THE MAJOR REVISION OF THE OPERATIONAL SCIAMACHY LEVEL 1B-2 OFF-LINE DATA PROCESSOR

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Abstract

Recently, the operational data processor chain for SCIAMACHY from Level 0 to Level 2 was subject to major revisions in each part including not only the Level 0-1b and Level 1b-2 data processing but also the IECF. In this contribution, we present the revisions and upgrades of the algorithms for the Level 1b-2 Off-line processing which had been applied to the derivation of products for Nadir and Limb back-scattered light observations as well. The results will be discussed briefly. In particular, the derivation of products from Nadir back-scattered light observations in the UV/VIS spectral region has been established by integration of most recently developments of state-of-the-art algorithms: The SDOAS algorithm of BIRA-IASB for the retrieval of column densities and the SACURA algorithm for the derivation of cloud-top height and cloud optical thickness based on cloud fraction provided by the DLR-IMF's OCRA algorithm. The combination of all three provides now the vertical column densities for Ozone and NO_2. It is worth to note, that the product list for cloud parameters is now substantially extended due to SACURA. The derivation of Ozone and NO_2 profiles from Limb back-scattered has been substituted by DLR-IMF's DRACULA retrieval package. Those in combination with optimised settings provide substantial improvements in profile information which are in very good agreement with scientific implementations of IFE Bremen. Additionally we present an overview about developments for future implementations. Beside an evolution scheme for the future, this holds for the evolution of the DRACULA package and for the retrieval of BrO profiles from Limb observations.

1 TOTAL COLUMN DENSITY DERIVATION FROM NADIR UV/VIS MEASUREMENTS

1.1 Upgrade DOAS Algorithm

The goal of the upgrade was two-fold: A state-of-the-art algorithm for the retrieval of total column densities of O_3 and NO_2 shall be established and very good agreement with operational GOME data products shall be achieved. Thus, parts of the GOME Data Processor Version 4.0 (GDP4) [1] have been selected for implementation baseline in SCIAMACHY Ground Processor Level 1b-2 Off-line (SGP) applying for the slant column density retrieval the GDOAS scheme of BIRA which has been adapted at BIRA to SCIAMACHY measurements (SDOAS) [2]. Slant column densities are combined together with air mass factors (AMF) which had been calculated from radiative transfer modelling using LIDORT V2.2. The iterative approach as implemented in GDP4 allows the determination of vertical total column content for O_3 and NO_2. In contrast to GDP4, the cloud parameters are derived applying the cloud cover algorithm OCRA [3] and the algorithm SACURA [4] to determine the cloud-top height and cloud optical thickness.

A schematic outline for the algorithm flow in the implementation is provided in Figure 1. A pre-processing of cloud parameters and of the climatology input is carried for each nadir state of the orbit simultaneously. The determination of slant column densities, air mass factors, and total column content is then performed as a sequence for each particular measurement.

1.2 Cloud Parameter Retrieval

The cloud coverage will be as before determined from the *rgb* PMD measurements, but the retrieval of cloud parameters is extended by IFE's SACURA [4]. SACURA has been specifically adapted for operational usage (SACURA-B) with the emphasis to those parameters which are relevant to the retrieval of trace gas total columns. Input to SACURA-B is the cloud cover derived from OCRA. The determination of cloud-top height and cloud optical thickness is based on the measurements of the top-of-atmosphere reflection function in the oxygen A-band. The cloud reflection function is extremely sensitive to cloud-top height in the centre of the O_2 absorption band. Since the problem is assumed as linear, a Taylor expansion of the reflection function with respect to the cloud-top height is considered for the determination of the parameter by means of least-squares.

1.3 Vertical Column Density Calculation

The vertical column density (VCD) is calculated as in GDP4 so that this part of the GDP4 algorithm kernel had been directly integrated. LIDORT Version 2.2 is used for the calculation of air mass factors. Cloud parameter input stems directly from OCRA (cloud fraction), or is converted from SACURA results applying climatological information (cloud-top pressure). Cloud-top albedo is derived from cloud optical thickness. Profile information is provided from climatology (Specific settings, see [5]) as the surface height and albedo. After determination of AMFs, the VCDs are determined iteratively based on AMF and SCD input and profile information from climatology (Settings see [5]). If no cloud parameters are available, the VCD computation is based on climatology input (ISCCP).

