Proposal Master Thesis

Validation of Carbon Monoxide retrieval from SCIAMACHY Near Infrared Nadir Spectra with NDACC/TCCON groundbased measurements

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Definition of the thesis framework

General

Measurements of trace gases from satellite based platforms are a common technique used today to derive global distributions. In comparison to ground based or airborne remote sensing techniques, satellite based measurements have the advantage of being able to cover most of the earth surface, hence delivering global maps of trace gases with reasonable resolution (spatially and temporally). Among others SCIAMACHY[1] aboard ENVISAT[2] is such a (passive) sensor which measured trace gases, aerosols, clouds etc. within the ultra violet (UV), visible light (VIS), near infrared (NIR) spectrum from 2002 - 2012.

An important task in combination with the analysis of satellite based measurements is the validation and verification process. Validation in that sense means comparing measurements acquired by satellite based instruments to other measurements utilizing different measuring methods, e.g. in situ measurements or ground based soundings. So validation asks for confirmation that the physical models implemented and solved are correct representations of the physical phenomena of interest. Beside validation, verification means

[1]Scanning Imaging Absorption Spectrometer for Atmospheric CHartographY
[2]Environmental Satellite

to determine precision and accuracy of models with the same datasets but different methodologies or implementations, e.g. comparing output of two radiative transfer codes with the same input data but another implementation of routines and/or physical processes. Basically this means to verify the accuracy of calculated results and of the error-free operation of the underlying software. With this definitions in mind, the thesis can be classified within the framework of validation of satellite based measurements by ground based measurements. The following two articles give an idea of how such an analysis (with SCIAMACHY data) can be performed (Schreier et al., 2014; Gimeno García et al., 2011).

Scope / Coverage

The main goal of the thesis is a validation and quality-check of the SCIAMACHY Channel-8 nadir measurements of CO (carbon monoxide) data processed from calibrated level-1b spectra at the Deutsches Zentrum für Luft- und Raumfahrt — Institut für Methodik der Fernerkundung — Atmospheric Processors (DLR-IMF-ATP). An appropriate approach to evaluate the quality of the dataset is to compare the satellite based level-2 data with ground-based measurements (Sussmann and Buchwitz, 2005). If time/data permits, even additional analysis on CH_4 (methane) from Channel-6 nadir measurements could be performed. Mainly due to technical reasons reliable SCIAMACHY channel-8 data is only available within the early years of the mission (approximately the first 3-4 years) but this should be enough for the projected analysis covered by this thesis. Additionally, it could be tried to retrieve data even until later stages of the mission (with some improvements/modifications of BIRRA (e.g. baseline, reflectivity, wavenumber-shift) which can then be compared to the ground based measurements.

NDACC and TCCON ground based measurements

To make datasets of two measurement methods (satellite based and ground based measurements) comparable to each other, both datasets have to fulfill certain citeria on retrieval quality (Dils et al., 2006). For satellite validation, a relatively uniform surrounding (in terms of altitude, surface albedo), remote from local pollution is preferable. Measurements provided by the Network for the Detection of Atmospheric Composition Change (NDACC)[3] would therefore be a good data resource because they provide calibrated long term

[3] http://www.ndsc.ncep.noaa.gov/

datasets from ground based stations. NDACC instruments which measure within the NIR - thermal infrared (TIR) are well distributed over the globe which is favourable for the planned analysis. As the focus of the thesis will be SCIAMACHY Channel-8 nadir measurements of CO which is sensitive in the near IR region (NIR) measurements from instruments supervised by the NDACC Infrared Working Group[4] (IRWG) are considered. Another pleasant fact of NDACC is that they have their own satellite working group[5].

A second resource for ground based measurements of carbon monoxide is the Total Carbon Column Observing Network (TCCON)[6] which is a network of ground based Fourier transform spectrometers recording direct solar spectra in the near-infrared spectral region. TCCON is affiliated with the NDACC Infrared Working Group (NDACC-IRWG) mentioned above. TCCON provides a comprehensive online documentation on their datasets with specific information updated for each measurement site as well as contact information. TCCON ensures that every site in their network processes data according to TCCON guidelines in order to make the products comparable within the network as well as externally. In that sense TCCON data should also be suitable for our validation. Further information in section 'Acquisition of data'.

