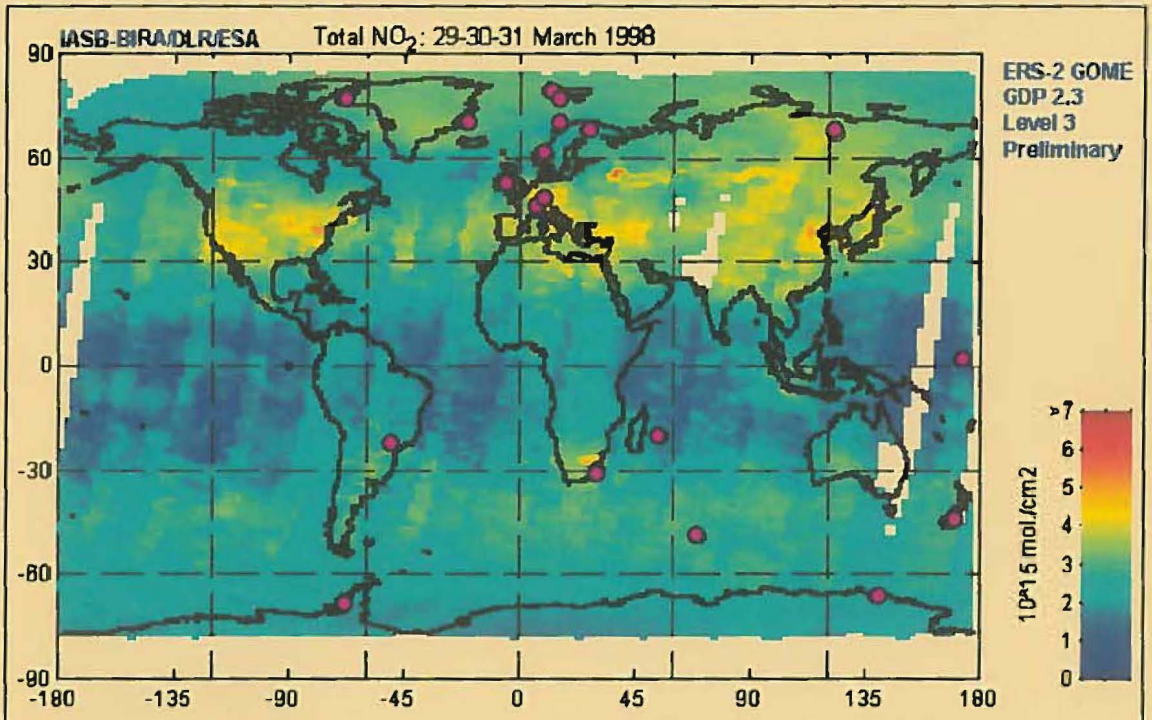
Geophysical validation and maturation of ERS-2 GOME level-2 products with ground-based observations from the NDSC and the SAOZ Network

ERS.AO2.B103/F114 Joint Final Report to ESA

August 1998



Global picture of NO_2 vertical column amount derived from ERS-2 GOME data in March 1998. The geophysical consistency of GOME NO_2 is investigated from pole to pole with correlative measurements from a ground-based network of SAOZ/UV-visible spectrometers, highlighted on the map.

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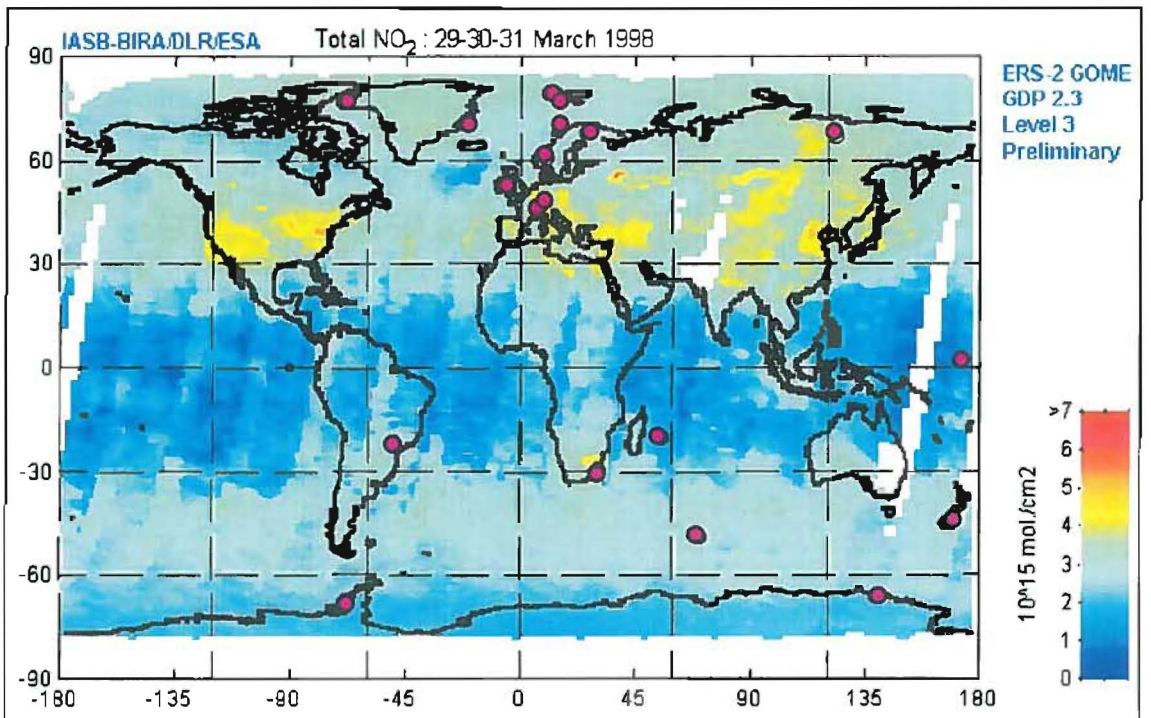

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ERS-2 GOME Level-2 Products Validation and Maturation:

AO2.B103/F114 Joint Final Report to the European Space Agency

Report title

Geophysical validation and maturation of ERS-2 GOME level-2 products with ground-based observations from the NDSC and the SAOZ Network.

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Project id.: **ESA ERS.AO2.B103**

Title: **GOME Data Product (Level-2) Validation by Ground-based Observations Performed at the NDSC/Alpine Stations**

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Project id: **ESA ERS.AO2.F114**

Title: **Validation of the ERS-2 GOME Products with the SAOZ Network**

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Geophysical validation and maturation of ERS-2 GOME level-2 products with ground-based observations from the NDSC and the SAOZ Network

Contents

Geophysical validation and maturation of ERS-2 GOME level-2 products with ground-based observations from the NDSC and the SAOZ Network

1. Objectives of the project

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 both the global composition and its long-term evolution are urgently needed to assess current and future changes. Remote sensing from a satellite platform provides unique access to the required continuous measurements of relevant atmospheric trace species on the global scale. Launched by ESA in April 1995 onboard its ERS-2 environmental satellite, the Global Ozone Monitoring Experiment (GOME) provides routinely the global picture of atmospheric ozone and nitrogen dioxide, as well as the abundance of other relevant trace species, such as BrO, OClO, SO_2, and CH_2O [ESA, 1995; Burrows *et al.*, 1998]. GOME carries on with the space-based, long-term mapping of the global distribution of atmospheric ozone started with the NASA Total Ozone Mapping Spectrometer (TOMS) onboard Nimbus-7 (October 1978 - May 1993), and continued with a second TOMS onboard Meteor-3 (August 1991 - December 1994) [Heath *et al.*, 1975; McPeters *et al.*, 1996]. Since July 1996, a third TOMS monitors total ozone onboard the Earth Probe platform (TOMS-EP), and a fourth TOMS operated aboard the Japanese ADEOS spacecraft (TOMS-AD) from September 1996 until the failure of ADEOS on June 29, 1997.

The geophysical exploitation of atmospheric chemistry data requires a high level of accuracy to be maintained over the lifetime of the experiment. Before using data from any satellite experiment, it is of prime importance to verify that they do respond to spatial, temporal, and quality requirements specific of the application for which the experiment has been designed. It is crucial to characterise, by means of intensive validation programmes relying on well-controlled correlative measurements, the sensitivity of both the measurement and the retrieval algorithms to a variety of instrumental as well as atmospheric parameters. The consistency between sensors operating on different platforms must also be studied.

The main objective of the ERS.AO2.B103 and ERS.AO2.F114 projects is to contribute to the geophysical validation of ERS-2 GOME level-2 data products. The B103 proposal relies on correlative studies using the ground-based stratospheric monitoring capabilities of the Alpine stations of the Network for the Detection of Stratospheric Change (NDSC). Targeted GOME products are the ozone total amounts and altitude profiles, NO_2 total amounts, and aerosol total amounts and vertical profiles. Intended studies include the validation of ozone retrieval algorithms. Ground-based observations are provided by UV-visible and Fourier transform infrared spectrometers, lidars, millimetre wave radiometers, and ozonesondes. In the F114 project, it is proposed to use the data of a homogeneous ground-based network of 14 SAOZ UV-visible spectrometers deployed from the Arctic to the Antarctic, and operating in the framework of the NDSC, to validate GOME level-2 products: a) total ozone during the 6 months commissioning phase; and b) other species as soon as they become available. Both projects include the regular provision of the stratospheric database at the Norwegian Institute for Air Research (NILU), with correlative data, and the comparison with those of GOME, as done in the past for the TOMS onboard Nimbus-7 and Meteor-3. It is also intended to identify the cause of possible systematic differences and to propose adequate solutions.

2. Overall assessment of the investigation

Since the early GOME validation studies, the AO2.B103 and AO2.F114 investigations have shown to be complementary. Therefore, they have been successfully achieved by a unique team gathering members from the Belgian and French groups and collaborators. For the sake of consistency, results obtained through the B103 and F114 projects are summarised hereinafter in a joint report, in agreement with the ERS Desk at ESA/ESRIN. Both projects have evolved from their original definition, according to the availability of GOME data and the scientific needs revealed by first validation results.

Total ozone and NO_2 studies reported here have played a major role, not only in the pole-to-pole characterisation of the GOME level-2 products, but also in the maturation of the GOME Data Processor's developmental versions (GDP 1.15, 1.20/1.21, 1.40, 1.50, and 1.60), of its first publicly available version (GDP 2.0), and in the preliminary evaluation of the current GDP 2.3, operational since January 1998. According to the needs, investigations have been extended to additional ground-based instruments, especially in the southern hemisphere, and to additional ozonesonde launch sites at northern middle latitudes. In order to study the needed link with the TOMS ozone sensor series, and to help identifying possible problems in both the GOME and the TOMS total ozone processing, the ground-based validation of GOME total ozone has also been successfully combined to that of both TOMS-EP and TOMS-AD. Reported activities are now prolonged and merged through the common ERS.AO3.356 proposal: 'Extended validation of the ERS-2 GOME ozone and NO_2 data using ground-based and balloon observations associated with the Network for the Detection of Stratospheric Change (NDSC)', J.-C. Lambert *et al.*

Due to the important delay in the development of ozone profile retrieval algorithms, only a limited set of preliminary height-resolved ozone, derived from GOME data with an early version of the Full Retrieval Method (FURM) developed at IFE/IUP, was evaluated with ozonesonde and lidar data. This preliminary validation exercise will be extended in the future to the most recent algorithm version and to a larger data set, through the ERS.AO3.377 project: 'Ozone Vertical Profile Retrieval from GOME/ERS-2: Optimization, Validation, and New Scientific Data Products', M. Weber *et al.*

No suitable aerosol products were available from GOME to achieve the planned aerosol studies.

Finally, the outcome of the project (strategy for the identification of problems, synergistic approach, scientific issues ...) has been valuable in the design of the validation strategy for the expected level-2 products from SCIAMACHY, GOMOS and MIPAS onboard ENVISAT-1, and has played a significant role in the elaboration of the validation requirements documents for those instruments [Kelder *et al.*, 1998; Wursteisen *et al.*, 1997].

3. Detailed description of the project and main achievements

3.1 Ground-based monitoring activities

As part of regular NDSC monitoring activities, preliminary correlative data listed in Table 1 have been acquired and validated for the entire reporting period. Most of them have been routinely stored into the NILU stratospheric database, within two weeks after acquisition. Pole-to-pole observations of total ozone and NO_2 have been provided by 17 UV-visible spectrometers: 14 SAOZ instruments (Système d'Analyse par Observation Zénithale) performing automated network operation [Pommereau and Goutail, 1988], two spectrometers of the SAOZ type designed at IASB-BIRA [Van Roozendael *et al.*, 1995] and NILU (SYMOCS, System for Monitoring Compounds in the Stratosphere), respectively, and one instrument designed at NIWA [McKenzie and Johnston, 1982]. Dobson and Brewer spectrophotometers operating at NDSC Alpine and Antarctic stations have also provided ozone column amounts. The vertical column abundance of a variety of molecules, including ozone and NO_2, has been retrieved from high-resolution infrared solar spectra recorded at the Jungfraujoch station by Fourier transform spectrometry (FTIR). The vertical distribution of ozone has been measured by ozonesondes, two stratospheric lidars, and two millimetre wave radiometers. Vertical profiles of aerosol backscatter ratio have been monitored by two aerosol lidars.

In order to control and improve their quality, to assess their accuracy, and to examine their consistency with other types of instruments, most of the instruments participated to intercomparison campaigns organised through the NDSC and the World Meteorological Organisation (WMO). The four Dobson and one Brewer involved in the B103 proposal participated to the WMO Dobson Intercalibration Campaign held at Arosa in July-August 1995 [WMO, 1995]. Major intercomparison campaigns of UV-visible zenith-sky spectrometers, including several instruments of the SAOZ network, were held in September 1994 at Camborne in UK [Vaughan *et al.*, 1997], and in June 1996 at the Observatoire de Haute Provence (OHP) in southern France [Roscoe *et al.*, 1998]. In March 1996, an intercomparison of ozonesondes, involving those used at three sites of the NDSC/Alpine station, was conducted in an environmental simulation chamber at Jülich in Germany [Smit *et al.*, 1998]. Research was also carried out by members of the team on atmospheric chemistry measurements by lidar and millimetre wave radiometry.

3.2 Validation strategy

Relying on the heritage of the TOMS and UARS validation exercises, the overall validation strategy has been designed according to potential scientific applications of GOME data. The geophysical consistency and the accuracy of the GOME level-2 products should be assessed over a variety of representative geophysical conditions (e.g., springtime polar ozone depletion, tropical convection, biomass burning emissions, midnight sun), during the entire mission. Correlative studies should be performed from pole to pole, and should investigate the dependence on the solar zenith angle (SZA), the latitude and the season, the time-dependent drifts, the dispersion, and the possible differences of sensitivity of the space-based sensors. Global ozone maps derived from GOME should be compared with those obtained from other satellite experiments. The impact of the validation results on specific scientific studies should be emphasised.

Partially based on the results of intercomparisons, and of studies specific of the project, investigations have been carried out to examine the capabilities and complementarity of the various ground-based sensors for the validation of satellite data in general, and GOME data in particular [Lambert *et al.*, 1998c]. A detailed error budget has been proposed for the ground-based total ozone sensors, highlighting their possible contributions to features such as SZA dependence and dispersion. An original comparison methodology has been proposed [Lambert *et al.*, 1995, 1998b], taking into account: (i) the error budget of the various correlative observation techniques; (ii) the differences in the air masses probed by the various space- and ground-based sensors; and (iii) the geophysical variability of the atmospheric constituent field. GOME ground pixels are selected such as the line of sight of the satellite (schematised in Figure 3-1) matches at best the actual location of the correlative ground-based measurements

Table 1 - Contributing stations, instruments and institutes.

