IMLM v6.3 algorithm description

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1. Introduction

This document describes the Iterative Maximum Likelihood Method (IMLM) developed at SRON for retrieval of total trace gas columns from near-infrared SCIAMACHY spectra. In contrast to most retrieval methods, this method is based on fitting a model of the expected detector signal to the measurements by varying the total amounts of the trace gases that play a role in the selected retrieval window. In other words, the forward model includes not only the atmospheric absorption but also the instrument characteristics. Since model results and measured detector counts can be directly compared, the influence of instrument peculiarities such as dark signal, pixel-to-pixel effects, etc. are more easily tracked. The use of the solar calibrations becomes slightly more complex.

The algorithm has been described extensively in Gloudemans et al. (2008).

2. Theoretical background and the forward model

The forward model computes first the atmospheric absorption for a given model atmosphere assuming the currently estimated values of the total slant columns. Spectroscopic data are taken from the HITRAN database (currently version 2004). Temperature and water vapour profiles are taken from ECMWF data. The trace gas profiles are assumed having a fixed dependence on pressure (the pressure distribution coming from the ECMWF data) and are derived from the US standard atmosphere (Anderson et al. 1986). The atmosphere is vertically divided in a number of layers. The optical density τ is calculated by applying the Voigt profiles corresponding to the temperature and pressure of each layer for each spectral line on a sufficiently fine wavenumber grid, and the sum is taken over all the layers.

A radiance spectrum is computed using a model solar spectrum I_0 at a distance of one astronomical unit, assuming the currently estimated values of the total slant columns and a fixed value of the surface albedo A assuming Lambertian reflection.

$$I(\nu) = I_0(\nu)e^{-\tau}\cos(\theta)A\pi^{-1}R_\odot^{-2}, \tag{1}$$

where $R_\odot$ is the distance Sun-Earth.

This spectrum is then fed into a model of the instrument yielding the modelled detector counts. This model accounts for the transmission of the optics, the dispersion by the grating, the detector quantum efficiency, and the analogue-to-digital converter. The result is multiplied by a closure term (a n-th order polynomial, where normally $n = 1$ for the CO/CH_4 retrieval window) in order to match the measured signal level and allow for low-frequency calibration errors, imperfect continuum modelling, and surface albedo wavelength dependence.

The SCIAMACHY measured solar spectrum cannot be applied directly in the IMLM algorithm, since it contains instrument effects such as spectral dispersion and damaged or noisy detector pixels which would spoil the forward model. In order to account for these instrument effects, a high-resolution ATMOS spectrum has been fed into the instrument model to obtain a solar spectrum on the SCIAMACHY detector pixel grid. Comparison of this modeled SCIAMACHY solar spectrum with the specially calibrated SCIAMACHY solar reference spectrum (provided by J. Frerick, ESA) leads to a correction factor for each detector pixel which is included in the forward model. Using daily measured SCIAMACHY solar spectra instead of the specially calibrated SCIAMACHY solar spectrum does not lead to significant improvements in the retrieved CO and CH_4 total columns.

The instrument model also computes the expected measurement noise by evaluating the various contributing noise sources: photoelectron shot noise, Johnson noise, detector read-out noise.

In addition, the forward model computes the derivatives of the expected counts with respect to the fitting parameters, i.e., the total columns and the terms of the polynomial closure term.

Detailed equations can be found in Gloudemans et al. (2008).

3. Fitting procedure

The fitting process aims at finding those values for the total trace gas columns (assuming a fixed vertical profile) and the coefficients of the polynomial scaling factor that correspond to maximal statistical likelihood for the measured detector counts. Because of the non-linear character of the model, this requires an iterative procedure. In each iteration the model and its derivatives must be recomputed.

