ERS-2 GOME Data Products Delta Characterisation Report 1999

Validation Report for GOME Data Processor Upgrade: Level-0-to-1 Version 2.0 and Level-1-to-2 Version 2.7

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Acronyms and Abbreviations

AMF	Air Mass Factor
BSDF	Bi-directional Scattering Distribution Function
COSE	Compilation of Atmospheric Observations in Support of Satellite Measurements over Europe
DFD/DLR	German Remote Sensing Data Centre/German Aerospace Centre
DISORT	DIScrete Ordinate Radiative Transfer model
DOAS	Differential Optical Absorption Spectroscopy
D-PAF	German Processing and Archiving Facility
ERS-2	European Remote Sensing Satellite-2
ESA/ESRIN	European Space Agency/European Space Research Institute
GDP	GOME Data Processor
GOME	Global Ozone Monitoring Experiment
HALOE	HALogen Occultation Experiment
IASB	Belgian Institute for Space Aeronomy
ICFA	Initial Cloud Fitting Algorithm
IFE	Institute of Remote Sensing (University of Bremen)
IUP	Institute of Environmental Physics (University of Heidelberg)
MPI	Max Planck Institute (University of Mainz)
NADIR	NILU's Atmospheric Database for Interactive Retrieval
NDSC	Network for the Detection of Stratospheric Change
NILU	Norwegian Institute for Air Research
NO_2	Nitrogen Dioxide
O_3	Ozone
PMD	Polarisation Monitoring Device
SAO	Smithsonian Astrophysical Observatory
SOLSTICE	Solar Stellar Irradiance Comparison Experiment
SPSU	Saint Petersburg State University
SZA	Solar Zenith Angle
TOA	Top Of Atmosphere
TOMS	Total Ozone Mapping Spectrometer
UARS	Upper Atmosphere Research Satellite

1. INTRODUCTION

1.1 GOME OPERATION AND OFF-LINE DATA PROCESSOR

Operating aboard the ESA ERS-2 polar platform launched in April 1995, the Global Ozone Monitoring Experiment (GOME) [1-3] is the successful predecessor of a series of new generation sensors aiming at the needed global measurement of key ozone-related species to assess current and future changes of the atmosphere. Providing the global picture of atmospheric ozone, GOME is also the first and currently the only spaceborne instrument having the capability to measure the vertical column amount of nitrogen dioxide (NO_2), a trace species playing a crucial role in the ozone photochemistry. Since August 1996, GOME total ozone and NO_2 data are routinely retrieved at the German Processing and Archiving Facility (D-PAF) on behalf of ESA with the off-line GOME Data Processor (GDP) [4-6].

The accurate derivation of total ozone and NO_2 from GOME data presents several difficulties and is still a matter of research. Since the release in summer 1995 of its first developmental version, GDP was upgraded on many occasions and the quality of both ozone and NO_2 products has improved significantly (e.g., [7]). Nevertheless, many studies have highlighted the need to revisit several aspects of the GDP retrieval algorithms. In spring 1999, DFD/DLR upgraded the level-0-to-1b (to version 2.0) and level-1b-to-2 (to version 2.7) segments of GDP, focusing on the processing throughput and the derivation of NO_2 slant column amount [8,9].

1.2 GOME DATA PROCESSOR DELTA VALIDATION CAMPAIGN 1999

The maturation of retrieval algorithms for atmospheric remote sensing is an iterative process, which benefits from validation exercises involving the scientific community having expertise in the algorithm development and the measurement of trace constituents from other relevant instrumentation. It requires detailed quality evaluation of both retrieval algorithms and data products, identification of possible source of uncertainty and solutions, and verification of expected improvements after each significant modification. In particular, before proceeding to the implementation of any major GDP changes in the operational processing chain, it is essential to verify the accuracy and effectiveness of the modification and to assess the quality of the new data product. Such 'delta' validation campaigns have been executed by a sub-group of the GOME Validation Group, with a limited but representative validation data set.

Supported by ESA/ESRIN through the contract No. 13554/99/I-DC, the Delta Validation Campaign 1999 was organised to provide an independent characterisation of the recent upgrades of the GDP level-0-to-1 and level-1-to-2 segments [8,9]. Main emphasis was given to the global quality assessment of new NO_2 column amounts, but other major GDP changes were investigated as well.

The main outcome of the campaign consists of:

- the characterisation of spectral solar irradiance level-1 data based on comparisons with UARS SOLSTICE measurements in the 240-400 nm spectral range, on auto-correlation studies of GOME data, and on comparisons with high-resolution solar spectrum atlas data;
- the characterisation of spectral earthshine radiance and polarisation level-1 data;
- the evaluation of changes in the ICFA determination of the cloud fraction;
- the characterisation of total nitrogen dioxide level-2 data by comparison with measurements from the ground-based Network for the Detection of Stratospheric Change and the spaceborne UARS HALOE, and by comparison of GDP retrievals with retrievals from independent DOAS algorithms;
- the characterisation of total ozone level-2 data by comparison with ground-based measurements from the Network for the Detection of Stratospheric Change and the Russian Ozone Monitoring Network;
- the update of the existing documentation on GDP data products quality.

The campaign involved the following institutes:

- ESRIN	European Space Research Institute, ESA, Frascati, Italy (coordinator)
- IASB	Belgian Institute for Space Aeronomy, Brussels, Belgium (coordinator)
- DFD	German Remote Sensing Data Centre, DLR, Oberpfaffenhofen, Germany
- IFE	Institute of Remote Sensing, University of Bremen, Germany
- IUP	Institute of Environmental Physics, University of Heidelberg, Germany
- KNMI	Royal Meteorological Institute of The Netherlands, De Bilt, The Netherlands
- SPSU	Department of Atmospheric Physics, Saint Petersburg State University, Russia

The composition of the team was defined according to the following objectives:

- to insure the availability of correlative data sets suitable for pseudo-global investigation;
- to insure the availability of independent level-1-to-2 retrieval algorithms;
- to get independent studies and data quality assessments;
- to combine complementary expertise.

The present document outlines the main outcome of the Delta Validation Campaign 1999. Results were discussed during dedicated meetings in May and July 1999 at ESRIN. Relevant GDP modifications are listed in Chapter 2. A more detailed description of the GDP upgrades is given in [9]. The issue of reference data sets for delta validation studies is addressed in Chapter 3, including a description of the data sets actually used during the present campaign. Individual contributions are reported in Chapters 4 to 6. Irradiance and radiance validation studies are reported in Chapters 4 and 5, respectively. Results of level-2 data studies are presented in Chapter 6, starting with investigations based on comparisons with ground-based network data and carrying on with comparisons with independent NO_2 retrievals. Updated documentation is provided in the Annexes.

1.3 REFERENCES

[1] GOME Interim Science Report, ESA SP-1151, 59 pp. (1993).

[2] GOME Users Manual, ESA SP-1182, 200 pp. (1995).

[3] Burrows, J.P., M. Weber, M. Buchwitz, V. Rozanov, V. Ladstätter-Weißenmayer, A. Richter, A. De Beek, R. Hoogen, K. Bramstedt, K.U. Eichmann, and M. Eisinger, The Global Ozone Monitoring Experiment (GOME): Mission concept and first Scientific Results, *J. Atmos. Sci.*, **56**, pp. 151-175 (1999).

[4] GOME Level 0 to 1 Algorithms Description (ER-TN-DLR-GO-0022, issue 4A, 9.8.1996).

[5] GOME Level 1 to 2 Algorithms Description (ER-TN-DLR-GO-0025, issue 2A, 9.8.1996).

[6] Product Specification Document of the GOME Data Processor (ER-PS-DLR-GO-0016, issue 3B, 29.7.1996).

[7] GOME Data Improvement Validation Report, B. Greco (Ed.), ESA/ESRIN APP/AEF/17/GB, 58 pp. (1998).

[8] Loyola, D., S. Slijkhuis, and W. Thomas, New GDP settings for the spectral fitting of NO_2, Report to the GOME Science Advisory Group (March 1999).

[9] Update Report for GDP 0-to-1 Version 2.0 and GDP 1-to-2 Version 2.7, ER-TN-DLR-GO-0043 (issue 1, 30.07.1999).

[10] GOME Geophysical Validation Campaign: Final Results Workshop Proceedings, ESA-ESRIN, Frascati 1996, ESA WPP-108, 268 pp. (1996).

2. SUMMARY OF THE GOME DATA PROCESSOR CHANGES

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The GDP level 0-to-1 system has been changed in two ways: There are processor changes (changes with impact on the binary level 1 product) and new options in the extractor software. The changes in the GDP level 1-to-2 system are changes in the algorithms and enhancements. The following listing gives an overview about the implemented updates and new algorithms.

2.1 GDP LEVEL 0-TO-1 PROCESSOR VERSION 2.0

- Updates based on Key data:
  - Modification of the BSDF asymmetric constant parameter.
  - Usage of degradation correction for the fractional polarisation of PMD detector #1.
- Wavelength calibration:
  - Change of the order of the polynomial function for measurement channel #1 and #2 in the current version of wavelength calibration to optimise parameterisation.
  - Introduction of a calibration algorithm based on cross-correlation and spectral lamp calibration to improve the wavelength calibration.
- System engineering changes in order to extent the capability of the software:
  - Update of commercial database software for calibration parameters.
  - Re-organisation of extractor software (performance improvement: 10%).

2.2 GDP LEVEL 0-TO-1 EXTRACTOR VERSION 2.0

- New option for degradation correction of the detector channels.
- New option for BSDF correction of seasonal effects.
- Correction of the Albedo option.

2.3 GDP LEVEL 1-TO-2 PROCESSOR VERSION 2.7

- Re-hosting of the GDP from SUN/SOLARIS on LINUX operating system for higher performance in reprocessing.
- Update of databases for NO_2 cross-sections (most recent revision of the flight model measurements - FM - provided by IFE Bremen).
- Inclusion of theoretical Ring spectrum for NO_2 fitting provided by SAO (K. Chance).
- Inclusion of undersampling correction spectra for NO_2.

- Implementation of tessellation algorithm to calculate area-weighted albedo and ground height, provided by SAO (R. Spurr).
- Simple check module for a valid wavelength calibration in the DOAS module chain.
- Improvement of Air Mass Factor calculation:
    - Revision of the software during porting step to the LINUX operating system.
    - Change of top of atmosphere from 60 to 70 km (affects also the TOA view angles).
    - Change of value for snow albedo (75% to 95%).
    - Change of reference albedo grid and height grid for the computation of the AMF look-up tables.
    - Change of reference days for the computation of the AMF look-up tables (15.10 to 15.07, 15.04 to 15.01).
- Changes in DOAS Module:
    - Inclusion of the fitting of H_2O in the NO_2 fitting.
    - Usage of error-weighted fitting.
    - Removal of redundant calculations.

3. REFERENCE DATA SETS

An important issue of any delta validation exercise is to provide reliable assessment covering a variety of relevant observation conditions, but with a limited data set in order to limit the effort and allow the fast release of the new version. Therefore, the determination of an optimal set of reference orbits and correlative data is a critical task.

3.1 GOME REFERENCE ORBITS

According to the scientific priorities relevant to GDP improvements in 1997, a list of about 330 GOME orbits was selected for the delta validation campaign of 1998, including every 15th orbit acquired in 1996 (see Loyola *et al.*, pp. 12-13, in ESA, 1998). A major objective of the campaign was to perform a quick verification at all latitudes of the improvement of GDP 2.0-to-2.3 total O_3 and NO_2 data, focusing on the consistency of GDP total NO_2 at northern middle latitudes. The following additional list of 36 orbits was selected to address more specific issues such as the seasonal variation of the solar zenith angle dependence of GOME total ozone in both the Arctic and the Antarctic or its column dependence:

Antarctic summertime		**Arctic summertime**	
Mid-morning	Midnight Sun	Mid-morning	Midnight Sun
61227225	61227143	60710096	60710200
70117000	70117134	60724092	60724192
70117215			
Antarctic springtime		**Arctic springtime**	
Inside vortex	Outside vortex	Inside vortex	Outside vortex
60831225	60917222	70115093	70118093
60902000	60917236	70122091	70207105
60902215	61008230	70119090	70207090
61026001		70122091	
61026216			
Southern Tropics		**Southern mid-latitudes**	
70322132	70427123	60709035	61109043
70429131	60903125	60718040	61226046
Alpine 3-month shift			
61227111	70104116		
61226115	70105112		

Table 1. Special orbits selected in 1998 for specific delta validation studies.

The scientific issues relevant to the improvement of GDP 2.0 and GDP 2.4 differ somewhat. For the present campaign focusing on improvements of the NO_2 spectral fitting, the following additional set of 79 orbits was selected to investigate more accurately NO_2 improvements at low latitudes:

70118130	70405223	70508215	70718126	70921222	71019225
70121130	70408224	70509126	70720216	70923130	71026223
70124131	70412203	70511216	70721131	70924223	71029223
70127131	70414124	70512131	70723220	70926130	71101224
70201204	70415204	70514221	70817222	70927223	71104224
70204204	70417126	70517203	70820222	70929132	71108204
70207205	70418204	70520203	70823223	70930224	71110125
70210205	70420126	70523204	70826224	71008215	71111204
70224215	70421205	70526204	70830203	71010223	71113131
70227216	70423130	70712124	70902204	71011216	71114205
70302220	70503125	70714214	70905204	71013223	71116130
70305221	70505215	70715126	70908205	71014220	71117206
70330222	70506126	70717215	70920125	71016224	71119132
70402223					

Table 2. Special orbits selected in 1999 (this work) for specific NO_2 delta validation studies at low latitudes.

The GOME orbit data set actually processed for the present campaign is a matter of concern. Due to changes in GDP level-0-to-1 in 1997, level-1-to-2 processing of GDP level-1 data during this period requires manual handling of individual GOME orbits. Manual handling requires important resources currently not available at DFD/DLR. To ensure fast achievement of intended activities, the data set was limited to the 1996 part of the 1998 campaign data set plus the 79 NO_2 orbits in 1997 selected for the present work. This decision impacts on the accuracy of the investigation and sometimes on the feasibility of particular studies. Indeed, ground-based instruments at several important locations operate only since 1997 or the end of 1996, and important correlative data (e.g., O_3 and NO_2 profiles measured from stratospheric balloons) are available only in 1997. The number of coincidences of the GOME orbits set with measurements at Russian stations is also too sparse.

The current data sets (GOME delta validation orbits + available ground-based data) available for the present campaign are suitable for the preliminary assessment reported hereafter. It might also allow a preliminary verification of future GDP improvements related to several relevant issues. However the current set of orbits is not completely satisfactory to address all current priorities with sufficient accuracy. It is vigorously recommended to include all orbits of 1997 of the delta validation campaign 1998 and to increase the number of coincidences with Russian measurements. It must also be kept in mind that the validation data set has to be defined according to the scientific needs, which are supposed to change with the version of GDP and with the molecule/product concerned by the GDP change.

3.2 CORRELATIVE DATA

The present campaign relies on high-quality ground-based measurements from the Network for the Detection of Stratospheric Change (NDSC) and the Russian ozone monitoring network. In the framework of several ERS AO projects coordinated by members of the team, preliminary ground-based total O_3 and NO_2 data have been stored in the NILU/NADIR database for the purpose of GOME validation. They often consist of individual values or daily means (Brewer, Dobson, and FTIR) or sunrise and sunset means (zenith-sky UV-visible spectrometers) retrieved in near real-time with standard spectral analysis and calibration, aiming at a quick evaluation and dissemination of preliminary data. High accuracy data are submitted later (typically within 2 years) to international databases (e.g., NDSC) with public access after reprocessing with a state-of-the-art calibration/analysis and proper validation.

Ground-based data sets to be used in a validation study depend on the nature of the study and on the GOME data set, which depend themselves on the scientific needs. As demonstrated on many occasions, the interpretation of comparison results is not straightforward and should be conducted by data providers/experts well aware of the information contained in the ground-based data, of its limitations, and of the history of the data sets.

It must be kept in mind that, although available for validation purposes through AO projects and international databases, ground-based data remain the property of the instrument PIs. The dissemination, use and publication of those data are regulated by protocols.

4. SOLAR IRRADIANCE

RESULTS FROM IASB

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VALIDATION OF GOME LEVEL-1 SOLAR IRRADIANCE

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Abstract: This short report summarises preliminary validation results of the GOME level-1 solar irradiance derived with GDP 2.0.

1. Data sets

The level-1 data has been provided by DFD-DLR on the CD-ROM `GDP_VAL_4_99_LVL1`. The CD-ROM contained 41 level-1 orbits from the 1st of January 1996 through the 19th November 1997. Two GDP_01 extraction programs were used. The latest officially released GDP_01 is labelled V 1.50 01/23/98 (from the file `version.h`). Data processed with this extraction program will be called "original" in the sequel. The GDP_01 provided by DLR specifically for this validation through their FTP server and labeled "2.00 02/26/99". This new extraction program allow for a degradation correction to be applied to the solar irradiance (option `-e parameter_file`). A parameter file has been provided by Ernst Egels from DFD/DLR (polynomial fitting coefficients). The SOLSTICE reference solar measurements are the version 12 "spline" data set provided by LASP.

2. Wavelength calibration

We have quickly checked the wavelength calibration of the new GDP 2.0 with respect to the AFGL83 high resolution spectrum (i.e. only in channel 1) using the same cross-correlation technique used in GDP 2.0. 10 windows were used in channel 1. The standard deviation of wavelength shift with respect to AFGL83 in channel 1 drop from 0.0049 to 0.0026 nm which is lower (better) than DLR first calibration results.

3. Comparison with SOLSTICE

The next two pages represent the ratio of GOME (all version) with respected to the coincident SOLSTICE solar spectrum for both channel 1 (Figure 1) and 2 (Figure 2). The solid line depicts the “original” v1.5 GDP_01, the diamonds show the GDP 2.0 without degradation correction and the triangles shows the same GDP 2.0 spectra with wavelength/time dependent correction applied. All spectra are normalised to 1 AU and convolved to a 1-nm grid centred on half nanometer using a triangular kernel.

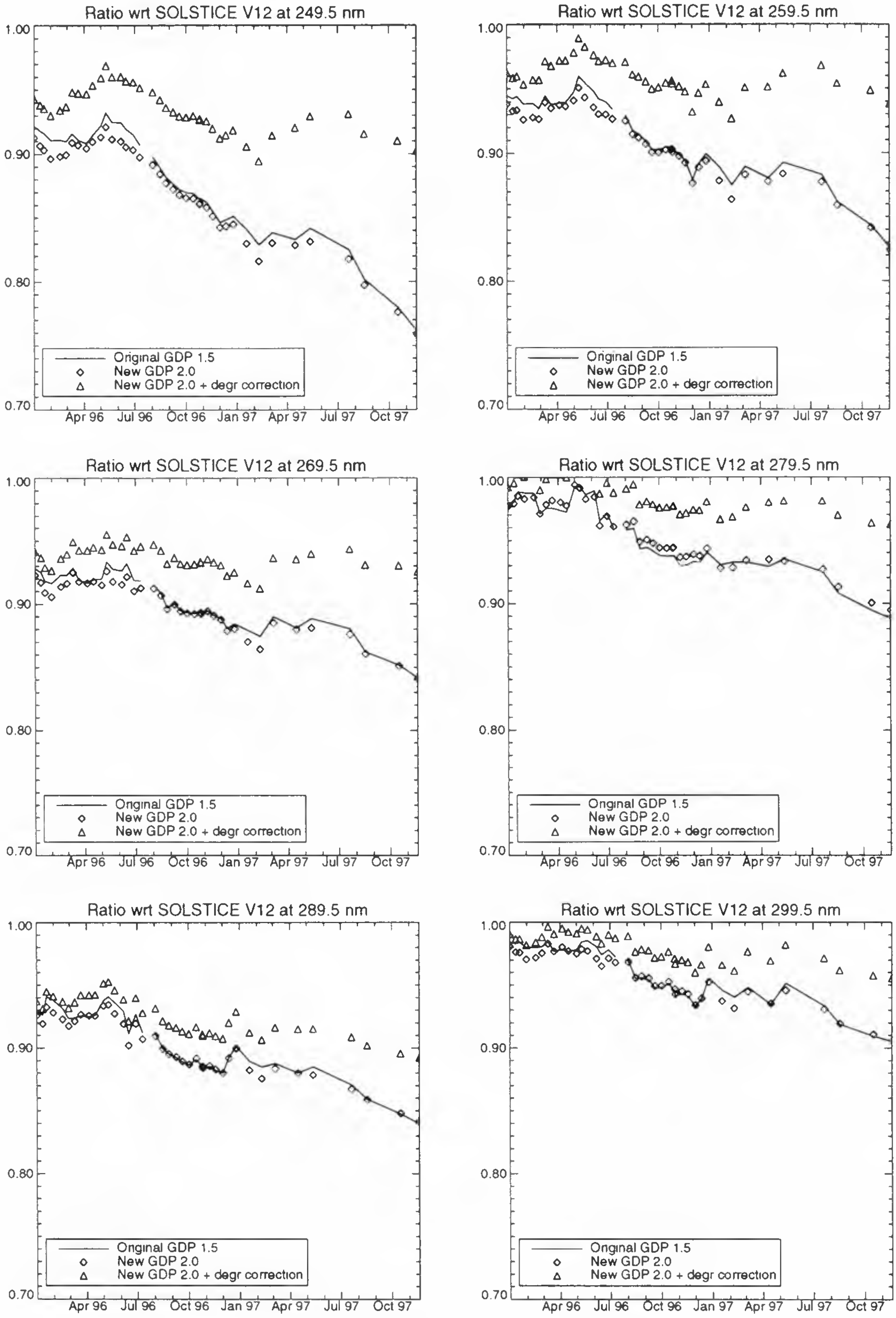


Figure 1. GOME/SOLSTICE ratio in GOME channel 1.