Lat.	Long.	Station	Instrument	Responsible Institution
79°N	12°E	Ny-Ålesund	SAOZ[+], SYMOCS[+] (except fall 1996)	NILU
78°N	15°E	Longyearbyen	SYMOCS[+] (fall 1996)	NILU
77°N	69°W	Thule	SAOZ	DMI
70°N	22°W	Scoresbysund	SAOZ	CNRS/DMI
67°N	27°E	Sodankylä	SAOZ	CNRS/FMI
67°N	123°E	Zhigansk	SAOZ	CNRS/CAO
63°N	9°E	Orlandet	Sondes	NILU
62°N	130°E	Yakutsk	Sondes	CAO
60°N	9°E	Gardermoen	Sondes	NILU
60°N	10°E	Harestua	IASB UV-visible[+]	IASB-BIRA
60°N	11°E	Oslo	SAOZ (August 1995)	NILU
56°N	38°E	Moscow	Sondes	CAO
52°N	4°W	Aberystwyth	SAOZ, sondes	U. Wales
48°N	11°E	Hohenpeißenberg	Dobson[D], Brewer[D], sondes, ozone lidar	DWD
48°N	11°E	Garmisch Partenkirchen	Aerosol lidar	IFU
47°N	7°E	Bern	Microwave	U. Bern
47°N	8°E	Jungfraujoch	SAOZ[+], FTIR	IASB-BIRA, U. Liège
46°N	7°E	Payerne	Sondes	SMI/ETH
46°N	9°E	Arosa	Dobson, Brewer	ETH
45°N	1°W	Bordeaux	Dobson[D], microwave	U. Bordeaux
44°N	6°E	Haute Provence	SAOZ, Dobson, sondes, ozone lidar, aerosol lidar	CNRS, U. Reims
1°N	173°E	Tarawa	SAOZ	CNRS
21°S	55°E	Reunion Island	SAOZ, sondes	CNRS/U. Reunion
22°S	49°W	Bauru	SAOZ (since November 1995)	CNRS/UNESP
45°S	170°E	Lauder	NIWA UV-visible	NIWA
49°S	70°E	Kerguelen Islands	SAOZ (since December 1995)	CNRS
65°S	64°W	Vernadsky/Faraday	Dobson[DZ], SAOZ[+] (until October 1995)	BAS/KTSU, BAS
67°S	140°E	Dumont d'Urville	SAOZ, sondes	CNRS
68°S	68°W	Rothera	SAOZ[+] (since November 1995)	BAS
76°S	27°W	Halley	Dobson[DZ]	BAS

[+]UV-visible zenith-sky data including the climatological treatment of the profile shape effect.
[D]daily means only; [Z]zenith-sky data included for cloudy days.

(schematised in Figure 3-2), resulting in several ground pixels a day. The method is particularly justified for the comparison of observations of nadir-scattered (GOME) and zenith-scattered (SAOZ) UV-visible radiation. The air mass effectively probed by both techniques can extend up to several hundred kilometres in direction of the sun, as depicted in Figure 3-3. In case of strong gradients in the constituent field, the comparison methodology can produce a significant reduction in the scatter arising from spatial differences in the sampled air masses, as illustrated in Figure 3-3. The scatter associated with difference in measurement time between SAOZ and GOME remains, however its contribution can be assessed by comparing twilight SAOZ data with co-located, direct sun Dobson/Brewer data recorded around the ERS-2 overpass. The comparison of satellite with Dobson, Brewer, and FTIR measurements is restricted to direct sun observations, except in Antarctica where zenith-sky Dobson data are included for cloudy days, and to data points co-located within 300 km and 3 hours between the ground-based measurement and the satellite overpass, except at stations where daily means only are available for the study. The comparison is performed with the direct GOME level-2 products, without spatial or temporal interpolation.

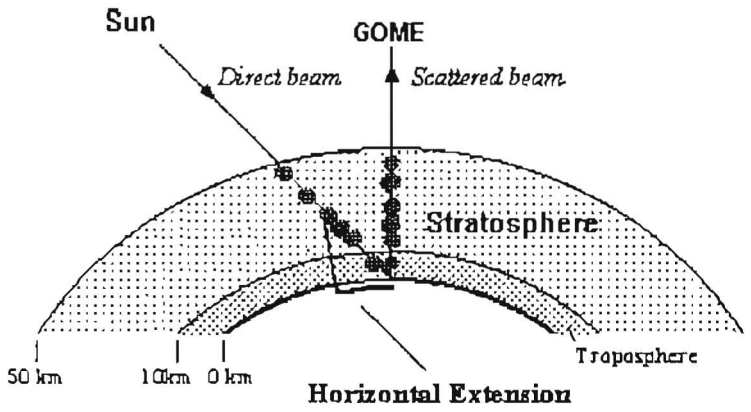

Figure 3-1 Line of sight of GOME at moderate SZA, and resulting horizontal extension of the sampled air mass.

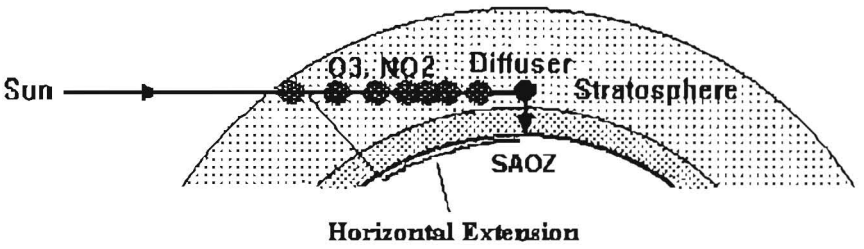

Figure 3-2 Line of sight of the zenith-sky instrument at twilight, and resulting horizontal extension of the sampled air mass.

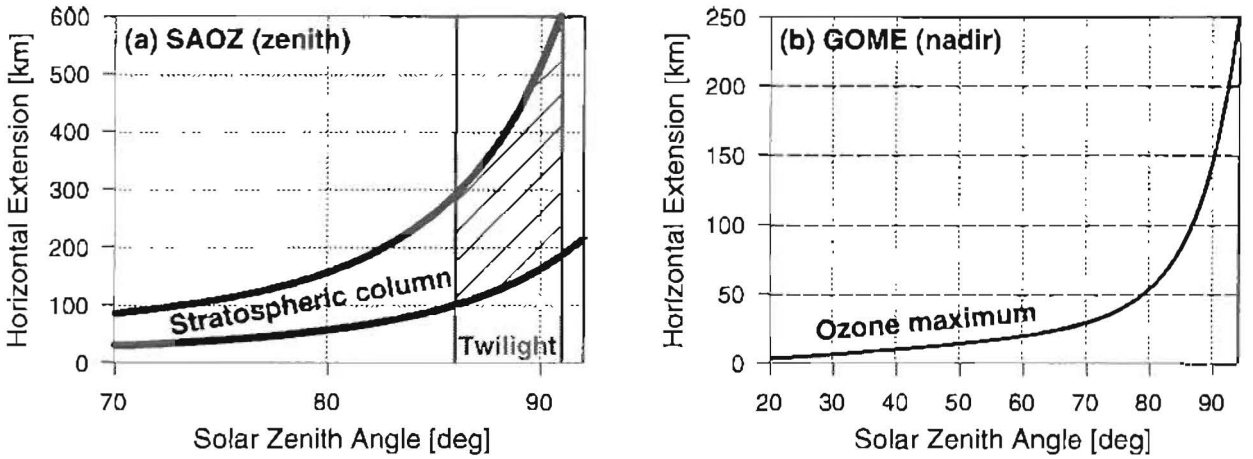

Figure 3-3 Horizontal extension of the air mass sampled by scattered-light instruments: (a) position, w.r.t. ground-based station, of the stratospheric ozone column probed by a UV-visible zenith-sky spectrometer (at 550 nm) during twilight; and (b) position in the direct beam (i.e., before scattering towards the nadir), w.r.t. satellite footprint, of the stratospheric ozone maximum observed by GOME (at 330 nm).

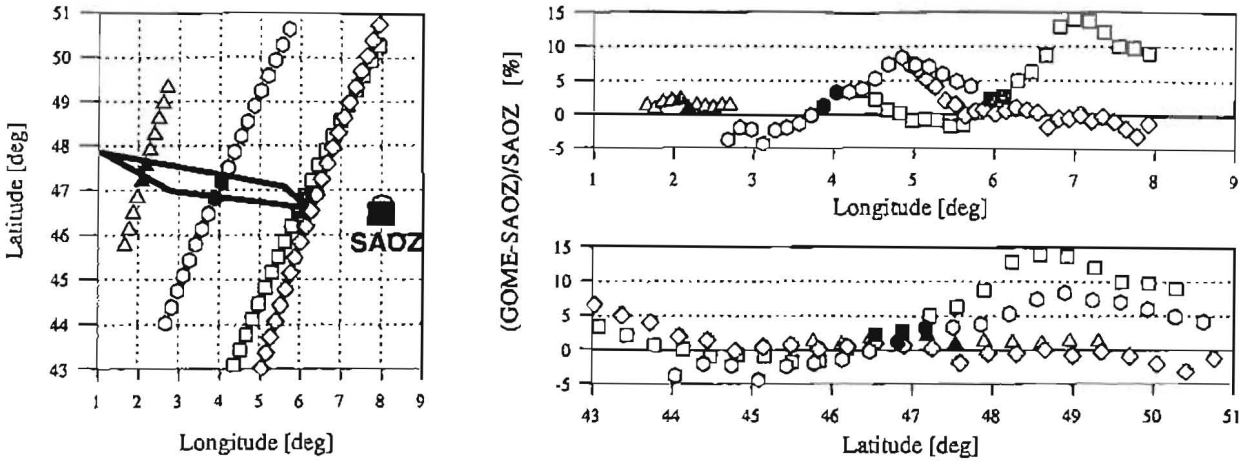

Figure 3-4 Comparison between the GOME and SAOZ total ozone at the Jungfraujoch on September 4, 1995. In the left-hand part, the horizontal projection of the GOME ground pixel centres up to 500 km from the ground-based station makes appear four tracks (triangles, hexagons, squares and diamonds) out of two different orbits. The SAOZ location and the horizontal projection of the stratospheric air mass probed by the SAOZ are schematised. GOME pixel centres intersecting with this projection are shaded. The right-hand part shows the percent relative differences between the GOME and SAOZ total ozone, as a function of the longitude (upper part) and of the latitude (lower part). The figure clearly demonstrates that the ±10% scatter introduced in the comparison by steep ozone gradients over the Alps can be reduced if only coincident geolocations are compared (from Lambert *et al.*, 1998b).

3.3 Commissioning phase

3.3.1 Early activities

In March 1995, prior to the launch of ERS-2, the B103/F114 team participated successfully to the GOME validation rehearsal, demonstrating its ability to handle and interpret quickly large amounts of data from satellites and ground-based networks. A similar exercise was performed a few weeks after the beginning of GOME operation in July 1995, with one orbit of GOME total ozone acquired on July 20. The real correlative studies started in fall 1995 with the release of a few days of GOME data processed with GDP 1.20 and 1.21. A general underestimation of total ozone by GOME, and a dependence on the solar zenith angle and on the total column, were already detectable, and reported during the GOME Geophysical Validation Campaign Meeting held in November 1995 at DFD/DLR (Oberpfaffenhofen, Germany). During this meeting, an obvious disagreement was also noticed between the first Antarctic ozone hole map presented by DLR/ESA, and ground-based SAOZ observations from Dumont d'Urville.

3.3.2 Ozone retrieval from GOME visible spectra: a test case study

The GOME ozone vertical column amounts retrieved during the commissioning phase for validation purposes were obtained by application of the DOAS method in the ultraviolet Huggins bands of ozone. GOME would be able to provide additional ozone determinations from the visible Chappuis bands, but the choice of the most relevant visible windows is a matter of discussion. Although the geometries of observation can be significantly different, the retrieval of total ozone in the visible region is rather similar for GOME and the ground-based instruments. Hence an additional interest of ground-based instruments in the context of the GOME validation is the potential for test case studies using ground-based data analysed in different spectral windows.

In this work, two different windows were selected for processing the SAOZ data recorded at the Jungfraujoch station during the commissioning phase: (i) the usual SAOZ window for ozone (470-540 nm) and, (ii) an ozone window suggested for GOME (510-550 nm). Figure 3-5-a shows the percent deviations in total ozone obtained when comparing the time series determined in both windows. The results show large differences in the retrieved ozone values (between 0% and 20%) accompanied by opposite differences in the O_4 amounts (figure 3-5-b), which suggests a possible correlation between the

spectral signatures of ozone and O_4 in one or both windows. The origin of the problem appears clearly when looking at the differential structures (figure 3-6). For the window 510-550 nm (figure 3-6-c,d), the correlation coefficient between ozone and O_4 is larger than 0.9. Additional tests using a slightly enlarged window (510-565 nm) give similar results and lead to the conclusion that the use of a restricted window to fit ozone in the visible is not suitable, at least for ground-based instruments. This conclusion might be extended to GOME as well, although the contribution of O_4 to the total absorption in the GOME geometry (nadir) is expected to be smaller.

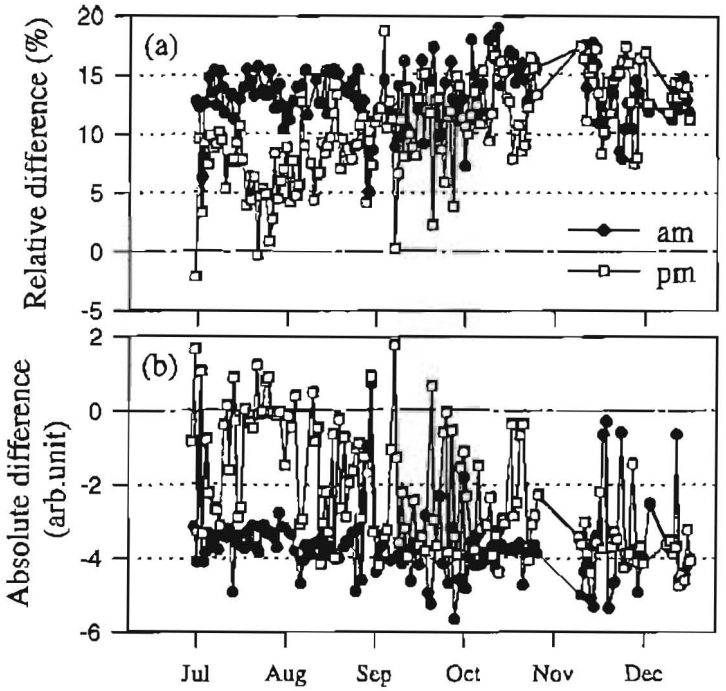

Figure 3-5 Comparison of O_3 and O_4 retrievals using two different spectral windows (see text); (a) percent deviations in total O_3, and (b) absolute deviations in O_4 slant columns.

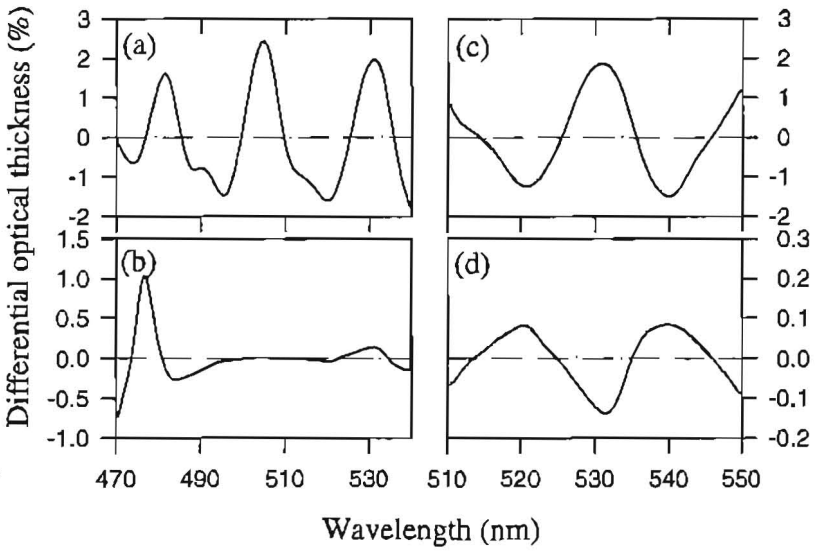

Figure 3-6 Differential optical thickness of O_3 (a,c) and O_4 (b,d) derived from least-squares analysis of SAOZ data (25.07.95, 88° SZA, PM) in two different spectral windows (see text).

