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SIX YEARS OF GROUND-BASED SUPPORT TO THE GOME MISSION : OVERVIEW AND PERSPECTIVES FOR ENVISAT

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INTRODUCTION

Operating aboard the ESA's ERS-2 heliosynchronous polar platform since 1995, the Global Ozone Monitoring Experiment (GOME) measures the solar irradiance and the earth radiance from 240 nm through 790 nm [1]. The atmospheric abundance of ozone and other key trace species – such as NO_2, BrO, OClO, CH_2O and SO_2 – is derived from GOME spectra using differential absorption spectroscopy techniques, which have been developed for several decades for ground-based remote sensing. GOME has proven to be a valuable component of the global observing system for atmospheric composition and climate. Getting on with the continuous global monitoring initiated in the 70s with the TOMS/BUV and SAGE series, it is the successful prototype of new-generation spaceborne sensors planned for the coming decade such as Envisat SCIAMACHY, EOS-Aura OMI, and the METOP GOME-2 series.

About three dozen groups involved in ground-based measurements of atmospheric composition have provided invaluable experimental and theoretical support to the GOME mission for nearly six years. The main purpose of the present overview is to highlight the unique role played by those groups in the development of GOME geophysical data products and related retrieval algorithms. The paper is not intended as an exhaustive review of all ground-based contributions. It is rather a tentative to digest and systemise the broad range of adopted approaches. Perspectives for adequate ground-based support to the Envisat mission are inferred from the experience acquainted with GOME.

SCIENTIFIC MEANING OF SATELLITE VALIDATION

Satellite missions such as GOME and Envisat are intended to provide access to the global distribution of the concentration of key trace species. This global monitoring is needed to address major scientific issues related to the chemistry and dynamics of the lower and middle atmosphere. Of primary concern are the budgets of odd oxygen, nitrogen, chlorine and hydrogen families and of water vapour, and the partitioning between specific molecules of these families; the long-term decrease of the ozone column at both high and middle latitudes; the strong springtime ozone depletion at high latitudes; the oxidising capacity of the atmosphere; the long-range transport of tropospheric pollutants. In this context, GOME has already yielded the global distribution and variation of several key constituents. The Envisat atmospheric chemistry payload will enhance significantly the GOME global monitoring capabilities. However, the measurements from space and the related retrieval algorithms are sensitive to a variety of instrumental as well as atmospheric sources of uncertainty. Satellite data may also be affected by time-dependent drifts arising from instrument degradation in the severe space environment and other instrumental effects. Therefore they need to be validated before any scientific use. Correlative studies based on comparisons with independent measurements are a common mean of investigating the actual performance of an orbiting sensor. But it must be stressed that so-called "validation" studies encompass a much broader scope than simple data intercomparisons. The primary purpose of validation is to determine if and how the satellite data can be used for science. In other words, one must:

1. Verify that the satellite data record does respond to spatial, temporal, and quality requirements specific of the scientific objectives which the experiment has been designed for;
2. 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 features. 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 need a study of the link with sensors operating on different platforms.

INVOLVEMENT IN THE GOME MISSION

Ground-based studies have contributed at many stages and many levels to the development and characterisation of GOME geophysical data products. They have addressed issues concerning not only the ESA-endorsed off-line GOME Data Processor (GDP) operated at DFD/DLR [2] and GOME Fast Delivery System (FD) operated at KNMI [3], but also several scientific products developed by independent groups.

Correlative data obtained by ground-based instrumentation have played a central role in the direct validation of the geophysical data products and related science:

- Basic validation: first correlative studies to assess the quality of total O_3 and NO_2, in support of the go/no go decision for public release after the commissioning phase [4] and in case of first public release [5]; quick verification of near real-time products such as preliminary O_3 profiles during Arctic winter campaigns [6];
- Main validation [e.g., 5-14]: detailed investigation of geophysical consistency, pole-to-pole study of accuracy and precision, detection and interpretation of dependences on atmospheric parameters etc.; consistency of GOME data records with other components of the global monitoring system for atmospheric composition and climate;
- Delta validation [e.g., 15,16]: after major improvement of a data product, verification of correctness of changes and assessment of actual improvement; preliminary quality assessment in case of public release of the new version;
- Long-term validation [e.g., 10-14]: routine monitoring of quality and operation; detection of trends and other time-varying features; discrimination of instrumental degradation related effects and other time-dependent artefacts from real geophysical features.