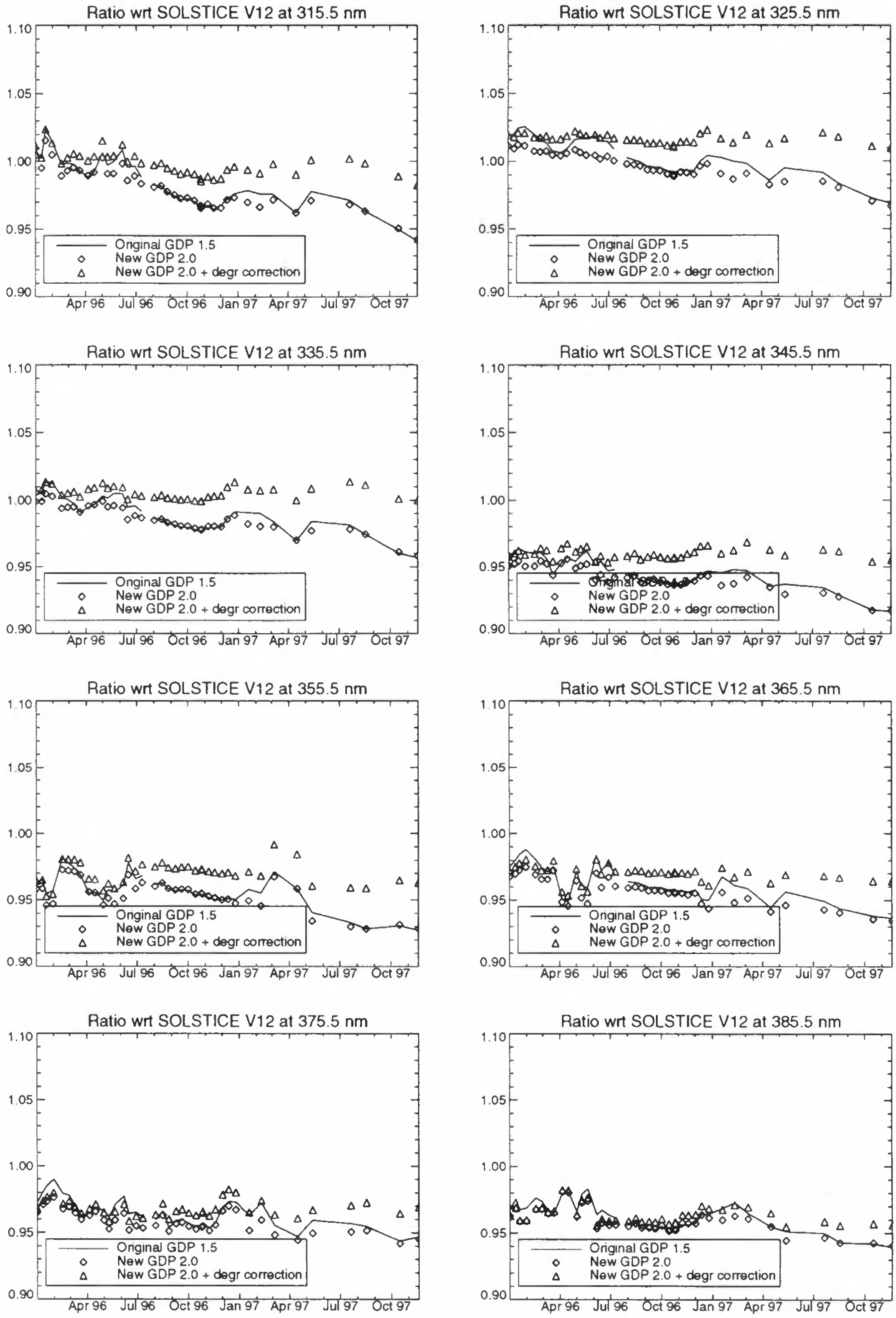


Figure 2. GOME/SOLSTICE ratio in GOME channel 2.

In term of temporal degradation, the new GDP 2.0 does not differ very much from the original (as expected). The degradation correction improved considerably the agreement with SOLSTICE by more than 10 % in channel 1 (as long as we consider SOLSTICE an accurate reference). However, GOME channel 1 irradiance is still much lower than SOLSTICE (from 10 to 5 %). In channel 2, the agreement is better but GOME accuracy is severely limited by the etalon features (modulation of +/- 2 %).

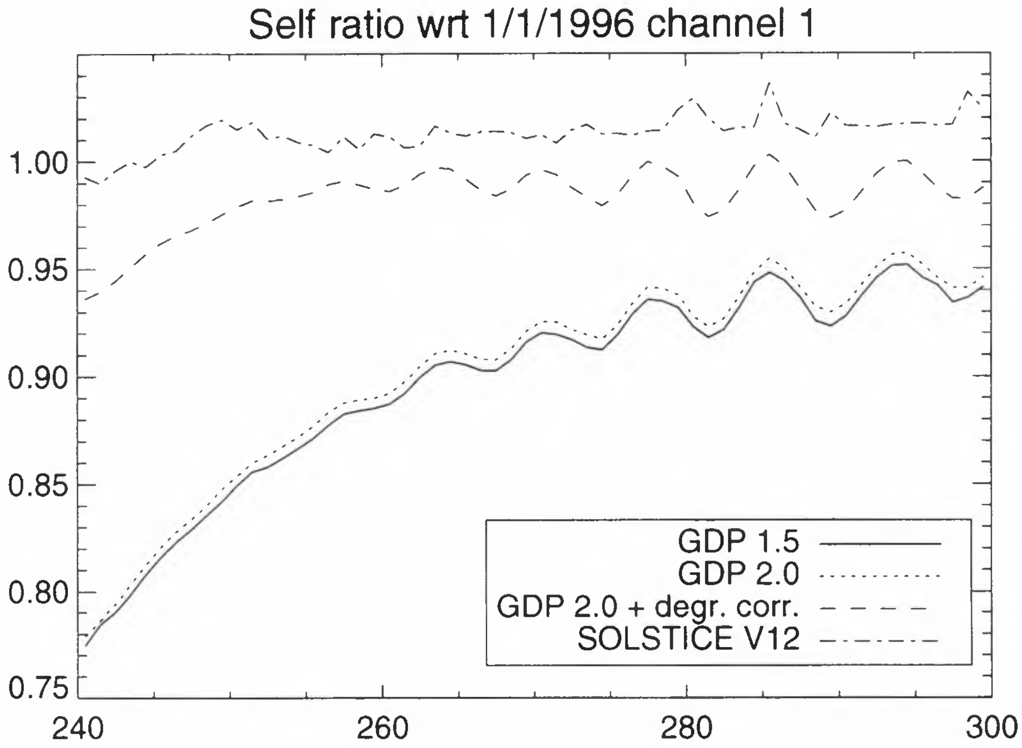
4. Cross-comparison

The ratio's of GOME irradiances has been compared with respect to a common reference date: 1st of January 1996 (Figure 3). The next two plots display the ratio for the original GDP 1.5, GDP 2.0--uncorrected and GDP 2.0--corrected for channels 1 and 2 for the spectrum acquired on 19th of November 1997 only. In addition SOLSTICE ratio is also plotted.

The degradation correction shows a substantial improvement in channel 1 (from -10% to -3% at 280 nm) but there remains a significant residual degradation left (both wavelength and time dependent). The situation is much better in channel 2.

Figure 4 gives the time variation of the GOME/GOME ratio at 250.5 nm.

For the record, Figure 5 depicts the cross comparison of the original GDP 1.5 spectra from mid 1995 to February 1999 in channel 1 only (reference spectrum: 3 July 1996). The wavelengths are indicated in the right margin. Notice the dramatic degradation acceleration in 1998 (in channel 1 only). Most of the spikes correspond to cooler switch on/off as shown in the next 2 plots for 295.5 and 240.5 nm (Figure 6).



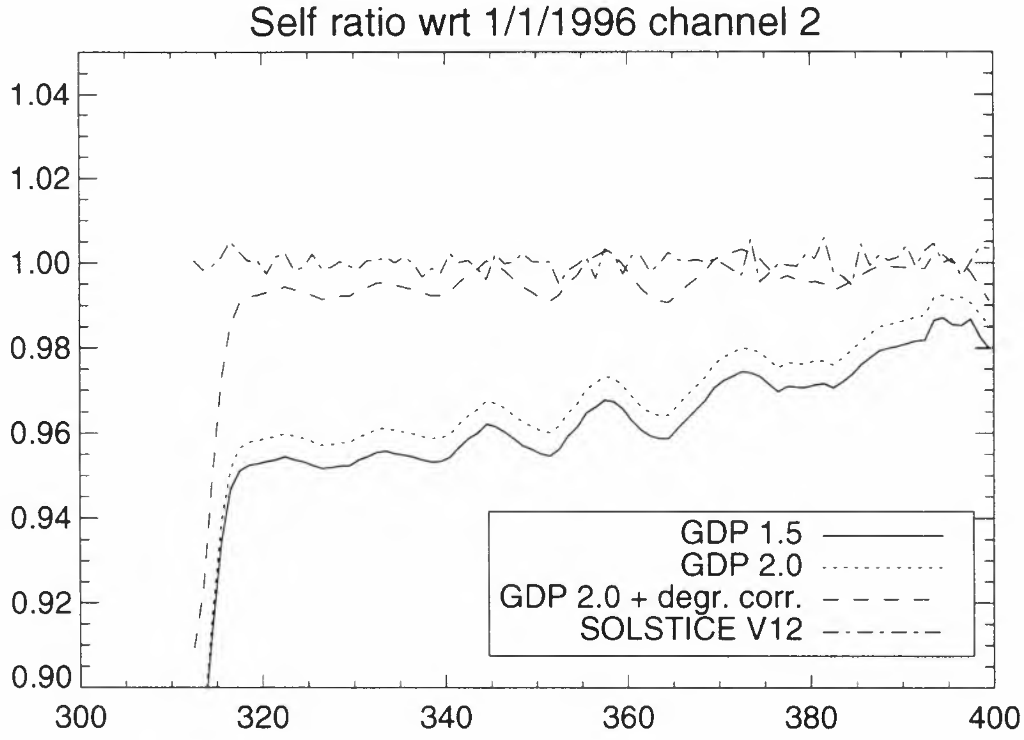


Figure 3. Irradiance ratio in channel 2 with respect to GOME spectrum of 1st of January 1996.

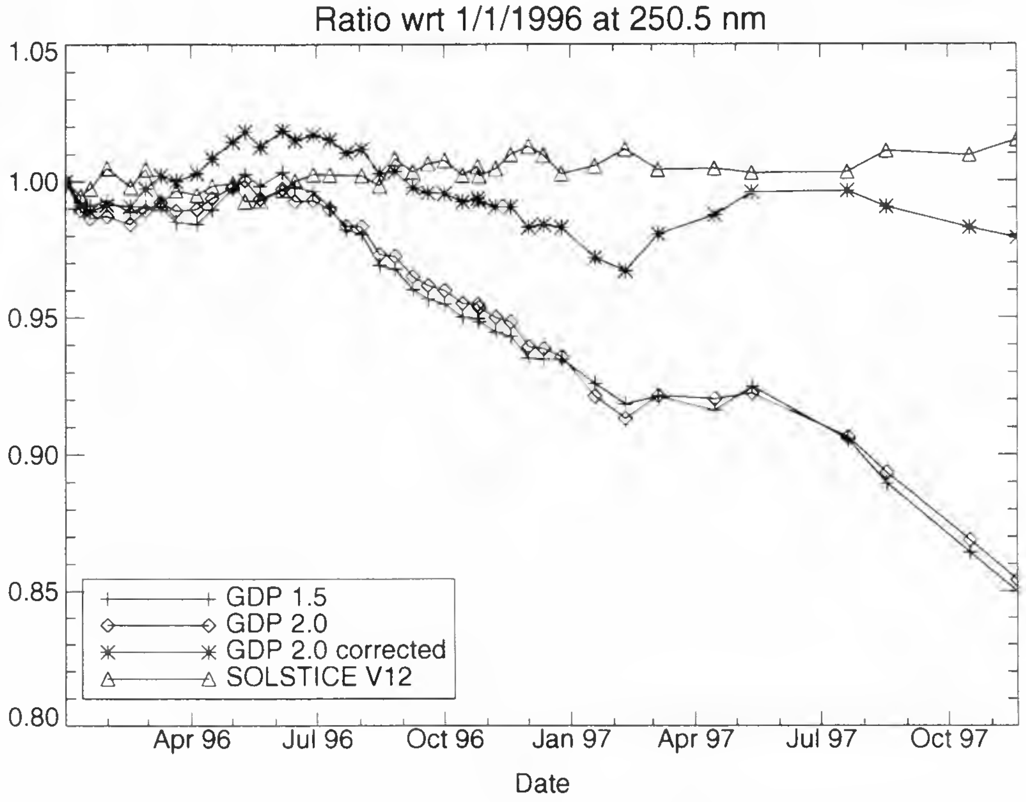


Figure 4. Time dependence of the ratio at 250.5 nm.

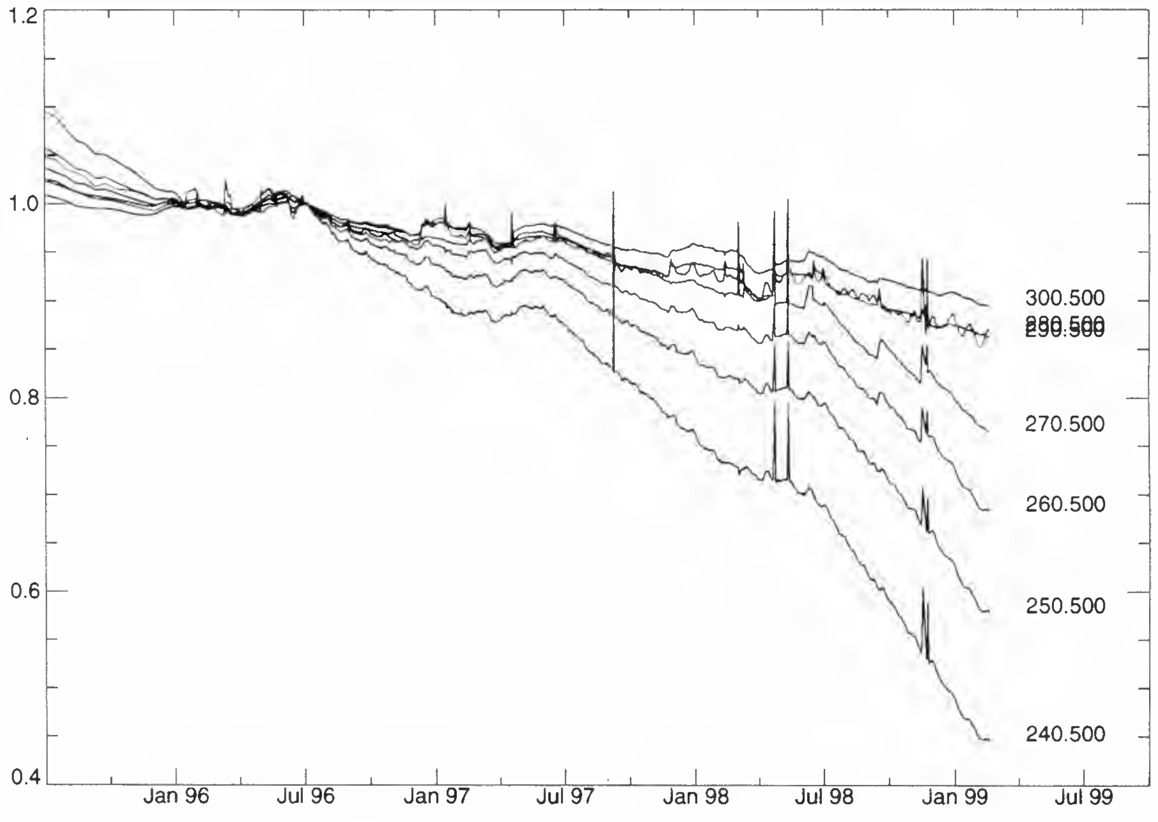


Figure 5. Original GDP 1.5 irradiance degradation in channel 1.

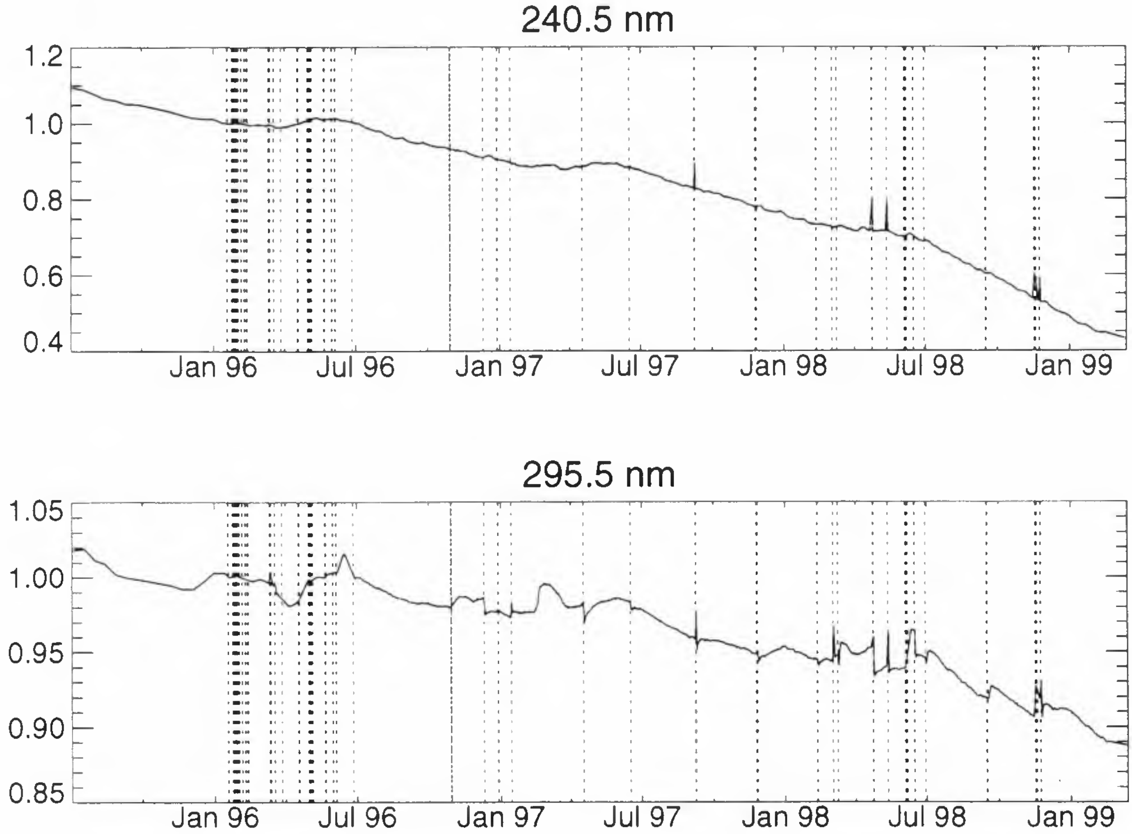


Figure 6. Same original GDP 1.5 irradiance degradation as in Figure 5, but at 240.5 and 295.5 nm. Each vertical bar corresponds to a cooler switch.