3.3.3 Evaluation of GDP 1.20-1.21

In December 1995, correlative studies of the GOME GDP 1.20 and 1.21 total ozone were extended to a data set of 45 days from July to December 1995. Comparisons conducted at northern middle latitudes using the NDSC Alpine station [Lambert *et al.*, 1996a], and at all latitudes using the SAOZ network [Lambert *et al.*, 1996b], were presented at the GOME Geophysical Validation Final Results Workshop held in January 1996 at ESA/ESRIN. Both exercises concluded to: i) a total ozone underestimation by GOME; ii) a significant SZA dependence at all latitudes compared to SAOZ : 5% underestimation on average at 45° SZA, 10% at 60° SZA and even much more beyond where multiple scattering was not considered in the GOME AMF calculation although significant; iii) a dependence of the relative difference between the GOME and the SAOZ total ozone, on the amplitude of total ozone amount, that is, a difference of sensitivity; and iv) an overestimation of the ozone column by 10%-20% at high latitudes in summer, as well as in ozone hole conditions in Antarctica. Figure 3-7 illustrates the SZA dependence of GDP 1.20-21 total ozone. Since the development of the GOME total NO_2 retrieval was still in progress, the quantification of the discrepancies between GOME and ground-based measurements of total NO_2 was irrelevant.

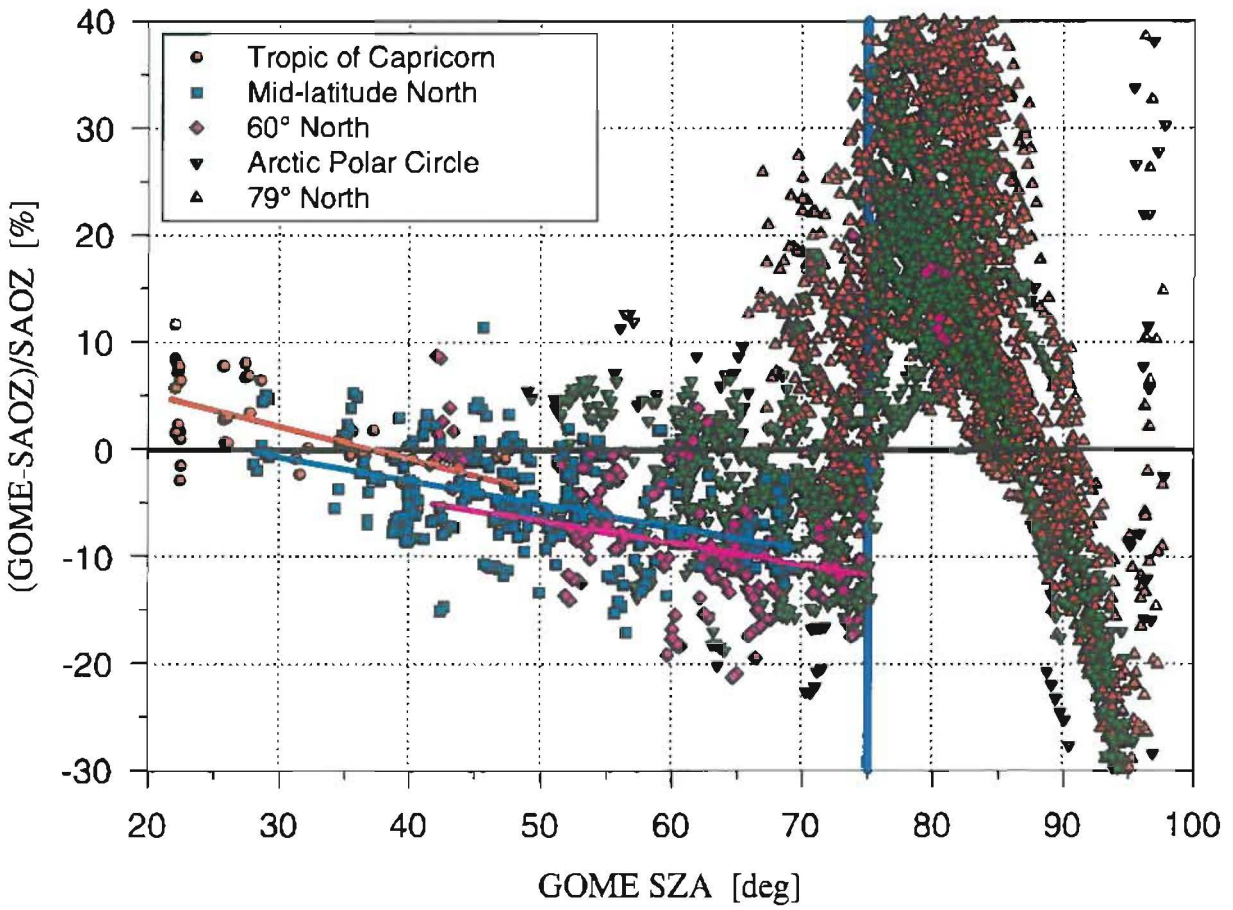

Figure 3-7 Solar Zenith Angle (SZA) dependence of the relative difference between GOME (GDP 1.20-1.21) and SAOZ total ozone. Ground-based stations are sorted into five latitude belts. Below 75° SZA, first order regressions are depicted (from Lambert *et al.*, 1996b).

3.3.4 GOME Tiger Team activities

Following the conclusions and recommendations drawn from the characterisation of GDP 1.20-1.21, the so-called 'GOME Tiger Team' was constituted, aiming at the needed improvement of the GDP before operational processing and public release of GOME data. Representing the B103/F114 and USA157 ('UARS Solstice Data as a Calibration and Validation of GOME', G Rottman *et al.*) groups, IASB-BIRA was selected as an effective member of this Tiger Team, together with DFD/DLR, ESA, KNMI, IFE/IUP, and NASA/GSFC. Within this framework, the GOME retrieval of ozone in the Huggins bands and of NO_2 was revisited. NDSC and SAOZ ground-based measurements were used to evaluate in detail the successive versions 1.40, 1.50 and 1.60 of GDP. GDP improvements for total ozone processing included the calculation of the GOME Air Mass Factors (AMF) at a more adequate wavelength (325 nm), the correction for multiple scattering up to 92° SZA, and a better treatment of the cloud cover. In July 1996, the general performance of GDP 1.60 was recognised as satisfactorily for public release. The team participated to the redaction of the GOME Data Disclaimer document to be provided to the GOME data users.

3.4 Operational phase

3.4.1 Characterisation of GDP 2.0 and TOMS v7 level-2 products

Following the public release of GDP 2.0 total ozone and NO_2, regular correlative studies of GOME data have been conducted using ground-based observations from the SAOZ/UV-visible network and from the Alpine and Antarctic stations of the NDSC. Total ozone measured from space by two NASA's Total Ozone Mapping Spectrometers onboard the Earth Probe (since July 1996) and ADEOS (September 1996 - June 1997) platforms has also been compared to ground-based observations. The total ozone comparisons with each spaceborne sensor have been combined altogether for investigating their respective performances. Studies have been carried out in collaboration with the TOMS/BUV team at NASA/GSFC. Results have been reported at many occasions during dedicated meetings, by fax and e-mail, and in international scientific journals. Current GOME time series processed with a single version of GDP are too limited to investigate long-term time-dependent drifts. Therefore, investigations have focused on the SZA dependence, the seasonal and latitudinal drifts, the dispersion, and the possible differences of sensitivity of the space-based sensors.

The total ozone studies [Van Roozendael *et al.*, 1998b; Lambert *et al.*, 1997a,b, 1998a,c,d,e] demonstrate a general better agreement between the GOME GDP 2.0 and the ground-based data. However, they also reveal significant systematic features for both the GOME and TOMS sensors, such as: (i) a SZA dependence with TOMS beyond 80°; (ii) a SZA dependence with GOME beyond 70°, changing with the season; (iii) a systematic bias of a few percent between satellite and SAOZ observations of low ozone columns in the southern tropics; (iv) a difference of sensitivity to ozone between the GOME and ground-based sensors at high latitudes; and (v) a pseudo-interhemispheric difference of TOMS with the ground-based observations.

GOME total NO_2 retrieved routinely with GDP 2.0 since June 28, 1996, has been compared to observations from the SAOZ/UV-visible network [Lambert *et al.*, 1997a, 1998e] and from the two FTIR spectrometers operating at the Jungfraujoch. GOME NO_2 measured between July 29 and October 15 in 1996 is irrelevant, due to a strong wavelength registration shift in the spectral channel 3 (where NO_2 is retrieved). Another major problem arose on December 17, 1997, when a 2-pixels shift occurred in channel 3 again. This problem disappeared after a switch-off of the instrument on February 11, 1998. Outside the two aforementioned periods when no GOME NO_2 can be retrieved, investigations point out major discrepancies between the GOME and ground-based data, as well as the geophysical inconsistency of GOME data in the northern hemisphere under several conditions. Correlative studies based on balloon data and 3D model results show that the major source of the problem is linked to the NO_2 vertical distributions used in the total column retrieval of GDP 2.0.

3.4.2 Preliminary evaluation of GDP 2.3

Following improvements of the GDP for total ozone and NO_2, a second Tiger Team exercise took place at the end of 1997, aiming at the evaluation of GDP 1.4 (level-0-to-1) and GDP 2.3 (level-1-to-2) before operational implementation. A GOME level-2 validation data set of about 330 orbits was processed with GDP 2.3, including every 15^{th} orbit acquired in 1996. Relying on the conclusions drawn from the ground-based evaluation of GDP 2.0 for total ozone and NO_2, a limited, but representative set of 36 additional orbits were selected by the B103/F114 team for processing in order to test improvements of the GDP under special conditions and to identify possible changes in the column-resolved SZA dependence of GOME total ozone. The study [Lambert and Simon, 1998f] was based partly on ground-based data provided by 24 instruments associated with the NDSC. Complementary information was provided by ozonesondes, lidars, ECMWF meteorological analyses, and the 3D chemical-transport model IMAGES of the troposphere [Müller and Brasseur, 1995]. The results and conclusions were presented at the GOME Tiger Team II Meeting held on 14 January 1998 at DFD/DLR.

4. Characterisation of GOME level-2 products

4.1 Combined analysis of GDP 2.0 and TOMS v7 total ozone

More than two years of GOME total ozone retrieved with GDP 2.0 (1996-1997) and GDP 2.3 (mid-1995 and early 1998), as well as total ozone measured by two NASA's TOMS onboard the Earth Probe (since July 1996) and ADEOS (September 1996 - June 1997) platforms, have been compared to high-quality ground-based observations listed in Table 1. For each ground-based data record, absolute and relative differences with satellite data have been investigated systematically with respect to relevant parameters, namely the SZA and the air mass factor of the space-based measurement, the ozone column value, the tropospheric cloud cover (GOME) or the reflectivity (TOMS), the possible occurrence of polar stratospheric clouds, the relative position of the polar vortex, and stratospheric temperatures. After taking properly into account the known biases of the ground-based total ozone time-series (e.g., seasonal/latitudinal variation of the AMF in real-time SAOZ data, or temperature dependence of the ozone absorption coefficients for the Dobson and Brewer instruments), comparison results based on different ground-based observation techniques generally are consistent within the accuracy level of the ground-based data. A consistency by latitude belt is also noticed.

4.1.1 General consistency

The key results of the comparisons are summarised in Table 2. The qualitative analysis of global ozone maps derived from GOME, TOMS-EP and TOMS-AD data, concludes that the three spaceborne sensors capture similarly the spatial structure of the total ozone field. The comparison of the space- and ground-based time-series leads to similar conclusions for the day-to-day variability of the ozone column, under normal conditions as well as during springtime polar ozone depletion. The quantitative comparison of time-series does not reveal any significant long-term drift.

Table 2 Summary of the consistency between space-based (ERS-2 GOME, TOMS-EP and TOMS-AD) and ground-based total ozone observations for various conditions (from Lambert *et al.*, 1998c).

	GOME	TOMS
Northern mid-latitudes	Good agreement, better than ±2 to 4%	Good agreement, better than ±2 to 3%
Arctic	Good agreement at moderate SZA: ±4%	Good agreement at moderate SZA: ±4%
	SZA dependence beyond 70° SZA	SZA dependence beyond 80° SZA
Southern hemisphere	Good general agreement in 'normal' conditions: ±2 to 4%	Systematic overestimation of about 5 to 10% at all latitudes
SZA dependence	Summer-fall: 5-10% underestimation between 70° and 85° SZA	5-10% underestimation beyond 80° SZA
	Winter-spring: 10% overestimation beyond 85° SZA	
	Small latitudinal variation	Small seasonal variation
Difference in sensitivity	High latitudes and southern Tropic: - overestimation of low ozone - relative differences correlate with the ozone column values	Overestimation of low ozone at the southern Tropic
Internal bias	In the Alps, small shift in GOME data every three months, and yearly drift	Small bias between TOMS-AD and TOMS-EP total ozone

The satellite data records are found to be globally consistent with ground-based measurements. In particular, the study demonstrates an average agreement to within ±2-4% between all space-borne and ground-based sensors at northern middle latitude, with a scatter of about ±2-3% (Figure 4-1). Similar results were obtained with the data records from TOMS onboard Nimbus-7 (1978-1993) and Meteor-3 (1991-1994). However, the comparisons reveal several discrepancies and systematic features. Some of them are common but not always similar among the two types of spaceborne sensors: the SZA dependence at high latitudes; discrepancies during springtime ozone hole in Antarctica; and the systematic bias between satellite and SAOZ observations of low ozone columns at the southern Tropic.

Although mutually consistent within a few percent, systematic differences are observed between TOMS-AD and TOMS-EP total ozone. They might be attributed partly to air mass differences in time (the orbits of ADEOS and Earth Probe are different) and in space (the lines of sight and resulting ground pixels are different), and partly to calibration uncertainties. The results obtained with both TOMS-AD and TOMS-EP also show a systematic pseudo-interhemispheric difference with the ground-based observations.

The results obtained with GOME do not reveal any significant interhemispheric feature, but: (i) a difference of sensitivity between the GOME and ground-based sensors at high latitudes, described in the next section, and (ii) internal inconsistencies in GOME data. Inconsistencies appear clearly in Figure 4-1, where GOME total ozone in the Alps (retrieved with both GDP 2.0 and 2.3) is compared with data from three independent ground-based instruments. Every three months, GOME data are shifted by a few percent, the sign and the amplitude of the shift depending on the season. This effect appears most clearly at the end of each year when the shift can exceed 5%. Three-months shifts might result from the combination of uncertainties in the seasonal AMF/profile climatology used in the GDP, with inadequate temporal interpolation of this climatology or the AMFs. The seasonal variation of the SZA dependence at high latitudes might be partly connected with this effect as well.

4.1.2 SZA dependence and difference of sensitivity

At high latitude, in both hemispheres, the mean agreement and the scatter vary with the SZA of the space observation, largely due to the retrieval method and its sensitivity to errors in the ozone profile shape. At first glance, the impact of the polar vortex is mainly an increase of the scatter during fast total ozone changes between the satellite and ground-based measurements. The dispersion of satellite data increases significantly beyond 85° SZA. The GOME total ozone increases systematically beyond 80° SZA, however its average SZA dependence is dominated by a seasonal variation resulting in negative mean deviations beyond 65-70° SZA in summer-fall (Figure 4-2-a) and in positive mean deviations beyond 80° SZA in winter-spring (Figure 4-2-b). Although a SZA dependence is also present in the TOMS data, its amplitude is smaller than that of the GOME, does not vary with the season, and is not significant below 80° SZA (Figure 4-2-c). The agreement between the GOME and the ground-based total ozone also depends on the ozone column, indicative of a difference of sensitivity. In particular, low ozone columns are overestimated by the GOME by a few percent at the tropics (Figure 4-3-a) and by more under springtime polar ozone depletion conditions in both the Arctic and the Antarctic (Figure 4-2-b and 4-4). Such a feature is not observed with the TOMS, except at the southern tropic (Figure 4-3-b). The SZA dependence and the difference of sensitivity must be kept in mind in studies based on satellite data recorded in polar areas during winter and spring. As an example, for an ozone loss assessment combining satellite total ozone measurements and trajectories modelling, the SZA dependence or the difference of sensitivity, if not taken properly into account, might both introduce large uncertainties in the ozone loss calculation since the studied air parcels travel through polar areas and hence can experience a wide range of SZA and total ozone.