Beyond those pure validation activities concentrating on the level-2 data, the development of GOME data products itself has benefited greatly from ground-based measurements, retrieval algorithms and related expertise in ground-based atmospheric remote sensing, among others through:

- Tiger Teams: advanced studies focusing on specific aspects of data retrieval; identification and testing of solutions; remarkable achievements in the development of O_3, NO_2, and BrO column products;
- Demonstration of GOME measurement capabilities and subsequent development of new data products;
- Mainly for O_3, NO_2, BrO and OClO columns and for O_3 profiles, intercomparison of GOME data and retrievals obtained with independent algorithms, using ground-based data as a reference or as a standard transfer;
- Especially for O_3 and NO_2 products, comparison of GOME with data and retrievals from other satellites (TOMS, HALOE, POAM-II, SAGE-II etc.) using ground-based data as a standard transfer.

Finally, the synergistic use of GOME, ground-based and other correlative data records has been valuable in enhancing their respective geophysical exploitation. Process studies during Arctic winter, investigation of tropospheric BrO issues, development of atmospheric NO_2 climatologies, and total ozone long-term trend assessments are a few illustrations of synergistic exploitation of complementary measurements. It must also be noted that, in turn, the satellite data have provided a valuable insight into the spatial and temporal homogeneity of ground-based data records and pointed out a few issues for the potential improvement of ground-based techniques.

CORRELATIVE STUDIES OF GEOPHYSICAL DATA PRODUCTS

Sources of Correlative Data

Ground- and balloon-based measurements have been the principal component of the systematic correlative database generated at the NILU Data Centre during the commissioning phase. The database has been extended since according to the needs. Correlative data have been acquired and/or collected from the following instruments and techniques:

- More than 30 SAOZ/DOAS UV-visible spectrometers for O_3, NO_2, BrO and OClO columns;
- More than 40 Dobson and Brewer UV spectrophotometers, 4 global UV radiometers (GUV), and about 10 UV filter spectrometers (M-124) for O_3 vertical columns;
- About 5 Fourier Transform Infrared (FTIR) spectrometers for NO_2 columns and additional species;
- About 10 lidars and 5 millimetre wave (MW) radiometers for stratospheric O_3 vertical distribution;
- More than 5 000 ozonesondes launched from 40 sites for O_3 vertical distribution from the ground up to 30 km;
- More than 40 flights of the SAOZ-balloon UV-visible instrument for O_3, NO_2, BrO and OClO profiles.

Various ground-based and balloonborne instruments have also acquired correlative information on the vertical distribution of pressure, temperature, aerosols and clouds. Most of the involved instruments contribute to the WMO's Global Atmospheric Watch (GAW) programme through participation in the Network for the Detection of Stratospheric Change (NDSC) and/or the World Ozone and Ultraviolet Data Center (WOUDC). GOME studies have benefited particularly from the experimental support offered by the NDSC for O_3 and NO_2 columns and O_3 profiles; the GAW, Norwegian and Russian ozone monitoring networks for O_3 columns; and EC-sponsored field campaigns – namely SESAME, THESEO and THESEO-2000 – for BrO columns, O_3 profiles, and additional measurements.

