END-TO-END VALIDATION OF EPS / METOP GOME-2 TRACE GAS DATA

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ABSTRACT

Within the next decade, the improved version 2 of Global Ozone Monitoring Experiment (GOME-2), a ultraviolet-visible spectrometer dedicated to the observation of key atmospheric trace species from space, will be launched successively on board three EUMETSAT Polar System (EPS) MetOp satellites. Starting with the launch of MetOp-1 scheduled for summer 2006, the GOME-2 series will extend till 2020 the global monitoring of atmospheric composition pioneered with ERS-2 GOME-1 since 1995 and enhanced with Envisat SCIAMACHY since 2002 and EOS-Aura OMI since 2004. For more than a decade, an international pool of scientific teams active in ground- and space-based ultraviolet-visible remote sensing have contributed to the successful post-launch validation of trace gas data products and the associated maturation of retrieval algorithms for the latter satellites, ensuring that geophysical data products are/become reliable and accurate enough for intended research and applications. Building on this experience, this consortium plans now to develop and carry out appropriate validation of a list of GOME-2 trace gas column data of both tropospheric and stratospheric relevance: nitrogen dioxide (NO_2), ozone (O_3), bromine monoxide (BrO), chlorine dioxide (OClO), formaldehyde (HCHO), and sulphur dioxide (SO_2). The proposed investigation will combine four complementary approaches resulting in an end-to-end validation of expected column data products.

1. INTRODUCTION

1.1. GOME-2

Global Ozone Monitoring Experiment 2 (GOME-2) is an ultraviolet-visible spectrometer operating from an orbiting platform. A scan mirror enables across-track scanning in nadir, as well as sideways viewing for polar coverage and instrument characterisation measurements. Raw data recorded by the instrument are transmitted to the ground where they are calibrated, geolocated and analysed by a suite of operational processors to retrieve the column abundance of key trace species absorbing in the UV-visible, such as O_3, NO_2, BrO, OClO, HCHO and SO_2, along with information on aerosols, clouds and surface properties. Current versions of the future operational retrieval algorithms are based on the Differential Optical Absorption Spectroscopy (DOAS), a technique developed since the 1970s for the analysis

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of ground-based UV-visible measurements [1-5], homogenised in the framework of the international Network for the Detection of Stratospheric Change (NDSC) [6,7] and related EC-sponsored research campaigns, and brought into space for the first time with ERS-2 GOME-1 [e.g. 8-10]. Three GOME-2 will be launched on board successive EUMETSAT Polar System (EPS) MetOp satellites, the launch of MetOp-1 being scheduled for summer 2006. The GOME-2 series will extend to 2020 the global monitoring of atmospheric composition pioneered with GOME-1 [8] since 1995 and enhanced with Envisat SCIAMACHY [11] since 2002 and EOS-Aura OMI [12] since 2004. Compared to the spatial footprint of its predecessor GOME-1 (320 km across track x 40 km along track), GOME-2 offers an improved spatial resolution of 80x40 km^2. Its wider swath width of 1920 km – instead of 960 km for GOME-1 – yields global coverage several times a day at high latitudes and 1.5 day near the Equator, instead of 3 days near the Equator for GOME-1.

1.2. General objectives of satellite validation

Satellite missions such as GOME-2 and its predecessors aim at measuring the concentration of key trace species on the global scale and in the long term. This global monitoring is required to address major scientific issues related to the chemistry and dynamics of the lower and middle atmosphere and their link with climate. However, measurements from space and related retrieval algorithms are sensitive to a list of uncertainties of instrumental, algorithmic and atmospheric origins. Time-dependent drifts arising from instrument degradation in the severe space environment and other instrumental effects may also affect satellite data. Therefore they need to be validated carefully before any scientific or operational use. Correlative studies based on independent measurements and retrievals are the most classical means of investigating the actual quality of satellite data. Nevertheless, it must be stressed that so-called "validation" studies encompass a much broader scope than straightforward comparisons of level-2 column data and associated statistics.

Indeed, the primary purpose of validation is to determine if and how the satellite data can be used for intended applications. In other words, one must:

- Verify that the satellite data record does respond to spatial, temporal, and quality requirements specific of the scientific/operational objectives which the experiment has been designed for;
- Identify the actual information content retrieved from the satellite radiometric measurements, test the geophysical soundness of the retrievals, and characterise any feature impacting the geophysical interpretation of the data.