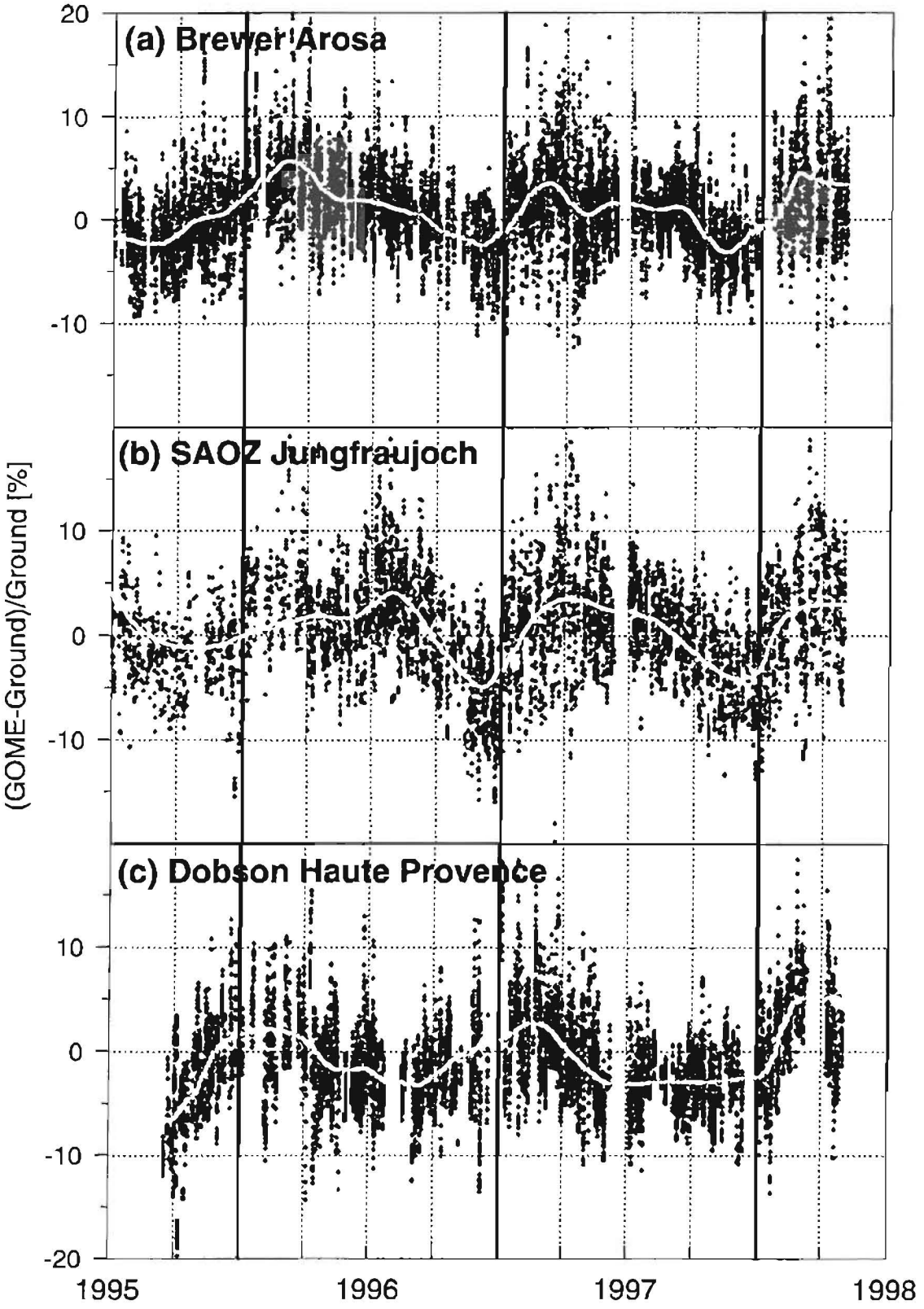

Figure 4-1 Percent relative difference between GOME total ozone retrieved with GDP 2.0 (1996-1997) and GDP 2.3 (1995 and 1998), and ground-based measurements from three independent instruments operating at the NDSC/Alpine station: (a) Brewer UV spectrophotometer at Arosa; (b) SAOZ UV-visible spectrometer at the Jungfraujoch; and (c) Dobson UV spectrophotometer at the Observatoire de Haute Provence. Time-series are low-pass filtered to discriminate the seasonal component. The monthly mean agreement is within ±2-4%, with a scatter of about 2-3% (1σ). No long-term drift can be detected after three years. However, comparison results in the Alps conclude to systematic features in GOME data, such as a slight drift with the time of the year, and a shift every three months, particularly clear at the end of each year when the shift can exceed 5%.

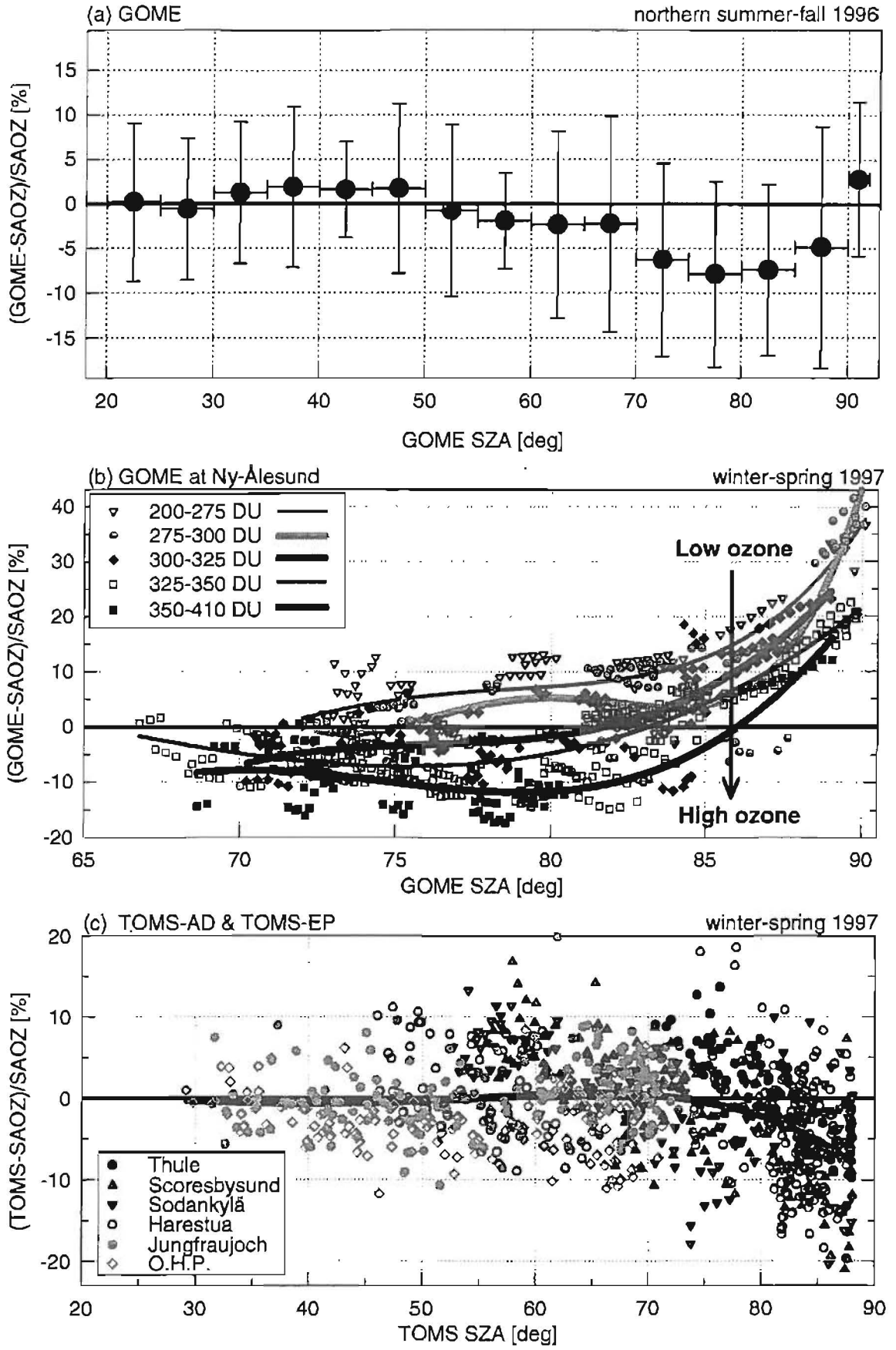

Figure 4-2 Solar zenith angle dependence of the difference in total ozone between the GOME, TOMS and SAOZ sensors: (a) average SZA dependence and scatter (2σ) with GOME in summer-fall, for eight stations in the northern hemisphere; (b) column-resolved SZA dependence with GOME in winter-spring, at Ny-Ålesund; and (c) SZA dependence with both TOMS-AD and TOMS-EP in winter-spring, at six stations in the northern hemisphere. Parts (b) and (c) are from Lambert et al., 1998d.

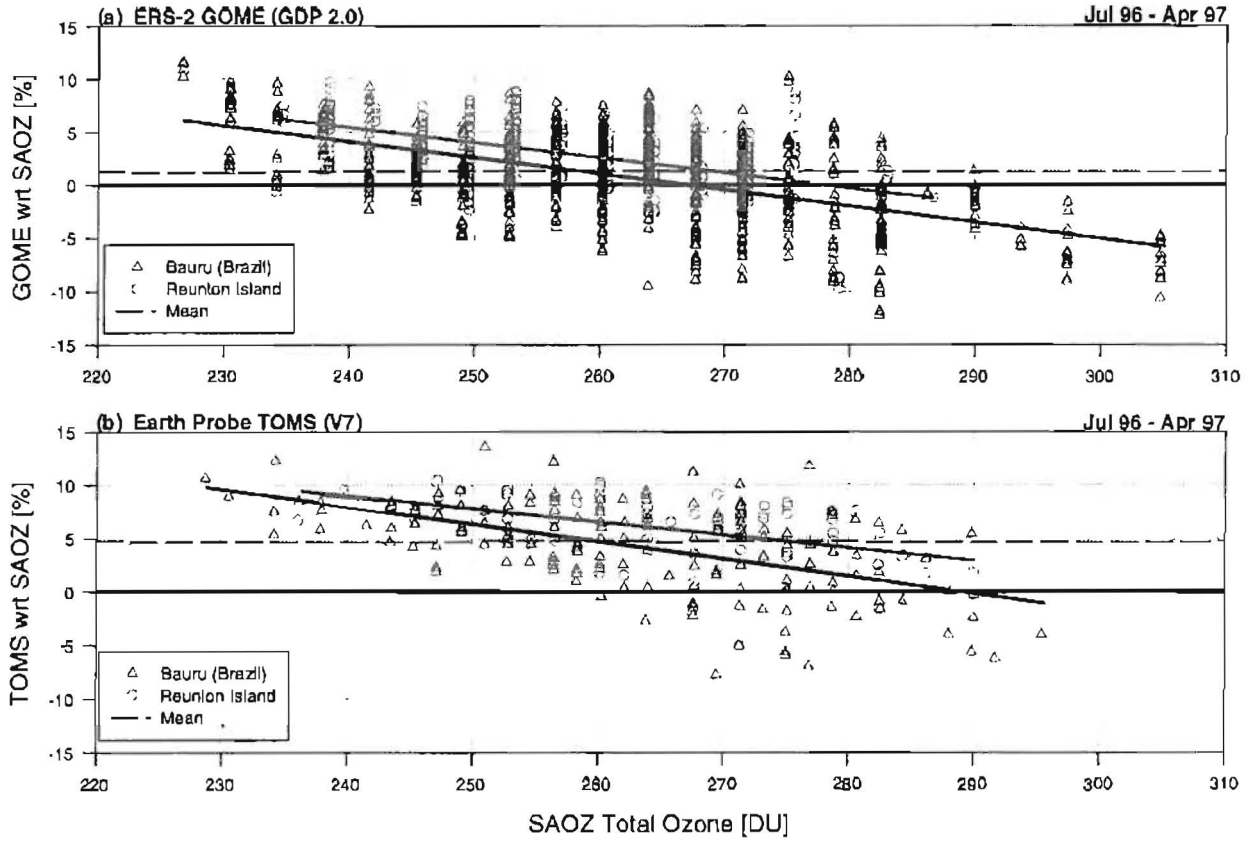

Figure 4-3 Difference of sensitivity to total ozone between SAOZ and space-based sensors at two stations on the southern Tropics: (a) ERS-2 GOME (GDP 2.0), and (b) Earth Probe TOMS (V7). First order regressions and the mean relative difference are also depicted.

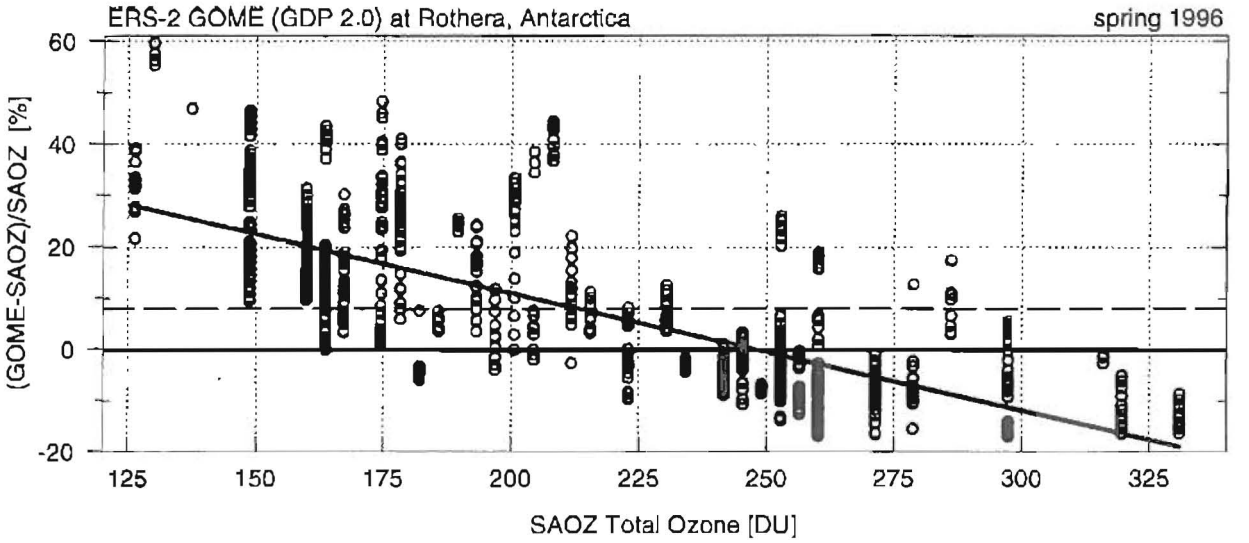

Figure 4-4 Difference of sensitivity to total ozone between GOME and SAOZ during the springtime 1996 ozone hole, at the Antarctic station of Rothera. First order regression and the mean relative difference are also depicted.

Seasonal/latitudinal biases peculiar to the ground-based measurements could contribute partly to the SZA dependence. However, they certainly can not account for the full systematic bias observed at high SZA, nor for the shape of the SZA dependence which, in addition, is different for GOME and for TOMS. The SZA dependence can be observed at high latitudes in the satellite data themselves, since in polar areas in summertime this dependence generates a systematic bias between satellite data of the descending and ascending orbits, that is around noon and under midnight sun. Ultraviolet radiance measurements at nadir are known to be sensitive to the shape of the ozone, pressure and temperature profiles. The difference between the GOME and the TOMS comparisons might arise from basic algorithm differences in the treatment of the profile shape effect. Indeed, in the one-step treatment of GDP 2.0, the profile is specified for a given latitude belt during a given season, while in the iterative approach of TOMS V7, the shape of the profile is optimized according to the latitude and the amplitude of the ozone column. The seasonal/latitudinal variation of the GOME SZA dependence might vindicate the use of a climatology based on real profile measurements, such as the TOMS V7 climatology. An overcorrection for multiple scattering, different for the GOME and TOMS algorithms, cannot be ruled out. The profile shape effect can also account partly for the correlation observed at high latitudes between the ozone column value and the difference of GOME with ground-based data. This difference of sensitivity might be related to the use of monthly atmospheric profiles in the GOME retrieval which cannot match the actual, highly variable atmospheric profile. The effect would be significantly reduced with TOMS since it uses a column-resolved climatology. In addition, at higher SZA, the TOMS algorithm uses measurements at the shorter wavelengths to optimize the combination of middle and high latitudes profiles. Since the apparent slant column amount of absorber increases with SZA, both the difference of sensitivity and the particular shape of the GOME SZA dependence might also result from the particular approach of DOAS adopted in GDP 2.0, and especially from: (i) the use of a single wavelength for the calculation of the GOME AMF, although this latter varies significantly over the fitting spectral window; (ii) a small wavelength registration shift between the GOME spectra and the laboratory cross-sections; (iii) the incorrect removal of the Fraunhofer solar lines; and (iv) an imperfect convolution of ozone cross-sections. Overall, the results shown are still too scarce to demonstrate a difference of sensitivity between the TOMS and ground-based instruments. An exception is the southern Tropic, where the three satellite instruments measure systematically higher values at low ozone. It remains to be seen if this could be explained by a combination of low signal-to-noise at low SZA, and profile shape effect in the spaceborne or ground-based sensors.