5. Preliminary conclusions and recommendations

The new wavelength calibration is an improvement (at least in channel 1) and should be implemented. We are more cautious about the degradation correction scheme. While it improves considerably the situation especially in channel 2, the residual bias in channel 1 remains significant. Efforts in this direction is definitely needed and this is a nice try in the right direction but it's not sufficient to give GOME solar irradiance radiometric precision enough credibility. The amount of solar data is however not sufficient to give a definitive recommendation (41 spectra over 2 years). The data plots in ER-TN-DLR-GO-0043 (p. 11) looks much nicer but include a full 3 years data set. The correction facility may be left in the new GDP_01 extraction program but a clear warning must be issued to the user of this facility, among others in the GOME data disclaimer.

5. EARTHSHINE RADIANCE, POLARISATION AND CLOUD FRACTION

RESULTS FROM KNMI

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GOME DELTA VALIDATION 1999 – RESULTS FROM KNMI

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1. Summary

The new GOME Data Processor (GDP) (version 2.0) results have been compared to the previous version for a limited data set of orbits from 1996 and 1997.

The following are our main findings:

1. The correction for the degradation of the fractional polarisation (p) of the PMDs goes in the right direction. The degraded p values of especially PMD1 are improved. However, the correction suffers from some overshoot;
2. Due to interpolation errors of the fractional polarisation occurring in the extraction software, a radiometric error of up to ≈ 5% in the UV exists;
3. The wavelength belonging to an individual detector pixel is unstable along an orbit. The wavelength pertaining to a certain detector pixel shows discrete steps of several times 0.01 nm along an orbit. This instability is probably a side-effect of the spectral calibration procedure using lamp lines;
4. The bias in ICFA cloud fractions as compared to ISCCP with respect to various surface types has been largely removed. However, the effective cloud fractions produced by ICFA are too low in absolute value, both for ICFA version 2.3 and 2.6 (version 2.6 ICFA values are even lower than 2.3);
5. We conclude that the reprocessing should continue, because of improvements regarding correction for degradation of polarisation measurements (level 1 data) and better NO_2 vertical columns (level 2 data).

However, we would like to stress that the GDP is far from perfect. We have concerns about the level 1 data regarding the wavelength calibration, the polarisation correction in the UV, strange artefacts, and about the level 2 data regarding processing speed, the Air Mass Factor calculation, the ICFA cloud detection results, the climatologies used, and missing or incomplete documentation.

2. Correction for degradation of polarisation measurements

Using eight (8) orbits of the 33 provided for Deltaval, we examined the (possible) temporal changes in the PMD fractional polarisations. For certain pixels of a GOME orbit, the viewing geometry is such that single scattering theory predicts a polarisation angle of 45°. It has been argued in the literature that multiple scattering will not substantially alter this angle. Hence, for selected pixels, the fractional polarisation is 0.5.

The aforementioned pixels were selected on basis of the criterium that $|p_7 - 0.5| \leq \varepsilon$, with $\varepsilon = 0.003$ for east and nadir pixels and $\varepsilon = 0.0015$ for west pixels. Under this assumption, the annual trend in p_7 (the theoretical point) is at most 0.09%. This trend should be zero, but any bias in the sampling of the data points will cause deviations thereof.

We first present the result for the old (v.1.3) GOME data processor. In Figure 1, the trend in p_2 (PMD 1) is shown for east, nadir and west. Trends in other PMDs are generally smaller. We have averaged over the selected pixels of each orbit. The straight line is a minimal χ^2 error fit. Both east and west pixels fail the χ-criterium (east, nadir and west have $\chi^2 = 114$, 1.9, 11.3 resp.), but a downward trend is nonetheless visible (it just cannot be appromated by a straight line). Our values are slightly larger than found by DLR and SRON.

We now present the result for the new (v.2.0) GOME data processor. In Figure 2, the trend in p_2 (PMD 1) is shown for east, nadir and west. Trends in other PMDs are generally smaller. Again we have averaged over selected pixels within one orbit. The straight line is a minimal χ^2 error fit. Only east pixels fail the χ-criterium (east, nadir and west have $\chi = 22$, 3.0, 2.3 resp.), but an upward trend seems apparent nonetheless. We conclude that for east and nadir viewing, the new processor seems to over-correct. Nevertheless, the annual changes have decreased.

So far we have averaged over pixels within one orbit, as this seems the accepted practice. We are not sure if this is a correct approach. More selected pixels within one orbit implies more reliability. By simpling averaging these pixels, this information is lost. The use of the standard deviation of p_2 for the selected pixels of one orbit as an error measure seems shaky, as this is only valid for large samples within each orbit. Furthermore, the annual trend in p_7 (!) is five times smaller when using each individual pixel than when averaging them. In Figure 3, the trend in p_2 (PMD 1) is shown for east, nadir and west. No χ^2 error test is possible, since we did not specify errors in individual measurements. Results agree with those in Figure 2 for east, but for nadir view the increase has doubled, while it has decreased for west.

Summarizing: we feel that in general the new processor improves the fractional polarisation measurments as compared to the old processor. Nevertheless, trends are still present in the form of an overcorrection for east and nadir. The precise annual increase depends on the chosen method of data representation (averaging over one orbit or not). Our data sample (eight orbits) is rather small, which may well bias our results.

We also want to point out that due to an inefficiency in the implementation of the interpolation scheme in the extractor software, errors in interpolated fractional polarisation can easily be as large as 0.06 (more than 10% of $p = 0.5$!) in the UV and 0.02 (little less than 5% of $p = 0.5$) for long wavelengths. Such errors can never be studied with the above method as the interpolation scheme works exceptionally (!) well for viewing geometries where $p \approx 0.5$.

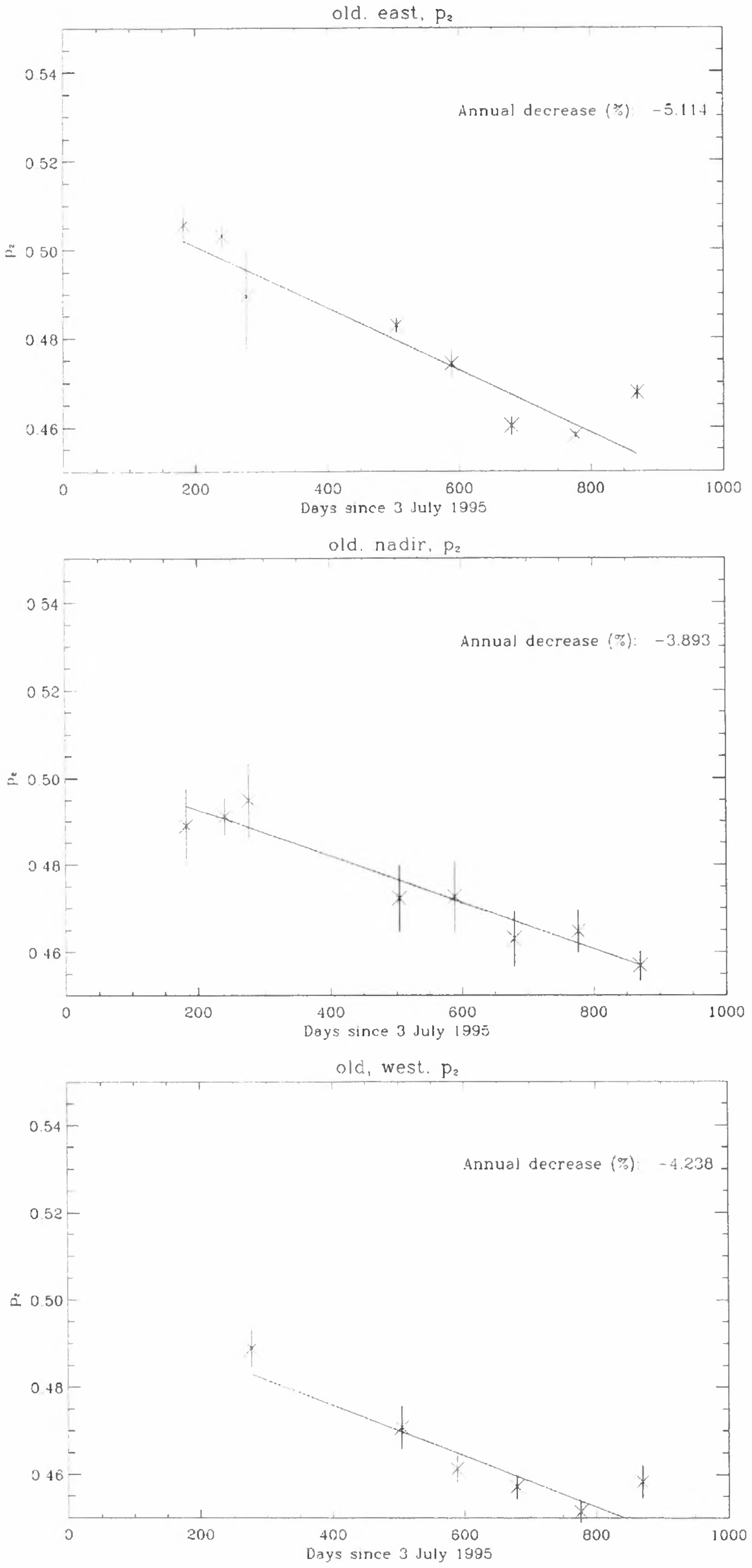

Figure 1. Temporal evolution of p_2 for cases where $p = 0.5$ on theoretical grounds. Averaged per orbit. Processor version 1.5 or lower (old).

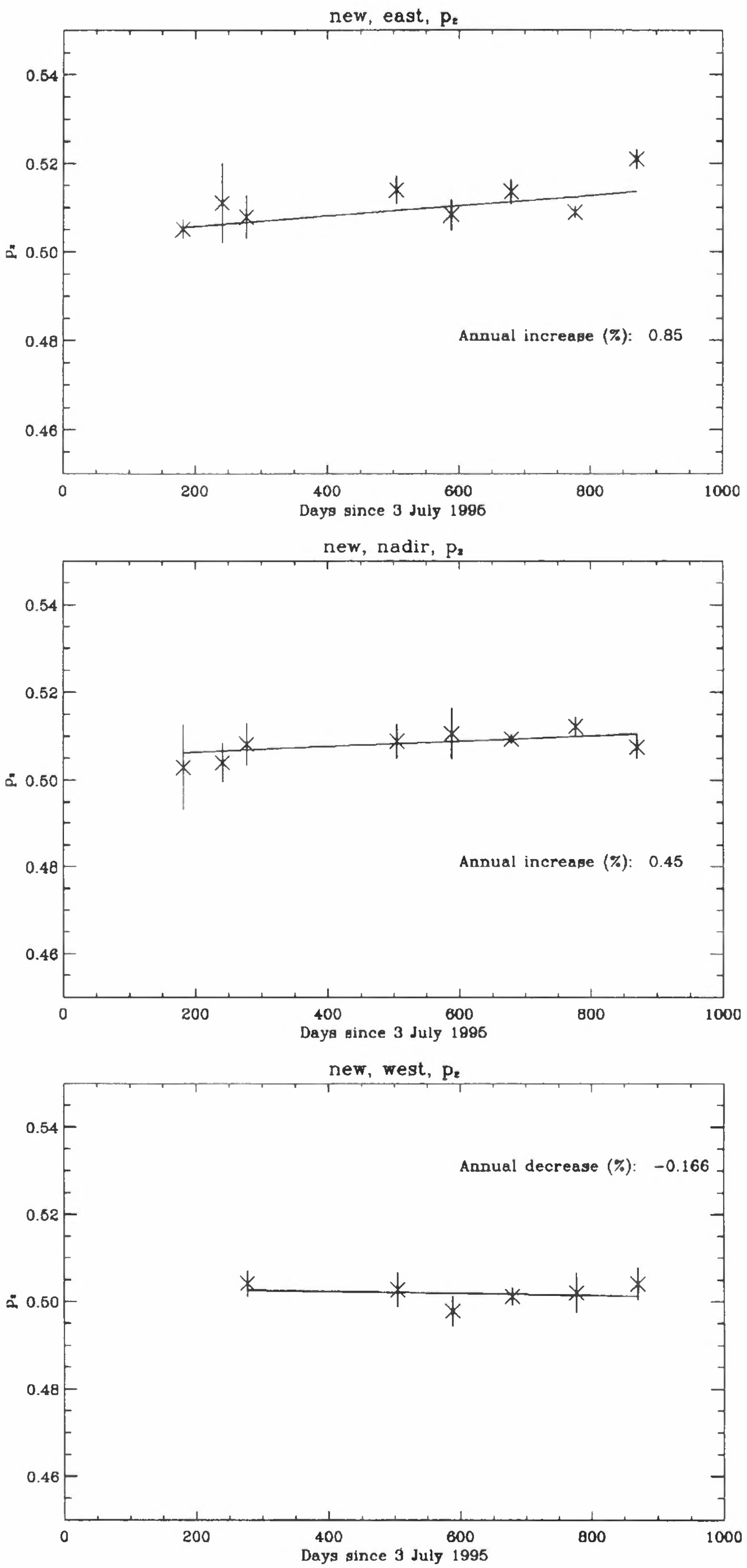

Figure 2. Temporal evolution of p_2 for cases where $p = 0.5$ on theoretical grounds. Averaged per orbit. Processor version 2.0 (new).

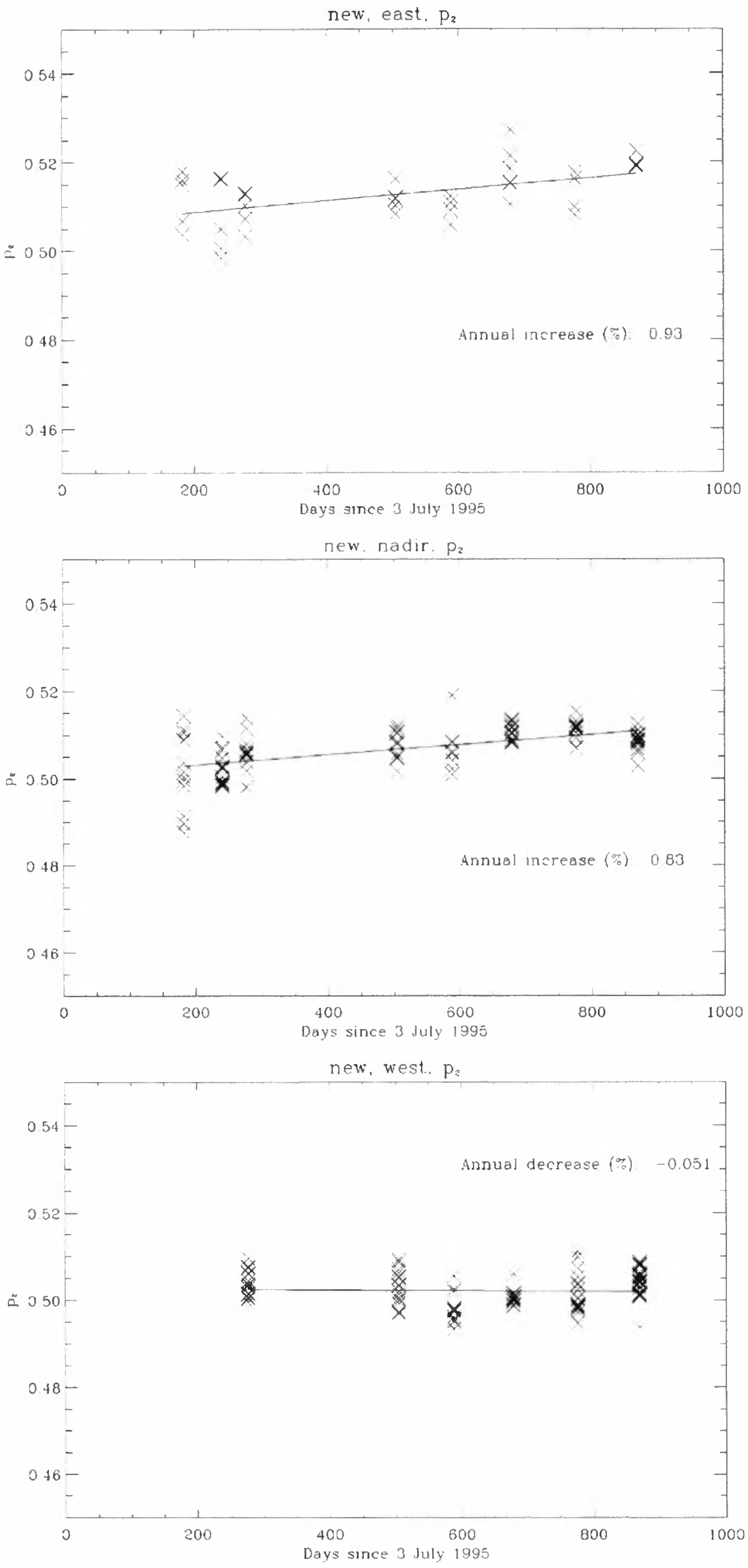

Figure 3. Temporal evolution of p_2 for cases where $p = 0.5$ on theoretical grounds. All pixels. Processor version 2.0 (new).

3. Errors in radiometric calibration due to polarisation effects

The absolute radiometric accuracy of the Earth's reflectivity (i.e., the ratio between Earth radiance and solar irradiance) in the UV is limited to about 5% because of the remaining effects of atmospheric polarisation. Work continues on improving the calibration in this regard.

This radiance error is due to an error in the polarisation-correction procedure implemented in the level 1 extractor software. The interpolation of the small p values in the region between 350 nm (measured PMD1 polarisation value) and 300 nm (theoretical polarisation value) is not correct. This has recently been found by Nick Schutgens at KNMI. We will, if possible, give an improvement in the near-future.

4. Spectral calibration

We investigated the wavelength calibration of the GOME Earth's radiances and Solar irradiances between 757 nm and 767 nm, using GOME level 1 data of GDP 0-1 version 2.0. Our conclusions are given below, in sections 4.1 and 4.2.

4.1 Variations in the wavelength calibration of the Earth's radiances along an orbit

We find that the wavelength calibration of the Earth's radiances sometimes shows unphysical discontinuities along an orbit of about 0.03 nm at 765 nm (see Figure 4, 5, and 6). In these figures, the heavy line at the right is the corresponding wavelength calibration of the Solar irradiance. The magnitude of these discontinuities increases as the wavelength increases, for example, if it is 0.018 nm at 757 nm, it is 0.029 nm at 765 nm. The wavelength discontinuities at various wavelenghts correlate well with eachother. These discontinuities were present in the old GDP level-1 data products, and are still present in the current processor, although the cross-correlation technique is used now.

4.2 Temporal variations in the wavelength calibration of the Solar irradiances

The wavelength calibration of the Solar irradiances shows some variation with time. Figure 7 shows as a function of time the Solar irradiance wavelength assigned to detector pixel 850 of GOME channel 4 (pixel 850 corresponds to about 758 nm). The blue points show data processed with GDP 0-1 processor version 2.0, the red points were processed with GDP 0-1 processor version 1.35 or lower. The absolute level of the wavelength calibration has changed by about 0.06 nm between the two processor versions. This is three times more than the the doppler shift of the Solar irradiance, which is about 0.02 nm at 758 nm. If we consider data extracted with the same processor, the wavelength calibration is rather stable between day-number 60 (1 March) and 274 (1 October). However, in November and December, wavelength changes of about 0.02 nm occur for this detector pixel. The changes for 1996 and 1997 show a similar pattern. The temporal variations are present in both processor versions.

