Geophysical Research Abstracts
Vol. 13, EGU2011-7767, 2011
EGU General Assembly 2011

Retrieval algorithms for TROPOMI – improving error estimates of retrieved quantities by using Optimal Estimation with explicit a priori data

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TROPOMI (TROPOspheric Monitoring Instrument) is a nadir-viewing shortwave spectrometer to measure the tropospheric composition for climate and air quality applications. The TROPOMI instrument, an initiative from the Netherlands and developed in co-operation with ESA, will be launched in December 2014 as a single payload on the Sentinel 5 Precursor mission. This mission is an important step forward from the current OMI (Ozone Monitoring Instrument) on NASA EOS Aura and SCIAMACHY on Envisat towards the operational Sentinel 5 mission that is planned around 2020.

TROPOMI will measure backscattered sunlight in the wavelength ranges 270-500, 710-770, and 2314-2382 nm, attain daily global coverage and has a small pixel size (7x7 km2 at nadir). Retrieval algorithms are used to translate the measured spectra into information of the composition of the atmosphere, such as ozone profile and columns of NO2, O3, BrO, HCHO, CH4, and CO, and information on clouds and aerosol.

In order to determine the composition of the atmosphere, a priori information is needed such as the spectral absorption cross sections of the different species, altitude profiles of the species, temperature profiles, and the surface albedo. In addition, information on cloud properties (cloud fraction, cloud albedo, cloud pressure) is needed because absorbing gases can be hidden below the clouds. Cloud properties are derived using a separate retrieval. Advanced use requires products in which the role of a priori data is included and transparent.

It is not sufficient to derive values of the parameters involved; the precision of the retrieval has also to be quantified. The Optimal Estimation method (Rodgers, 2000) is the mathematical framework that has been developed for these kinds of retrieval problems. The uncertainty in the measured radiances and the uncertainty in the a-priori information are translated into an uncertainty in the retrieved parameter values. Sometimes retrieved parameters are highly correlated, such as cloud fraction and cloud albedo which can have a correlation coefficient larger than 0.99. Such correlations should be taken into account as they affect the error estimate in the final product.

At least some of the retrieval algorithms for TROPOMI will be based on Optimal Estimation which will provide improved error estimates compared to older algorithms that are currently used for OMI. For that purpose prototype software has been developed which can be used to evaluate retrieval algorithms and their sensitivity to measurement noise, bias in the measured radiance, bias in the a priori information, and bias in the model atmosphere used. The simulation software has an Optimal Estimation module and a radiative transfer module. Currently, the simulation software is being extended so that retrievals can be applied to OMI measurements since 2004 in order to test the retrievals on measured instead of simulated data.

Results of simulated retrievals will be presented. The importance of good error estimates will be stressed because such error estimates are essential for validation/verification studies and for further processing (e.g. data assimilation). Finally, it is argued that inconsistencies between the a priori data and the measured values can lead to poor convergence or no solution at all. This means that the use of the Optimal Estimation method has an in-build consistency check with regard to a priori information. Such a consistency check is usually not available for traditional retrieval algorithms.