4.1.3 Dispersion

After removal of the average difference as a function of time, the dispersion of satellite data with respect to ground-based observations is similar for GOME and TOMS. It increases from ±2-3% in the tropics and at middle latitudes, up to ±10% at high latitudes in winter and also at high SZA. A first contribution to this scatter is related to the spatial and temporal difference in air masses probed by the spaceborne and the ground-based instruments, combined with the presence of horizontal gradients and of variability [Lambert et al., 1998b]. The scatter is smaller with Dobson and Brewer measurements performed within about three hours around the GOME and TOMS overpasses. It increases with UV-visible zenith-sky observations at twilight, partly due to the difference of measurement time, and the large horizontal extension of the zenith-sky air mass (about 350 km towards the sun at twilight) compared to the direct sun air mass. At low sun elevation, a lower scatter might be expected between nadir-viewing spaceborne and zenith-sky ground-based observations, since both measure, within a few hours, coincident air masses extending over several hundred kilometers in the same direction. However, the opposite is observed, partly due to the low sensitivity of UV nadir measurements at high SZA to the lower atmosphere, and partly due to the uncertainty on radiative transfer modeling in the ultraviolet when SZA increases. Another important source of scatter originates in deviations of the actual ozone, pressure and temperature profiles, from those in use in the retrievals. Other possible contributions are related to the cloud cover: (a) perturbations generated in the ground-based measurements (mainly the SAOZ) by tropospheric multiple scattering in presence of dense clouds or haze, combined with local ozone changes; (b) uncertainties in the cloud treatment in the satellite retrieval (e.g., uncertainties in optical properties of clouds, or the use of a climatological database for cloud top pressure); (c)

perturbations due to dense (type II) polar stratospheric clouds in winter polar regions; and (d) clouds mask the tropospheric contribution of the satellite measurements.

4.1.4 Investigation of the impact of convolution errors at large SZA

Total ozone is derived from GOME nadir radiance measurements between 325 and 335 nm, by means of the DOAS technique. This latter consists in studying narrow absorption features generated in the atmospheric spectra by atmospheric absorbers, after removal of the broad band signal due to Mie and Rayleigh scattering processes. With the standard DOAS approach adopted in GDP, the observed differential optical depth is correlated with differential absorption cross sections measured in the laboratory, yielding apparent slant column amounts. Slant columns are converted into vertical column amounts by means of a geometrical enhancement factor, or Air Mass Factor (AMF). The GOME retrieval is based on the use of absorption cross sections measured with the Flight Model (FM) before launching the instrument in space, thus avoiding the need for (imperfectly) convolving higher resolution data with the slit function of GOME. However, the use of cross sections measured with the FM in the laboratory under condition of relatively small optical thickness and with a light source quite different from the sun, could possibly lead to errors in the total ozone retrieval at large SZA because of the large atmospheric optical thickness encountered in the ultraviolet region.

Investigations were carried out to clarify this issue, based on high-resolution simulations of the ultraviolet nadir radiance, further convolved to the GOME resolution, and then analysed with the DOAS technique [Van Roozendael, 1997]. Tests included spectral analysis with both the standard DOAS procedure (retrieval of the slant column amount, followed by the division by a single-wavelength AMF to obtain the vertical column abundance) and the 'modified' DOAS approach (direct fitting of the vertical column amount, using a wavelength-varying AMF in the fitting procedure). The study concludes that the main source of error on total ozone in the standard DOAS fitting procedure is related to the spectral dependence of the AMF. Once this effect is taken into account with the 'modified' DOAS approach, the quality of the spectral analysis improves significantly, and remaining errors due to convolution approximation appear as regular small features, smaller than 1% at all SZA.

4.1.5 Interhemispheric difference of TOMS with ground-based data

The pole-to-pole comparison points out a clear north/south difference in the agreement between the TOMS and ground-based data. Figure 4-5 reveals a systematic bias of TOMS-EP total ozone compared to SAOZ and Dobson observations at seven stations in the southern hemisphere. In particular, both TOMS overestimate the ground-based columns in Antarctica by 8-12%, while the agreement is reasonable in the Arctic. This pseudo-interhemispheric difference might arise from the climatology of ozone and temperature profiles used in the TOMS V7 algorithm. These profiles are derived from a composite climatology of Stratospheric Aerosol and Gas Experiment II (SAGE II) and ozonesonde data sets. The TOMS V7 climatology is hence somewhat biased towards the northern hemisphere. In addition, higher altitudes are poorly represented at polar latitudes since there are very few SAGE II measurements beyond the polar circle. The interhemispheric consistency of GOME seems to vindicate a separate treatment of each hemisphere. But further investigation is needed for a better understanding of the problem, among others to determine if the difference is really interhemispheric, or varies rather with, e.g., the latitude belt of the TOMS climatology. At Antarctic stations, both the cloud cover fraction (GOME) and the reflectivity (TOMS) indicate an almost permanent overcast. The tropospheric contribution to the satellite measurement is partly masked and a climatological ozone profile below clouds must be used, which can also introduce an offset in the satellite data. Small errors of the TOMS calibration in the southern hemisphere can not be excluded. Calibration uncertainties might partly explain small differences between TOMS-AD and TOMS-EP data as well. The recent re-calibration and subsequent reprocessing of the entire TOMS-AD data record should help addressing this issue in the near future.

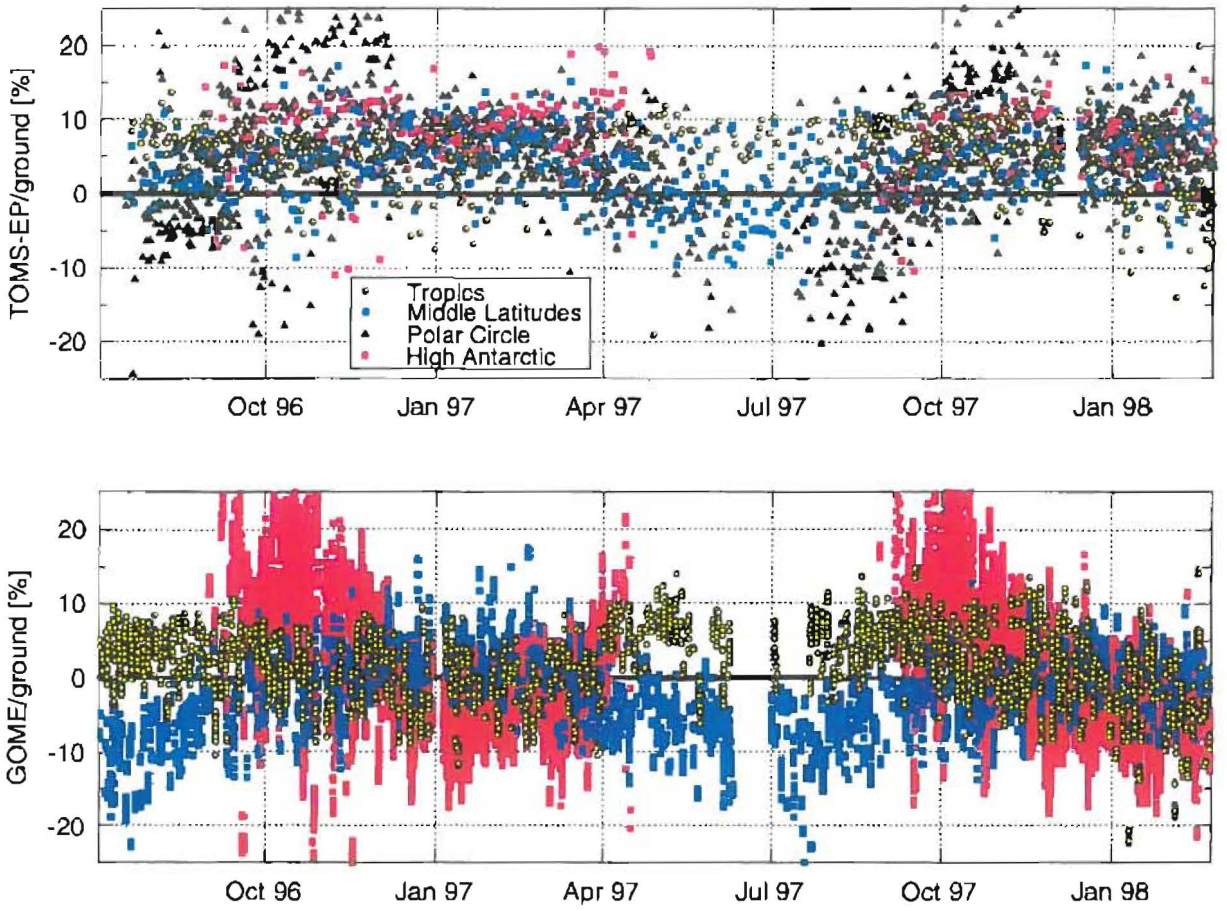

Figure 4-5 Percent relative difference between space- and ground-based total ozone in the southern hemisphere. Whatever the latitude belt, TOMS-EP (upper panel) reports systematically higher total ozone values, except at large SZA due to its SZA dependence. Other features are visible in the figure, such as the enhanced dispersion around the Antarctic polar circle from August through November, associated with high ozone variability at the border of the polar vortex. The lower panel shows the comparison with GOME (since they agree very well with high Antarctic data, polar circle data have been omitted for clarity). Cyclic signatures are clearly visible in the relative difference, which are related mainly to the seasonal SZA dependence of GOME, and to its difference of sensitivity combined with the seasonal variation of the ozone column. At middle latitudes (Kerguelen), the profile shape effect, not taken into account in the real-time SAOZ data, contributes also to the seasonal variation. However, no real year-round, systematic difference is to date with GOME data.

4.1.6 Conclusions on GDP 2.0, TOMS-EP and TOMS-AD total ozone

The global picture of total ozone provided from summer 1996 through April 1997 by the three space-based sensors studied in this work, is globally consistent with high quality ground-based observations associated with the NDSC. Nevertheless, the present analysis highlights major problems of accuracy of the space-based total ozone measurements, requiring further investigations. Several issues should be addressed, such as: (i) an iterative treatment of the profile shape effect with the GOME, using (ii) a column-resolved climatology (iii) based on real profile measurements; (iv) refinements of the current DOAS approach used in GOME; (v) improvement of temporal interpolation of GOME AMFs; (vi) the hemispheric separation of the TOMS V7 climatology; and (vii) possible calibration problems with both TOMS-EP and TOMS-AD, especially in the southern hemisphere.

4.2 Analysis of GDP 2.0 total nitrogen dioxide

4.2.1 General consistency

Two years (1996-1997) of GOME total NO_2 were retrieved routinely at DFD/DLR with GDP 2.0. The geophysical consistency of this global total NO_2 record has been investigated from pole to pole by means of correlative ground-based observations from the SAOZ/UV-visible network and from the two Fourier Transform infrared spectrometers operating at the Jungfraujoch. Figure 4-6 illustrates the comparison at representative stations in the Arctic, the Alps, and the Indian Ocean. Main findings are summarised in Table 3. GOME NO_2 measured in 1996 between July 29 and October 15 is irrelevant, due to a strong wavelength registration shift in the GOME spectral channel 3 (where NO_2 is retrieved). Outside this period, the analysis reveals: (i) the frequent occurrence of aberrant individual values in the vertical column amounts (negative, or too high by one and even two orders of magnitude) and the slant column amounts (negative, or quantified); (ii) the high dispersion of GOME data from pixel to pixel and from day to day; (iii) a general underestimation of ground-based observations by the GOME; (iv) a significant shift in the GOME data and in their agreement with the ground, every three months; (v) the poor general consistency in the northern hemisphere; (vi) the strong variation of this consistency with the season and the latitude; and (vi) the better agreement (10%-20%) at southern latitudes, although GOME yields lower total NO_2 values systematically.

Table 3 Summary of the consistency between ERS-2 GOME and ground-based total nitrogen dioxide data.

	Northern hemisphere	Southern hemisphere
General agreement	Underestimation of ground-based data.	Underestimation of ground-based data.
	Strong seasonal dependence	Good consistency up to 50°S; beyond, good only in winter.
Seasonal variation of total NO_2	Phase: excellent agreement.	Phase: excellent agreement.
	Amplitude: smoother.	Amplitude: excellent up to 50°S; smoother beyond.
Midnight Sun conditions	Sharp increase in GOME total NO_2.	No evidence of increase in total NO_2.
Inconsistent values	Higher by 0.5-4 10^{15} cm^{-2}: - at middle latitudes in fall; - at higher latitudes in fall and winter.	Lower by 1-4 10^{15} cm^{-2}: - at high latitudes in summer.
Aberrant values	Frequent occurrence of negative values or beyond 10 to 100 10^{15} cm^{-2}.	Frequent occurrence of negative values or beyond 10 to 100 10^{15} cm^{-2}.

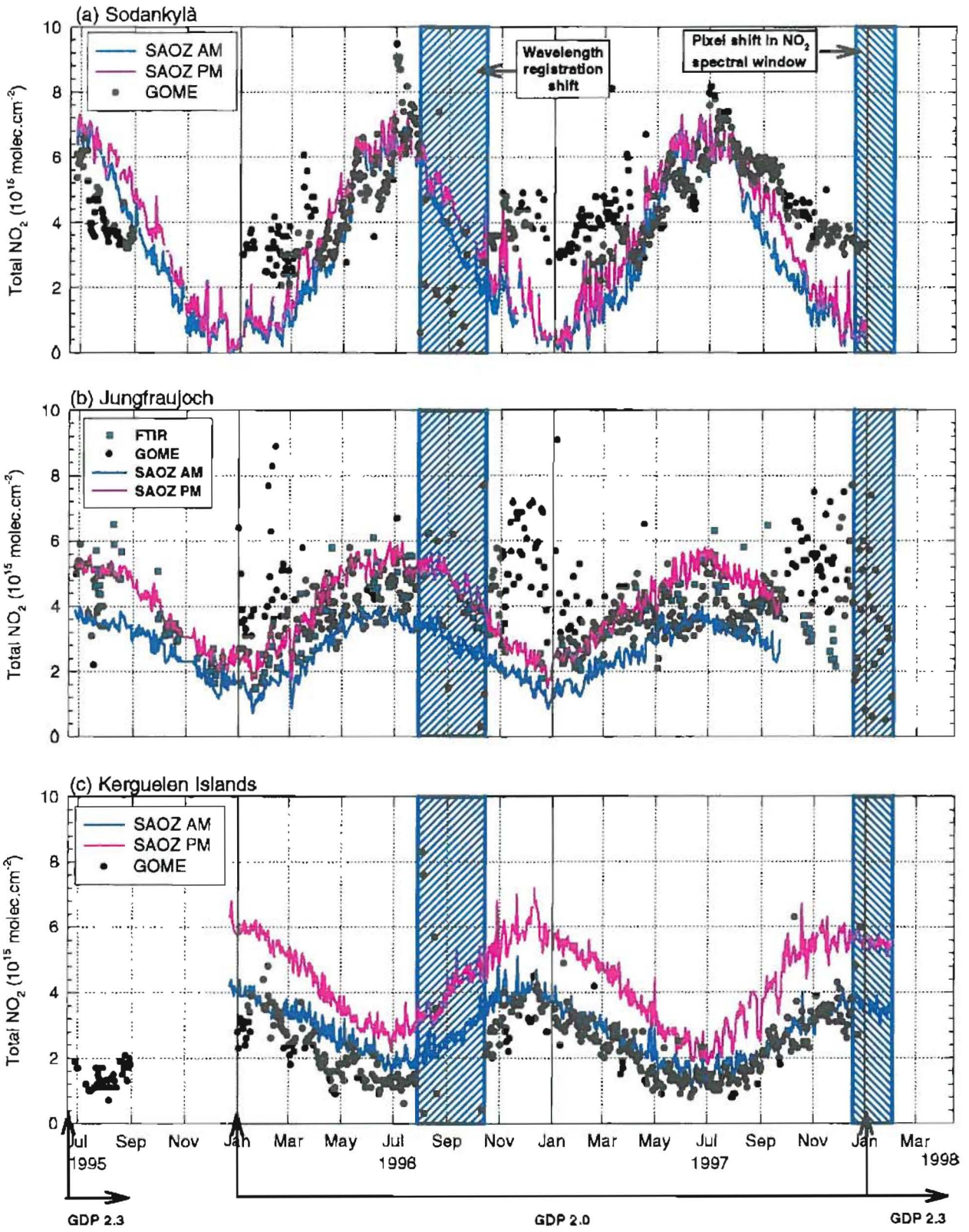

Figure 4-6 Comparison between GOME and ground-based total NO_2 at: (a) Sodankylä (Finland, Arctic polar circle); (b) the Jungfraujoch (Swiss Alps, 47°N); and (c) Kerguelen Islands (Indian Ocean, 49°S). GOME data processing with GDP 2.0 and 2.3 is identified, as well as the two periods of problems with radiometric measurements in the GOME channel 3.