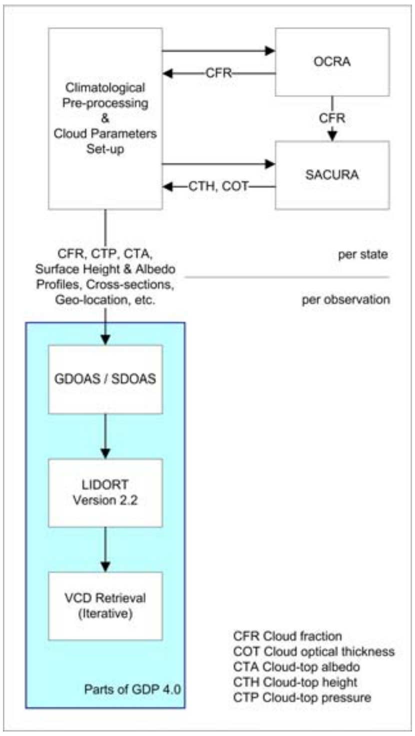

Figure 1 Outline of the algorithm flow in SGP for the retrieval of total column content of O_3 and NO_2

1.4 Verification

Verification had been carried out for the total column density determination against the SDOAS reference in a first step. Since SDOAS makes use of FRESCO cloud parameters, the SGP had been prepared to use the FRESCO data used at BIRA as input. A sample of 60 orbits out of the year 2003 had been taken. For ozone, a slight mean deviation (-0.1% with std.dev. of 0.05%) has been observed; AMFs (mean dev. 0.38%, std.dev. 3.9%) and VCD (mean dev. -0.4%, std. dev. 4.1%) show a stronger discrepancy which is for a high amount due to the fact that in SGP profile extraction from climatology is extracted by interpolation over geo-location and season; in contrast SDOAS performs a nearest-neighbour search. In total, 97% of the SCDs are within 0.2% deviation and 97% of VCD within 1%. For NO2 deviation of SCDs are around -0.4% (std.dev. 3.9%); in case of VCD a mean deviation of around -0.25% (std.dev. 4.1%) is observed. Cloud parameter had been verified against IFE's original implementation taking the same sample as baseline. For cloud-top height, 93% of the sample can be found within ±250 m and about ±98% within 750 m. Evaluation of cloud optical thickness showed the same quality of agreement, around 97% are found within $\pm 1\sigma$. Deviations are explained by usage of different surface database between reference system and processor. As final step, the impact of the different cloud scheme used for AMF retrieval in the processor has been studied. These results are more detailed presented in an additional poster (see poster [5]) demonstrating that no impact could be observed for NO2 but some enhancement (mean deviation of around 0.4%-0.6%) for ozone VCDs. Finally, the sample of 54 orbits computed with the coming operational implementation of SGP had been provided to BIRA for an inter-comparison study which is also presented in this session (see poster [6]). Here, a comparison to GDP4 is also presented which shows a very good agreement between SGP and GDP4.

2 IMPLEMENTATION OF NEW LIMB RETRIEVAL ALGORITHM PACKAGE

In order to be prepared for a flexible limb retrieval package within SGP, DLR-IMF decided to substitute the original approach (Version 2.5) with which the extension was not possible. As alternative proxies, the Iterative Gauss-Newton Regularization with bound constraints (IRGN) and the Tikhonov Regularization had been integrated into one system with the opportunity to apply different schemes for the set-up of the regularization matrix, the choice and the alteration of the regularization parameters during each iteration step. Note that different kind of schemes can be applied for the determination and alteration of the regularization parameters during iteration. The implemented solvers are on one side a trust-region method with bounds constraints and as alternative a classical Gauss-Newton iteration scheme.