Comparison Techniques

The accurate comparison and interpretation of geophysical quantities obtained by atmospheric remote sounding raise several issues. Different observation methods and retrieval techniques offer different time/space resolution, sampling and sensitivity; hence, they do not measure the same air mass. Due to the finite resolution and the difference in air mass, the comparison between ground-based and satellite measurements may be seriously corrupted by small-scale gradients, dynamic variability and, if any, diurnal (photochemical) variation of the measured atmospheric field. Geometry-, time- and frequency-domain artefacts may arise from cycles linked, e.g., to the orbit properties and the observation geometry, often convolving with real periodic atmospheric features. Satellite and correlative measurements may have correlated errors arising, e.g., from the use of similar spectroscopic databases, retrieval approach, or a priori information on atmospheric properties. The precision and accuracy of the correlative measurement are also necessarily limited and must be estimated and properly taken into account in the interpretation of the comparisons.

For GOME validation, the adopted comparison methodology has often been restricted to direct comparisons of columns and profiles following a basic data selection. A typical example of basic data selection relies on time/space distance criteria based on an arbitrary space/time window – spanning in the GOME validation literature from 150 to 600 km and from 2 hours to 1 day. Assuming that space- and ground-based measurements offer the same resolution and are concentric when the satellite overpasses the station, the presumed objective of this easy-going method is to reduce the time and distance differences in air mass. Unfortunately, it may underestimate the impact of differences in resolution and sensitivity and it does not take into account the actual properties of the atmosphere. For total O_3 comparisons, it leads to increase the scatter by a few percent at middle latitudes and a few ten percent near the polar vortex edge. Stronger effects have been observed for NO_2 and BrO. It may also generate systematic biases when the probed air masses are separated by a quasi-permanent gradient such as those associated with the wintertime polar vortex.

More sophisticated methods have been studied to deal not only with variability and spatial gradients, but also with photochemical variation during the day or along the line of sight, or the lack of knowledge about the vertical distribution of the constituent. Among the refinements which have proved to be efficient, we may cite: estimation of effectively probed air mass using a ray tracing model; methodical identification and rejection of comparison points affected by large atmospheric variability; studies of slant columns using chemical and radiative transfer tools; degradation of highest resolution profiles to match the lowest resolution, e.g., using averaging kernels. Results obtained with different ground-based techniques have also been combined to take advantage of their complementarity in terms of altitude range, spatial and temporal resolution, sources of uncertainties etc.

Examination of Geophysical Data Records

Fields of Investigation

Another matter of concern of correlative studies is the massive amount of satellite data and the broad range of quantities and scales which may be looked at: vertical columns or distributions, absolute or relative differences, yearly means or individual footprints, time-varying features or sensitivity to measurement parameters etc. For GOME, correlative studies have covered four main fields of investigation: the geophysical consistency; the assessment of accuracy and precision; the sensitivity; and the internal consistency of the data records.

1. Geophysical consistency: Many studies have concentrated on the geophysical soundness of the GOME measurement. Time-series, two-dimensional maps and four-dimensional animations have been examined to verify that GOME and correlative instruments capture similarly temporal and spatial features of the geophysical field such as daily means, day-to-day variability, small-scale spatial gradients, seasonal variations, global and regional patterns, peculiar events of concern etc. Further comparisons have pointed out features that can not always have a geophysical origin, such as dependences on solar zenith angle, line-of-sight, type of scan, integrated column amount, temperature, clouds, and aerosols.

2. Accuracy and precision: Most validation groups have calculated statistical quantities such as the mean difference between GOME and correlative data, and the scatter at 1σ level of the differences around this mean agreement. Those quantities may be considered as crude indicators of GOME accuracy and precision, respectively, on condition that the adopted comparison methodology addresses properly the aforementioned issues. In particular, the interpretation of comparisons must take into consideration accurate error budgets of the measurements, error correlations, and estimates of the actual atmospheric characteristics (state, gradients, variability etc.), in order to discriminate between features of atmospheric, retrieval and instrumental origin.
3. Internal consistency: Careful look at the comparison time-series has revealed internal inconsistencies in the GOME data records: gaps, shifts, systematic biases between data acquired at two different angles of nadir scan, drifts, cycles etc. Most of internal inconsistencies are not expected to affect dramatically the geophysical interpretation of the data but they may be symptomatic of problems in the retrieval and the processing chain.
4. Sensitivity: Remote sensing from space is of limited, altitude-varying sensitivity because of clouds, aerosols, and other physical limitations, such as optical thickness and line broadening. The retrieval methods themselves introduce some limitation of the sensitivity. Therefore, sensitivity studies have been conducted to assess to which extent the retrieved quantities are related to the actual atmospheric quantities, whatever the apparent agreement with correlative measurements can be.