In this sense of scientific usability, the validation work requires careful investigation of many topics. E.g., polar ozone loss assessments relying on successive satellite measurements along isentropic trajectories are affected by any dependence on the solar zenith angle (SZA) and column amount, requiring a detailed characterisation of such dependences. Global and regional families budgets may be altered by fictitious spatial structures and temporal signals in the data records. Climatological studies and long-term change assessments relying on the combination of contiguous measurement data records acquired by different satellites need a study of the link with sensors operating on different platforms.

1.3. Objectives and scope of this project

The overall objective of the present project is to develop and carry out end-to-end validation/maturation of GOME-2 trace gas column products, representative of major geophysical states, at a hierarchy of spatial and temporal scales, with a focus on the intended use of the products. The study will start with studies of stratospheric columns of NO_2 and BrO. O_3 total column validation will be envisaged where specific capabilities of the project add significantly to the current validation plans made by the O3SAF. New methods will have to be explored for the validation of tropospheric column products such as HCHO and SO_2 columns.

Four complementary approaches lead to the proposed end-to-end validation. They will interact closely in the course of the project:

A. Study of the feedback between level-0 and level-1 data quality and level-2 data quality;
B. Comparisons of independently retrieved GOME-2 level-2 products;
C. Ground-based validation of level-2 data against NDACC/UV-visible network measurements;
D. Satellite-based validation of level-2 data against GOME-1, SCIAMACHY and OMI.

The following Sections describe for each approach the methodology and anticipated results.

3. APPROACH A: FEEDBACK BETWEEN LEVEL 0-1 DATA QUALITY AND LEVEL 2 DATA QUALITY

The influence of instrument characteristics or level-1 processing algorithms on the quality of the level-2 retrieval will be investigated. On one hand we propose a "bottom up" approach: we will study selected level-0 or level-1 characteristics that may have a critical influence on level-2 data quality. Based on our experience with the GOME-1 and SCIAMACHY instruments, we have selected three fields of instrument characterisation which, to our knowledge, are not covered by the standard ESA/EUMETSAT Cal/Val activities, at least not to the level of details we propose. We will address: (i) characterisation of in-flight sun diffuser properties; (ii) influence of data spikes in the South Atlantic Anomaly (SAA); and (iii) errors due to residual polarisation structures in level-1b data after polarisation correction.

On the other hand we propose a "top down" approach, where any suspected anomalies in the level-2 data are traced down to properties of the level-0 or level-1 data. The details will depend on the eventuality of anomalies, revealed either by monitoring of the level-2 data or by geophysical and algorithmic validation studies. By nature, it is not possible to predict beforehand whether, and what kind of, anomalies may turn out.

4. APPROACH B: COMPARISONS WITH INDEPENDENT RETRIEVALS

Operational GOME-2 total column products are based on DOAS-type algorithms. As stressed in the "GOME-2 Calibration and Validation Plan", it is vitally important to continue the development of new and improved algorithms to derive more accurate products and to better characterise their errors. This is especially true for trace gas products for which the retrieval is still affected by a list of uncertainties. Therefore we propose:

- To apply independent DOAS-type algorithms to GOME-2 level-1b data for the retrieval of trace species.
- To develop an alternative algorithm methodology.
- To validate newly produced GOME-2 trace gas products against correlative data, and to compare these validations with those obtained from the official products.

The use of other DOAS-type algorithms and the development of an alternative algorithm methodology will allow more flexibility and independence in: (a) characterising error sources, generating comprehensive error budgets, and improving accuracy; (b) optimising spectral window choices for individual species; and (c) extending the range of options for retrievals.

Several team members have developed their own DOAS-type algorithms in the context of the NDSC (see Section 5), GOME-1 or SCIAMACHY. These well-characterised algorithms will be applied now on a test-case basis to GOME-2 level-1b data, with the aim to investigate several aspects of the retrieval accuracy for NO_2, BrO, HCHO, SO_2 and O_3 columns. DOAS-type algorithms first derive apparent slant columns from a least-squares spectral fit based on the Beer-Lambert extinction law, and then assign an Air Mass Factor (AMF) to convert slant columns into vertical columns. The consistency between GOME-2 operational data products and our independent retrievals will be verified in terms of both slant column fitting and AMF calculation. The sensitivity of DOAS retrievals to potential sources of errors will be considered. For NO_2, several approaches developed in Europe to retrieve tropospheric columns will be contrasted.