We denote the result of the forward model as the vector $\mathbf{I}(\mathbf{p}) = I_1(p_1 ... p_M) ... I_K(p_1 ... p_M)$, thus consisting of K elements I_k each depending on M parameters p_m. The measurements are represented by the vector of K elements $\mathbf{N}$ and a measurement covariance matrix Σ. Then in the i-th iteration an updated value of $\mathbf{p}$ is computed as

$$\mathbf{p}_{i+1} = \mathbf{p}_i + (\mathbf{D}^\mathbf{T} \Sigma^{-\mathbf{1}} \mathbf{D})^{-\mathbf{1}} \cdot \mathbf{D}^\mathbf{T} \Sigma^{-\mathbf{1}} \cdot (\mathbf{N} - \mathbf{I}(\mathbf{p}_i)) \quad (2)$$

where $\mathbf{D}$ is the $K \times M$ matrix with elements $D_{km} = \partial I_k / \partial p_m$. The covariance of the estimated parameters (i.e., the error due to the instrument noise) is

$$(\mathbf{D}^\mathbf{T} \Sigma^{-\mathbf{1}} \mathbf{D})^{-\mathbf{1}}. \quad (3)$$

These expressions can be evaluated by standard numerical procedures, based on Cholesky decomposition.

The starting values for the total trace gas columns can be conveniently taken as zero. Convergence is reached within 4 iteration steps.

The total vertical columns are computed assuming a geometrical air mass factor computed from the solar zenith angle and the line-of-sight viewing angle in a spherical geometry.

4. Auxiliary data

The cloud cover is estimated on the basis of the 32 Hz PMD readings, using the PMD channels B, C, D, and E. The procedure is described in Krijger et al. (2005).

Temperature and water vapour profiles and surface pressure are taken from data from the European Centre for Medium-Range Weather Forecasts (ECMWF) (http://www.ecmwf.int). Three-hourly forecast data on a 0.5° by 0.5° grid have been interpolated to the satellite overpass time and footprint (cf. http://www.knmi.nl/samenw/tosti/).

5. Sensitivity and error analysis

Results of an early sensitivity analysis for SCIAMACHY channel 8 done before launch were reported by Schrijver (1999). There the use of the entire channel 8 was assumed. The growth of an ice layer made the latter impossible. The use of microwindows has the consequence of lowering the sensitivity by a considerable factor. The loss of detector window transmission due to the ice layer and the loss of useful photons caused by scattering in this layer further reduce the sensitivity. On top of that, the growing number of bad and dead detector pixels has a negative effect on the sensitivity (Kleipool 2004, Kleipool et al. 2007).

The sensitivity depends of course strongly on the signal level, and thus on the surface albedo. There is also dependence on solar zenith angle and integration time since both influence the signal level. As an example, Figure 1 gives the estimated noise-related errors for the currently used retrieval window in channel 8. A global distribution of the random instrument-noise error can be found in de Laat et al. (2006, 2007) and Gloudemans et al. (2008).

An extensive sensitivity study has been performed by Gloudemans et al. (2008) including effects of fixed trace gas profiles, surface pressure, spectroscopy, aerosols, and polarization.

6. Algorithm validation

The algorithm has been tested extensively on a number of synthetic spectra. It has been shown to be robust, and to return the total columns used as input for the computation of the spectra. The results do not depend on the initial values in the iteration.

Deviations from the trace gas profiles assumed in the forward model have an influence on the retrieved columns. These effects can be quantified by total column averaging kernels using the same method as described in Buchwitz et al. (2004). The total column averaging kernels are found to be close to one from the surface up to pressure levels of about 200 hPa thus showing good sensitivity throughout the troposphere (Gloudemans et al. 2008).

The effects of the various calibrations on the quality of the results have been reviewed by Gloudemans et al. (2005).

The CO results have been validated against model results by de Laat et al. (2006, 2007).