Pixel 800 of channel 4 (about 747 nm) shows a similar behaviour as pixel 850, but with a change in the absolute level of the wavelength calibration of about 0.02 nm instead of 0.06 between the two processor versions (see Figure 8). Also, the change in calibration for November and December is smaller (0.01 instead of 0.02). This clearly indicates that the lack of lamp lines for wavelenghts larger than 754.6122 nm in channel 4 leads to large wavelength calibration errors, even for wavelengths close to the last line.

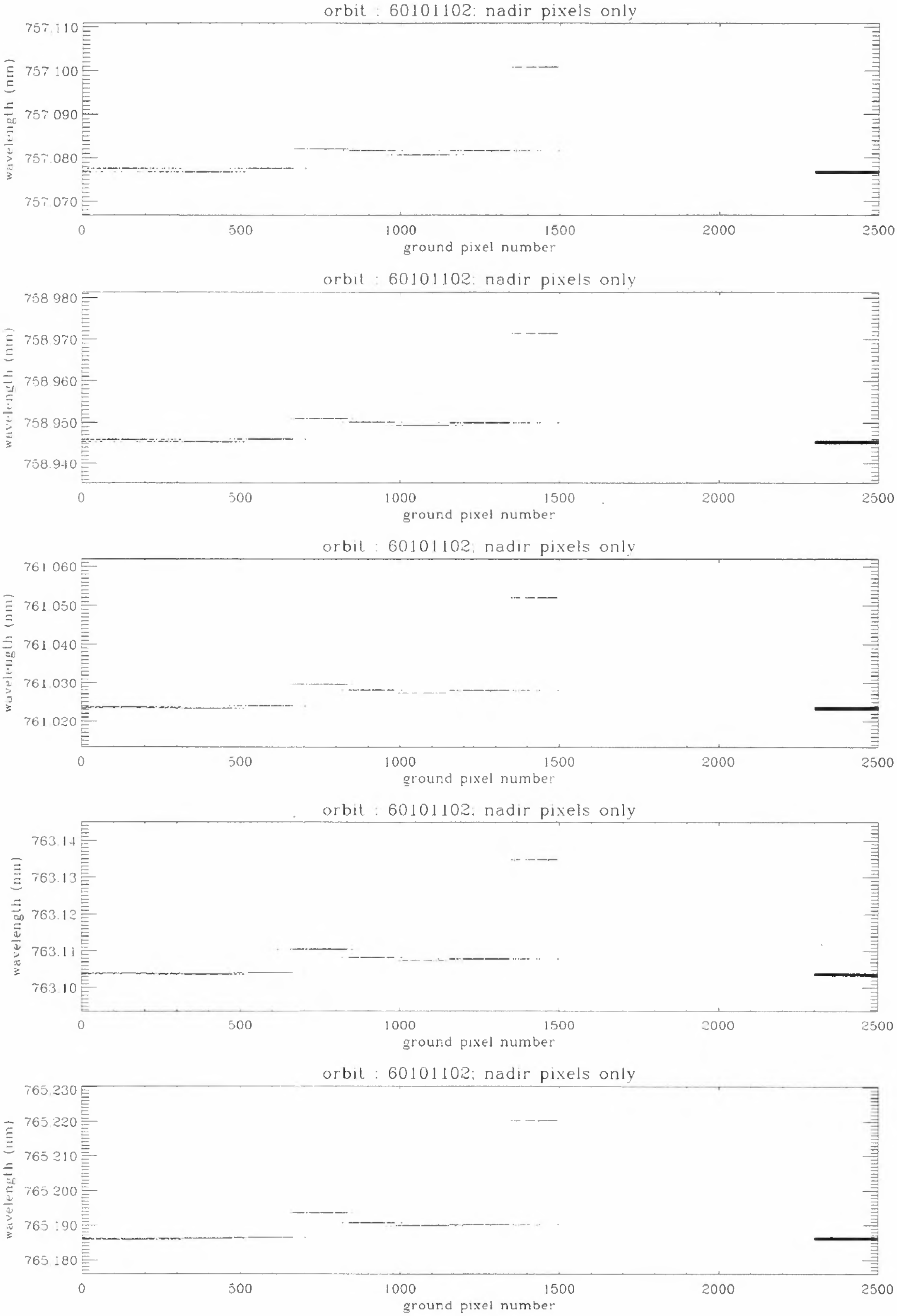

Figure 4. Variations in the spectral calibration of individual diode-array pixels along orbit 60101102. Processor version 2.0 (new).

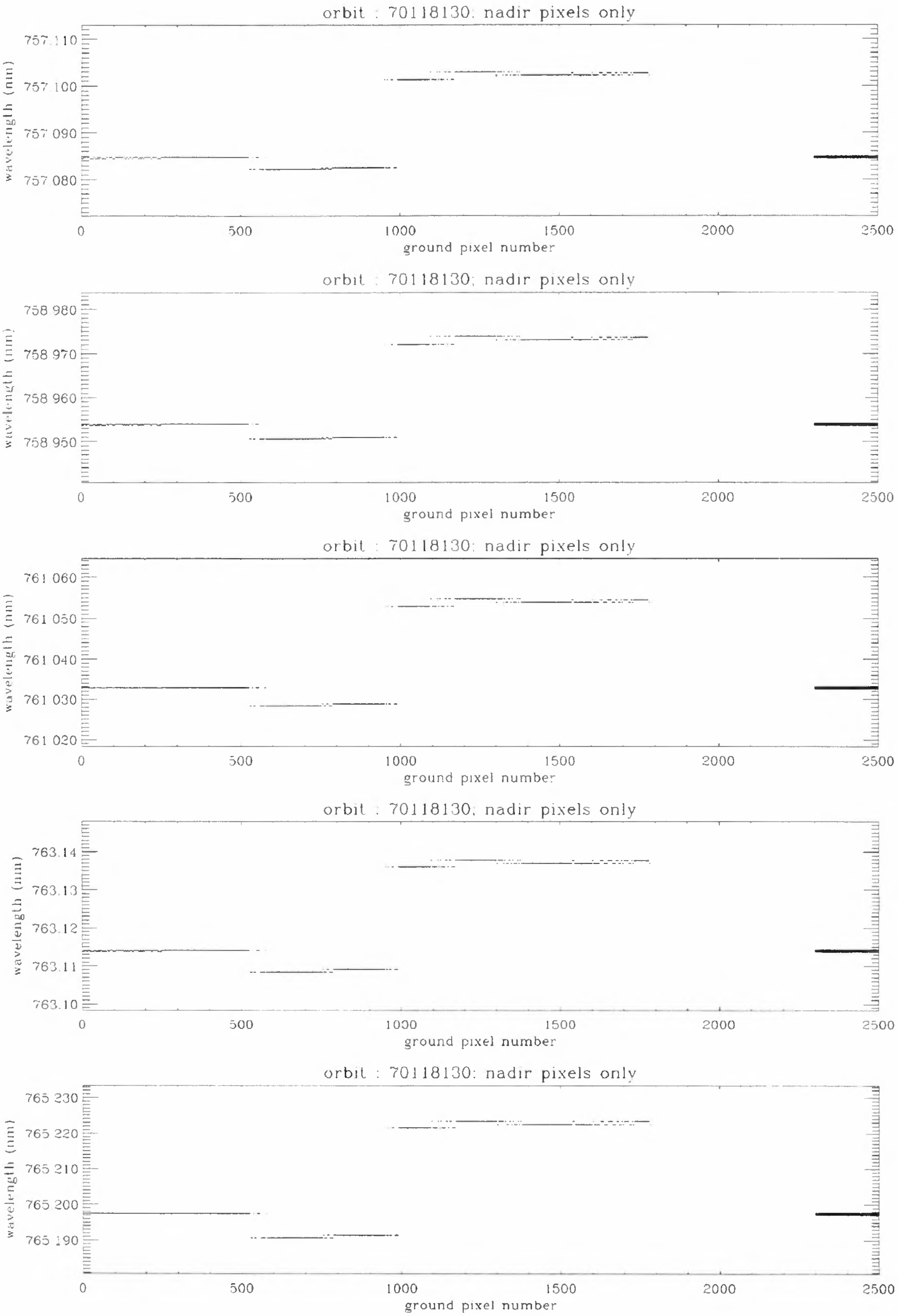

Figure 5. Variations in the spectral calibration of individual diode-array pixels along orbit 70118130. Processor version 2.0 (new).

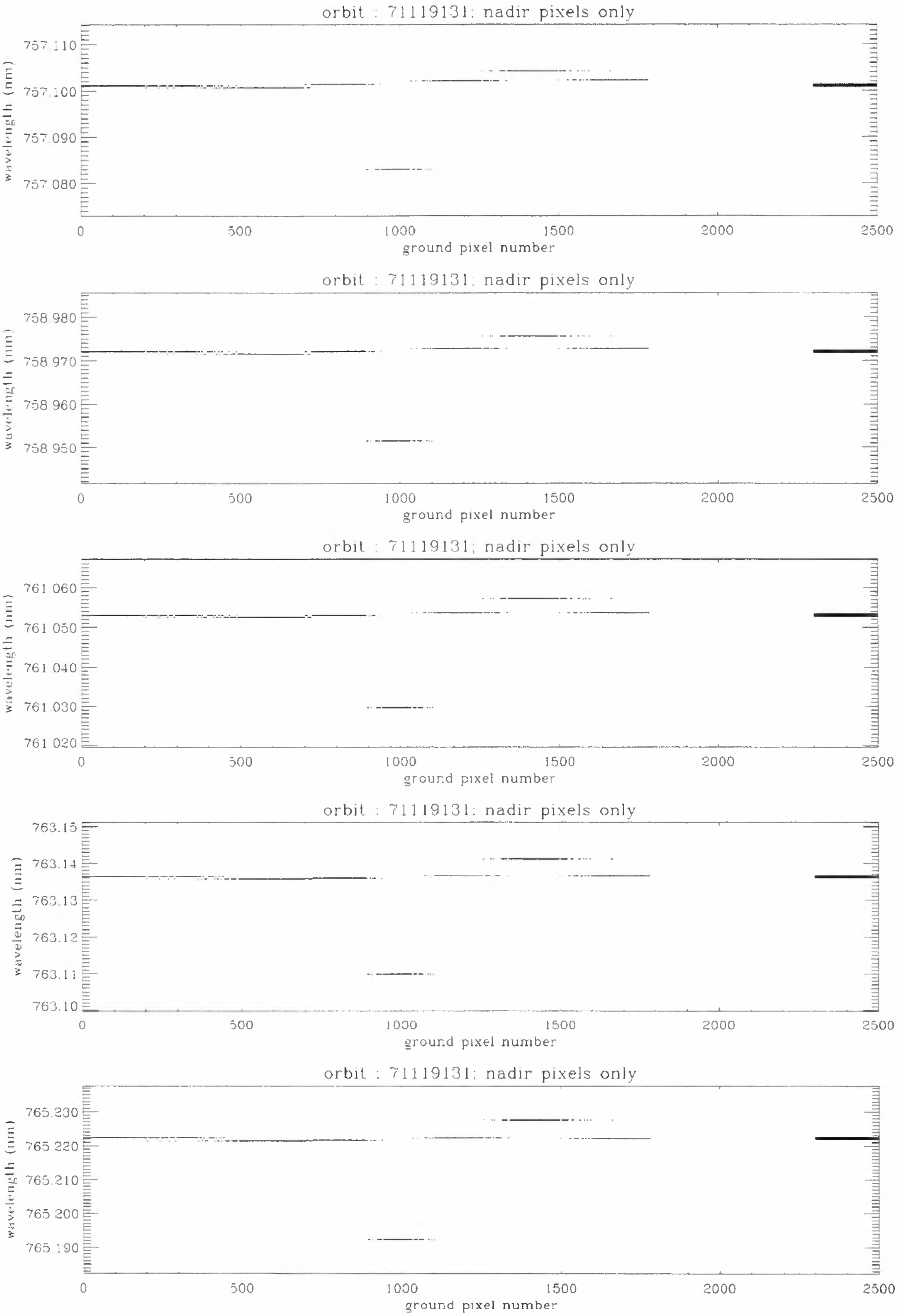

Figure 6. Variations in the spectral calibration of individual diode-array pixels along orbit 71119131. Processor version 2.0 (new).

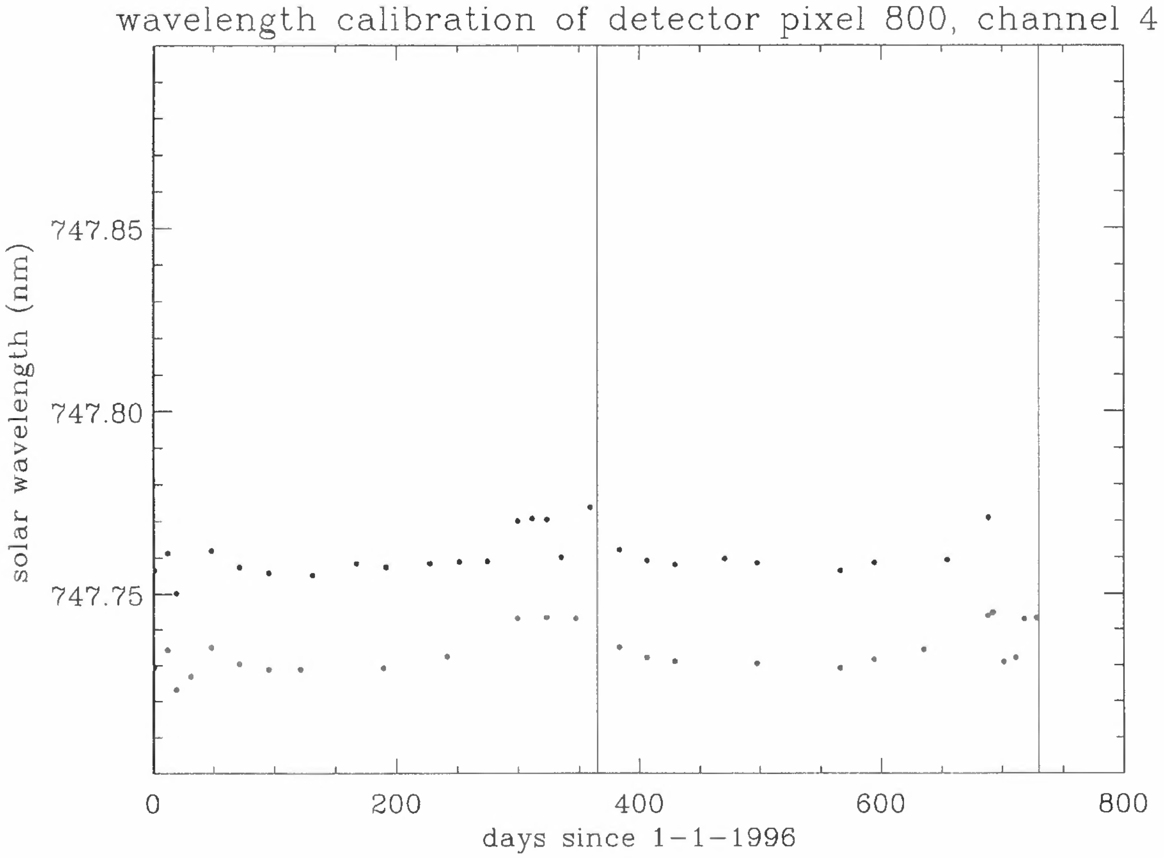

Figure 7. Temporal variation in the spectral calibration of the solar irradiance at pixel 850 of channel 4. Blue points: processor version 2.0 (new); red points: processor version 1.35 or lower (old).

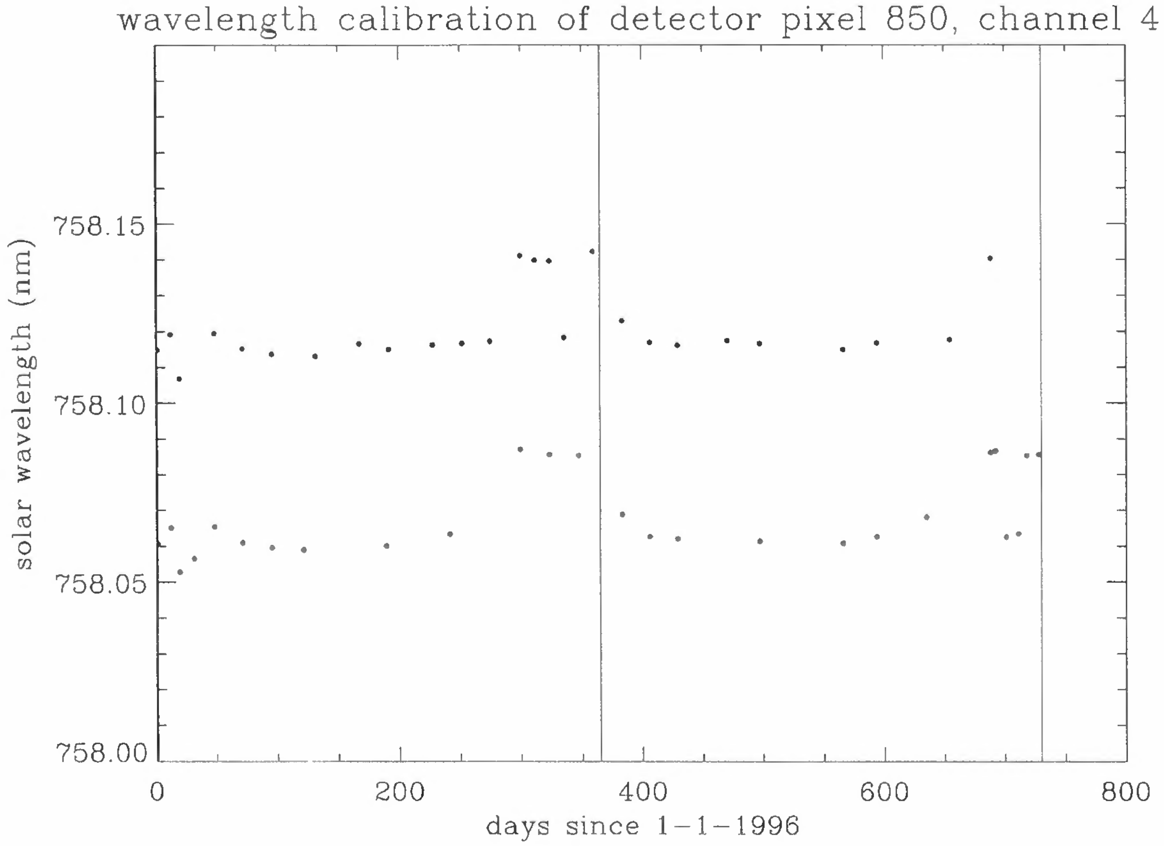

Figure 8. Temporal variation in the spectral calibration of the solar irradiance at pixel 800 of channel 4. Blue points: processor version 2.0 (new); red points: processor version 1.35 or lower (old).

ICFA cloud fraction

It has been found by Andreas Richter (IUP, Bremen) that in the new GDP 1-2 processor (v 2.6) ICFA cloud fractions are lower than in the previous version (v 2.3), in particular over bright surfaces, whereas over ocean the cloud fraction is only slightly lower. Consequently, the bias in ICFA cloud fractions with respect to various surface types as compared to ISCCP is now largely removed.

In general, however, the effective cloud fraction values produced by ICFA were already too low in absolute value in the previous version (v 2.3); in v 2.6 it is even lower. The global average ICFA effective cloud fraction was 0.24 in v 2.3, and has decreased to about 0.22 in v 2.6. This should be at least 0.30 to represent clouds with an optical thickness of 20, which is assumed in the AMF calculations. Furthermore, for individual orbits, still errors in ICFA cloud fractions are present due to errors in the assumed cloud top pressure.

