Development, Validation, and Exploitation of Ers-2 Gome Satellite Data: Overview and Perspectives for Envisat

Jean-Christopher Lambert - Michel Van Roozendael - Martine De Mazière
lambert@oma.be

Institut d'Aéronomie Spatiale de Belgique (IASB-BIRA)
Avenue Circulaire 3,
Brussels, 1180, Belgium

INTRODUCTION

The global composition of the Earth's atmosphere is changing due to the increasing anthropogenic release of chemically and radiatively active species. A better knowledge of the global composition of the atmosphere and of its long-term evolution is needed to assess current and future changes. Issues of primary concern are the evolution of the stratospheric ozone layer both in polar regions and at mid-latitudes, understanding the budgets of main stratospheric species including odd oxygen, nitrogen, chlorine and hydrogen families and water vapour; the oxidising capacity of the troposphere; and the long-range transport of tropospheric pollutants.

Only remote sensing from a satellite platform can provide the required continuous measurements of relevant atmospheric trace species on the global scale. Getting on with the continuous global monitoring initiated in the 70s with the NASA's TOMS/BUV and SAGE series, the ESA's Global Ozone Monitoring Experiment (GOME) is the successful prototype of a new generation of spaceborne sensors planned for the coming decade and beyond: SCIAMACHY aboard ESA's Envisat (2002-2006), OMI aboard NASA's EOS-Aura (2003-2008), and the EUMETSAT METOP GOME-2 series (from 2005). Operating aboard the ERS-2 heliosynchronous polar satellite since April 1995, GOME measures the solar irradiance and the earthshine radiance backscattered at nadir from 240 nm to 790 nm [Burrows *et al.*, 1999]. The atmospheric abundance of ozone (O_3) and other key trace species – such as NO_2, BrO, OClO, CH_2O and SO_2 – is derived from GOME spectra by differential optical absorption spectroscopy (DOAS), a technique first developed in the late seventies for ground-based remote sensing [Platt, 1994, and references therein]. GOME has proven to be a valuable component of the global observing system for atmospheric composition and climate. Moreover, GOME has also paved the way for tropospheric remote sensing from space.

Since the early stage of GOME operation, a group of scientists from the *Institut d'Aéronomie Spatiale de Belgique/Belgisch Instituut voor Ruimte-Aëronomie* (IASB-BIRA), involved for many years in UV-visible remote sensing of atmospheric composition, have provided experimental and theoretical support to the GOME mission. The present overview illustrates several of their achievements in the development of GOME geophysical data products and related retrieval algorithms, and in the use of GOME and other measurement systems for geophysical studies. The central role played by ground-based monitoring networks such as the international Network for the Detection of Stratospheric Change (NDSC) [Lambert *et al.*, 1999a; Zander *et al.*, 1999], in support of GOME and other satellite systems is highlighted. Sections 2 and 3 report on the geophysical validation of operational products and their subsequent refinement. Section 4 summarises the development of a global climatology of stratospheric nitrogen dioxide (NO_2) based on the integrated use of many different sensors including GOME. Sections 5 and 6 describe two scientific data products developed at IASB-BIRA from GOME, tropospheric NO_2 columns and bromine monoxide (BrO) columns. In sections 7 and 8 the work performed in preparation of the upcoming Envisat mission is highlighted. This includes progress achieved towards the development of an advanced correlative database facility and general issues concerning plans for adequate ground-based support to the Envisat mission.

GEOPHYSICAL VALIDATION OF OPERATIONAL DATA PROCESSORS

The Purpose of Satellite Validation

GOME ozone columns are delivered on an operational basis by two data processors endorsed by ESA: the off-line GOME Data Processor (GDP) hosted at DFD/DLR [Loyola *et al.*, 1997] and the GOME Fast Delivery System (FD) hosted at KNMI [Valks *et al.*, 2002]. The GDP also provides routinely the vertical column of nitrogen dioxide as well as information on the cloud cover. However, measurements from space and related retrieval algorithms are known to be sensitive to a variety of atmospheric as well as spectrometric sources of uncertainty. 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 and characterised before any scientific use. The primary purpose of those so-called validation studies is to determine if and how the satellite data can be used for science. Correlative studies based on comparisons with independent measurements are an efficient mean of investigating the actual scientific usability of an orbiting sensor.

Correlative Data

The quality control and validation of GOME measurements, on the global scale as well as in the long term, has been coordinated at IASB-BIRA using ground-based observations from the NDSC, in which Belgian scientists are particularly active. On top of a NO_2 global field derived from GOME measurements, Figure 1 shows the location of the NDSC stations operating UV-visible and FTIR NO_2 sensors. Many other NDSC instruments not represented on the figure have also been used for ozone studies, such as lidars, microwave radiometers, Dobson spectrophotometers, and ozonesondes. Most of the involved instruments contribute to the WMO's Global Atmospheric Watch (GAW) programme through participation in the NDSC and/or the World Ozone and Ultraviolet Data Centre (WOUDC) [Basher, 1995]. Recent EC-sponsored field campaigns (SESAME, THESEO and THESEO-2000) have provided complementary BrO columns, O_3 profiles, and additional measurements. The ground-based data sets are the principal component of the correlative database generated at the NILU Data Centre during the commissioning phase of GOME.

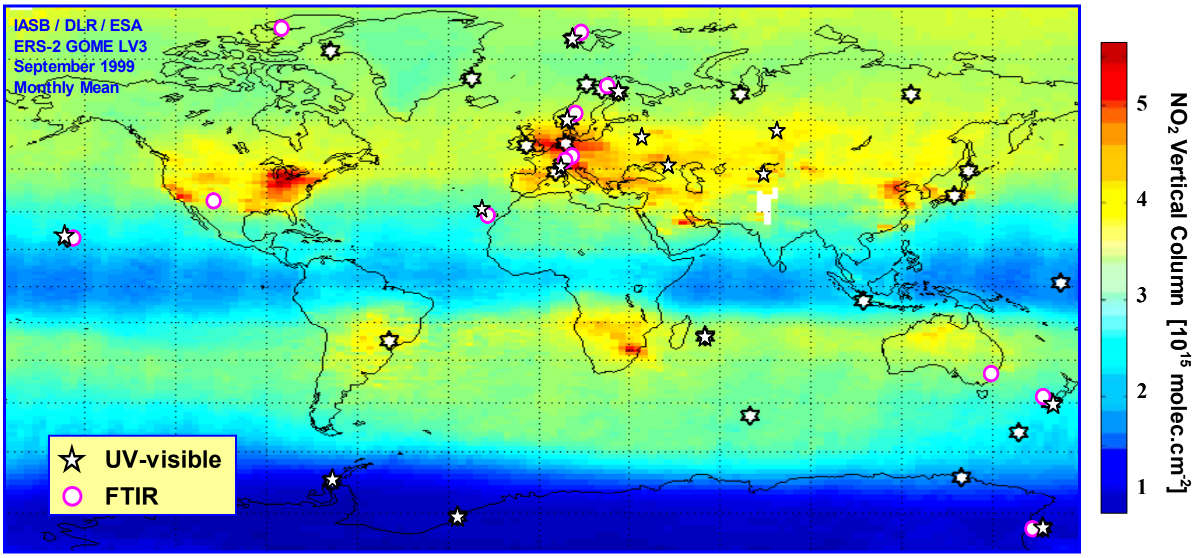


Figure 1. NDSC total NO_2 sensors highlighted on the September 1999 mean NO_2 field derived from GOME observations. The geographical distribution of stations allows to address a variety of geophysical conditions of major interest, such as polar denoxification prior to the Antarctic ozone hole, tropical lows, differences between polluted/clean sites, latitude distribution.