Classical DOAS slant column fitting uses radiance ratios, implying a non-linear fitting procedure. We propose to apply also a direct fitting retrieval method to GOME-2 spectral data. The key idea here is that all vertical columns are retrieved directly from an iterative least-squares fitting of simulated and measured sun-normalized radiances – there is no more two-step DOAS approach. In addition, all multiple-scatter radiative transfer is done from first principles, without the use of Look-Up-Tables – this allows for greater flexibility. The radiative transfer models will be based on the LIDORT family, and will include a complete weighting function capability for total column and other Jacobians, and the ability to deal with full atmospheric sphericity concomitant with the wide-angle off-nadir viewing conditions encountered with GOME-2 (1920 km swath width). The direct fitting technique is not restricted to windows where optical absorption is thin, enabling us to use it anywhere in the ultraviolet.

5. APPROACH C: COMPARISONS WITH GROUND-BASED OBSERVATIONS

The third and fourth (next Section) validation approaches rely on the classical concept of correlative studies using independent observations. Ground-based measurements of stratospheric relevance will be acquired at, and collected from, a network of well-controlled UV-visible DOAS spectrometers measuring zenith-scattered sunlight from pole to pole. Most of contributing instruments have been certified for the WMO/GAW/UNEP Network for the Detection of Atmospheric Composition Change (NDACC), formerly known as the NDSC. The techniques and instruments are well documented ([3-7] and references therein; see also http://www.ndsc.ws) and their quality is controlled regularly through participation to field and/or algorithm intercomparison campaigns. About 30 NDACC/UV-visible instruments measure the vertical column of NO_2 twice daily at twilight. In unpolluted areas, the zenith-sky viewing geometry – mostly sensitive to the stratosphere – will provide an accurate validation of GOME-2 NO_2 total/stratospheric columns, which is a prerequisite for the validation of NO_2 tropospheric columns derived by residual methods. The geographical distribution of total NO_2 sensors covers major stratospheric states, from the Arctic to the Antarctic, with some zonal sampling in the highly variable polar and middle latitude stratospheres. A smaller network measures the column abundance of BrO at different latitudes. In case of chlorine activation, these BrO instruments also measure the column abundance of OClO. Two-dozen zenith-sky spectrometers monitor total O_3 year-round up to the polar circles, adding towards high latitudes and high solar zenith angles to the O_3 column validation planned by the O3SAF (based currently on the use of Dobson and Brewer ultraviolet spectrophotometers). In addition to standard zenith-sky data, newly developed multi-axis DOAS (MAX-DOAS) instruments available at a few stations offer profiling capabilities in the troposphere [e.g. 13,14]. Ground-based validation of SO_2 is not presently available, and the focus here will be on algorithm verification.

Depending on the geophysical characteristics of the species (e.g. amplitude of natural variability, diurnal variation and tropospheric burden) and on the differences in viewing and sensitivity between GOME-2 and the ground-based instruments, appropriate comparison methods will be applied on a case-by-case basis to derive and discuss representative indicators of GOME-2 data quality: temporal signals and meridian structures, dependence on the solar zenith angle and total column amount, and long-term stability. This will enable us to assess the geophysical usability of GOME-2 data products. We also intend to investigate new methods for the validation of tropospheric columns, based among others on the synergy between zenith-sky and multi-axis DOAS measurements. Interpretation of the results will be supported by a hierarchy of chemical-transport and radiative transfer models.

6. APPROACH D: COMPARISONS WITH SATELLITE-BASED OBSERVATIONS

Several team members are also involved in the validation and processing of level 2-data products from GOME-1 and SCIAMACHY [e.g. 9-11]. More than 10 years into the mission, GOME-1 measurements have become less readily available due to on-board recorder problems first encountered in 2003, and data quality has deteriorated due to instrument degradation. Therefore validations based on GOME-1 are hypothetical. Four years after launch, a few products from SCIAMACHY have not yet reached release status (e.g. HCHO, SO_2) but could be available when GOME-2 will start operation. If not, it will still be possible to use in-house DOAS algorithms to process SCIAMACHY level-1b data and generate total column products for collocated orbits and ground stations. OMI was launched in summer 2004 and first validations are in progress. Comparisons with validated OMI data are expected to be possible for several years after the beginning of GOME-2 operation. Later it would be possible to take on board also validation against U.S. OMPS data.

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