6. TOTAL OZONE AND NITROGEN DIOXIDE

RESULTS FROM IASB... **34**

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RESULTS FROM SPSU... **61**

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RESULTS FROM IUP... **87**

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DELTA CHARACTERISATION OF GOME LEVEL-2 DATA PRODUCTS VERSION 2.7 USING NDSC AND HALOE CORRELATIVE MEASUREMENTS

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Abstract: This report summarises preliminary delta validation results of the version 2.7 of GOME level-2 total ozone and nitrogen dioxide data, using ground-based measurements from the Network for the Detection of Stratospheric Change (NDSC) and space-based data from the UARS Halogen Occultation Experiment (HALOE).

1. Introduction

During the first half of 1999, the level-1-to-2 segment of the operational GOME Data Processor (GDP) established at DFD/DLR was upgraded from its version 2.4 to version 2.7. A Delta Validation Campaign was organised to provide an independent verification and characterisation of the upgrades. Main emphasis was given to the global quality assessment of new NO_2 column amounts. Other major GDP changes had to be investigated as well.

This document reports on delta validation studies carried out during this campaign by means of correlative ground-based observations associated with the Network for the Detection of Stratospheric Change (NDSC) and space-based observations from the UARS Halogen Occultation Experiment (HALOE). Data sets and methodology are described in Section 2. Based on previous validation results using the same instrumentation, current performances of GDP 2.4 data products are summarised in Section 3. The effect of changes from GDP 2.4 to GDP 2.7 is investigated in Section 4. In Section 5, extended ozonesonde data records acquired at various NDSC stations are used to assess the impact of the GDP atmospheric profile database on the accuracy of the GDP ozone air mass factors.

2. Data sets and methodology

2.1. GOME level-2 data

A GOME level-2 validation data set of about 400 orbits has been processed at DFD/DLR with GDP 2.7. It consists mainly of the 1996 part of the data set selected for the last delta validation campaign (ESA, 1998), plus an additional set of 79 orbits (Table 2-1) selected to enhance NO_2 data investigation by means of NDSC data at low latitudes. It must be noted that, although suitable for the preliminary quality assessment reported hereafter, the set of orbits available for the present delta validation campaign is not completely satisfactorily to address all current priorities of GDP development with sufficient accuracy.

70118130
70121130
70124131
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70408224
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70415204
70417126
70418204
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70421205
70423130
70503125
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70511216
70512131
70514221
70517203
70520203
70523204
70526204
70712124
70714214
70715126
70717215
70718126
70720216
70721131
70723220
70817222
70820222
70823223
70826224
70830203
70902204
70905204
70908205
70920125
70921222
70923130
70924223
70926130
70927223
70929132
70930224
71008215
71010223
71011216
71013223
71014220
71016224
71019225
71026223
71029223
71101224
71104224
71108204
71110125
71111204
71113131
71114205
71116130
71117206
71119132

Table 2-1. Orbits (level-2 data file names) selected for specific NO_2 delta validation studies at low latitudes.

2.2. Correlative measurements

Studies reported here rely mainly on comparisons of GOME data with ground-based measurements from the NDSC. Contributing instruments are listed in Table 2-2.

Measurements of the NO_2 vertical column amount at sunrise and sunset have been collected from about 20 zenith-sky UV-visible spectrometers using differential absorption spectroscopy (DOAS): (a) 5 scanning instruments developed by NIWA since the late 1970s (McKenzie and Johnston, 1982); (b) 15 SAOZ grating instruments (Système d'Analyse par Observation Zénithale) developed by CNRS and performing automated network operation since the late 1980s (Pommereau and Goutail, 1988); and 3 spectrometers of a similar design developed at (c) IASB (Van Roozendael *et al.*, 1995), (d) IFE (Richter *et al.*, 1998), and (e) NILU (Arlander *et al.*, 1998), respectively. Using high-resolution Fourier transform infrared (FTIR) solar spectrometry, the NO_2 column amount throughout the day has also been measured at the Jungfraujoch station by the University of Liège, as part of its monitoring activities initiated in the 1950s (Delbouille and Roland, 1995). Most of the contributing UV-visible sensors have been certified for the NDSC after fruitful participation to major intercomparison campaigns organised through the NDSC or the EC Environment Programme. During such campaigns, the agreement between the various instruments generally falls within 5% to 10% (e.g., Vaughan *et al.*, 1997; Roscoe *et al.*, 1999). Long-term comparisons of nearly co-located instruments conclude to a mean agreement of 3% in summer and 9% in winter (e.g., Koike *et al.*, 1999). The figure is consistent with an estimated 5-10% accuracy of the retrieved slant column amount taking into account the 5% uncertainty of the NO_2 absorption cross-sections (Merienne *et al.*, 1995), their temperature dependence (Harwood and Jones, 1994; Coquart *et al.*, 1995), and the average 1.5% one sigma confidence level of the least-squares spectral fit. Vertical columns are derived from measured slant columns by means of a geometrical enhancement factor, or air mass factor (AMF). The zenith-sky NO_2 AMF exhibits periodic signatures related to seasonal, latitudinal, and sunrise/sunset change of the vertical distribution of atmospheric constituents. Not taken into account in the ground-based data processing yet, those features generate in the resulting vertical columns fictitious cyclic signatures of a few percent, superimposed on the real total NO_2 variations observed by the instrument. As shown in an NDSC-based study of GOME NO_2 data (Lambert *et al.*, 1999d), those cyclic biases should not affect conclusions of current GOME validation studies.

Sunrise and sunset NO_2 columns have also been derived from stratospheric profiles measured by the UARS Halogen Occultation Experiment (HALOE, Russell *et al.*, 1993). Integrated stratospheric profiles have been completed with a tropospheric column representative of an unpolluted troposphere, estimated by the 3D chemical-transport model IMAGES (Müller and Brasseur, 1995).

Station	Location	Lat.	Long.	Institute	Instruments
Ny-Ålesund	Spitsbergen	79°N	12°E	NILU, IFE	DOAS, SAOZ
Longyearbyen	Spitsbergen	78°N	16°E	NILU	DOAS
Thulé	Western Greenland	77°N	69°W	DMI	SAOZ
Scoresbysund	Eastern Greenland	70°N	22°W	CNRS/DMI	SAOZ
Sodankylä	Finland	67°N	27°E	CNRS/FMI	SAOZ
Zhigansk	Eastern Siberia	67°N	123°E	CNRS/CAO	SAOZ
Harestua	Southern Norway	60°N	10°E	IASB	DOAS
Aberystwyth	Wales	52°N	4°W	U. Wales	SAOZ
Hohenpeißenberg	Germany	48°N	11°E	DWD	Brewer, Dobson
Jungfraujoch	Swiss Alps	47°N	8°E	IASB, U. Liège	FTIR, SAOZ
Arosa	Swiss Alps	46°N	9°E	ETH	Brewer, Dobson
Bordeaux	France	46°N	1°W	U. Bordeaux	Dobson
OHP	French Alps	44°N	6°E	CNRS, U. Reims	Dobson, SAOZ
Mauna Loa	Hawaii	20°N	156°W	NIWA	NIWA
Tarawa	Kiribati	01°N	172°E	CNRS, NIWA	NIWA, SAOZ
Saint-Denis	Reunion Island	21°S	55°E	U. Réunion	SAOZ
Bauru	Brazil	22°S	48°W	CNRS/UNESP	SAOZ
Lauder	New Zealand	45°S	170°E	NIWA	NIWA
Kerguelen	Indian Ocean	49°S	70°E	CNRS	SAOZ
Macquarie	Southern Pacific	55°S	159°E	NIWA	NIWA
Faraday	Antarctic Peninsula	65°S	64°W	BAS/KTSU, BAS	Dobson, SAOZ
Dumont d'Urville	Antarctica	66°S	140°E	CNRS	SAOZ
Rothera	Antarctic Peninsula	68°S	68°W	BAS	SAOZ
Halley	Antarctica	76°S	27°W	BAS	Dobson
Arrival Heights	Antarctica	78°S	167°E	NIWA	NIWA

Table 2-2. Characteristics of NDSC total ozone and nitrogen dioxide monitoring instruments contributing to the present study: station name, geographical location, coordinates, responsible institute, and type of instrument.

Measurements of the ozone vertical column amount at twilight have been collected from about 15 DOAS spectrometers associated with the SAOZ/UV-visible network of the NDSC (Pommereau and Goutail, 1988; Roscoe *et al.*, 1999). Total ozone data throughout the day have been monitored at NDSC Alpine and Antarctic sites by Dobson and Brewer ultraviolet spectrophotometers. Combined together, the various ozone observation techniques used in the frame of the NDSC provide powerful complementary information for satellite validation, each observation technique extending capabilities of the others.

2.3. Method of investigation

Changes in ozone and nitrogen dioxide data products have been characterised first for a set of 24 individual orbits consisting of one orbit every fortnight in 1996. Cross-correlation of the two versions of GDP has been carried out along track and also at representative NDSC stations. Not only total columns but also intermediate products (slant columns and air mass factors) have been investigated as a function of latitude, time, and geophysical conditions. The internal characterisation of GDP changes has been followed by an assessment of the improvement with respect to NDSC measurements involving the whole set of GOME delta validation orbits.

Comparisons with total ozone data from the pole-to-pole SAOZ/UV-visible network of the NDSC yield a homogeneous global picture of GDP ozone data improvement. Complementary comparisons at the Alpine and Antarctic stations with independent Dobson and Brewer measurements confirm UV-visible results and add significantly to their statistical significance.

Comparisons with nitrogen dioxide data from about 20 UV-visible spectrometers of the NDSC including those from the SAOZ and NIWA networks yield a homogeneous global picture of GDP NO_2 data improvement. More sporadic HALOE and FTIR data are used to confirm results obtained with continuous UV-visible time-series. At each latitude, redundant correlative measurements obtained with different types of instrument (e.g., SAOZ instrument, NIWA system, and HALOE) allow permanent quality control and internal validation prior to the comparison with GOME data.

The comparison of mid-morning GOME data with sunrise and sunset data from NDSC/UV-visible spectrometers and from HALOE is not straightforward due to the photochemical variation of NO_2 throughout the day. In addition, compared to the observation geometry of the other instruments used in the study, the geometry of GOME enhances its sensitivity to the troposphere. At stations where tropospheric NO_2 is not abundant, GOME data acquired in the mid-morning are expected to lie between sunrise and sunset vertical columns. At high latitudes, the comparison is easier during midnight sun conditions and near the terminator, that is, when GOME data are acquired at low sun elevation and consequently are comparable with sunrise and sunset measurements. Finally, to assess to what extent the diurnal variation of NO_2 impacts on comparisons with twilight data in the Alps, mid-morning FTIR data at the Jungfraujoch have been extracted with the strict selection criterion of 1.5 hour around the GOME overpass time.

3. Current performances of GDP 2.4

3.1. Total ozone

Observations acquired with the same instrumentation at the same NDSC stations have been used to carry out a combined validation of total ozone measured for several years by GOME, TOMS-EP and TOMS-AD (Lambert *et al.*, 1999a-c). Long-term comparisons demonstrate a good average agreement to within ±2-4% between all spaceborne and ground-based instruments at northern middle latitudes but also highlight three-month shifts of a few percent in GOME data. At high latitudes in both hemispheres, the mean agreement and the scatter vary with the solar zenith angle of the space observation, largely due to the retrieval method and its sensitivity to errors in the ozone profile shape. GDP 2.4 total ozone increases systematically beyond 80° SZA, however its average SZA dependence is dominated by a seasonal variation resulting in positive mean deviations beyond 80° SZA in winter-spring and in negative mean deviations beyond 70° SZA in summer-fall. The dispersion of satellite data increases significantly beyond 85° SZA. 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 and by much more under polar springtime ozone depletion. Conclusions based on comparisons with NDSC data are in excellent agreement with independent studies based on other monitoring network such as the Norwegian ozone monitoring network (Hansen *et al.*, 1999).

3.2. Total nitrogen dioxide

The current GOME total NO_2 data record inferred routinely with GDP 2.3 and 2.4 has been investigated under a variety of relevant geophysical conditions by means of correlative observations performed by the same ground-based network of NDSC UV-visible spectrometers as used here (Lambert and Simon, 1998; Lambert *et al.*, 1999d). Compared to the previous version 2.0 of GDP, GDP 2.3/2.4 provides a consistent NO_2 data product. The calculation of GOME AMFs using the AFGL US Standard NO_2 profile instead of MPI modeling results constitutes clearly an improvement. However, due to significant variations of the actual profile shape in both the stratosphere and the troposphere, the use of the single US Standard profile generates in the retrieved vertical columns fictitious signatures superimposed on the real total NO_2 variations observed by GOME. AMF studies relying on a more sophisticated database of atmospheric NO_2 derived from real measurements (Lambert *et al.*, 1999d, 2000) have highlighted the need to improve the GDP NO_2 database with seasonal/latitudinal stratospheric features and a consistent tropospheric background to get accurate AMFs under unpolluted conditions. Accurate AMF evaluation under polluted conditions remains a major issue. The agreement with NDSC measurements varies with the latitude and the season, largest discrepancies being observed at low latitudes and during pollution events at all latitudes. The observed bias between the GOME and ground-based total NO_2 time-series persists or increases after deduction of the stratospheric profile shape effect on both the GOME and ground-based data records. This latter finding suggests that other issues related to the retrieval of the slant column amount remain to be addressed, among others, the quality of the DOAS fitting procedure, or the impact of the temperature dependence of the NO_2 absorption cross-sections.

4. Characterisation of changes from GDP 2.4 to GDP 2.7

4.1. Total ozone

Cross-correlation of GDP ozone data along track

Figure 4-1 depicts GDP 2.4 and 2.7 ozone data along track for two individual orbits in February and June 1996. Similar results are obtained with the 24 orbits studied here. Changes in the vertical column generally fall within ±3% at latitudes below 45°-60° but can increase up to ±6% at low sun elevation. Vertical column patterns along track are unchanged. Changes in the slant columns are smaller than 0.5%, except for end-of-orbit measurements when the sun is near or below the horizon. In this latter case, the GDP 2.7/GDP 2.4 slant column ratio increases by a few percent as the sun elevation decreases.

As illustrated in Figure 4-1, the major contribution to changes in the vertical column arises from changes in the air mass factor. The analysis of the 24 orbits highlights two different behaviours presented in the figure. Creased patterns along track shown in Figures 4-1-h and 4-1-j are observed from April through September while smoother patterns in Figures 4-1-c and 4-1-e are observed from October through March.

Cross-correlation of GDP ozone data at NDSC stations

A closer look at GDP ozone data around NDSC stations at all latitudes confirms the results of along-track cross-correlation studies. Slant columns do not change significantly from GDP 2.4 to 2.7, as illustrated in Figure 4-2 for northern and southern mid-latitude sites. Vertical columns correlate very well at all latitudes (Figure 4-3): $r^2>0.98$, the slope of the regression is close to unity, and the intercept is of a few Dobson. The conclusion is that GDP 2.4-to-2.7 upgrades result mainly in a systematic shift in the total ozone data.

In general, correlation plots at individual stations (Figure 4-3) highlight two trails of similar slope but characterised by intercepts differing by a few Dobson. This bimodal nature of the difference between GDP 2.4 and 2.7 total ozone reflects the aforementioned behaviour of the GDP 2.7/GDP 2.4 air mass factor ratio. A shift in the air mass factor ratio occurs in April and October (Figure 4-4), which affects directly vertical columns by a similar shift (Figure 4-5). This is to be attributed to change of reference days for the computation of the GDP air mass factor look-up tables.

Comparison with NDSC ground-based data

Changes in the agreement between GDP and NDSC data at seven representative stations are displayed in Figure 4-6. As expected from the cross-correlation studies, neither real improvement nor marked deterioration of GDP total ozone data is to date. Note that average change in the agreement with NDSC data depends on the temporal sampling of the delta validation data sets, since GDP upgrades are associated with time-dependent features such as the 6-month shift of the GDP 2.7/GDP 2.4 AMF ratio.

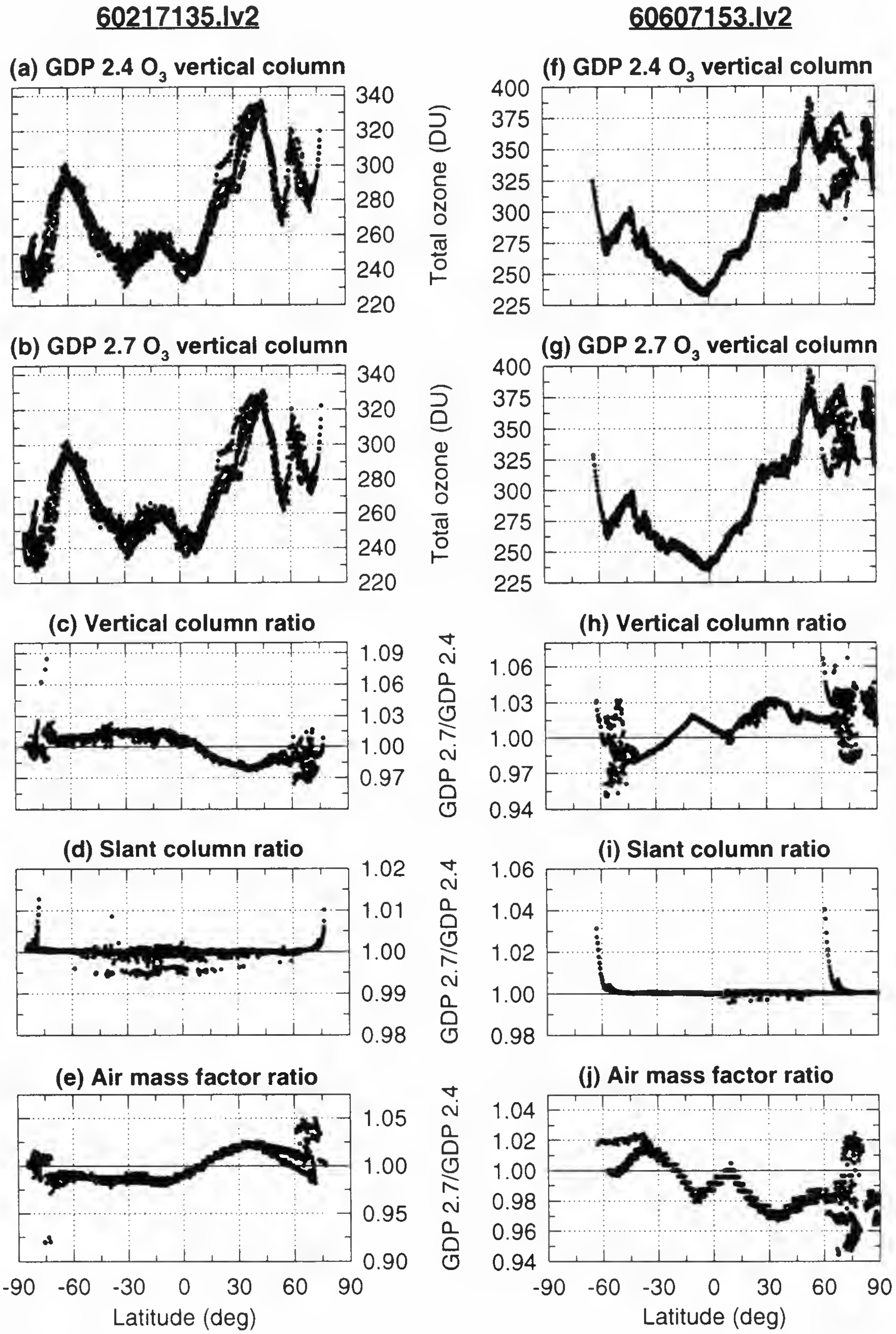


Figure 4-1. Comparison of GOME ozone data derived with GDP 2.4 and GDP 2.7 for two individual orbits in 1996: GDP 2.4 (a,f) and GDP 2.7 (b,g) O_3 vertical column amounts; and GDP 2.7/GDP 2.4 ratio of: (c,h) O_3 vertical columns; (d,i) slant columns; and (e,j) air mass factors. (a-e): orbit 60217135.lv2 of February 17, and (f-j): orbit 60607153.lv2 of June 7.