Development of Adequate 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. Figure 2 illustrates some of those differences. 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.

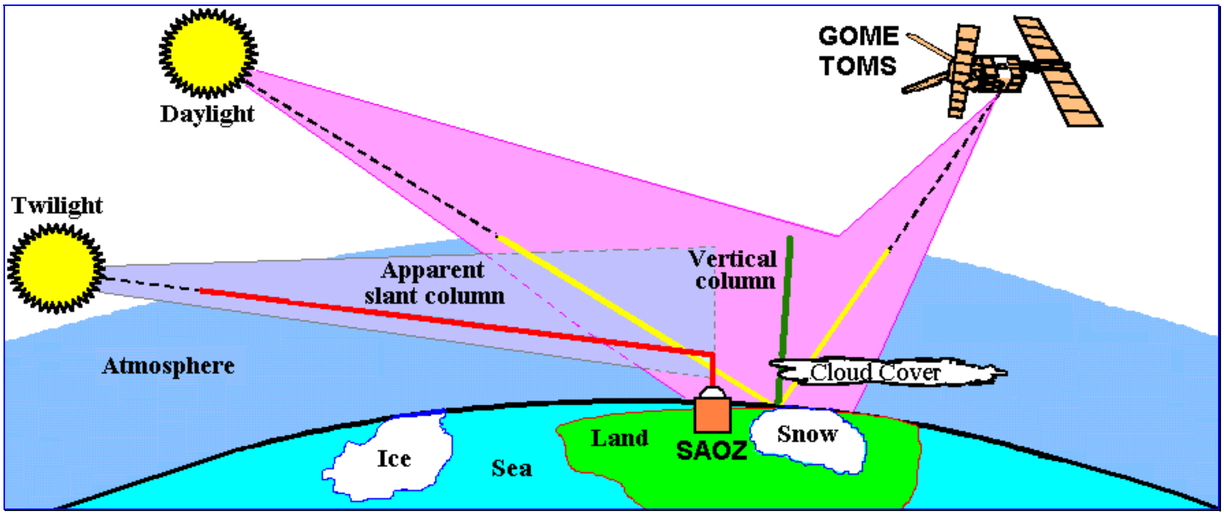


Figure 2. Schematic illustration of the difference in air mass probed by nadir-viewing satellites (e.g. GOME and TOMS) and a ground-based spectrometer (SAOZ). Each instrument has a different perception of atmospheric properties, clouds, surface reflectivity, natural variability etc. that must be taken into account in the comparisons and in the integrated exploitation.

In many studies, 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, this simple method reduces the time and distance differences in air mass. However neither the impact of differences in resolution and sensitivity nor the actual properties of the atmosphere are taken into account. For total O_3 comparisons, this 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. Straight comparisons 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.

Therefore more sophisticated methods have been developed at IASB-BIRA in order to deal with variability and spatial gradients, with photochemical variation during the day or along the line of sight, and with 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.

Impact of Validation on Geophysical Studies

Through correlative studies, the usability of GOME for addressing several scientific issues of interest has been investigated in details [e.g., Lambert *et al.*, 1997, 1999, 2000a]. E.g., an efficient method to assess polar ozone loss in the Arctic winter consists in studying successive satellite measurements along isentropic trajectories. Such studies will be affected by any dependence on the solar zenith angle (SZA) of the satellite measurement and on the ozone column amount, requiring a detailed characterisation of such features. Global and regional families budgets may be altered by fictitious spatial structures and temporal signals introduced by the algorithms in the data records, as those illustrated in Figure 3. 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. For example, the comparison performed between GOME and TOMS total ozone data records, using NDSC as a transfer standard, is illustrated in Figure 3.

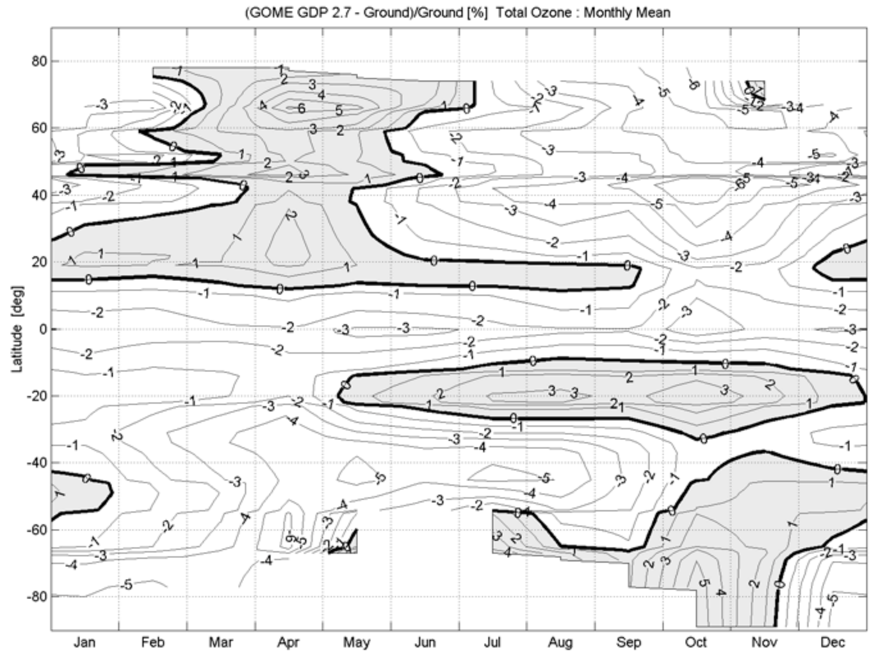


Figure 3-a. Percent difference between ESA's GOME GDP 2.7 [Von Bargen and Thomas, 1999] and NDSC total ozone, as a function of the season and latitude (1996-1999 average). Shaded areas represent positive deviations. A recent upgrade of the GDP algorithm is expected to reduce most of the seasonal and meridian features.

