RECENT ADVANCES IN SCIAMACHY NEAR INFRARED NADIR LEVEL 2 ALGORITHM DEVELOPMENT

Franz Schreier, Michael Hess, Adrian Doicu, Thomas Schröder, and Albrecht von Bargen

DLR — German Aerospace Center, Remote Sensing Technology Institute, Oberpfaffenhofen, 82234 Wessling, Germany

Abstract

The near infrared channels of SCIAMACHY onboard ENVISAT can be used to derive information on CO, CH₄, N₂O, and H₂O. A core element of the current operational level 2 data processor for nadir observations is the BIAS (Basic Infrared Absorption Spectroscopy) algorithm using a DOAS–type approach with a standard nonlinear least squares fit. Here we present work on recent advances towards a “Better InfraRed Retrieval Algorithm”, covering both the forward modelling and inversion aspect, nb.

• Nonlinear least squares exploiting special structure of the forward model
• Flexible choice of additional fit parameters besides molecular columns
• Option for ‘online’ line-by-line absorption cross section computation and continua

First results of the improved algorithm for SCIAMACHY near infrared nadir processing are presented.

1. INTRODUCTION

Nadir sounding of vertical column densities of atmospheric gases is well established in remote sensing. For UV instruments such as SCIAMACHY [1] the analysis is traditionally based on a DOAS–type methodology. This approach has also been successfully applied for analysis of SCIAMACHY’s near infrared channels [2, 3, 4, 5] and is the basis of the BIAS (Basic Infrared Absorption Spectroscopy) nonlinear least squares algorithm, a core element of the current operational level 2 data processor [6]. In addition to the column scale factors for the molecular densities a one-parameter “closure term” is fitted to account for any other effects such as (single or multiple) scattering, surface reflection, or instrumental artefacts. However, recent sensitivity studies have shown the importance of adequate modelling the instrumental slit function; in particular an under- or overestimate of the slit function half width can have a significant impact on the retrieved columns. Furthermore, in BIAS molecular absorption is taken into account using look–up tables that have been calculated for a coarse altitude grid version of the US standard atmosphere [7] and a dated set of spectroscopic line parameters. Likewise the slant path optical depth is interpolated from look–up tables generated for a finite set of path geometries.

In order to gain much greater flexibility in the forward modelling (radiative transfer and instrument) and a more efficient and robust least squares inversion scheme, work on further improvement of the SCIAMACHY near infrared nadir processing is ongoing. The methodological background and implementation of a “Better InfraRed Retrieval Algorithm” (BIRRA) are described in the following section and results are presented in section 3.

2. THEORY

2.1. Near Infrared Radiative Transfer

The intensity (radiance) $I$ at wavenumber $\nu$ received by an instrument at $s = 0$ can be described by the integral form of the equation of radiative transfer [8]

$$ I(\nu) = I_b(\nu) - \int_0^\infty ds' J(\nu) \frac{\partial T(\nu; s')}{\partial s'}, $$

(1)
where \( I_b \) is a background contribution and \( J \) is the source function, that in general comprises thermal emission, single and multiple scattering contributions. In the near infrared contributions from reflected sunlight become important, whereas thermal emission is negligible. Furthermore scattering can be neglected for clear sky (cloud free) observations. Thus the radiative transfer equation simplifies to

\[
I(\nu) = r I_{\text{sun}}(\nu) T_1(\nu) T_2(\nu)
\]

where \( r \) is the reflection factor and \( T_1 \) and \( T_2 \) denote the transmission between reflection point (e.g. Earth surface) and observer and between sun and reflection point, respectively.

The monochromatic transmission \( T \) (relative to the observer) is given according to Beer’s law by

\[
T(\nu, s) = \exp \left[ -\int_0^s \alpha(\nu, s') \, ds' \right]
\]

(3)

\[
\alpha(\nu, s) = \sum_m k_m(\nu, s) n_m(s) + \alpha^{(c)}(\nu, s)
\]

where \( \alpha \) is the volume absorption coefficient, \( k_m \) and \( n_m \) are the absorption cross section and density of molecule \( m \), and \( \alpha^{(c)} \) the continuum absorption coefficient. Note that the absorption cross section is a function of (altitude dependant) pressure and temperature, i.e., \( k(\nu, z) = k(\nu, p(z), T(z)) \).

The instrumental response is taken into account by convolution of the monochromatic intensity spectrum (1) with an spectral response function \( S \) (a.k.a. instrumental line shape function ILS)

\[
\tilde{I}(\nu) \equiv \langle I \otimes S \rangle(\nu) = \int_{-\infty}^{\infty} I(\nu') \times S(\nu - \nu') \, d\nu'
\]

(5)

(in general a further convolution will be required to account for the finite field of view, however, this is usually negligible for nadir viewing). For SCIAMACHY NIR measurements Gaussian, hyperbolic, or Voigt profiles are commonly used,

\[
S_G(\nu, \gamma) = \frac{1}{\gamma} \left( \frac{\ln 2}{\pi} \right)^{1/2} \cdot \exp \left[ -\ln 2 \left( \frac{\nu - \nu'}{\gamma D} \right)^2 \right]
\]

(6)

\[
S_H(\nu, \gamma) = \frac{\sqrt{2} \gamma^3 / \pi}{\nu^2 + \gamma^4}
\]

(7)

\[
S_V(\nu, \gamma_L, \gamma_G) = S_L(\nu, \gamma_L) \otimes S_G(\nu, \gamma_G)
\]

(8)

where the Voigt profile is a convolution of the Gaussian with a Lorentzian profile \( S_L(\nu, \gamma) = \gamma / [\pi (\nu^2 + \gamma^2)] \).