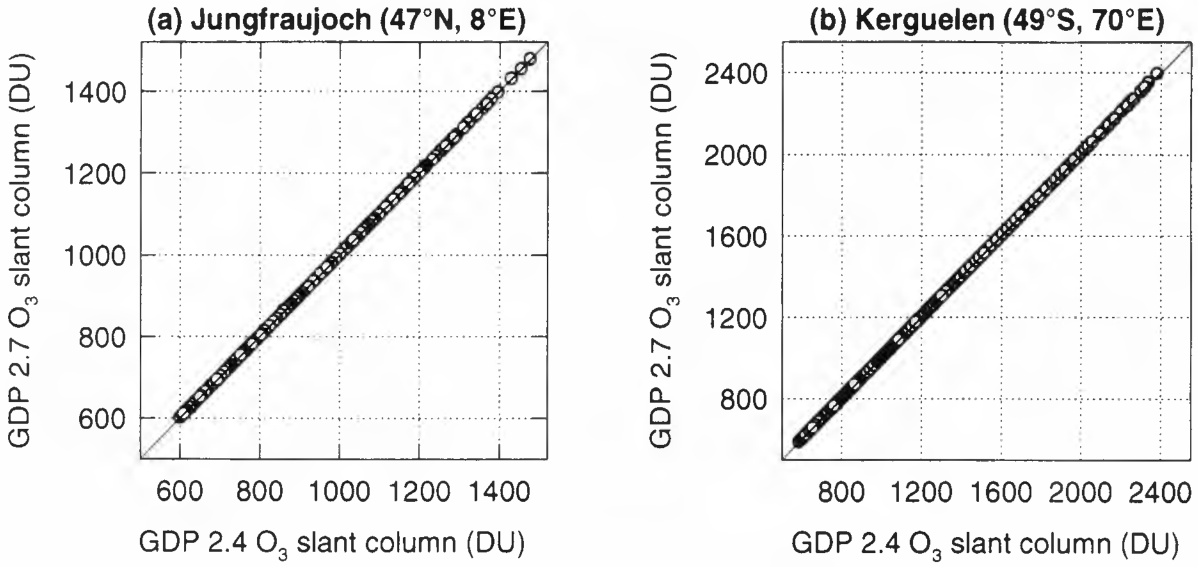


Figure 4-2. Correlation of GOME ozone slant column amounts derived with GDP 2.4 and GDP 2.7 at the mid-latitude NDSC stations of (a) the Jungfraujoch (Swiss Alps) and (b) Kerguelen Island (Indian Ocean). For both stations, $r^2 \approx 1$, $a_1 \approx 1.01$, and $a_0 < 10$DU. Straight line: GDP 2.4 = GDP 2.7.

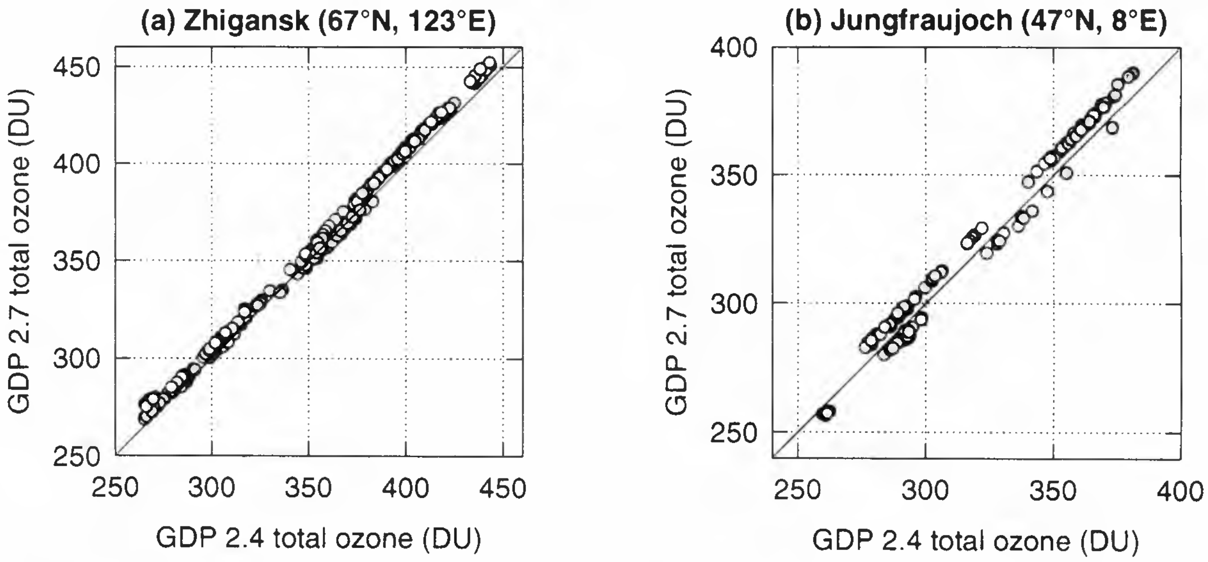


Figure 4-3. Correlation of GOME ozone vertical column amounts derived with GDP 2.4 and GDP 2.7 at the northern NDSC stations of (a) Zhigansk (Western Siberia) and (b) the Jungfraujoch (Swiss Alps).

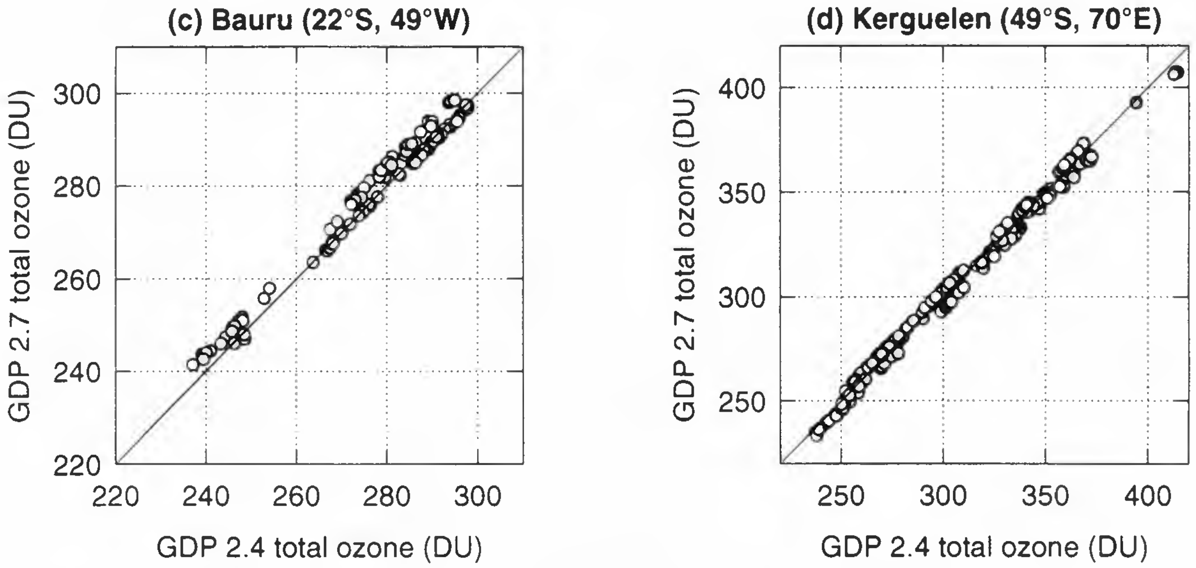


Figure 4-3. (continued) Correlation of GOME ozone vertical column amounts derived with GDP 2.4 and GDP 2.7 at the southern NDSC stations of (c) Bauru (Brazil) and (d) Kerguelen (Indian Ocean).

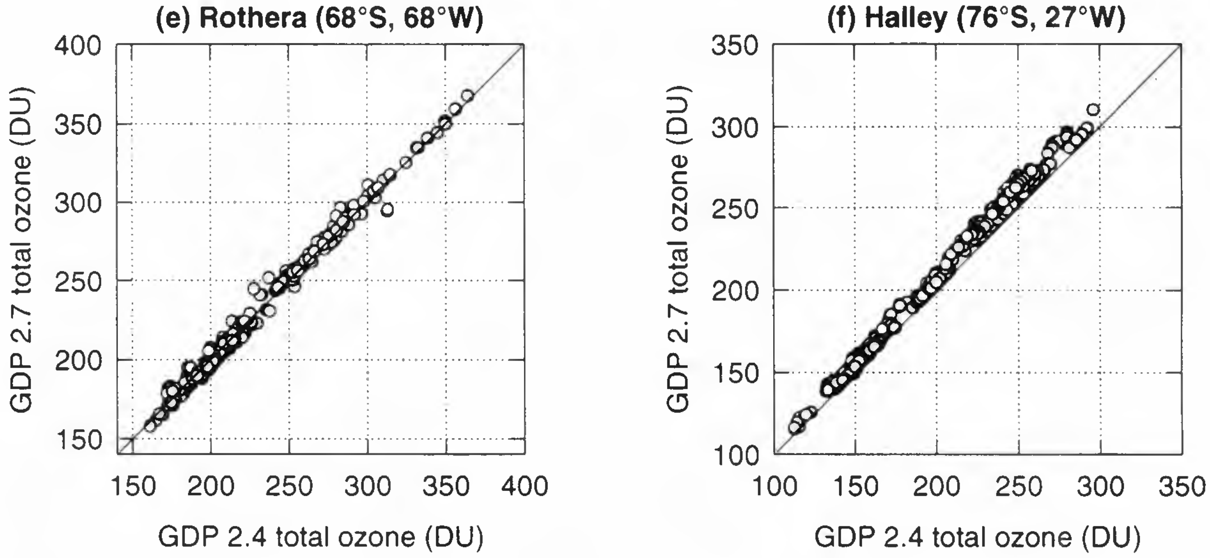


Figure 4-3. (continued) Correlation of GOME ozone vertical column amounts derived with GDP 2.4 and GDP 2.7 at the Antarctic NDSC stations of (e) Rothera and (f) Halley.

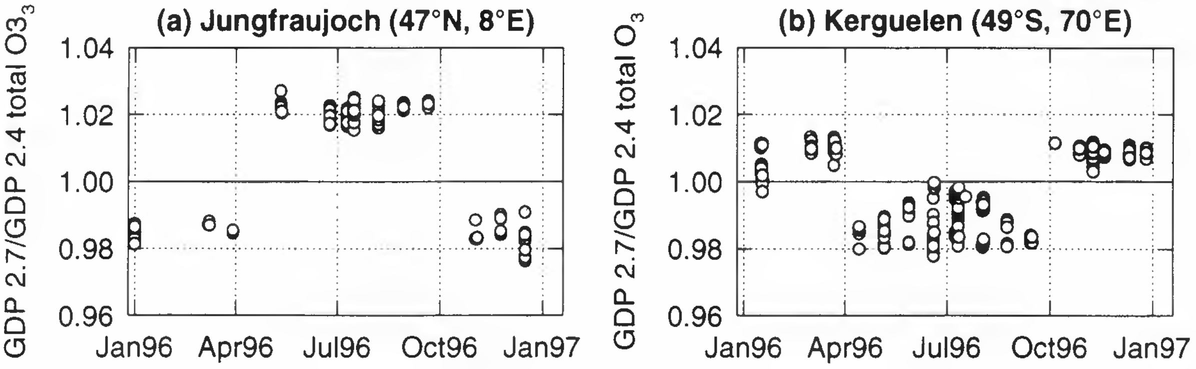


Figure 4-4. Ratio of GDP ozone vertical columns at the mid-latitude NDSC stations of (a) the Jungfraujoch (Swiss Alps) and (b) Kerguelen Island (Indian Ocean).

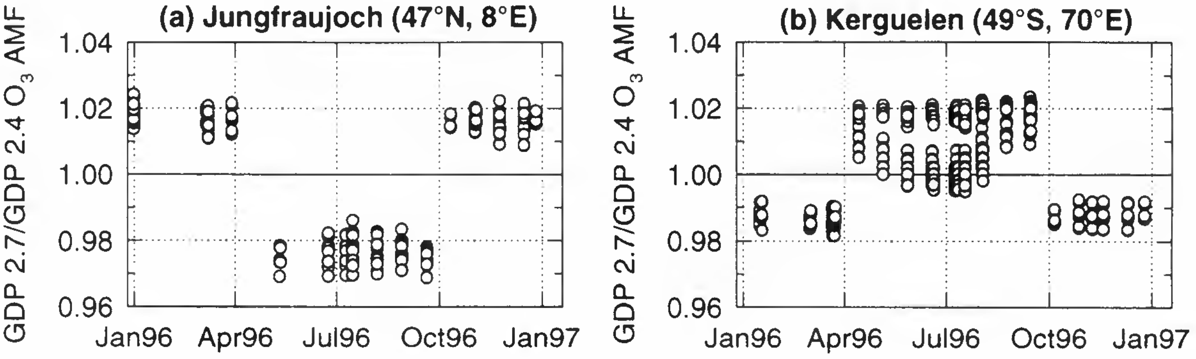


Figure 4-5. Ratio of GDP ozone air mass factors at the same mid-latitude stations as in Figure 4-4.

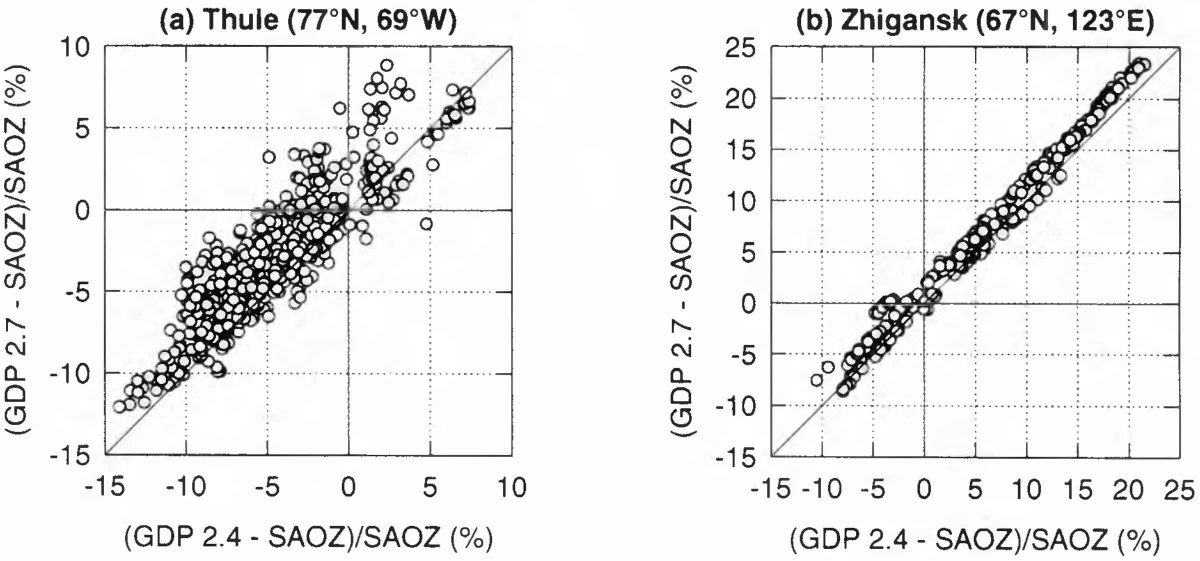


Figure 4-6. Change in the agreement between GDP and NDSC total ozone: correlation of the relative difference at the Arctic NDSC sites of (a) Thulé (Western Greenland) and (b) Zhigansk (Eastern Siberia). The mean agreement has improved at Thulé but has deteriorated at Zhigansk, at both sites by a few percent.

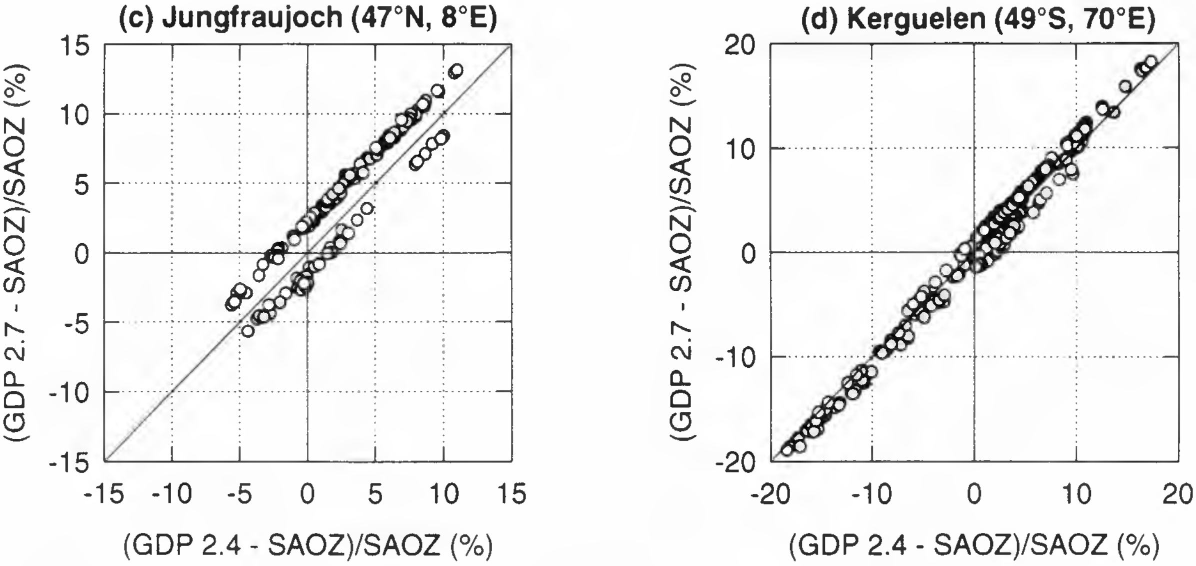


Figure 4-6. (continued) Correlation at the mid-latitude NDSC sites of (c) the Jungfraujoch (Swiss Alps) and (d) Kerguelen Island (Indian Ocean). The wider range of difference values at Kerguelen arises partly from the SZA and column dependence of GDP data, which is observed already at 49°S but not discernible at 47°N yet.

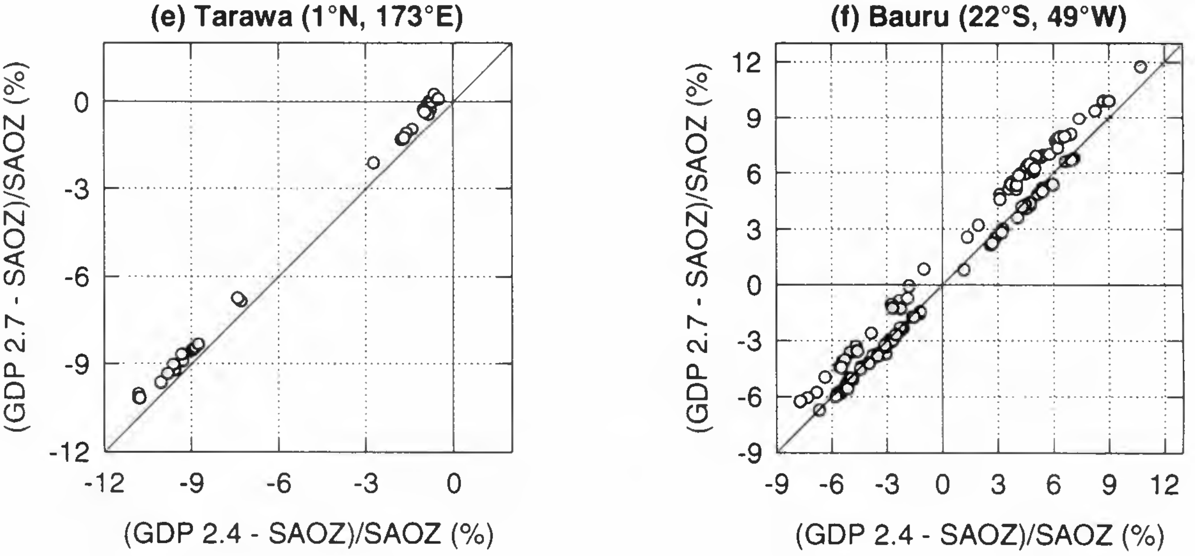


Figure 4-6. (continued) Correlation at the equatorial and tropical NDSC sites of (e) Tarawa (Central Pacific) and (f) Bauru (Brazil).