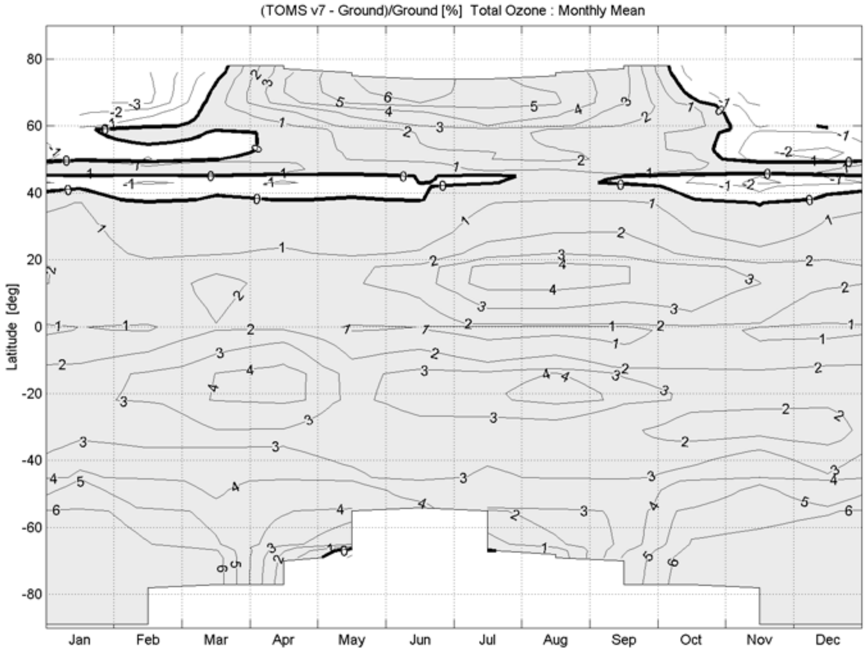


Figure 3-b. Percent relative difference between NASA's TOMS V7 [McPeters and Labow, 1996] and NDSC total ozone, as a function of season and latitude (1996-1999 average). Fictitious seasonal and meridian variations are less pronounced than with the version 2.7 of GOME GDP, but a nearly global, systematic offset is observed.

SUPPORT TO THE DEVELOPMENT OF OPERATIONAL DATA PROCESSORS

The GOME data processing chain incorporates different modules from which intermediate results are combined together to obtain the final geophysical data 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 correlative measurements. Beyond the aforementioned validation activities concentrating on the geophysical data products, the development of GOME data products itself has greatly benefited from ground-based measurements, retrieval algorithms and related expertise of IASB-BIRA in ground-based atmospheric remote sensing, among others through:

- Participation to many "GOME Tiger Teams", focusing on specific aspects of data retrieval [e.g., Loyola *et al.*, 1998; Lambert *et al.*, 1999c];
- Demonstration of GOME measurement capabilities and subsequent development of new approaches;
- Intercomparison of GOME data and retrievals obtained with independent algorithms, using ground-based data as a reference or as a transfer standard;
- Comparison of GOME with data from other satellites (TOMS, HALOE, POAM-II/III, SAGE-II etc.) and from models using ground-based data as a transfer standard [e.g., Lambert *et al.*, 1999a, 2000a].

An illustration of the support provided by validation teams to the development of GOME algorithms is described below. In the operational GDP 2.7 and FD 3.0 for O_3 and NO_2 columns, a differential absorption technique (DOAS) is used which 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 effective optical path, or apparent slant columns (*SC*), are derived by an iterative least squares procedure, fitting the observed differential optical thickness with reference absorption cross-sections measured in the laboratory. Apparent slant columns are converted into vertical columns (*VC*) 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 (*CF*) 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 (*GCV*) hidden by the clouds is estimated from climatological grounds. The vertical column is calculated from those intermediate parameters as follows:

$$VC = \frac{SC + CF.AMF_{cloud}.GVC}{CF.AMF_{cloud} + (1 - CF).AMF_{ground}}$$

Ground-based measurement records have provided a valuable experimental support to test the determination of absorption cross-sections, air mass factors, 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 air mass factors 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.

GLOBAL CLIMATOLOGY OF STRATOSPHERIC NITROGEN DIOXIDE

NO_x species (NO + NO_2) play a crucial role in the photochemistry of stratospheric ozone. Since the late 1970s, several generations of ground-based and satellite sensors have provided high quality data sets of the NO_2 vertical distribution and vertical column. These were used in many studies to explore the latitudinal and seasonal behaviour of stratospheric NO_2. Generally concentrating on a single type of observation technique or platform, the results of such studies are necessarily limited to the temporal sampling, altitude range, and geographical coverage specific of the technique and the platform. Various applications would however require climatology of atmospheric nitrogen dioxide (NO_2) covering the entire stratosphere. The problem is that combining data records obtained by different type of sensors is far from being straightforward due to harsh differences in time/altitude/latitude sampling, accuracy, and resolution, and the photochemical variation of NO_2 throughout the day. Table 1 outlines some of these differences.

Instrument	**Technique**	Time of the day	**Latitude Sampling**	**Time Sampling**	**Altitude Range**
UARS HALOE, ERBS SAGE-II	Solar occultation	Sunset, sunrise	80°N to 80°S (high inclination orbit)	2 (poles) to 8 (Tropics) 1-week periods a year	25(20)-50 km profile
SPOT-3 POAM-II, SPOT-4 POAM-III	Solar occultation	Sunset, sunrise	55°-71°N / 63°-88°S (low inclination orbit)	Year-round	20-40 km profile
ERS-2 GOME	Nadir-scattered sunlight	Mid-morning	Global (daylight side only)	Daily (poles) to 3-day (Tropics)	Total column
NDSC/UV-visible	Zenith-scattered sunlight	Sunset, sunrise	About 30 sites from pole to pole	Daily, year-round up to polar circles	Total column
NDSC/FTIR	Direct sun	Daylight	About 15 sites	Weather permitting	Total column
SAOZ-balloon	Solar occultation	Ascent (descent), sunset (sunrise)	Arctic, European mid-latitudes, Brazil	About 10 flights a year	8-30 km profile

Table 1. Spatial and temporal characteristics of major NO_2 data records.

To address these issues, we have developed a frequency-domain method based on the harmonic decomposition of the spatial and temporal features of NO_2 on the global scale [Lambert *et al.*, 1999b]. This new method allows detailed investigation of the geophysical consistency of two different sensors despite the poor latitude/time/altitude coincidence of the data records. The method also allows the unification of the data records into a composite climatology taking advantage of their complementarity.

