Algorithm Document (AD)

Product: Methane column averaged mixing ratios
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Forward model

The forward model used for the retrieval neglects scattering and uses the Lambert-Beer law and geometrical air-mass factors (using line of sight and solar zenith angle) to calculate radiances at high spectral resolution (line by line, typically 0.005 nm resolution). These are subsequently convoluted with the instrumental slit function (Gaussian, FWHM approx. 1.35 nm) and interpolated to instrumental resolution. More Details can be found in Frankenberg et al, 2005a,b.

Inversion procedure

The inversion is based on the classical DOAS approach, i.e. the deviations between log(I/I0) and modeled differential optical densities are minimized. ECMWF pressure, temperature and water vapor profiles are used as prior input. For CH_4 and CO_2, TM5 and CarbonTracker model profiles are applied as prior profiles, respectively. Both models are optimally consistent with the ground based measurement network and ensure that deviations from the prior are as small as possible.
For CH_4 and CO_2, only the lowermost layer (about 10% of the entire atmospheric mass) are fitted in an unconstrained least-squares sense while the other layers are strictly constrained to the prior profiles. This technique ensures very similar averaging kernels for both species in the main region of variation, i.e. the lowermost troposphere (be it due to true variations or, more strongly, due to the presence of fractional clouds or aerosol layers).
The final product, viz. the column averaged volume mixing ratio of methane, is the ratio of the CH_4 and the CO_2 vertical column densities multiplied with the column averaged mixing ratio of CO_2. This can be either taken from climatologies or models, CarbonTracker output is provided with this dataset (we don't grant permission to actually use the CarbonTRacker data in scientific work. For terms of use please contact the CarbonTracker team or visit their website:
http://www.esrl.noaa.gov/gmd/ccgg/carbontracker/.

Sensitivity and error analysis / Algorithm validation

A detailed error analysis is carried out in Frankenberg et al, 2006. Statistical fit errors are, depending on surface albedo, on the order of 1-2%. Systematic errors can be introduced by differences in the light path distribution between the CH_4 and the CO_2 retrieval window. These are estimated to be below 3% (see Frankenberg et al, 2006). Another error source are unaccounted variations in CO_2 while they are expected to be within +/- 1.5%. Systematic errors of the algorithm are analysed in Frankenberg et al, 2005a. Further, the sensitivity of the algorithm is tested using a comprehensive set of simulated measurements.
Initial validation of the previous dataset (IMAPv1.1) has been performed in Dils et al. (2006).

Auxiliary data

A priori profiles of atmospheric variables are taken from ECMWF, interpolated to SCIAMACHY overpass time. The data are provided by KNMI, for details see http://www.knmi.nl/samenw/tosti/.
Spectral line parameters of CO_2 are taken from a recent study of Toth et al, 2007. Parameters of methane are determined using laboratory spectra recorded at several different ambient pressure levels (Frankenberg et al, 2008a).
Water vapor parameters are adapted from the Bxl-Reims database (http://www.ulb.ac.be/cpm/data.html), with changes as explained in Frankenberg et al, 2008b.

Recommendations for product validation

When validating the algorithm, it should be considered that it is not a pure methane product but the ratio between the vertical column densities of methane and carbon dioxide. Although variations in CO_2 are supposed to be far smaller, they can exhibit a large seasonal signal, especially in northern midlatitudes. The CarbonTracker model should eliminate most of this error but it might not be perfect at all locations, especially in regions where ground-based measurements assimilated by CarbonTracker are sparse or non-existent. Further, it should be noted that small biases depending on air-mass factors could still be present (due to small remaining errors in spectroscopy or instrumental line shapes).
An ideal validation would include methane and carbon dioxide total column measurements. For validation purposes, it should also be noted that the instrument sensitivity (averaging kernels) should be taken into account when comparing SCIAMACHY with different instruments.

B. Dils, M. De Mazière, J. F. Müller, T. Blumenstock, M. Buchwitz, R. de Beek, P. Demoulin, P. Duchatelet, H. Fast, C. Frankenberg, A. Gloudemans, D. Griffith, N. Jones, T. Kerzenmacher, I. Kramer, E. Mahieu, J. Mellqvist, R. L. Mittermeier, J. Notholt, C. P. Rinsland, H. Schrijver, D. Smale, A. Strandberg, A. G. Straume, W. Stremme, K. Strong, R. Sussmann, J. Taylor, M. van den Broek, V. Velazco, T. Wagner, T. Warneke, A. Wiacek, and S. Wood, *Atmos. Chem. Phys.*, **6**, 1953-1976, 2006.

Frankenberg, C., Meirink, J. F., van Weele, M., Platt, U.,and Wagner, T.: Assessing Methane Emissions from Global Space-Borne Observations, *Science*, **308**, 1010–1014, doi:10.1126/science.1106644, 2005a.

Frankenberg, C., Platt, U., and Wagner, T.: Iterative maximum a posteriori (IMAP)-DOAS for retrieval of strongly absorbing trace gases: Model studies for CH_4 and CO_2 retrieval from near infrared spectra of SCIAMACHY onboard ENVISAT, *Atmos. Chem. Phys.*, **5**, 9–22, 2005b.

Frankenberg, C., Retrieval of methane and carbon monoxide using near infrared spectra recorded by SCIAMACHY onboard ENVISAT : Algorithm Development and data analysis, PhD thesis (http://www.ub.uni-heidelberg.de/archiv/6016), 2005c

Frankenberg, C., Meirink, J. F., Bergamaschi, P., Goede, A. P. H., Heimann, M., Koerner, S., Platt, U., van Weele, M., and Wagner, T.: Satellite chartography of atmospheric methane from SCIAMACHY on board ENVISAT: Analysis of the years 2003 and 2004, *J. Geophys. Res.*, **111**, D07303, doi:10.1029/ 2005JD006235, 2006.

Frankenberg, C., T. Warneke, A. Butz, I. Aben, F. Hase, P. Spietz, and L. R. Brown, Pressure broadening in the 2ν3 band of methane and its implication on atmospheric retrievals, *Atmos. Chem. Phys*., **8**, 5061-5075, 2008a

Frankenberg, C., Bergamaschi, P., Butz, A., Houweling, S., Meirink, J. F., Petersen, K., Schrijver, H.,Warneke, T., and Aben, I.: Tropical methane emissions: A revised view from SCIAMACHY onboard ENVISAT, Geophys. Res. Lett., 35, L15811, doi:10.1029/2008GL034300, 2008b.

Toth, R. A., L. R. Brown, C. E. Miller, V. M. Devi, and D. C. Benner, Spectroscopic database of CO^2 line parameters: 4300–7000 cm^{-1}, *J. Quant. Spectrosc. Radiat. Transfer*, **109(6)**, 906–921, doi:10.1016/j.jqsrt.2007.12.004, 2007