Geographical Domain

Correlative studies of GOME data have covered a hierarchy of geographical domains from single sounding stations to pole-to-pole monitoring networks. Local studies carried out at individual stations constitute the preferred approach to detailed investigation. They benefit from local research and excellent understanding of local geophysical particulars; they assure full control of the instrumentation and the availability of adequate ancillary data; and, last but not least, the amount of data to be studied remains reasonably low, allowing careful examination. Studies exploiting the capabilities of regional networks – such as the Norwegian and Swiss ozone monitoring networks – have added to the investigation by increasing the statistical significance of comparisons and/or by extending the variation range of parameters such as SZA, latitude, O_3 column, and meteorological states.

Complementarily, regional and pseudo-global correlative studies based on the integrated use of network data records yield access to patterns, sensitivity and spatial/temporal structures on the global scale. In turn, they give insight into the homogeneity of the network data through detection of controversial stations. Network data have also been used as reference/standard transfer for GOME comparisons with other satellite sensors and with modelling results. The massive amount of data often prevents from detailed investigation of all details, but improves the derivation of statistical quantities. It must be stressed that all aforementioned reservations remain valid, even for statistical studies.

SOUNDNESS AND CORRECTNESS OF LEVEL-1B-TO-2 RETRIEVAL

Exchange of Experience in Atmospheric Remote Sounding

During the past decades, ground-based experimentators have gained a high level of expertise in the retrieval of geophysical quantities from radiometric measurements. This expertise has been shared with developers of the GOME retrieval algorithms for the further improvement of existing retrieval chains, among others through intercomparisons of retrievals. Such intercomparisons provide an opportunity to improve the analysis for each group and to highlight the sources of errors in the instrumentation, calibration, input to the analysis and the spectral analysis itself. Intercomparisons of measurements and retrievals constitute a commitment for affiliation to the WMO Global Atmospheric Watch Programme and they are regularly carried out within the Dobson/Brewer network and the NDSC [e.g., 17-19]. Intercomparisons with independent retrievals have been particularly valuable in the framework of O_3 and NO_2 Tiger Team studies [15,16]. Ground-based expertise has also contributed to feasibility and/or development studies of new data products such as BrO, OClO, SO_2, HCHO, and O_3 from the visible part of the spectrum. The development of GOME BrO products [e.g., 14 and references therein] has benefited from the major intercomparison exercise of ground-based BrO spectral analysis [20] performed during the major NDSC field intercomparison campaign in 1996.

A Priori Assumptions and Intermediate Parameters

The GOME level-1b-to-2 processing chains incorporate different modules from which intermediate results are combined together to obtain the final level-2 product. Several of those intermediate results may be sensitive to uncertainties in a list of input parameters and a priori assumptions that can be tested using ground-based measurements.

To illustrate, in the operational GDP 2.x and FD 3.0 for O_3 and NO_2 columns, a differential optical thickness is calculated as the logarithm of the ratio between the actual nadir earthshine spectrum containing absorption signatures and the solar irradiance spectrum recorded as a reference out of the atmosphere. The adopted retrieval method, referred to as the Differential Optical Absorption Spectroscopy (DOAS), consists of studying the narrow absorption features of the species, after removal of the broad band signal due to scattering processes. Column densities along the optical path, or apparent slant columns, are derived by an iterative least squares procedure, fitting the observed differential optical thickness with high resolution differential absorption cross-sections measured in the laboratory. Apparent slant columns are then converted into vertical columns using a geometrical enhancement factor, or air mass factor (*AMF*), as well as information related to clouds. *AMFs* down to the ground and down to the clouds are calculated with a radiative transfer model assuming vertical distributions of the target absorber and of the atmospheric parameters controlling the path of the solar radiation into the atmosphere. The cloud fractional cover of the ground pixel is derived from GOME measurements of the O_2 A-band around 760 nm. The so-called 'ghost' vertical column amount hidden by the clouds is estimated from climatological grounds.