Comparisons with FTIR stations have been performed by Dils et al. (2006)

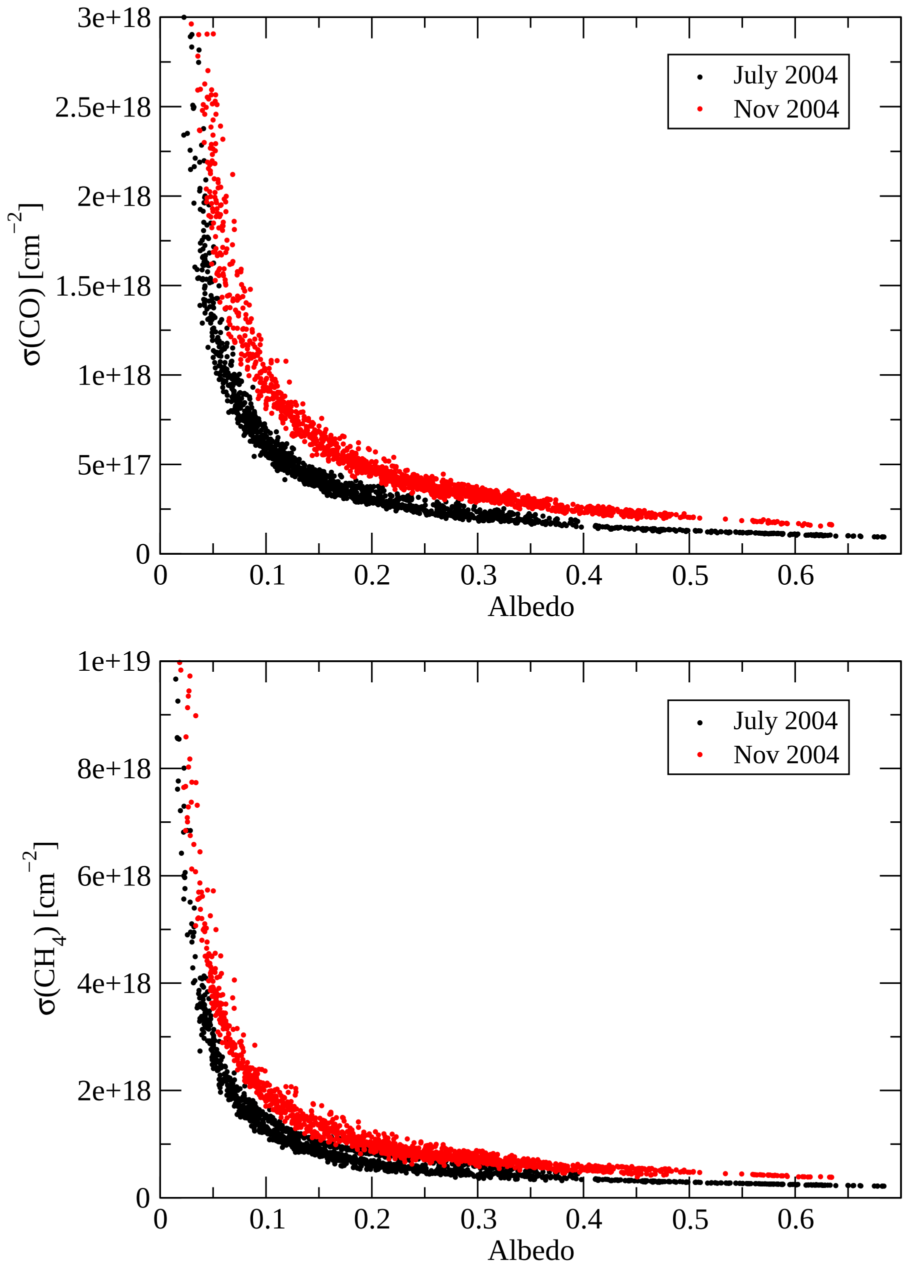

Figure 1. Noise-related errors as function of surface albedo for CO (upper panel) and CH_4 (lower panel) for two dates: July 2004 (shortly after decontamination) and November 2004 (four months after decontamination).

7. Recommendations for product validation

Validation measurements should be representative for the extent of the SCIAMACHY ground scene. The use of measurements taken above oceans, in coastal regions, at high surface elevation, or at high latitudes ($> 70^\circ$N or $< 70^\circ$S) is therefore not recommended.

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