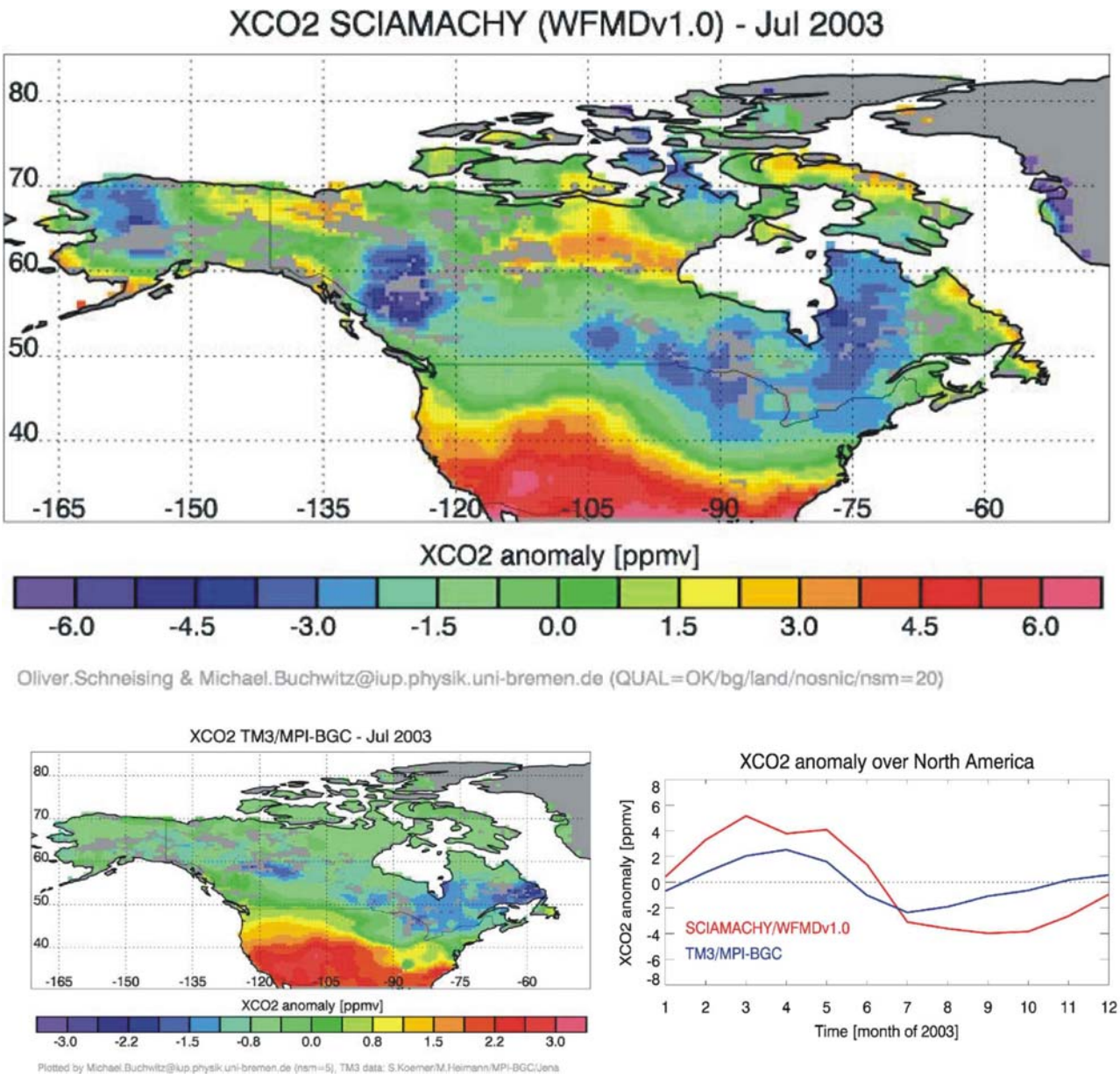

Fig. 4: Top: Carbon dioxide column averaged mixing ratios as retrieved from SCIAMACHY using WFM-DOAS version 1.0 over North America. Bottom left: Corresponding TM3 model simulations (courtesy S. Körner and M. Heimann, MPI-Biogeochemistry, Jena, Germany). Bottom right: Time dependence of the average CO_2 over North America as measured by SCIAMACHY (red) compared to TM3 (blue) (shown as anomalies, i.e., the mean values have been subtracted; the difference between the mean values is about 2%). The SCIAMACHY averaging kernels have not been applied to TM3.

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