In this poster, we outline the algorithm flow which will be applied in the operational chain and, in addition, the implemented alternative of Tikhonov Regularization, both given in Figure 2. The algorithm behind and the theoretical background is explained within this poster session in an additional poster (see poster [7]).

The operational processing will be carried from version 3.0 on with the method IRGN. A major issue is the preparation of the global regularization matrix and the weighting of regularization parameters. L-curve criteria is applied in every iteration of the trust region solver compiling a descending sequence of regularization parameters. The original Tikhonov regularization method differs in some details: The regularization parameters are kept constant so that the solver performs the solution determination without any coupling to an additional regularization parameter change. Usually, no boundary conditions are introduced.

2.1 Verification

A verification campaign had been carried out by IFE Bremen twice for the retrieval of Ozone vertical profiles in the Huggins band and NO2 vertical profiles in the visible spectral region: Once to check out the different approaches for operational usage, an additional one at the beginning of this year to study the impact of the new Level 1b product version (IPF 6.0) and the correction with respect to tangent height correction. For the latter, the processing system is now coupled for off-line processing with the input of attitude corrections with higher precision (AUX_FRA) and an additional elevation correction has been introduced to correct for a constant off-set of around 1.1 km.

The verification exercises showed that between 15 km and 30 km both sets of data differ within ±10%; to higher layers (40 km) differences in the partial columns are until 20% for ozone. Both retrieval schemes, IFE's and the SGP one's, can resolve the tangent height correction showing both the same amount of shift in the profiles.

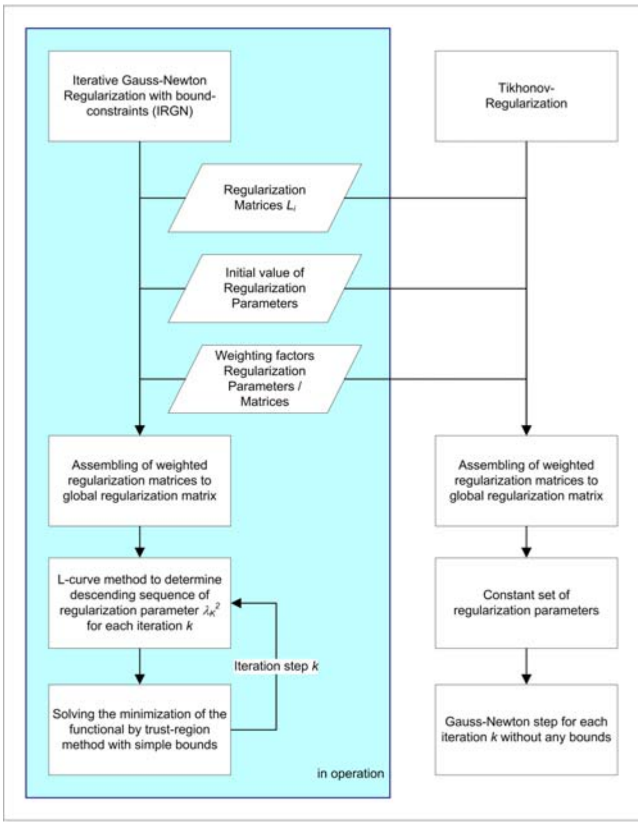

Figure 2 Outline of the algorithm flow in SGP for the retrieval of vertical profile content of O3 and NO2. The left light-blue panel covers the part of the implementation which will be used in the operational SGP (from version 3.0 on). One of the alternative approaches is the Tikhonov regularization shown in the right part of the sketch

3 FUTURE WORK

Since the limb retrieval scheme shows a high sensitivity to tangent height deviations, an extension of the limb retrieval scheme is now in the experimental status to include the influence of the tangent height in the retrieval as an error source as additional retrieval parameter (see posters [7] & [8]) which is not a retrieval of the tangent height. Furthermore, an application to BrO is planned.

Since SCIAMACHY provides also measurements from the SWIR spectral region, a fast retrieval scheme had been developed and is under internal verification (see poster [9]). Note that for the retrieval of SWIR chain in the operational chain some calibration issues had been solved.

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