The consistency study concludes to a reasonable agreement between POAM-II, POAM-III and HALOE satellites, and with the ground-based NDSC network. Those instruments capture main stratospheric features – such as the latitudinal and seasonal variation, dawn-to-dusk ratio, and wintertime polar denoxification – similarly. Individual

HALOE and POAM profiles are in reasonable agreement with co-located SAOZ-balloon measurements [Pommereau and Piquard, 1994]. Modelling results obtained with the coupled PSC-box/SlimCat model often give a consistent description of the NO_2 field. Over regions with high tropospheric NO_x amounts, the NO_2 enhancement observed by GOME generally is consistent with the enhancement predicted by the IMAGES model. SAGE-II satellite v5.94 is found to overestimate dramatically the other data sets by at least 30%. The agreement is much better with SAGE-II v6.1, but an overestimation persists.

The outcome of the consistency study constitutes the basis for a robust global climatological description of the vertical, seasonal, latitudinal, and dawn-to-dusk distribution of stratospheric NO_2. This climatological reference atmosphere takes advantage of the complementarity of the various data sets in terms of geographical, temporal and altitude sampling. NO_2 profile data as measured by the HALOE and POAM satellites cover altitudes spanning from above the stratopause down to 20-25 km. But their occultation measurement mode leads to a sparse latitude/time sampling (see Table 1). Ground-based monitoring offers well-controlled continuous time-series of stratospheric NO_2 column but at a limited number of stations only (see Figure 1). Balloon measurements have their best accuracy and vertical resolution in the 8-30 km region, but they are limited to a few flights a year. GOME offers global coverage in three days but the accuracy of the retrieved stratospheric data is hampered over areas with enhanced tropospheric NO_2.

The construction principle of the composite climatology is illustrated in Figure 4. A harmonic decomposition is applied to low-pass filtered HALOE and POAM NO_2 time-series at each altitude. Decomposition functions are derived from climatological characteristics of the stratospheric NO_2 column observed by the NDSC/UV-visible network and by GOME. Limited to altitudes above 25 km, the climatology is extrapolated down to the tropopause using tropospheric NO_2 fields derived by the IMAGES chemical-transport model [Müller and Brasseur, 1995]. NO_2 profiles measured by the SAOZ-balloon experiment are used to constrain this extrapolation at altitudes where the accuracy of both satellite profile data and IMAGES model results might degrade. For the sake of comparison, Figure 4 also displays the US Standard Atmosphere NO_2 profile.

The resulting NO_2 climatological model has been validated against major components of the global observing systems. Figure 5 shows the annual mean and annual variation of sunset stratospheric NO_2.

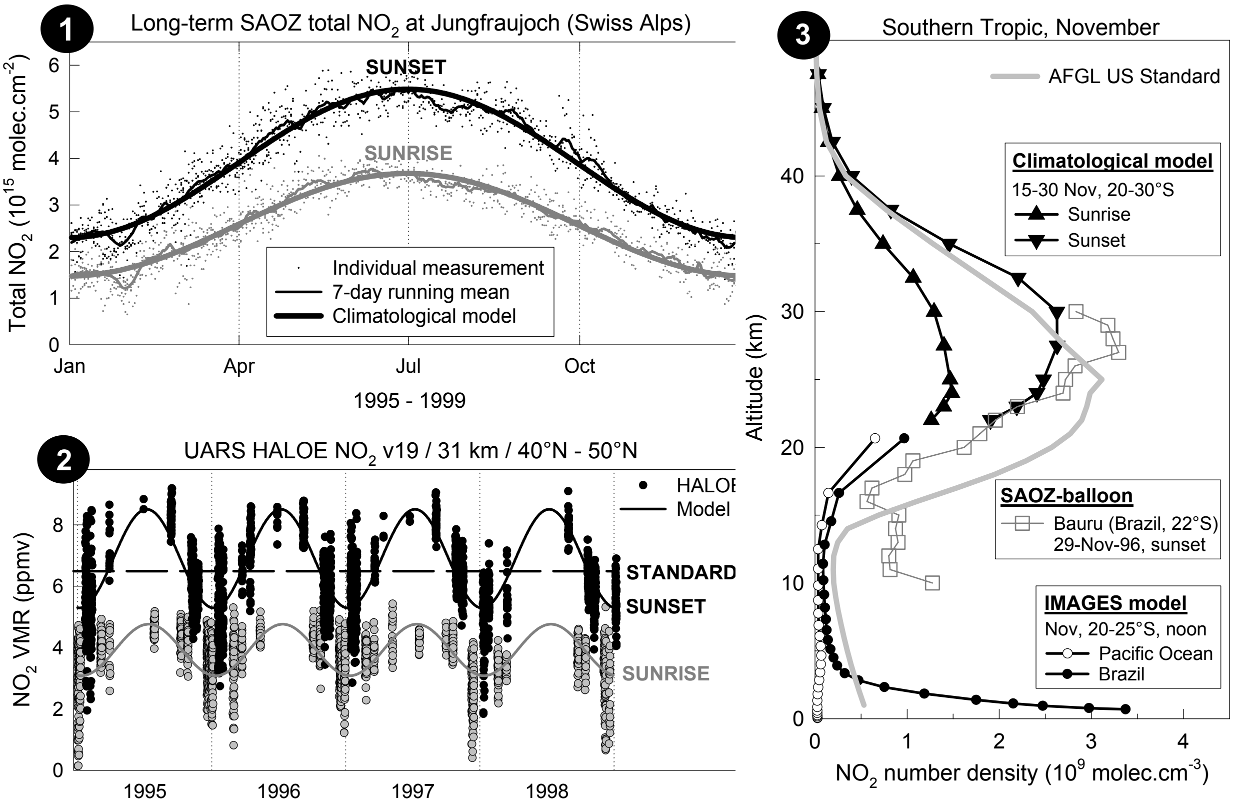


Figure 4. Construction of the composite NO_2 profile database: (1) ground-based determination of NO_2 climatological characteristics; (2) at each altitude, fitting of satellite data with functions inspired from the ground-based harmonic decomposition; (3) use of IMAGES tropospheric model results and of SAOZ-balloon observations to complete the profile down to the ground. US Standard Atmosphere values are depicted for comparison.