Ground-based measurement records have provided a valuable experimental support to test the determination of absorption cross-sections, *AMFs*, cloud top pressure, and ghost columns, as well as the sensitivity of those quantities to input parameters and a priori assumptions. In particular, ground- and balloon-based profile data sets have been combined together to review the relevance of atmospheric profile databases used in GDP and FD for the estimation of *AMFs* and absorption cross-section temperatures. Ozone ghost columns have been estimated independently from profile measurements of temperature, pressure and O_3 combined with meteorological information about cloud fractional cover. The type of investigation and relevant parameters will obviously depend on characteristics of the studied specie.

PERSPECTIVES AND RECOMMENDATIONS FOR ENVISAT

The large-scale Envisat validation campaign, combining the effort and expertise of many groups, should be invaluable in getting a comprehensive, initial global picture of data quality. Further improvement of the data products is foreseen through the constitution of smaller groups of experts, which have proved to be key to efficiency. Current plans for correlative data collection are expected to address most of major issues. However, it must be stressed that validation activities planned during the 3-month commissioning phase campaign are not satisfactory from both geophysical and operational point of view. One year of data is a minimum to cover a sufficient number of geophysical events of interest and to detect seasonally varying biases.

According to the experience gained with GOME, there is no doubt that correlative data sets contributing to the Cal/Val Plan will lead to a successful validation of stratospheric GOME-type products. There is more concern about the validation of tropospheric products, for which GOME paved the way. Tropospheric ozone profiles will be measured by ozonesondes and lidars, and promising ground-based techniques yielding tropospheric observation are being developed such as off-axis UV-visible measurements or height-resolved FTIR retrievals. However, there is a general lack of tropospheric data sources in the current measurement plan. The experience in validation of tropospheric products might also be somewhat poor. Ancillary atmospheric data (e.g., pressure, temperature, and backward trajectories) needed for the interpretation of comparisons and the verification of retrieval algorithms would be available, among others through ECMWF and dedicated measurements. Correlative measurements of the spectral properties of the surface, which may alter dramatically the radiation field, do not seem to be taken accordingly into consideration.

Some more effort should be brought into techniques of comparison. Simple comparison techniques are proved to be suitable for first validation of O_3 columns and profiles. However, they may lack of accuracy and precision for further studies and are not adapted to constituents exhibiting strong spatial gradients and photochemical variation during the day or along the line of sight. Promising results have been obtained with comparison techniques taking into account the remote sensing origin of the data and the geophysical nature of the measured field, such as those based on differential slant columns or using averaging kernels. Further developments of comparison techniques are still needed, especially for new products. Data assimilation tools are also expected to offer support to ground-based validation.

The current version of the Envisat Cal/Val Plan as well as tools provided during the rehearsal concentrate on accuracy estimates – which are purely speculative if relying exclusively on ground-based comparisons – and would not reflect sufficiently the scientific objectives of validation. There are a much larger variety of relevant parameters to be looked at. This requires co-ordination of the studies to enhance the efficiency of the validation campaign as well as fast exchange of results during the commissioning and main validation phases. Developers of Envisat level-1b-to-2 processors are requested to provide the Cal/Val community with detailed description of the processing chains and with access to auxiliary databases, in order to foster examination of a priori information and intermediate parameters. A clear documentation – description of level-1b-to-2 retrieval algorithms and processing chains, history of processor changes, survey of major instrumental problems etc. – should be maintained throughout the Envisat lifetime.

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