4.2.2 Climatology of NO_2 density profiles and Air Mass Factors

Major inconsistencies noticed in the GOME total NO_2, as well as the seasonal and latitudinal dependence of the agreement with ground-based data, point out two main source of problems in GDP 2.0: significant bugs in the GDP itself (e.g., negative values, or quantified slant columns), and the use of inadequate NO_2 vertical distributions in the calculation of the GOME AMFs. The comparison at the Jungfraujoch displayed in detail in Figures 4-7 and 4-8 highlights the most representative problems. Except the specific problem of the quantified slant columns, most of the discrepancies observed in Figure 4-7 can be partly explained by studying the related AMF time-series as depicted in Figure 4-8.

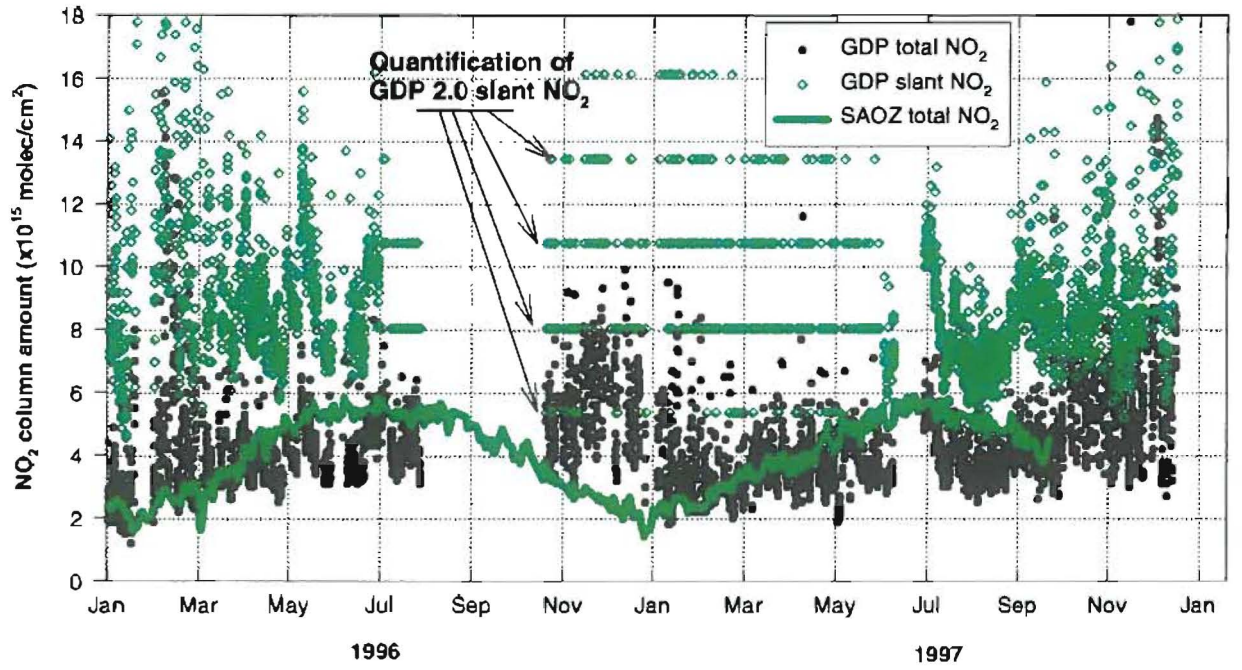

Figure 4-7 NO_2 time-series at the Jungfraujoch: (i) vertical and slant column amounts extracted from GDP 2.0 level-2 data files; (ii) sunrise/sunset average of SAOZ total NO_2.

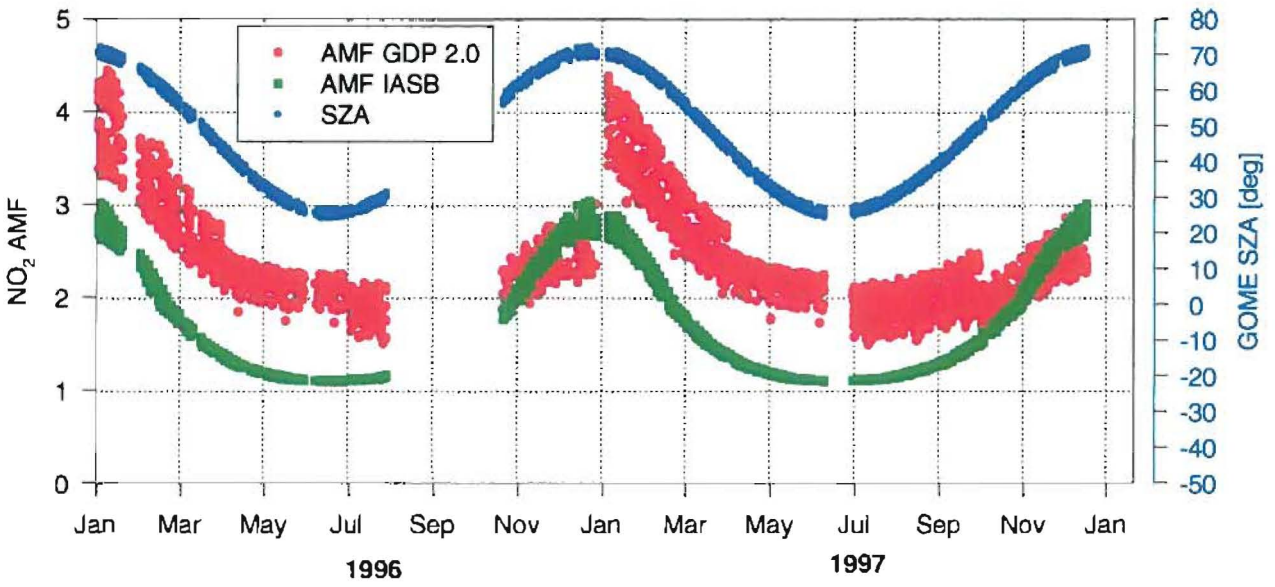

Figure 4-8 Time-series of nadir NO_2 AMFs at the Jungfraujoch: (i) GOME AMFs (middle curve) and SZA (upper curve) extracted from the level-2 data files, and (ii) related AMFs calculated with the IASB AMF processor and the US Standard NO_2 climatology (lower curve).

The evident inconsistency of the GOME AMFs originates in the NO_2 vertical distributions used in their calculation. While the ground-based retrieval algorithms use NO_2 density profiles measured during the MAP/GLOBUS campaign in 1982 [Pommereau *et al.*, 1987], or from the US the Standard climatology, GOME AMFs are based on the results of a two-dimensional chemical-transport model of the atmosphere developed at the Max Planck Institute [Crutzen and Gidel, 1983; Bruehl, 1991], hereafter referred to as MPI-2D profiles. Those latter profiles are characterised in the northern hemisphere by unreasonably high NO_2 densities in the low troposphere and low densities in the middle troposphere. Figure 4-9 shows the MPI-2D profiles in the 40°-50°N latitude belt, which are those used for GOME AMFs at the Jungfraujoch. Their more realistic tropospheric content in the southern hemisphere explains the better agreement with ground-based data in this part of the globe. In many cases, MPI-2D profiles in the northern hemisphere are found inconsistent with the US Standard profiles, with real NO_2 density profiles measured with SAOZ-balloon sondes, and with 3D model results (see next sections). Investigations based on GOME data retrieved at IASB-BIRA with US Standard NO_2 profiles - more consistent with SAOZ-balloon data, and implemented in the newly operational GDP 2.3 - show a better general agreement between GOME and SAOZ total NO_2 [Lambert *et al.*, 1997a].

The scatter and the day-to-day fluctuations, both especially enhanced in polluted areas, originate partly in the high sensitivity of the GOME observation (nadir geometry) to the tropospheric NO_2 content - which can exhibit sharp gradients and fast variations - compared to the ground-based zenith-sky observations at twilight. Since the relative contribution of a given atmospheric layer is constrained in the AMF calculation by the input profile, the sensitivity to tropospheric NO_2 is reinforced in the northern hemisphere due to the enhanced tropospheric content in MPI-2D.

4.2.3 Comparison with the IMAGES tropospheric model

A three-dimensional chemical-transport model of the troposphere, named Intermediate Model of Global Evolution of Species (IMAGES) [Müller and Brasseur, 1995], has been developed jointly at IASB-BIRA and at the National Center for Atmospheric Research (NCAR) to study the global distributions, budgets and trends of 41 chemical compounds, including ozone and nitrogen oxides. IMAGES distributions of nitrogen oxides and of other species are found to be generally in good agreement with correlative airborne in situ measurements. IMAGES has been run to provide monthly vertical distributions of NO_2 onto a 5° x 5° grid. At 45° (Figure 4-9) and 65° north, the comparison of MPI-2D with IMAGES profiles confirms the significant overestimation by MPI-2D of NO_2 density values in the low and middle troposphere, particularly in fall. This overestimation in the most dense layers, characteristic of northern middle latitudes, might be the main source of the aberrant seasonal variation of GOME total NO_2 observed in the northern hemisphere. Modelled global distribution of NO_2 (e.g., Figure 4-10) demonstrates that, for an instrument such as the GOME, strong zonal gradients in the NO_2 field - that can vary from 100 pptv up to 50 ppbv over less than 500 km - make any 2D model inadequate to reach a reasonable level of accuracy. Modelled meridional gradients also suggest that a 10° longitude resolution (approximately 1110 km at sea level) would be too coarse. Moreover, the enhanced variability of tropospheric NO_2 in fall and winter might make a set of input profiles based on monthly means preferable to a seasonal set.

4.2.4 Comparison with SAOZ-balloon soundings

The critical analysis of the NO_2 database used in the GDP 2.0 has been completed by a comparison carried out in the upper troposphere and in the stratosphere with 25 NO_2 density vertical distributions measured with the SAOZ-balloon experiment [Pommereau and Piquard, 1994] at mid and high northern latitudes, in various seasons. Figure 4-11 illustrates the comparison for midnight sun conditions in the Arctic. At mid-latitudes, MPI-2D and SAOZ-balloon number densities present a reasonable agreement in the middle stratosphere, but MPI-2D underestimates balloon measurements by a factor two in the lower stratosphere and upper troposphere. A similar systematic underestimation in this altitude range is observed in the Arctic under midnight Sun conditions, while modelled and measured profiles are at first glance mutually consistent in winter. In the upper troposphere, the comparison between IMAGES and SAOZ-balloon profiles at 45°N and 65°N shows a general reasonable agreement whatever the season.

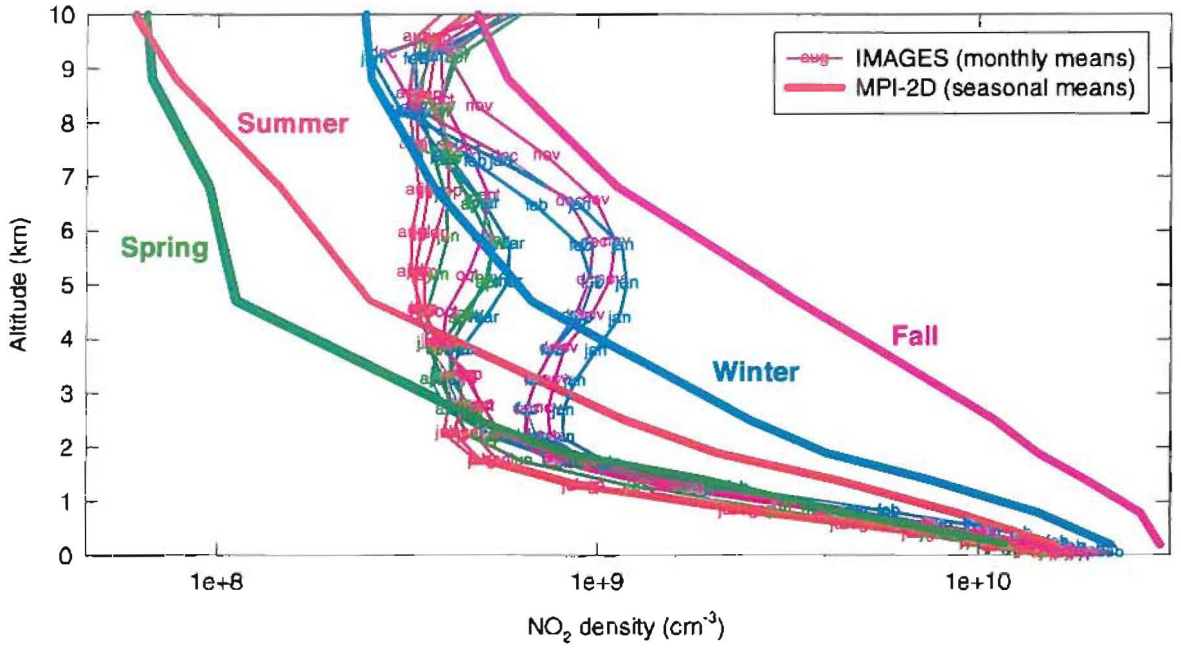

Figure 4-9 Year-round comparison of seasonal MPI-2D and monthly IMAGES-3D NO_2 density profiles, calculated at 45°N for both models and at 5°W for IMAGES.

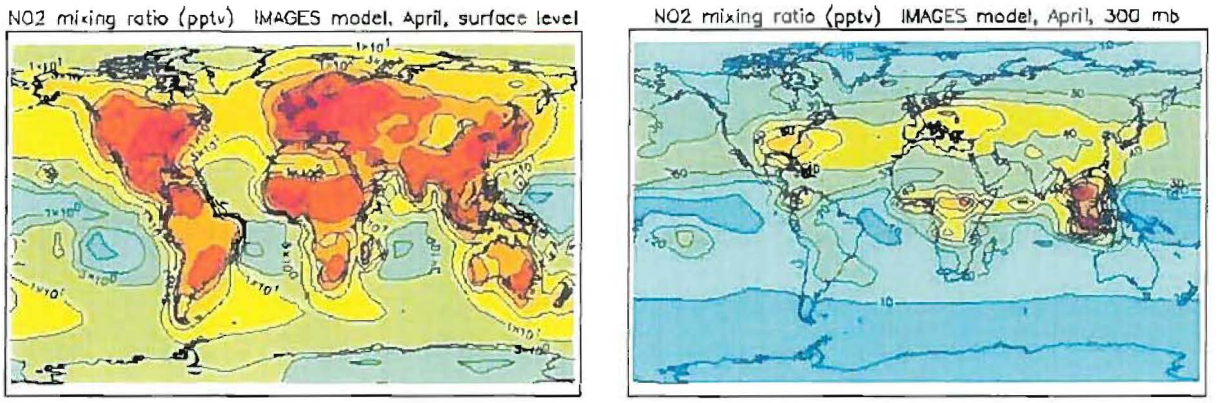

Figure 4-10 Modelled global distribution of NO_2 mixing ratio at the surface and at 300 hPa for April. Although attenuating with increasing altitude, structures observed at the surface propagate through the troposphere.