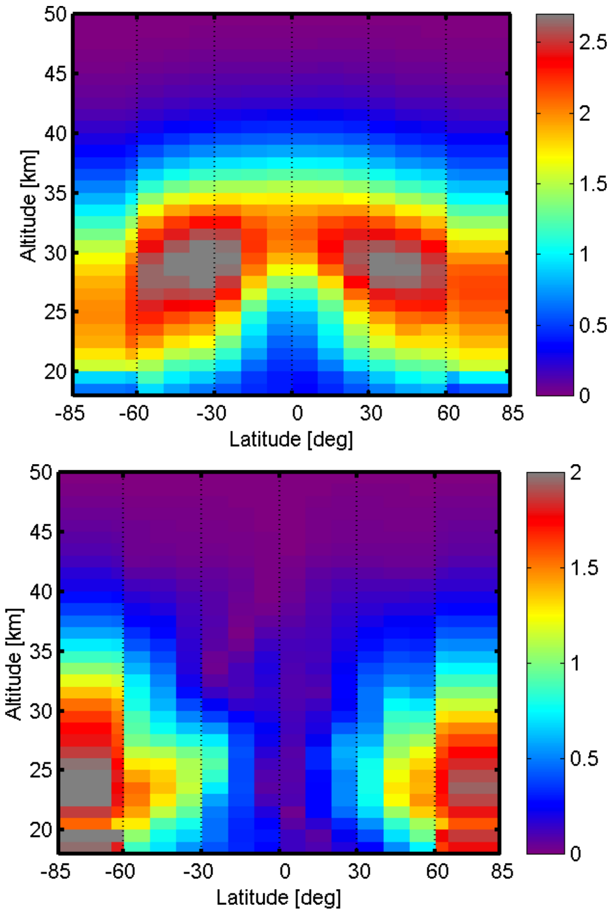


Figure 5. Composite NO_2 climatology: altitude/latitude cross-section of the annual mean (left plate) and annual variation amplitude (right plate) of the sunset NO_2 number density, in 10^9 molec.cm^{-3}. The annual variation reaches its maximum in polar regions where low winter values due to denoxification processes alternate with high summer values resulting from the permanent illumination of the poles.

DEVELOPMENT OF A TROPOSPHERIC NITROGEN DIOXIDE PRODUCT

NO_x species also play a major role in the photochemistry of the troposphere. However, very little is known about their global distribution and variability. Inspired by the tropospheric ozone residual technique pioneered by Fishman *et al.* [1986], we have developed a method for the retrieval of tropospheric NO_2 from operational GOME NO_2 total columns [Lambert *et al.*, 2000b]. The methodology consists of a data pre-processing (quality verification, selection of cloud-free ground pixels, statistical analysis, gridding) followed by the estimation and removal of the stratospheric contribution to the total column. Figure 6 shows preliminary results of tropospheric NO_2 residual columns for October 1997. The spatial distribution and month-to-month variation of major features are clearly identifiable in monthly mean data records, such as air pollution from large urban and industrial areas, tropical biomass burning, and long-range transport of NO_x from their sources. In general, GOME-derived and IMAGES-modelled NO_2 fields are qualitatively consistent.

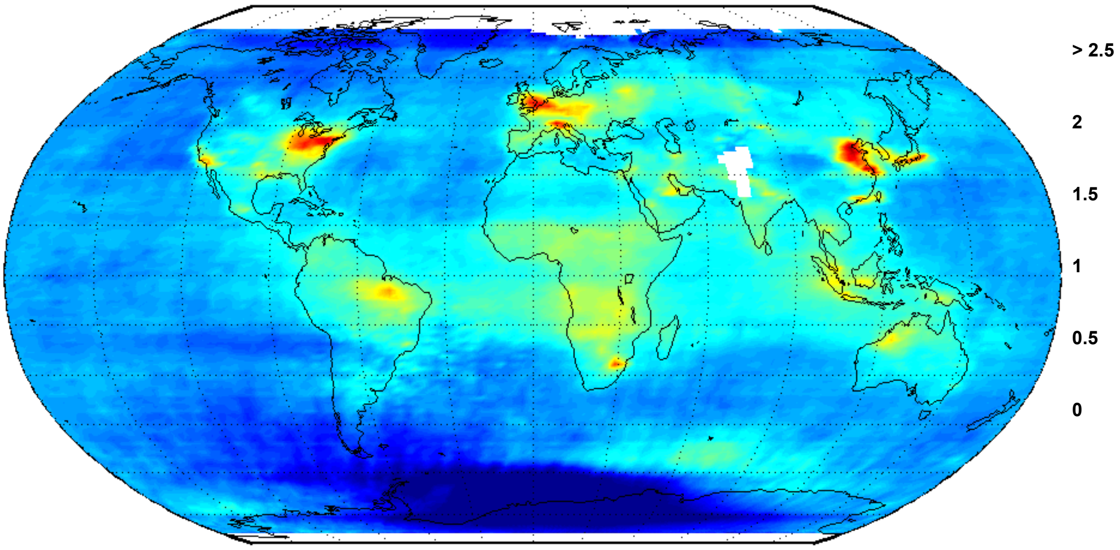


Figure 6. Global picture of the tropospheric NO_2 column (in 10^{15} molec.cm^{-2}) for October 1997 derived from GOME measurements. Emission sources are clearly discernible, such as major cities, large industrial regions, and tropical biomass burning. Long-range transport across the oceans is also visible. Enhanced NO_2 in the Southern Indian Ocean arises from an algorithm artefact that will be fixed in a future version.

DEVELOPMENT OF A BROMINE MONOXIDE PRODUCT

As mentioned in section 2, operational GOME data products delivered by the GDP are limited to O_3 and NO_2 total columns, and cloud fractions. Hence retrieval algorithms for other species measurable by GOME (OClO, SO_2, H_2O, HCHO and BrO), not under responsibility of ESA, have been progressively developed on a scientific basis by several Universities and Institutes in Europe, among them IASB-BIRA. Over the last few years, IASB-BIRA has taken an active part in the development and quality assessment of the GOME BrO product.

Inorganic Bromine in the Atmosphere

Despite their low abundance in the atmosphere (a few pptv), inorganic bromine species play a key role in the ozone chemistry because of their large efficiency as catalyst of the ozone destruction. In the stratosphere, bromine oxide is known to be responsible for approximately 50% of the seasonal polar spring O_3 loss, through the ClO-BrO catalytic cycle [McElroy *et al.*, 1986]. In the troposphere, it has been established that severe ozone depletion events occurring in the Arctic and Antarctic boundary layer during springtime are due to the seasonal release of large amounts of BrO (up to 30 pptv) from sea-ice and sea-salt aerosol [e.g., Wagner and Platt, 1998; Richter *et al.*, 1997]. Furthermore, recent observations indicate that BrO is also present (although in smaller quantities) in the free-troposphere at all latitudes and seasons with possible impact on the tropospheric ozone chemistry at the global scale [Platt, 2000].