SCIAMACHY data processing

To derive for example vertical column densities of trace gases from level-1b measurements retrieval algorithms have to be applied on the acquired spectrum. At DLR-IMF-ATP the Beer InfraRed Retrieval Algorithm (BIRRA) is such an algorithm performing an inversion of measurements to derive a state vector (Gimeno García et al., 2011) . BIRRA is based on the forward model Generic Atmospheric Radiative Transfer Line-by-Line Infrared Code (GARLIC) (Schreier et al., 2014) which was also developed at DLR-IMF-ATP. Instrument specific parameters (in context with the inversion often known as 'auxiliary' parameters) have to be assessed which are critical for the upcoming retrieval process once measurements are delivered. These parameters have then to be modeled within the forward model $\Phi(\boldsymbol{x})$. The state vector $\boldsymbol{x} = (\boldsymbol{\alpha}, \boldsymbol{r}, \boldsymbol{b})$ is fitted within the retrieval process. Some of these parameters are linear within the forward model ($\boldsymbol{r}$, $\boldsymbol{b}$) while others are non linear ($\boldsymbol{\alpha}$),

[4]http://www.acd.ucar.edu/irwg/index.html
[5]http://accsatellites.aeronomie.be/
[6]http://www.tccon.caltech.edu/

so describing the non-linear dependency between the measured values $\boldsymbol{y}(\nu)$ and the elements of the state vector $\boldsymbol{x}$ in the model. This can be expressed as follows

$$\Phi(\boldsymbol{x}) \equiv \hat{I}(\nu) = (I \otimes S)(\nu) \tag{1}$$

which is the forward model for the measured intensity spectrum $\hat{I}(\nu)$. So we represent the measured values $\boldsymbol{y}(\nu)$ as

$$\boldsymbol{y}(\nu) \quad = \quad \hat{I}(\nu) \tag{2}$$

with

$$\hat{I}(\nu) \quad = \quad \frac{\boldsymbol{r(\nu)}}{\pi} \mu_{\odot} I_{\text{sun}}(\nu) \exp\left(-\sum_m \alpha_m \tau_m(\nu)\right) \otimes S(\nu, \varsigma) + \boldsymbol{b}(\nu). \tag{3}$$

τ_m stands for the two way (sun - earth - sat) optical depth of a certain molecule and $S(\nu, \varsigma)$ represents the instrument response function. α_m is called the molecular scaling factor and as a parameter of the state vector $\boldsymbol{x}$ adjusts the a-prior profile. Beside the molecular scaling factor additional parameters of the state vector have to be determined and fitted, e.g. surface albedo $\boldsymbol{r}(\nu)$ and an optional baseline correction $\boldsymbol{b}(\nu)$ (in BIRRA both modeled by a polynomial depending on wavenumber with the coefficients as fit parameters). These are critical steps within the level-2 processing because the forward model, which simulates the measured spectrum acquired by the satellite, constitues an integral part of the retrieval algorithm (e.g. within BIRRA). At DLR-IMF-ATP all tools and datasets are accessible to make a comprehensive analysis of the SCIAMACHY data.

Prerequisites

Before starting with SCIAMACHY level-2 processing for the comparison with ground based measurements we have to figure out what kind of datasets (e.g. which level, calibrations applied, ...) NDACC and TCCON are providing to users. As I have already found out most of these questions can be answered with the information provided on their websites, but contacting a specific site in case of ambiguity is possible. Also checking if NDACC sites which are finally used (selected) for comparison are retrieving CO at the same or similar wavelength interval compared to that of SCIAMACHY Channel-8 [4191 - 4426 cm^{-1}] is favorable before starting simulations. Finally our analysis will be based on the 'as-is' state of the products provided by the two networks and we will compare them to different (modified) BIRRA runs based on SCIAMACHY data.

Acquisition of data

Contact has been established with Ralf Sussmann from the Karlsruher Institut für Technologie (KIT), collaborator (PI) of the Garmisch / Zugspitze spectrometers (awaiting answer soon). If questions arise on data for other stations contact will be established. Data from more than one station within NDACC/TCCON are intended to be used for validation. Prefered sites for validation are those remotely located within homogeneous terrain. Among others, stations which provide measurements on CO and CH_4 for the years from 2002 through 2006 or later are Kiruna, Lauder[7], Jungfrau, Mauna Loa.

Datasets of stations processed with a-priori information of the National Centers for Environmental Prediction (NCEP) can be found under the following link[8]. Datasets from NDACC are free accessible and provided as Hierarchical Data Format (HDF) files. These files can be read with Python libraries such as *pytable*[9] or *vitables*[10]. The HDF datasets are also readable with the software package *Level2*, a subpackage of *anaLiza*, at DLR-IMF-ATP.

For TCCON sites data can be found here[11]. There is a web interface from which one can filter data on quality, time, solar zenith angle (SZA) and other parameters for each station. TCCON is providing the data in tables which can be viewed with any text editor.

[7] ftp://ftp.cpc.ncep.noaa.gov/ndacc/station/lauder/hdf/ftir/
[8] http://www.ncep.noaa.gov/
[9] http://www.pytables.org/moin
[10] http://vitables.org/
[11] http://tccon.ipac.caltech.edu/

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