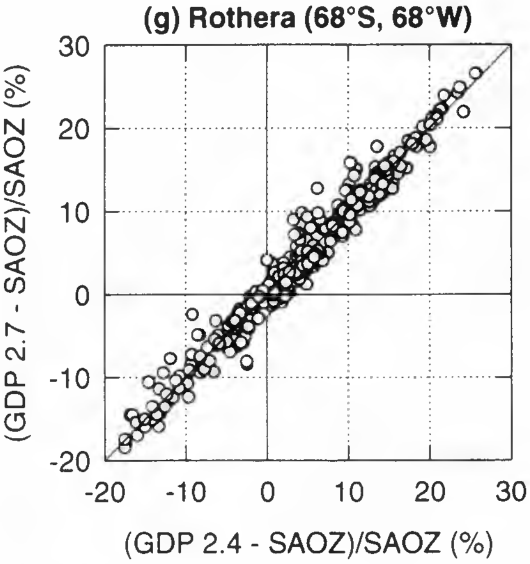


Figure 4-6. (continued) Correlation at the Antarctic NDSC site of Rothera.

Solar zenith angle dependence

No significant change of the solar zenith angle dependence is expected from current GDP upgrades. This is confirmed in Figure 4-7 where mid-morning (moderate SZA) and midnight sun (high SZA) GOME data are compared with ground-based measurements in the Artcic summer.

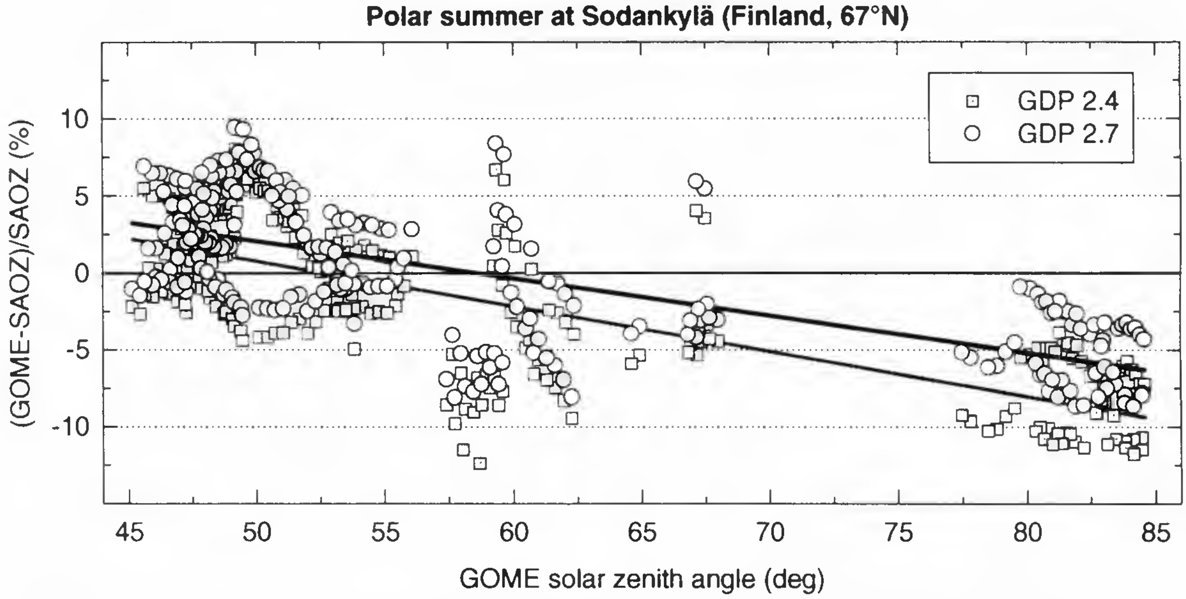


Figure 4-7. Percent relative difference between GOME (GDP 2.4 and 2.7) and SAOZ total ozone in Arctic summer as a function of the GOME solar zenith angle (SZA). Using ground-based data as a transfer, the systematic bias of -8% between GDP 2.4 data at moderate (mid-morning) and high (midnight Sun) SZA persists with GDP 2.7.

Total column dependence

Figure 4-8 show the column dependence of GDP total ozone compared to NDSC data in the springtime Antarctic ozone hole, where the ozone column range is the widest. Although the overestimation of low columns seems to persist with GDP 2.7, the scarcity of the current data set prevents from accurate investigation. However, some information can be retrieved from the correlation between GDP 2.7 and 2.4 total ozone data. Figure 4-3 shows such correlation at the Arctic and Antarctic Polar Circles and at the Southern Tropics. Several trails appear in the correlation plots, which are associated with similar GDP AMF shifts as those appearing in Figure 4-4. However the straight and the slope of the various correlation lines are consistent over an extended range of total ozone values including the lowest and highest values. This consistency indicates that the two versions of GDP exhibit the same sensitivity to the ozone column. This is also to be expected according to the changes from GDP 2.4 to 2.7. Hence it can be concluded that the ozone column dependence of GOME total ozone data persists with GDP 2.7.

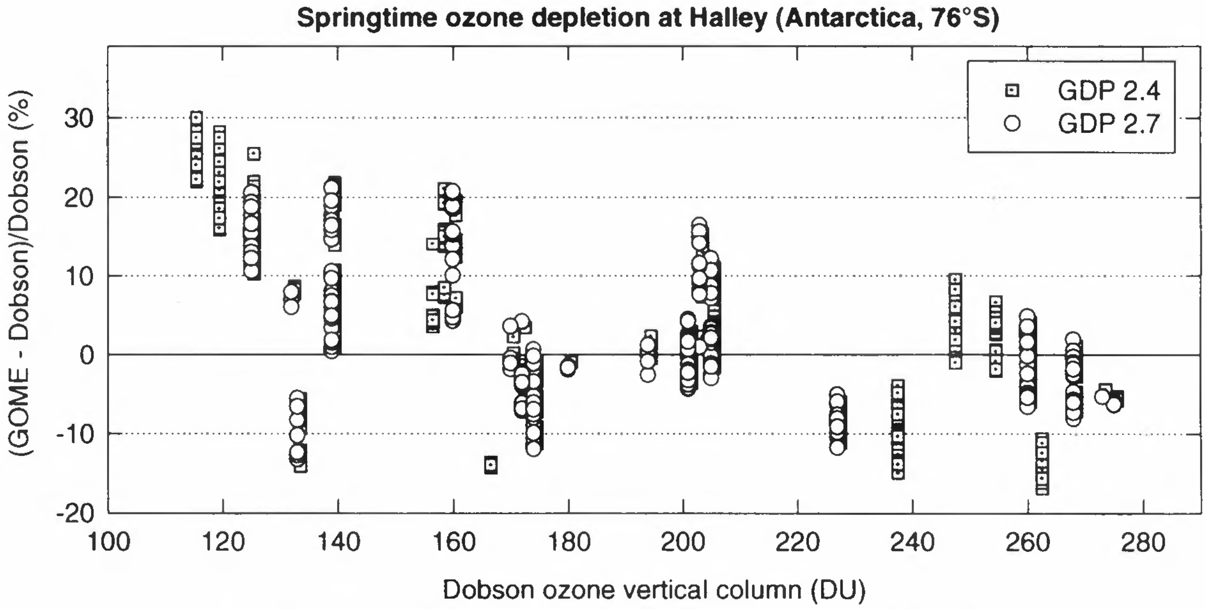


Figure 4-8. Percent relative difference between the GOME (GDP 2.4 and 2.7) and Dobson total ozone during springtime ozone depletion at the Antarctic station of Halley (76°S), as a function of the Dobson ozone column. The overestimation of low ozone column values by GDP 2.4 persists with GDP 2.7.

4.2. Total nitrogen dioxide

Cross-correlation of GDP nitrogen dioxide data along track

Figure 4-9 depicts GDP 2.4/2.7 NO_2 data along track for two individual orbits in February (60215135.lv2 data file) and June (60607153.lv2) 1996. The two orbits contain most of the interesting features identified in the 24 orbits studied here. Although spatial structures along track look similar, changes in the vertical column are clearly visible for all orbits. Total NO_2 values increase from a few 10^{14} molec.cm^{-2} at the poles to several 10^{15} molec.cm^{-2} at low latitudes. Negative and out-of-range values frequently observed in subtropical GDP 2.4 data have mostly disappeared with GDP 2.7. However irrelevant values persist in the South Atlantic Anomaly (SAA) as shown in the February orbit which overpasses the SAA area. At middle and high latitudes, the improvement is noticeable although less striking. The scatter along track at low latitudes has somewhat decreased but it is still enhanced.

Changes in the vertical columns are linked essentially to changes in the slant columns, as confirmed by the obvious similarity between ratios of the vertical column amounts (panels c and h of Figure 4-9) and ratios of the corresponding slant column amounts (panels d and i). Changes in the air mass factor account only for a maximum of about 2%.

Comparison with NDSC ground-based data

The general increase of NO_2 values derived with GDP 2.7 improves not only the consistency of the GOME total NO_2 data product at low latitudes but also its agreement with correlative NDSC/UV-visible data. Figure 4-10 shows evidence that mid-morning GOME data fit now much better between sunrise and sunset values reported by ground-based NDSC instruments and by the space-based HALOE. Subtropical GDP 2.7 total NO_2 is also in better agreement with NO_2 levels reported in the literature (e.g., Noxon, 1979; Denis *et al.*, 1997; Senne *et al.*, 1996). At the equatorial and tropical stations of Tarawa and Bauru (Figure 4-10-a,b), small seasonal and day-to-day variations typical of those latitudes are well reproduced. Although still high for such stations, the scatter within 500 km has somewhat decreased from about 2.10^{15} molec.cm^{-2} to less than 10^{15} molec.cm^{-2}. At Bauru, the seasonal variation is well reproduced and the mean agreement is reasonable but here GOME data are dramatically affected by measurement problems linked to the situation of the station near the South Atlantic Anomaly of the radiation belts.

At higher latitudes in the Southern Hemisphere, a reasonable consistency had been reported with GDP 2.4, although GDP 2.4 data had been found to underestimate systematically NDSC values. Again, the general increase in total NO_2 yielded by GDP 2.7 improves the agreement with NDSC data (Figure 4-11). The improvement appears clearly at all southern mid-latitude stations where GOME data lay now between sunrise and sunset values reported by other instruments. The improvement is less striking at high latitudes but still noticeable. Some outlying GDP data are detected during polar summer under midnight sun conditions, which are associated with high SZA measurement. Similar outlying data are detected in the Arctic summer. It is not clear whether they can be attributed to the real diurnal variation of NO_2 or to any retrieval artefact such as SZA dependence.

Similarly, the increase in NO_2 levels yielded by GDP 2.7 seems to improve somewhat the overall agreement at high latitudes in the Northern Hemisphere (Figure 4-12).

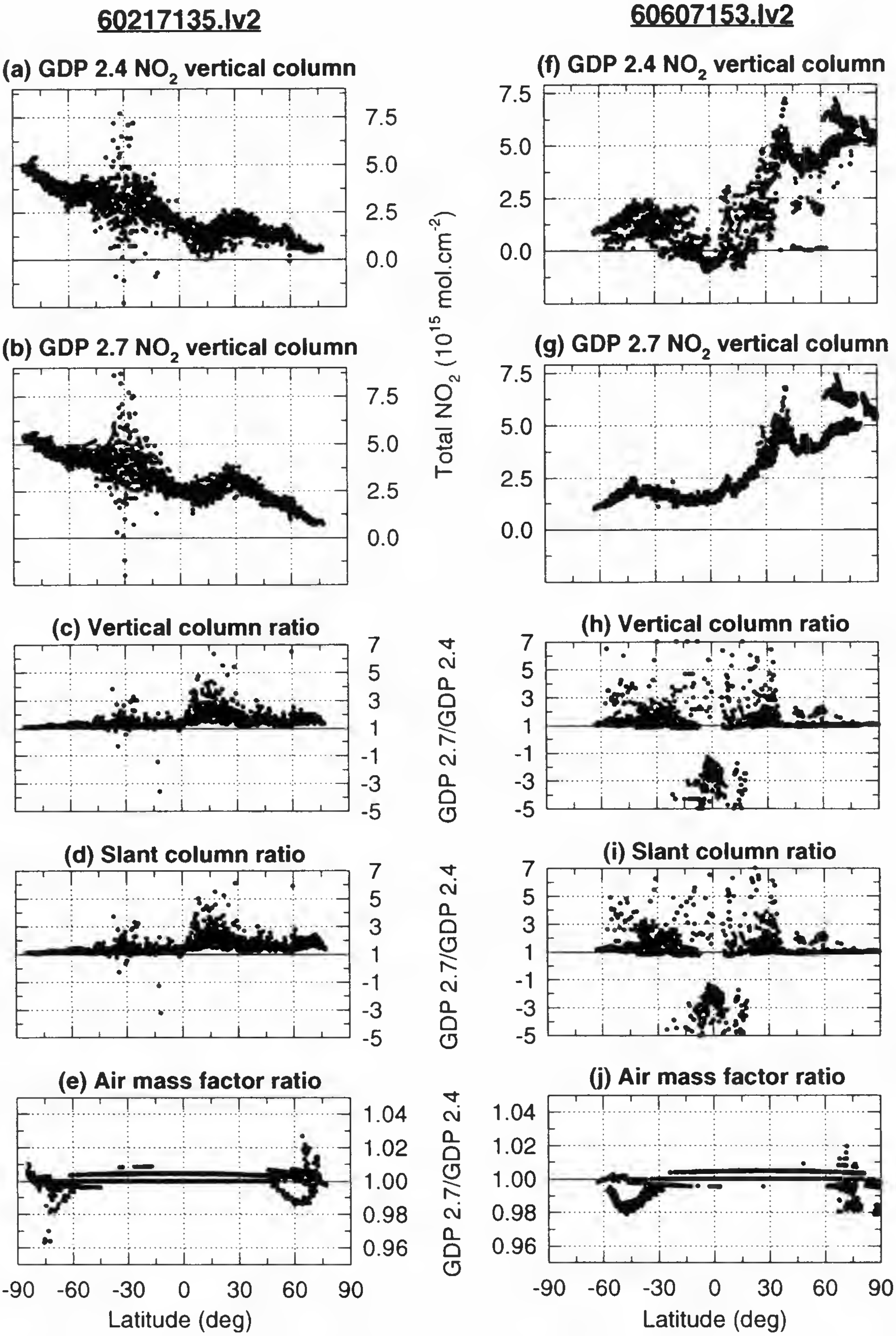
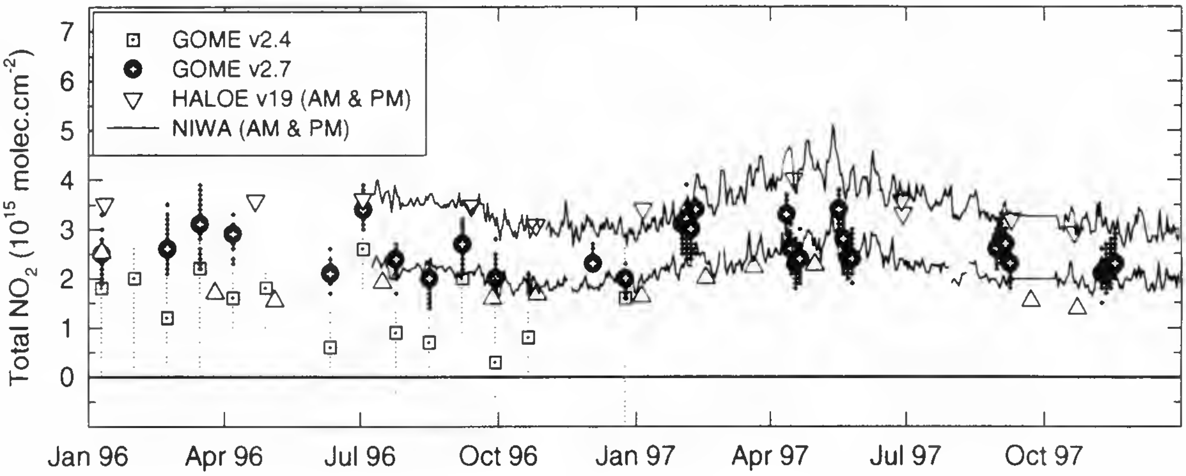
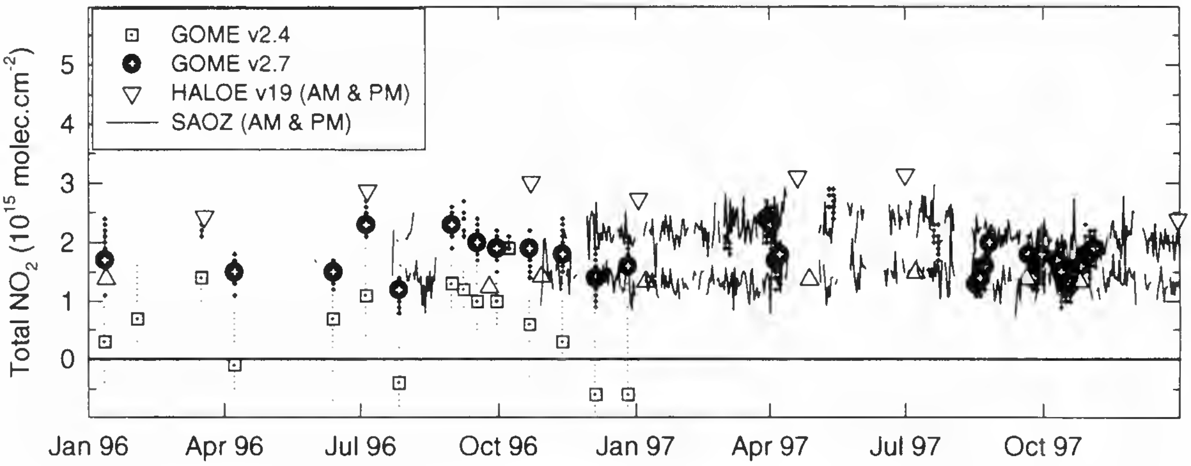


Figure 4-9. Comparison of GOME nitrogen dioxide data derived with GDP 2.4 and GDP 2.7 for two individual orbits in 1996: GDP 2.4 (a,f) and GDP 2.7 (b,g) NO_2 vertical column amounts; and GDP 2.7/GDP 2.4 ratio of : (c,h) NO_2 vertical columns; (d,i) slant columns; and (e,j) air mass factors. (a-e): orbit 60217135.lv2 of February 17 and (f-j): orbit 60607153.lv2 of June 7.