GOME BrO Retrieval

BrO total columns can be retrieved from GOME nadir earthshine spectra by DOAS analysis in the 344-360 nm wavelength region. The spectral retrieval algorithm used at IASB-BIRA (WinDOAS) has been developed over the 1990s for ground-based applications and thoroughly validated through participation at several intercomparison exercises [e.g. Hofmann *et al.*, 1995; Roscoe *et al.*, 1999; Aliwell *et al.*, 2002]. In the current state of the algorithm used for GOME BrO retrieval, the inversion is performed in the 344.7-359 nm spectral range. The BrO slant column retrieval includes many refinements [Van Roozendael *et al.*, 1999] as needed for optimal determination of minor absorbers by the DOAS technique (the typical BrO signal to be retrieved is of the order of a few tens of a percent). BrO vertical columns are currently derived using AMFs calculated under the assumption that BrO is located in the stratosphere. Tropospheric AMFs are generally smaller than corresponding stratospheric AMFs, which means that our BrO product generally underestimates the BrO columns where contribution from the troposphere is significant.

This effect is largest at low sun near the terminator. An improved retrieval algorithm accounting better for tropospheric BrO AMFs is currently under development (see below).

BrO Product Validation

The quality of the IASB-BIRA GOME BrO product has been tested in several ways, mainly as part of a recent European project coordinated at IASB-BIRA (THESEO-Stratospheric BrO; coordinator, M. Van Roozendael). GOME BrO validation activities included direct comparison of GOME analysis results performed at different Institutes (IASB-BIRA, University of Bremen, University of Heidelberg, and SAO/Harvard University). BrO vertical columns derived from GOME were also compared to BrO measurements from ground-based and balloon instruments at different locations and time [Van Roozendael *et al.*, 2002]. In some cases, more direct comparisons of BrO differential slant column amounts simultaneously measured from the ground and from GOME were also possible, as illustrated in Figure 7 based on the IASB-BIRA measurements at Harestua, Norway, 60°N. Slant columns are the natural product of optical remote sensing measurements, corresponding to integrated amount of the measured species along the line-of-sight. Absolute slant columns cannot be obtained in a direct way from the ground, because of the impossibility to measure the extraterrestrial solar spectrum.

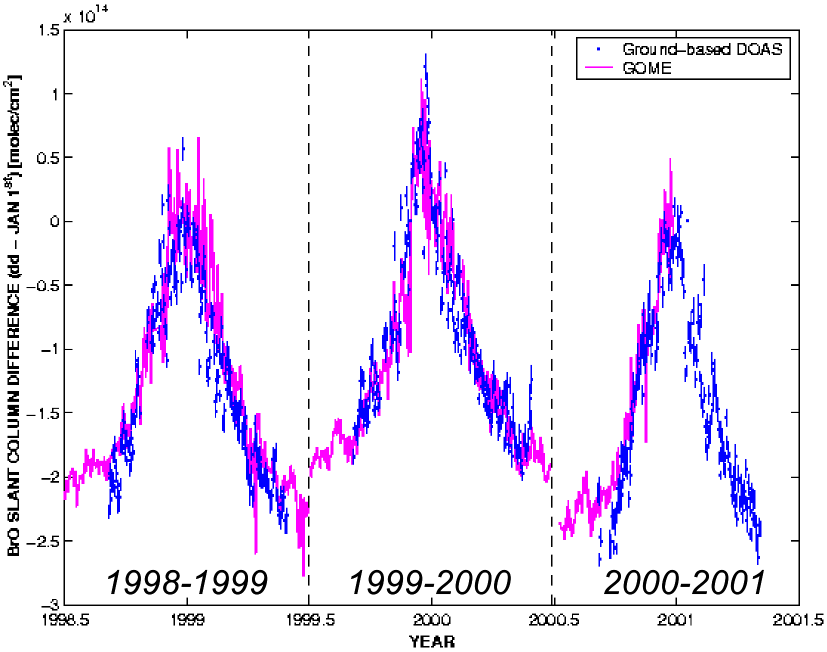


Figure 7. Comparison between BrO differential slant columns amounts (taken relative to 1st January on each year) simultaneously measured by GOME and by the spectrometer operated by IASB-BIRA at the Harestua station (Norway, 60°N). The large seasonal variation of the measured BrO differential slant columns is mainly due to the seasonal variation of the local solar zenith angle.

In summary it can be concluded from the different validation exercises that, when accounting for the BrO diurnal variation and the differences in sensitivity between ground-based, balloon and satellite observations, measurements from all platforms can be made consistent within their error bars. Validation results also confirm the suggested presence of a tropospheric BrO background of 1-3 10^{13} molec/cm^2 extending over middle and high latitudes [Van Roozendael *et al.*, 2002].

On-going Developments

Like NO_2, BrO is present in both the stratosphere and the troposphere. The development of an algorithm allowing the separation of both contributions is therefore highly desirable. This could in principle be obtained by a residual technique such as that described in Section 5 for tropospheric NO_2. However, in contrast to NO_2, the sources of BrO in the troposphere (currently the subject of scientific debates) are not localised above continents so that the stratospheric BrO column cannot be easily estimated from GOME data themselves. In order to try and overcome this difficulty, work is currently under way to develop a combined retrieval/modelling approach using validated three dimensional chemistry-transport model (3D CTM) calculations to provide the stratospheric BrO column reference. The principle of the approach is illustrated in Figure 8 for a monthly-average map of BrO on March 1997. In this example, modelled stratospheric BrO columns are based on the 3D CTM SLIMCAT developed by University of Leeds [Chipperfield, 1999]. This model has been recently validated for bromine chemistry [Sinnhuber *et al.*, 2002]. In the future, assimilation of stratospheric BrO profile measurements by e.g. SCIAMACHY onboard Envisat will be considered as a further step in the algorithm development.