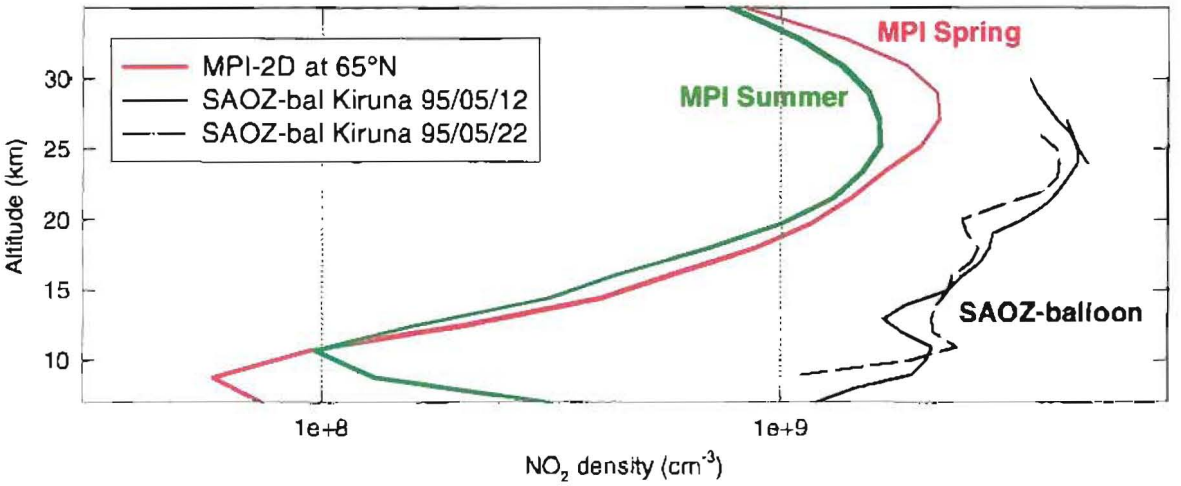

Figure 4-11 Comparison of SAOZ-balloon measurements at Kiruna (68°N) under midnight sun conditions, with MPI-2D NO_2 density profiles calculated at 65°N.

4.2.5 Conclusions on GDP 2.0 total nitrogen dioxide

The two years of GOME total NO_2 retrieved with GDP 2.0. should be used with care. If data at low and middle latitudes in the southern hemisphere are geophysically consistent, data in the northern hemisphere are mostly irrelevant. The main sources of inconsistency in the GOME total NO_2, and of discrepancy with correlative data, are clearly: (a) major bugs in the GDP 2.0, and (b) the NO_2 profiles used for the calculation of AMFs. A preliminary comparison of GDP 2.0 with GDP 2.3 (see next section), based on a limited data set, reveals that the use of the US Standard NO_2 database improves significantly the geophysical consistency of GOME data, as well as their agreement with ground-based observations. Although the overall quality of GOME total NO_2 does not appear to be satisfactorily, the results of the investigation are encouraging: there is no apparent, significant problem with the GOME NO_2 slant column retrieval. Major problems arise from the AMFs. It is therefore vigorously recommended to investigate in detail the sensitivity of the GOME retrieval to the NO_2 profile shape errors, for both the troposphere and the stratosphere, and consequently to revisit the GDP NO_2 profile database.

4.3 Preliminary evaluation of GDP 2.3

4.3.1 Total ozone

GOME total ozone data out of a level-2 validation set of 370 orbits have been compared to correlative ground-based observations. From pole to pole, the average agreement with GDP 2.3 is found similar to that observed with GDP 2.0. Changes often are within a few percent, that is within the accuracy level of ground-based measurements. When looking in more details at the influence of the cloud fraction or the AMF, it appears that modifications to the Initial Cloud Fitting Algorithm (ICFA) or to the AMF computation (e.g., new combined time/latitude interpolation scheme, multiple scattering look-up table computed with GOMETRAN v2.0, parabolic weighting of AMFs) in GDP 2.3 do not affect significantly the GOME total ozone and its agreement with ground-based observations. Due to the lack of GOME data at northern mid-latitude, investigations related to the 3-months shifts do not yield relevant results.

The seasonal SZA dependence of GOME at high latitude persists with GDP 2.3, in both hemisphere. In Figure 4-12, GOME data acquired in summer at mid-morning (descending orbit, moderate SZA) and under midnight Sun (ascending orbit, high SZA) are compared to SAOZ data at Sodankylä. This figure shows a similar summer SZA dependence for both GDP 2.0 and 2.3. The winter SZA dependence at Sodankylä is illustrated in Figure 4-13, showing no significant improvement. Figure 4-13 also shows that the SZA dependence is still column-resolved. Investigations in the Tropics, at southern middle latitude and under springtime ozone depletion in both the Arctic and the Antarctic confirm that the difference of sensitivity of GOME remains unchanged. Additional investigations were carried out on the possible influence of PSCs or the effect produced by the change in GDP in the determination of the Bass-Paur temperature. However, those effects are masked by the strong SZA/column dependence and cannot be studied with the limited validation data set.

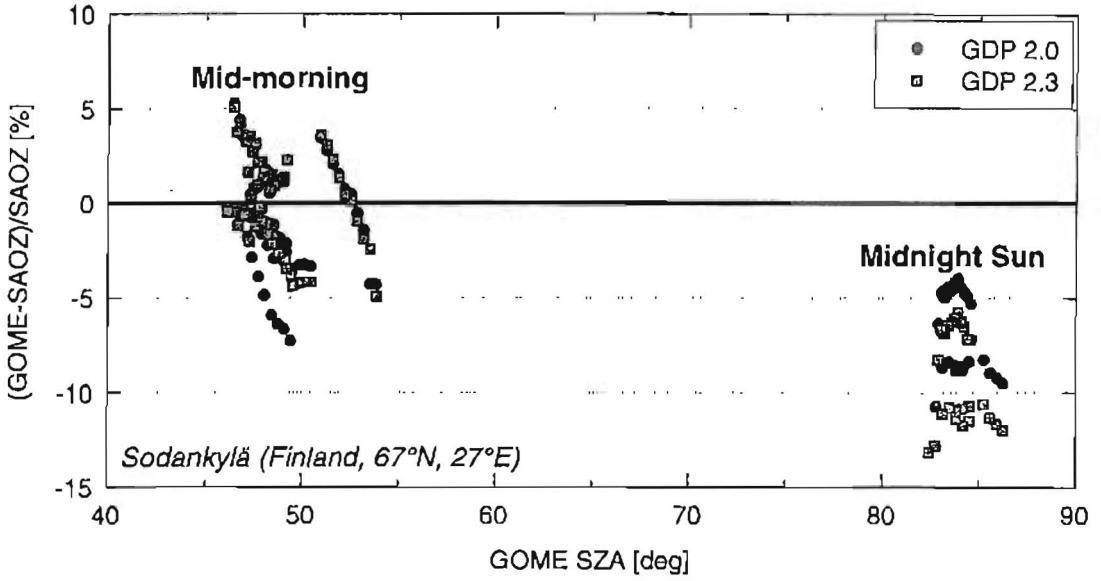

Figure 4-12 Summer SZA dependence of the relative difference between the GOME and SAOZ total ozone in the Arctic : comparison between mid-morning (moderate SZA) and midnight Sun (high SZA) data at Sodankylä on July 10 and 24, 1996.

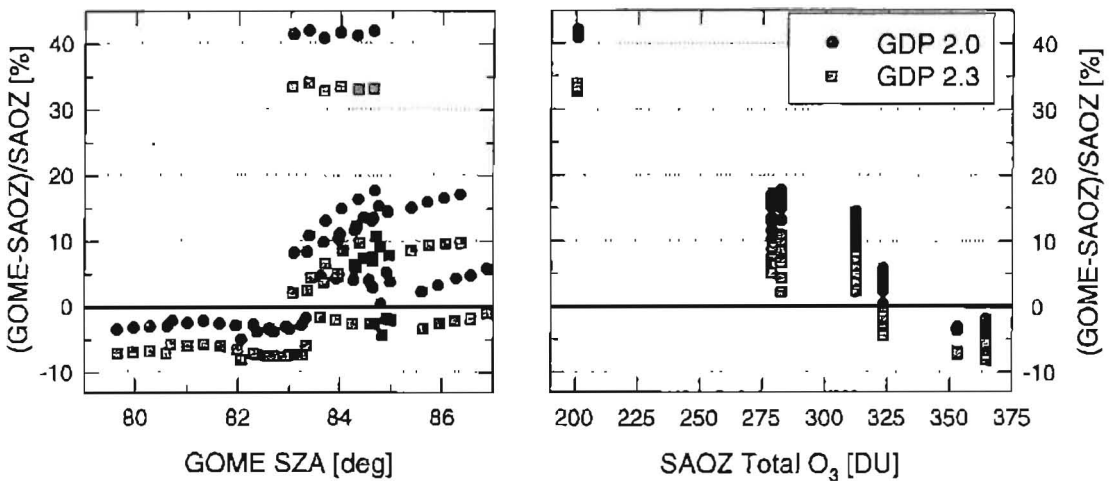

Figure 4-13 Winter column-resolved SZA dependence of the relative difference between the GOME and SAOZ total ozone in the Arctic: comparison at Sodankylä for 7 days in January and February 1997, as a function of GOME SZA (left panel) and of SAOZ total ozone (right panel).

4.3.2 Total nitrogen dioxide

The 370 orbits of the GDP 2.3 evaluation data set have been analysed with respect to ground-based observations and modelling results. A special care has been given to the 36 additional orbits representing special conditions. The data set of GOME total NO_2 is found to be 'cleaner' with GDP 2.3 than with GDP 2.0. The occurrence of anomalous values of total column beyond 10 x 10^{15} molec.cm^{-2} - and even beyond 100 x 10^{15} molec.cm^{-2} in extreme cases - is reduced by a large factor, and errors on the DOAS fit, given in the level-2 data files, look more reasonable. Due to the limited data set, it is difficult to estimate the relevance of the day-to-day variation, but the scatter between adjacent ground pixels is more reasonable according to the sensitivity of GOME to the troposphere. There are less unreasonable scenes with enhanced pollution. In general, the geophysical consistency of GOME total NO_2 retrieved with GDP 2.3 is improved. The seasonal and latitudinal variations of GOME total NO_2 are in much better agreement with ground-based observations. Figure 4-14 shows that GDP 2.3 data generally are less scattered. The inconsistent sharp increase of total NO_2 beyond 40°N towards the pole is reduced down to a more realistic slope, however anomalous behaviour under midnight Sun conditions persists. Figure 4-15 illustrates the better geophysical consistency obtained with GDP 2.3, especially in the Tropics and the southern hemisphere. At northern middle latitudes, both total NO_2 and its scatter along track are more consistent. The general improvement is attributed mainly to the use of the NO_2 vertical distribution from US Standard climatology, which was recommended by the team as a first step towards a geophysically consistent NO_2 product. E.g., the reduction of the NO_2 column observed at northern latitudes in Figure 4-14 between GDP 2.0 and 2.3 is related to the relevant reduction in tropospheric content of the US Standard climatology compared to that of the MPI profiles used in GDP 2.0. Although the benefit of GDP 2.3 compared to GDP 2.0 is clear, it must be kept in mind that: (a) the use of the US Standard climatology generates probably significant seasonal and latitudinal biases in the GDP 2.3 total NO_2 data set; (b) several major source of uncertainties remain; and (c) significant improvements of the GDP are still required.

4.3.3 Preliminary conclusions on GDP 2.3

While there is no major difference between GDP 2.0 and GDP 2.3 for total ozone retrieval, the improvement of the geophysical consistency of total NO_2 and the implementation of the polar viewing mode processing in GDP 2.3 vindicate its use for operational processing. However, it must be kept in mind that significant improvements are still needed for both total ozone and NO_2 data. For the total ozone retrieval, the same problems as detected with GDP 2.0 remain. Possible solutions are already well identified. The use in GDP of the so-called 'modified DOAS' approach, as well as a column-resolved climatology based on real ozone profile measurements like that used in the TOMS algorithm, could reduce both the seasonal SZA dependence of the GOME and its difference of sensitivity. For the total NO_2 retrieval, it is recommended to revisit the NO_2 profile data base used in the AMF calculation. The sensitivity of GOME retrieval to the NO_2 profile shape errors should be studied in detail, for both the troposphere and the stratosphere.

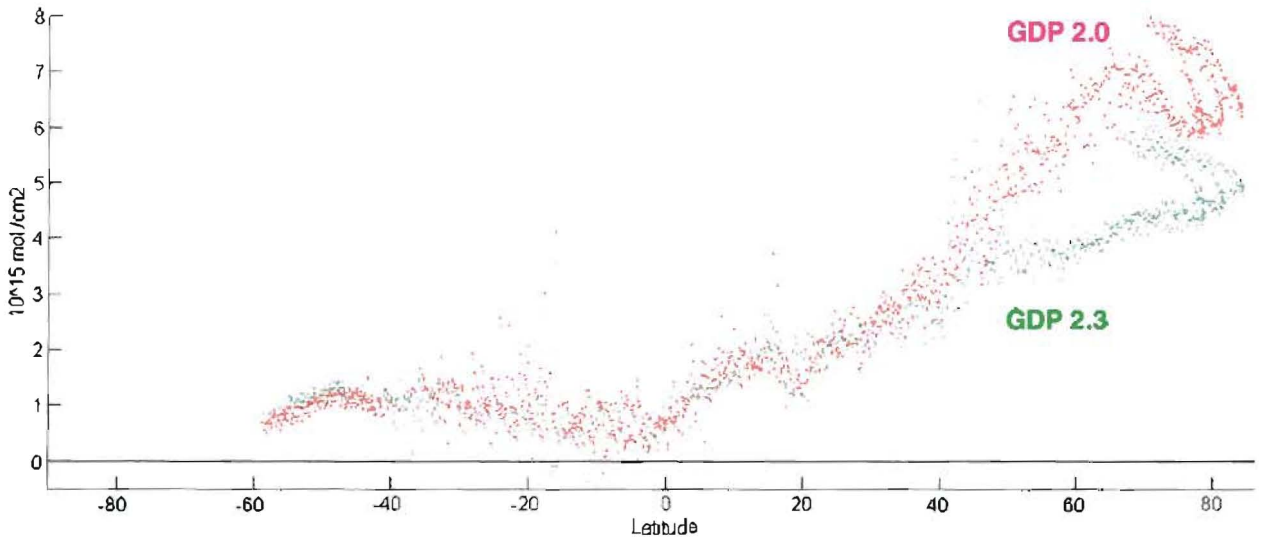

Figure 4-14 Comparison of GOME total NO_2 retrieved with GDP 2.0 (in red) and GDP 2.3 (in green) for an individual orbit on 16 July 1996 (60716100.lv2). The inconsistent, sharp increase of total NO_2 beyond 40°N towards the pole is reduced down to a more realistic slope. However, the anomalous behaviour observed under midnight sun conditions persists.