### 2.2. Forward Model

The forward model is based on the MIRART (Modular InfraRed Atmospheric Radiative Transfer) code, a set of programs for high resolution infrared atmospheric radiative transfer calculations developed with emphasis on efficient and reliable numerical algorithms and a modular approach appropriate for simulation and/or retrieval in a variety of applications [9]. Molecular spectroscopic parameters can be read from HITRAN [10], GEISA [11], or IPI [12] databases. Continuum corrections to the absorption coefficient are supported, e.g. the CKD continuum [13]. In contrast to other line–by–line codes MIRART solves the integral forms of Beer’s and Schwarzschild’s equation by means of numerical quadrature schemes for arbitrarily spaced abscissas. Derivatives of transmission and/or radiance spectra with respect to the atmospheric state vector are obtained by means of algorithmic (automatic) differentiation [14]. Arbitrary observation geometry (up or downlooking, limb) and instrumental field-of-view and line shape for heterodyne, Fourier transform, Fabry-Perot, and grating sensors are supported. MIRART has been extensively verified by intercomparisons with other codes, nb. in the AMIL2DA (Advanced MIpaS Level 2 Data Analysis) project devoted to infrared limb emission sounding [15] and in the IRTM Workshop series covering up–, down–, and limbviewing in the microwave spectral range [16].

### 2.3. The inverse problem — nonlinear least squares

The objective of SCIAMACHY near infrared measurements in nadir viewing geometry is to retrieve information on the vertical distribution of trace gases such as \( \text{N}_2\text{O}, \text{CH}_4, \text{or CO} \), e.g., the volume mixing ratio \( q_X(z) \) or number density...
where the unknown state vector \( \mathbf{x} \) is comprised of the geophysical and instrumental parameters \( c, \gamma, r \) and an optional additive baseline correction \( b \) (more generally a polynomial in wavenumber).

For the solution of the nonlinear least squares problem (9) we use solvers provided in the PORT Optimization Library \([17, 18]\) that are based on a scaled trust region strategy. In some cases the iteration might lead to negative values for physical quantities such as column densities. Hence BIRRA provides the option to use alternatively a nonlinear least squares with simple bounds (e.g., nonnegativity).

Note that the surface reflectivity \( r \) and the baseline correction(s) \( b \) enter the forward model \( \mathbf{F} \equiv \mathcal{I}(\nu; \ldots) \), Eq. (11), linearly. Due to this special structure of the forward model the least squares problem (9) can be reduced to a separable nonlinear least squares problem \([19]\) that has several advantages: a modified nonlinear least squares containing only the nonlinear parameters has to be solved, the Jacobian of the forward model has to be calculated for these nonlinear parameters only, and no iteration and accordingly no initial guess is required for the linear parameters. Furthermore experience has shown that frequently the separable nonlinear least-squares solver converges in fewer iterations.

### 3. RESULTS

The BIRRA code now offers both “standard” and separable nonlinear least squares solvers with and without bounds. As shown in Fig. 1, the different methods lead to the same results except for a few observations. These differences are attributed to problems with the observed spectra, e.g. cloud coverage or bad/dead pixels.

The essential idea of least squares is the minimization of the residual. A comparison of the residual norm between the new and the old algorithm is given in Fig. 2.

Molecular spectroscopic data are a critical input for successful analysis of atmospheric spectra, and line parameter databases are updated frequently. The recent 2004 version of the HITRAN \([10]\) database has brought a significant change of \( \mathrm{H}_2\mathrm{O}, \mathrm{CH}_4, \) and \( \mathrm{N}_2\mathrm{O} \) data compared to 2000. Although the number of \( \mathrm{CH}_4 \) lines has increased dramatically (due to inclusion of numerous weak lines), the most severe changes are due to water vapor. In Fig. 3 retrieval results using the latest two HITRAN editions are compared.

The BIAS algorithm uses a “distilled” version of the US standard atmosphere \([7]\) using 17 levels up to 57.6 km. Beside the coarse resolution and reduced altitude range the use of this atmospheric model globally might be problematic. In Fig. 4 column density scale factors and reflection are compared for two different atmospheric models and observations of orbit 2509, state 3 located in the arctic.
4. SUMMARY AND OUTLOOK

A significant upgrade of the SCIAMACHY near infrared nadir level 2 algorithm from “BIAS” to “BIRRA” has been presented and results showing the performance and flexibility of the new implementation have been shown. Careful analysis and verification of the data by intercomparisons is ongoing.
Figure 3. Application window 2: Comparison of column density fits (plots on left) using different versions of HITRAN (line strengths and cross sections on right side). Orbit 2509, State 03; Separable nonlinear least squares without bounds.

Figure 4. Application window 2: Comparison of column density fits for different atmospheres: “BIAS atmosphere” vs. “Subarctic Summer Atmosphere” (50 levels up to 120 km). Orbit 2509, State 03; Separable nonlinear least squares with bounds.

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REFERENCES