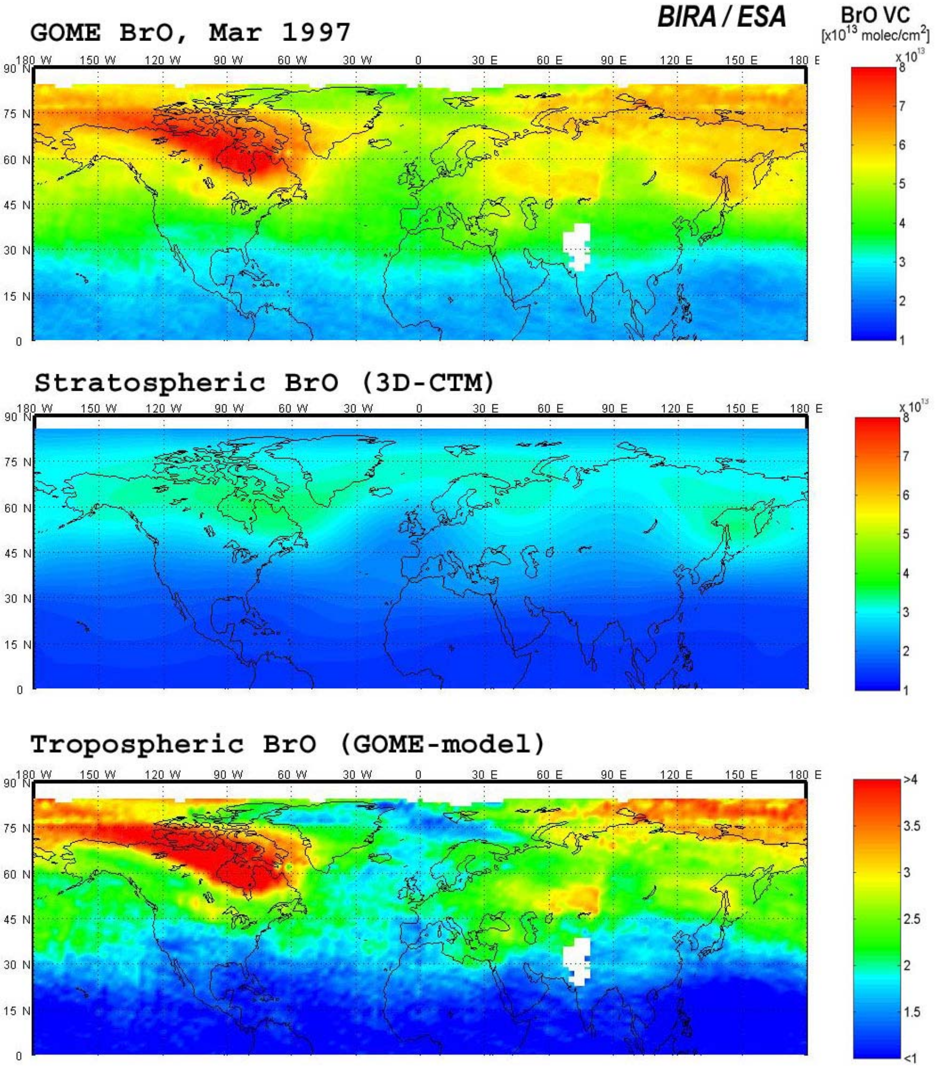


Figure 8. Total vertical column of BrO over the Northern Hemisphere for March 1997, derived from GOME measurements (upper map), stratospheric BrO column from the 3D-CTM SLIMCAT (middle map), and estimated residual tropospheric BrO column (lower map).

DEVELOPMENT OF A CORRELATIVE DATA BASE FOR ENVISAT

The previous chapters have demonstrated the central role of independent data sets for validation and support of satellite experiments; ground-based network data represent a major part herein. Therefore, the EC project COSE, Compilation of atmospheric Observations in support of Satellite measurements over Europe (1998-2000; coordinator, M. De Mazière), has addressed the issues of data accessibility, data documentation and enhanced data exploitation, focusing on the European contributions to the NDSC.

Data retrieval algorithms have been improved, in particular as to the vertical inversions of UV-visible DOAS and FTIR spectral data; some more details are given in De Mazière *et al.* (this volume). To enhance synergistic exploitation of various data types, in particular for satellite validation activities, an appropriate harmonised data format and related relational database with catalogue have been established. This initiative has led to the development of the Envisat CAL/VAL database at NILU (Norwegian Institute for Air Research), in which the COSE concepts have been extended to encompass data from a broader range of instrument types covering a multitude of geophysical parameters, from atmospheric to oceanographic science. This database concept is intended as the overall standard for future data collection activities at the NADIR/NILU data centre (NILU's Atmospheric Database for Interactive Retrieval, http://nadir.nilu.no).

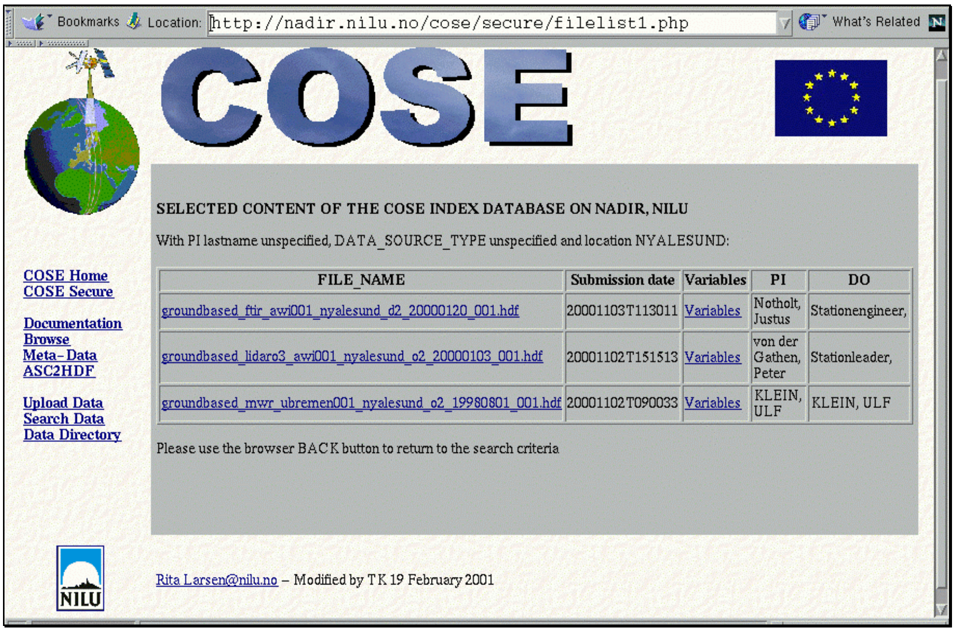
The Envisat CAL/VAL database has been developed in close collaboration with NILU, ESA, and the Envisat Atmospheric Chemistry Validation Team (ACVT). ESA has decided to adopt the HDF version 4.1.3 format for all correlative data submitted to the database. HDF is a binary format, contrary to the commonly used NASA-Ames ASCII format, but it has a number of advantages that make it more suitable for a wide utilisation and easy data exchange:

- HDF data files are machine-independent: the same file can be read on machines having different ways of storing integers, floating point numbers, etc.
- Transfer over the net is no problem;
- Data are stored in binary form, but the HDF interface insulates the user from the underlying binary structure;
- HDF is self-describing: the file itself contains the information that is in it (via the attributes);
- Software for manipulating or displaying data is available, e.g., IDL, MATLAB,…
- The HDF format makes it easy to build a searchable catalogue of the data content of a collection of HDF files.

A very important property of HDF is that its structure allows including all data characteristics. The HDF structure is based on variable definitions (name, data type, number of dimensions, sizes,...), and a collection of data elements is defined in terms of a variable. The data files consist internally of 2 parts: (1) one part containing the data (any dimension, any type: from scalar to n-dimensional arrays, text, integer, float,…), (2) a second part containing data and file attributes (metadata, data base dictionary). The attributes can be of any type and dimension, e.g., model run parameters, data precision and accuracy information, ancillary data used, … As such the HDF data file includes documentation of the data that is necessary for a correct exploitation by any user. The adoption of HDF allows the data providers and users to, (i), include/find all data attributes included in the data files, (ii), to benefit from existing software to handle the data, and (iii), to create/search a relational database with quasi-automatic cataloguing.