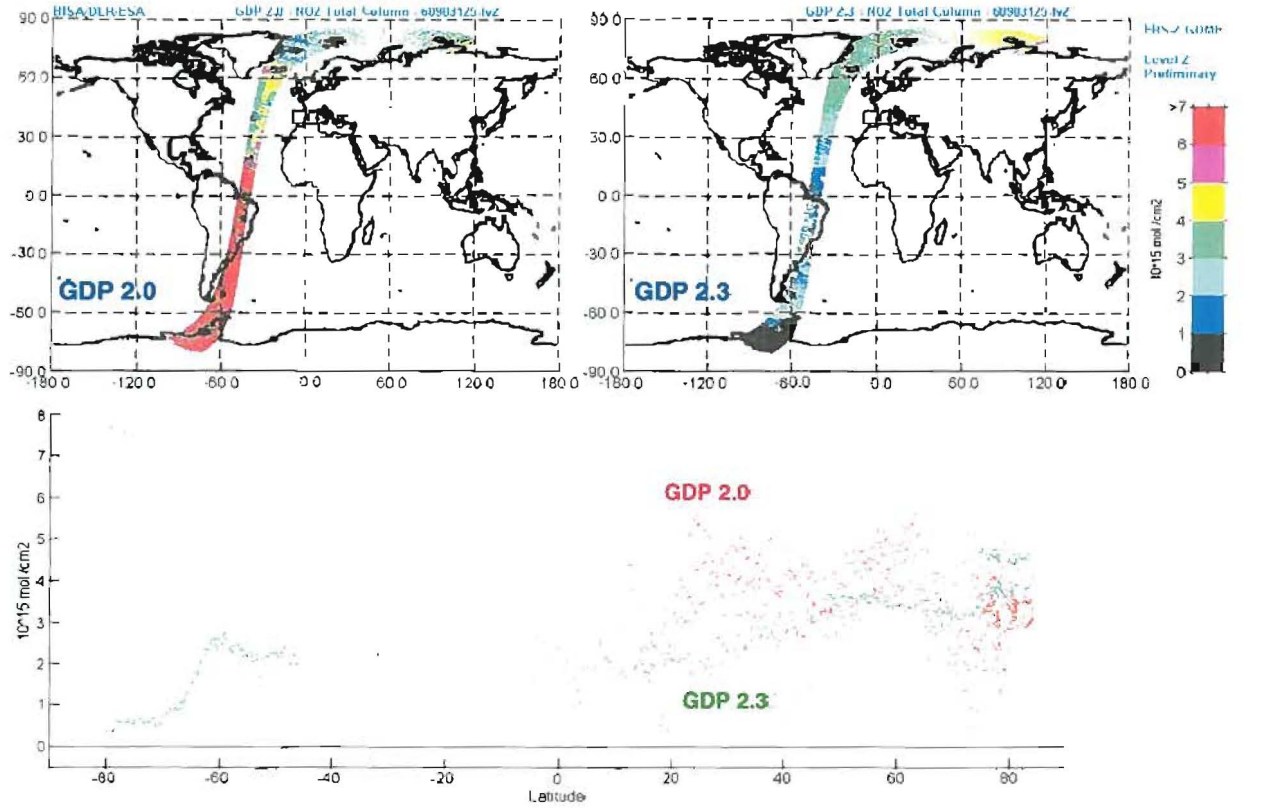

Figure 4-15 Comparison of GOME total NO_2 retrieved with GDP 2.0 (in red) and GDP 2.3 (in green), for an individual orbit on 3 September 1996 (60903125.lv2). The figure illustrates the better geophysical consistency obtained with GDP 2.3. In the Tropics and the southern hemisphere, aberrant total NO_2 values of $10\text{-}100.10^{15}$ molec.cm^{-2} obtained previously with GDP 2.0, appear now only in a few cases and are associated with extremely large errors in the GOME spectral analysis. In the northern hemisphere, both the NO_2 vertical column and its scatter along track are more realistic.

4.4 First analysis of preliminary NRT ozone profiles

From a joint effort of IFE/IUP, DFD/DLR and ESA, a set of preliminary GOME ozone vertical distributions were available in 'near-real time' (NRT) from 24 January to 31 March 1997, in support to the 1997 Arctic winter campaign [Eichmann *et al.*, 1997]. Ozone concentration was derived from GOME spectra with the Full Retrieval Method (FURM) developed at IFE/IUP, and integrated within predefined atmospheric layers (0-10, 10-20, 20-27, 27-33, 33-40, 40-48 and 48-60 km). To investigate the relevance of these NRT profiles, a quick comparison was carried out with correlative ozone density profiles measured by ozonesondes launched from the stations listed in Table 1 [Lambert *et al.*, 1997b]. Recent improvements in the FURM at IFE/IUP, not available at the time of this study, might modify the conclusion, and will be tested in the frame of the aforementioned ERS.AO3.377 project (Weber *et al.*).

Preliminary NRT GOME ozone profiles consist of ozone concentrations integrated within seven broad layers from ground to 60 km, reflecting the limited vertical resolution of the ozone profile retrieval from nadir measurements. When a coincidence of at least 3° latitude and 8° longitude occurs between the GOME ground pixel centre and the ground-based launch site, correlative profiles are integrated through the four lowest NRT GOME layers (0-10, 10-20, 20-27, and 27-33 km) and then compared to satellite data. Figure 4-16 illustrates the comparison at Aberystwyth on February 4 for three successive ground pixels along track. It must be noted that the GOME information delivered in NRT was limited to a sparse data set of clear-sky GOME pixels, resulting in a poor spatial coverage. Therefore, only a few coincidences were found, and conclusions summarised here should be considered as preliminary and subject to change.

The average agreement between NRT GOME and ozone soundings in the stratospheric layer from 20 to 27 km is reasonable, between 10% and 15% ([GOME-sonde]/sonde), although scattered. Larger deviations up to 30-40 % and more can occur in the tropospheric and lowest stratospheric layers, where comparison results are also more scattered. Systematic offsets are observed in the troposphere (-15% in February and from +30% to +55% in March) and at 27-33 km (+23%). Above 33 km, uncertainties on ozonesonde data deteriorate the reliability of the comparison.

The observed discrepancies can be partly explained by the large variability of ozone between the GOME and the ozonesonde measurement time, as well as sharp horizontal and vertical ozone gradients within the field of view of GOME. The influence of natural variability appears clearly in the comparison at Aberystwyth on 4 February 1997 (e.g., Figure 4-16) where four adjacent coincidences are found. Depending on the ground pixel, the agreement varies on this day from +12% to -4% in the 10-20 km layer and from -9% to +4% at 20-27 km. These results are consistent with those obtained when studying ozonesonde profiles measured at the same site within a few hours. Indeed, at several occasions in winter-spring 1994 to 1997, two or three ozonesondes were launched at Aberystwyth the same day within a few hours. For each set of these ozone soundings, the difference between the two or three ozone density profiles integrated in the lowest NRT GOME layer ranges from 0.05 to 0.3 10^{12} molecules cm^{-3} (that is 5% on average, with an extreme case of 25%).

The systematic biases observed in the tropospheric layer arise likely from inaccuracies in the climatological profiles used as a priori in the NRT algorithm, combined with the poor sensitivity of the NRT retrieval algorithm to the actual ozone vertical distribution. This is supported by the fact that the retrieved tropospheric content is always close to the tropospheric content of the *a priori* profile. The same reason might also explain the striking degradation of the agreement in the troposphere between February (when the *a priori* was close to the actual ozone profiles), and March (when the *a priori* overestimated significantly the ozonesonde measurements). The general agreement between the NRT GOME and the various ozone soundings is also found to be constrained by the shape of the actual ozone vertical distribution inside the GOME layer. For layers between 10 and 27 km, largest deviations are usually observed in presence of sharp laminae. To a less extent, the agreement in the 0-10 km layer is better when tropopause and its related increase of ozone density are located outside or not too deeply inside the layer.

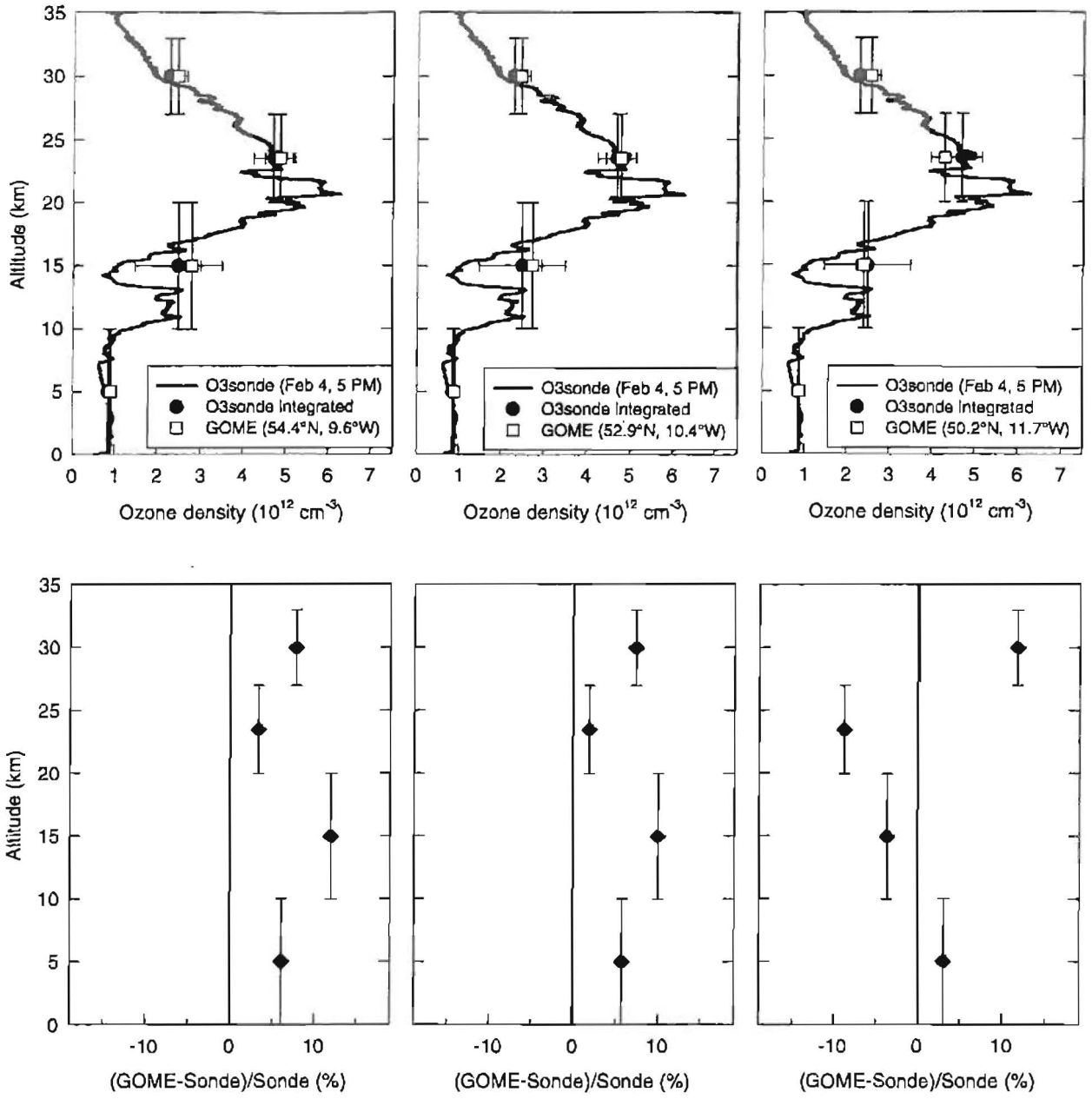

Figure 4-16 Comparison of the ozone vertical distribution at Aberystwyth (52.4°N, 4.1°W) measured by an ECC ozonesonde and retrieved from GOME measurements on 4 February 1997. Horizontal error bars give the standard deviation of ozone density within the GOME layer. Ozone density profile and related difference are depicted for three adjacent GOME ground pixels along track, illustrating the influence of the difference in air mass.

The impact of the tropopause altitude and of sharp ozone laminae on the agreement suggests that the use of too broad, predefined atmospheric layers, fitted to the vertical resolution of the profile retrieval, might lack of accuracy. This is particularly true for the retrieved tropospheric layer (0-10 km) which contains limited information from the lower troposphere (due to the strong attenuation of solar radiation through the stratospheric ozone bulk and the dense lowermost layers) and partial information from higher altitudes (due to the large averaging kernels of the profile retrieval method). In addition, such broad layers are not suitable for scientific studies which require conversion to other height co-ordinates, such as isentropic or isobaric levels. Since the FURM algorithm retrieves ozone at a much higher vertical resolution, it is recommended to produce GOME ozone profiles at higher altitude resolution, e.g., every kilometre.

5. Recommendations

Correlative studies carried out in the framework of the B103 and F114 projects have demonstrated the geophysical consistency of the GOME total ozone and NO_2, under standard atmospheric conditions, but also the persistence of major problems in the successive versions of the GDP for a variety of relevant geophysical conditions. Possible causes have been identified, and solutions have been proposed. The conclusions reported here for the level-1b-to-2 data processing of ERS-2 GOME apply directly to improved versions of the experiment programmed after 2001 (e.g., GOME-2 for METOP) and to the SCIAMACHY nadir observations, and thereby to the scientific interpretation of interleaved nadir/limb measurements from SCIAMACHY. Therefore, it is vigorously recommended to carry on with the needed maturation of the GOME level-1b-to-2 retrieval algorithms.

For total ozone, refinements of both the slant column DOAS retrieval and the AMF calculation are required. As demonstrated by IFE/IUP [communication to the GOME Tiger Team, June 1996] and confirmed by Van Roozendael [1997], the implementation of the so-called 'modified DOAS' approach should reduce the SZA dependence at large SZA. An iterative retrieval algorithm, using a column-resolved climatology based on real ozone profile measurements like that used in the TOMS V7 algorithm, would reduce both the seasonal SZA dependence of the GOME total ozone and its difference of sensitivity. But before using a column-resolved climatology similar to that used by the TOMS, it is recommended to investigate more deeply the sensitivity of the GOME retrieval to the ozone profile shape errors as well as the pseudo-interhemispheric difference between TOMS and ground-based data.

The geophysical consistency of the GOME total nitrogen dioxide was recently improved after implementation of the US Standard NO_2 climatology in the AMF calculation (GDP 2.3). Despite this recent improvement, it is still recommended to revisit the NO_2 profile data base used in the GDP. The sensitivity of the GOME measurement to the tropospheric NO_2 should be investigated with care. Test case studies with a 3D model suggest that a 2D climatology might be inadequate for nadir observations, partly due to the sharp gradients of the tropospheric NO_2 field.

A limitation of the GOME data accuracy is inherent in the large span of its ground pixels. This significant spatial extension combines with atmospheric inhomogeneities in the field of view of the instrument, to increase the uncertainty in the retrieval of critical parameters such as the AMF or cloud information. The derivation of sub-pixel information (via the PMDs) is therefore recommended.

Preliminary NRT GOME ozone profiles consist of ozone concentrations integrated within only seven broad layers from ground to 60 km, reflecting the limited vertical resolution of the ozone profile retrieval from nadir measurements. The correlative study reported here calls for further improvement of the retrieval of tropospheric abundances, and it reveals a significant influence of the tropopause altitude and of sharp ozone laminae, suggesting that the use of wide, predefined atmospheric layers would lack of accuracy. In addition, broad layers are not suitable for conversion to other height co-ordinates required by several scientific studies, such as isentropic or isobaric levels. Ozone concentrations at intermediate altitude levels (e.g., every kilometre) should be preferred, although it must be kept in mind that the actual vertical resolution of the GOME measurement is limited physically to 5-8 km.

The organisation of regular GOME/SCIAMACHY scientific workshops has proved to nourish motivation and to support valuable communication among the various groups interested in GOME. For the sake of efficiency, the team also encourages, if needed in the future, the constitution of dedicated 'Tiger Teams', working on specific problems with a limited, representative data set.

From an operational point of view, a critical limiting step of the GDP maturation consists of the inappropriate computing resources available for data processing. As experienced with many spaceborne instruments, and confirmed now with GOME, the development of advanced processing algorithms is an iterative process which requires several re-processing and subsequent validation during the instrument lifetime and even after (e.g., the TOMS series with 7 versions, or the UARS HALOE with 18 versions). A rational expansion of the operational computing power is highly recommended, not only for ERS-2 GOME, but also for any future atmospheric chemistry instrument.

6. List of contributors and acknowledgements

For providing high quality data in near real time and for fruitful scientific discussions, the authors of the report address all their acknowledgements to the contributing PIs and instrument operators of the NDSC and the SAOZ/UV-visible network, to Georg Hansen (NILU) and Rob Koopman (RIVM, ESA/ESRIN, now at ESA/ESTEC), and to J.F. Gleason from the TOMS/BUV team at NASA/GSFC. They greatly appreciate the invaluable, computational and logistic support provided by Pierre Gerard and José Granville from IASB and Jack Hottier from CNRS. The achievement of both projects benefited from collaboration with ERS.AO2 proposals B105 (de Muer and Debruyn), CH101 (Staehelin and Gamma), F109 (Brogniez et al.), and N102 (Hansen et al.).

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