A large effort was devoted to the definition of the HDF format specifications, in particular to the standardisation of the metadata for the atmospheric sciences community. IASB-BIRA has played a leading role in the Envisat Atmospheric Chemistry Validation Team to establish the metadata guidelines and the relational database structure. NILU has implemented the database and all associated formatting and data QA/QC tools. The relational metadata index and file structure will allow extensive quality assurance and quality control of files submitted to the Envisat CAL/VAL database, while also enabling easy data mining and data retrieval from the Figures 9 and 10 show the Web interface to access the COSE Database (the prototype for the Envisat CAL/VAL database, http://nadir.nilu.no/calval). Figure 9 shows the results of a search for all data from the location of Ny-Ålesund (Spitsbergen), and Figure 10 shows the information about the data content of one of the files resulting from the search (satisfying the query).

The final release of the Envisat CAL/VAL metadata guidelines and associated database structure is expected by early March 2002.



http://nadir.nilu.no/cose/secure/filelist1.php

SELECTED CONTENT OF THE COSE INDEX DATABASE ON NADIR, NILU

With PI lastname unspecified, DATA_SOURCE_TYPE unspecified and location NYALESUND:

FILE_NAME	Submission date	Variables	PI	DO
groundbased_ftir_awi001_nyalesund_d2_20000120_001.hdf	20001103T113011	Variables	Notholt, Justus	Stationengineer,
groundbased_lidaro3_awi001_nyalesund_o2_20000103_001.hdf	20001102T151513	Variables	von der Gathen, Peter	Stationleader,
groundbased_mwr_ubremen001_nyalesund_o2_19980801_001.hdf	20001102T090033	Variables	KLEIN, ULF	KLEIN, ULF

Please use the browser BACK button to return to the search criteria

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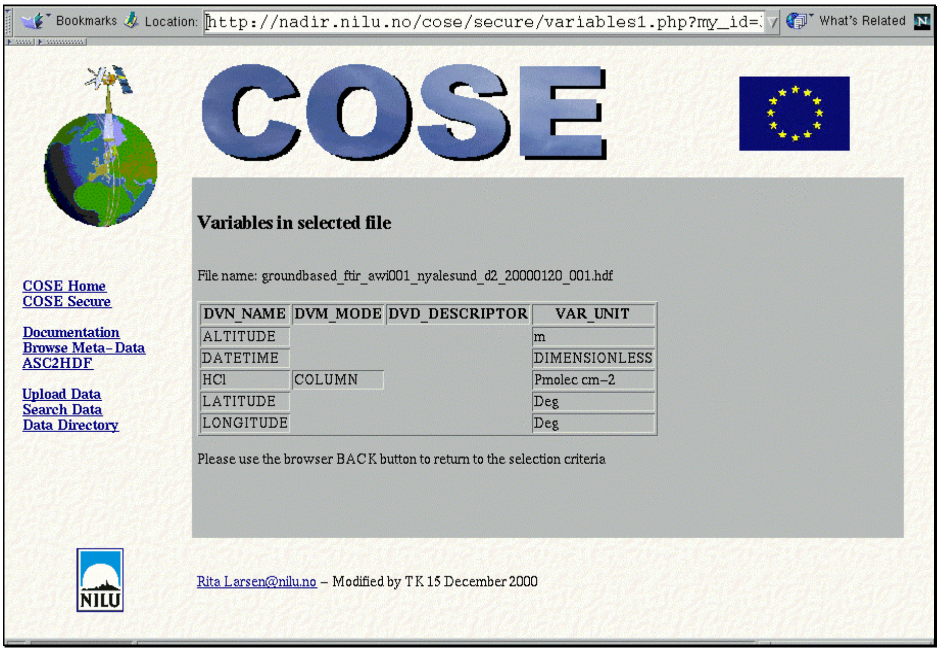
Figure 9. The result of the search for data at Ny-Ålesund (Spitsbergen, 79°N). The search gave three resulting files. These files can then be downloaded to the local computer by clicking on the filename to the left in the table, or one can browse the variables found in the file by clicking in the column designated "Variables". Clicking on this table cell for the first file leads to the output shown in the next figure.



http://nadir.nilu.no/cose/secure/variables1.php?my_id=

Variables in selected file

File name: groundbased_ftir_awi001_nyalesund_d2_20000120_001.hdf

DVN_NAME	DVM_MODE	DVD_DESCRIPTOR	VAR_UNIT
ALTITUDE			m
DATETIME			DIMENSIONLESS
HCl	COLUMN		Pmolec cm–2
LATITUDE			Deg
LONGITUDE			Deg

Please use the browser BACK button to return to the selection criteria

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Figure 10. The variables contained in the first file that appears in the list of query results shown in the previous figure.

PERSPECTIVES FOR THE ENVISAT MISSION

As mentioned in the introduction, GOME is the successful predecessor of several satellite sensors planned for the next decade and beyond. The expertise acquainted and the methods developed with GOME will be extended very soon to SCIAMACHY and to the other Envisat instruments. IASB-BIRA will contribute to the validation and exploitation of the geophysical products from the three atmospheric chemistry instruments on Envisat, namely SCIAMACHY, GOMOS and MIPAS. In particular, IASB-BIRA is deeply involved in the development of geophysical data products from SCIAMACHY, as a logical continuation of the effort invested in the GOME mission.

A large-scale Envisat calibration/validation campaign has been set up by ESA, combining the effort and expertise of many groups. Within this framework, IASB-BIRA co-ordinates several projects relying on the integrated use of NDSC correlative observations obtained by a variety of ground-based instrumentation. This coordinated campaign should be invaluable in getting a comprehensive, initial global picture of data quality. Further improvement of the data products is foreseen through the participation to smaller groups of experts focusing on details of the retrieval. 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-months 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. Long-term investigation is also required. Therefore, IASB-BIRA and OSTC have agreed on an extended programme ensuring the quality of SCIAMACHY data throughout the satellite lifetime.

According to the experience gained with GOME, there is no doubt that correlative data sets contributing to the Envisat Cal/Val Plan will lead to a successful development and validation of stratospheric GOME-type products. There is more concern about the tropospheric products. Tropospheric ozone profiles will be measured by ozonesondes and lidars, and promising ground-based techniques yielding tropospheric observations are being developed (notably at IASB-BIRA) such as off-axis UV-visible DOAS 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 and remains to be developed. 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 combined use on which validation and climatological studies rely. Such techniques are often neglected since apparently far away from the geophysical objectives of the work. 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 interpretation techniques are still needed, especially for new products. Data assimilation tools are also expected to offer valuable support.

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