(a) Tropic of Cancer: Mauna Loa (Hawaii, 20°N)



(b) Equator: Tarawa (Kiribati, 1°N)



(c) Tropic of Capricorn: Bauru (Brazil, 22°S)

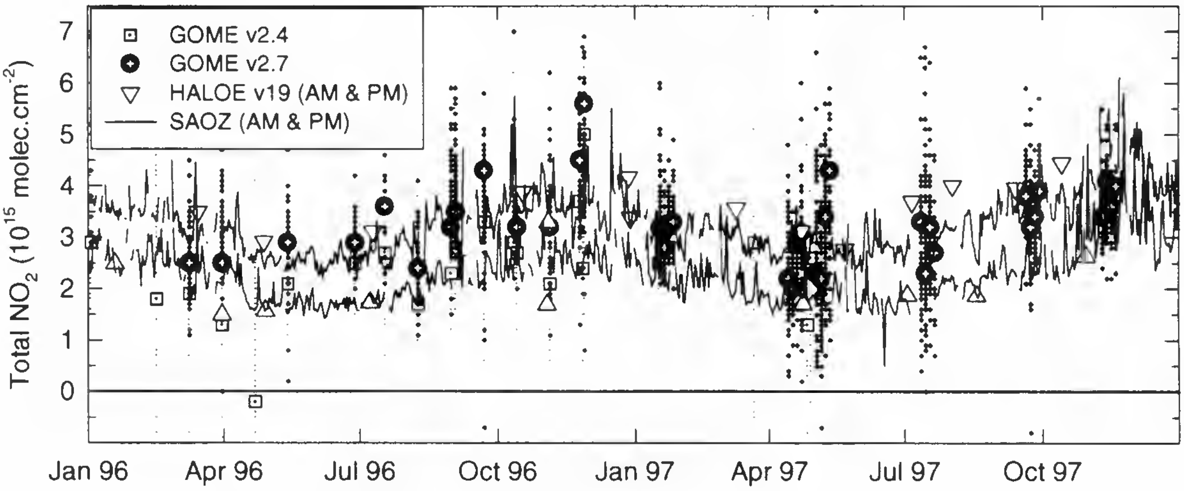
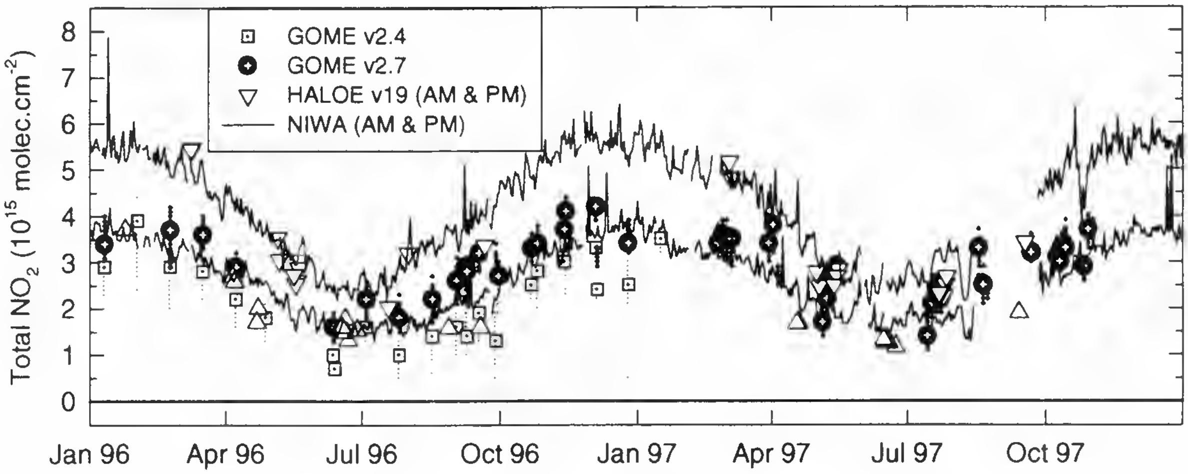
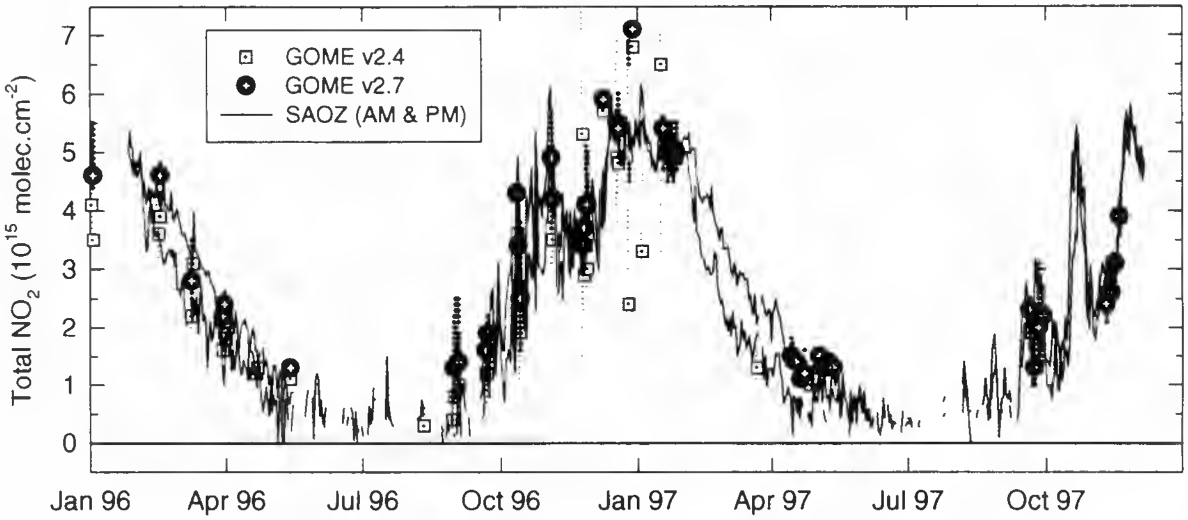


Figure 4-10. GOME GDP 2.4 and 2.7 (large symbols: average of closest five ground pixels; small dots: all individual pixels within 500 km), HALOE (integrated stratospheric profiles completed by modelled tropospheric column) and NDSC (NIWA and SAOZ UV-visible data) total NO_2 at low latitudes. The general improvement gained with GDP 2.7 is obvious at Mauna Loa (a) and Tarawa (b). At Bauru (c), GOME data are affected by measurement problems linked to the South Atlantic Anomaly and by tropospheric pollution events.

(a) Lauder (New Zealand, 45°S)



(b) Rothera (Antarctic Peninsula, 68°S)



(c) Arrival Heights (Antarctica, 78°S)

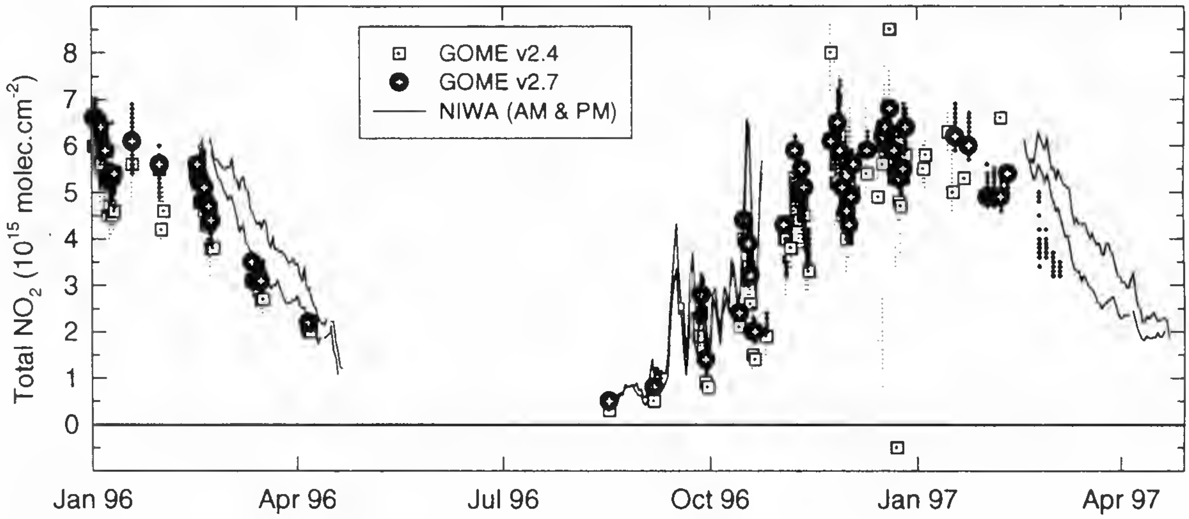
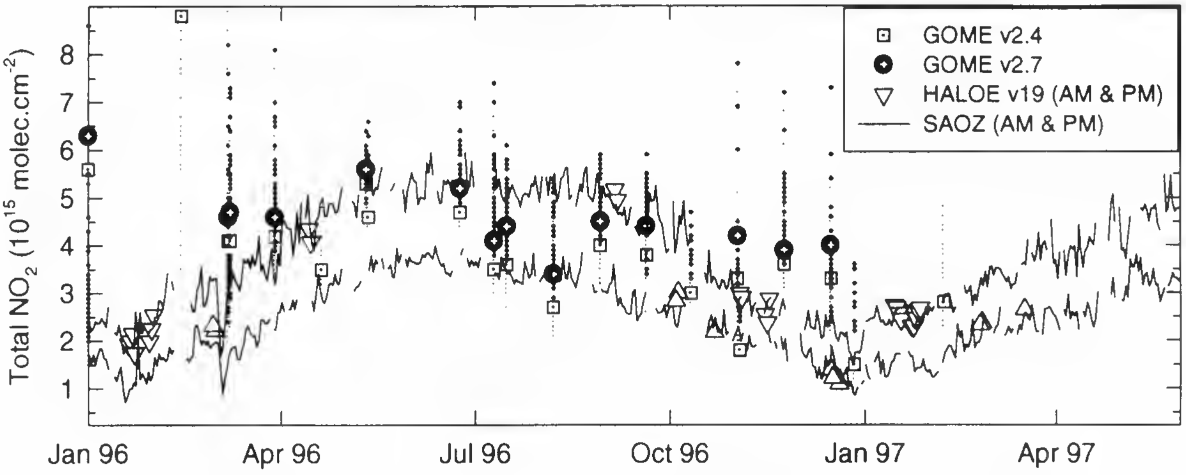
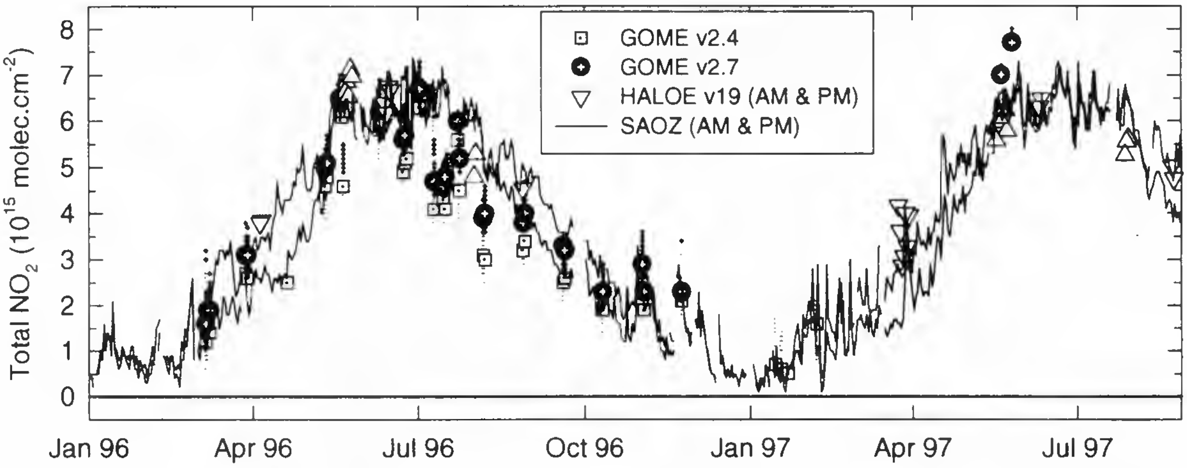


Figure 4-11. Same as Figure 4-10, but at higher latitudes in the Southern Hemisphere.

(a) Jungfraujoch (Swiss Alps, 47°N)



(b) Sodankylä (Finland, 67°N)



(c) Thulé (Western Greenland, 77°N)

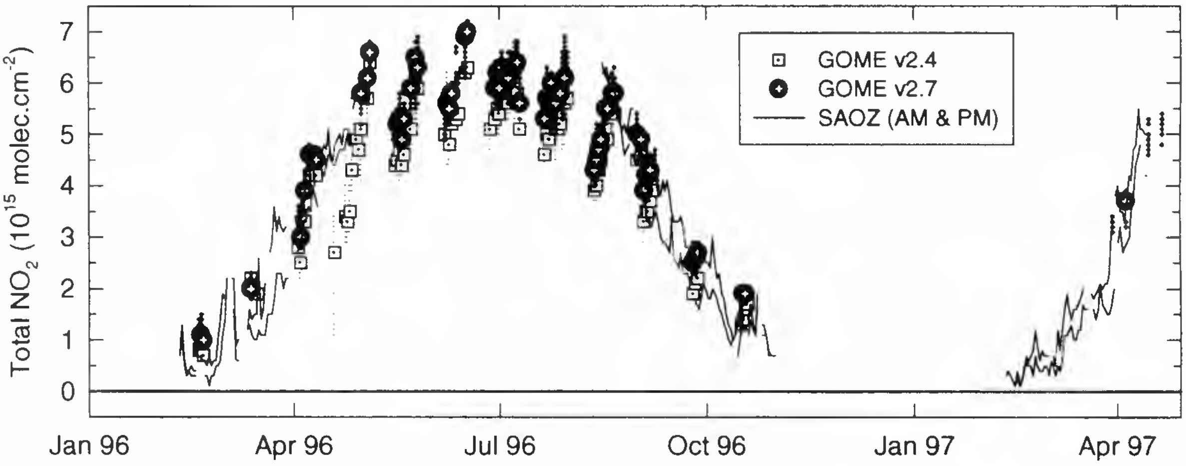


Figure 4-12. Same as Figure 4-10, but at higher latitudes in the Northern Hemisphere. Outlying GDP data observed during polar summer are associated with midnight sun conditions, that is, at low sun elevation.

While the improvement is general in the Southern Hemisphere and at high and low latitudes in the Northern Hemisphere, the situation is much less clear at northern middle latitudes. The consistency between GOME and NDSC data at northern middle latitudes was already a matter of concern with GDP 2.4. Figure 4-12-a shows that the general NO_2 increase from GDP 2.4 to 2.7 deteriorates the mean agreement with ground-based UV-visible and satellite HALOE observations. Figure 4-13 shows that the use of ground-based FTIR measurements selected strictly within 1.5 hour around the GOME overpass does not improve the comparison: the agreement seems better in summer but deteriorates in spring and fall. The particular behaviour of GOME over mid-latitude Western Europe might reflect the enhanced sensitivity of its measurement to tropospheric pollution while all the other techniques are mainly sensitive to the stratosphere. The accuracy of GDP NO_2 AMF under polluted conditions is also known to be very poor. Problems related to the ground albedo might be argued for a high altitude station such as the Jungfraujoch, but similar results are obtained at the middle latitude sites of Aberystwyth and OHP (this study), Zvenigorod (Timofeyev *et al.*, this issue), and Bremen (Richter *et al.*, this issue), where high albedo due to snow is less frequent. Further investigation of GOME data quality at northern mid-latitudes is needed.

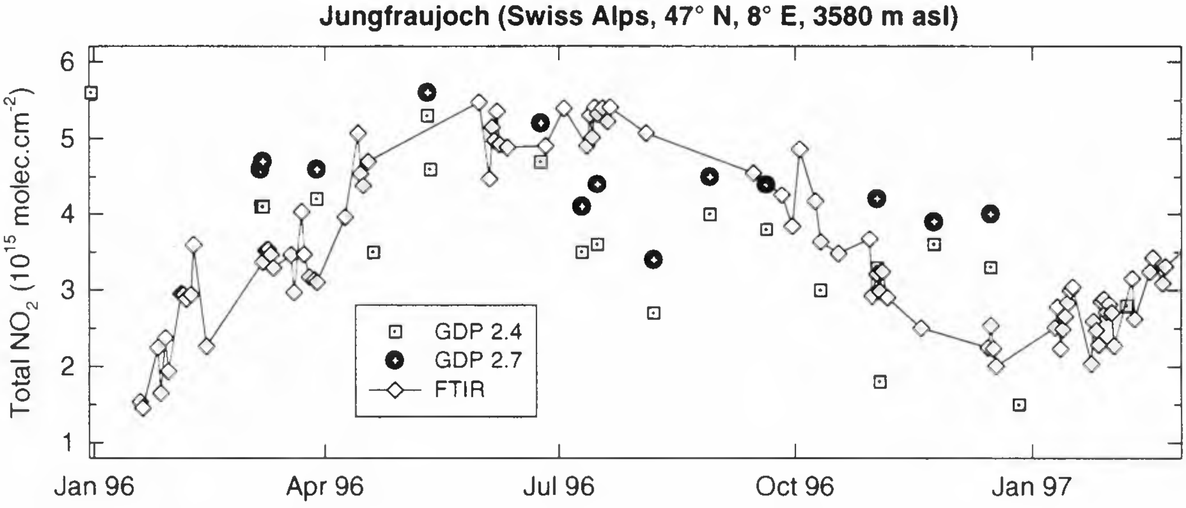


Figure 4-13. Comparison of mid-morning total nitrogen dioxide at the Jungfraujoch derived from GOME data (GDP 2.4 and 2.7) and from FTIR measurements. GOME and FTIR observations depicted in the figure do not differ by more than 1.5 hour.

5. Consistency of GDP atmospheric database for ozone air mass factors

The accuracy of the GOME total ozone depends on the atmospheric database used in the retrieval. Air mass factors are known to be sensitive to the vertical distribution of the atmospheric constituents controlling the path of the solar radiation through the atmosphere. In addition, temperature-dependent ozone absorption cross-sections used in the DOAS fitting of GOME spectra are taken at the temperature of the ozone density maximum, a quantity that is also retrieved from the atmospheric database. Any uncertainty in the temperature should affect the accuracy of the retrieved slant column amounts rather than the quality of the spectral fitting since the temperature effect on the absorption cross-sections consists of a scaling of the differential structures rather than a spectral distortion. In the present section, extended ozonesonde data records at various NDSC stations have been used to investigate how the GDP atmospheric profiles database impacts on GOME ozone AMFs. Multiple scattering AMFs have been calculated with the IASB AMF processor (Lambert *et al.*, 1999d, 2000) based on a pseudo-spherical adaptation of DISORT (Dahlback and Stamnes, 1991).

5.1. Ozone, pressure and temperature profiles

Contributing ozonesonde data records are listed in Table 5-1. Flights with uncertain data quality or too low burst altitude have been omitted in the study. At altitudes beyond burst point, ozone, pressure and temperature profiles have been extended by means of the COSPAR Reference Atmosphere. Monthly means of ozone-weighted average temperature, or effective ozone temperatures, have also been calculated at representative stations, data set permitting.

Station	**Location**	**Latitude**	**Institute**	**Flights**	**Years**
Ny-Ålesund	Spitsbergen	79°N	AWI	256	1994-1998
Thulé	Western Greenland	77°N	DMI	110	1993-1998
Bear Island	Arctic Norway	74°N	NILU	121	1993-1997
Scoresbysund	Eastern Greenland	70°N	DMI	223	1994-1998
Sodankylä	Finland	67°N	FMI	274	1994-1998
Yakutsk	Eastern Siberia	62°N	CAO	117	1995-1998
Gardermoen	Southern Norway	60°N	NILU	172	1994-1998
Aberystwyth	Wales	52°N	U. Wales	177	1994-1998
Debilt	Netherlands	52°N	KNMI	125	1995-1997
Uccle	Belgium	51°N	IRM-KMI	230	1994-1997
Hohenpeißenberg	German Alps	48°N	DWD	625	1991-1998
Payerne	Swiss Alps	47°N	SMI, ETH	612	1991-1998
OHP	French Alps	44°N	CNRS	120	1993-1997
Saint-Denis	Reunion Island	21°S	CNRS, LPA	20	1993-1994
Lauder	New Zealand	45°S	NIWA	208	1994-1996
Dumont d'Urville	Antarctica	66°S	CNRS	123	1990-1997

Table 5-1. Characteristics of NDSC ozonesonde data records contributing to the present study: station name, geographical location, latitude, responsible institute, number of selected flights, and time period. Note that launches concentrate in winter and spring for several high latitude sites.

Figure 5-1 shows climatological ozone and temperature profiles derived from ozonesonde data at two northern stations. Corresponding profiles retrieved from the GDP database (MPI profiles) are depicted for comparison. The agreement between the two data sets is clearly questionable and raises some concern about the accuracy of the AMFs. Similar differences are observed at other stations and latitudes. Compared to the effective ozone temperatures also depicted in Figure 5-1, mean temperatures at the ozone density maximum derived from MPI profiles would be too low in the springtime Alps and too high in the wintertime high Arctic by more than 5 K. More generally, confrontation of GDP atmospheric databases with real data reveal uncertainties which might impact on the accuracy of both the ozone slant column fitting and the conversion to vertical columns.

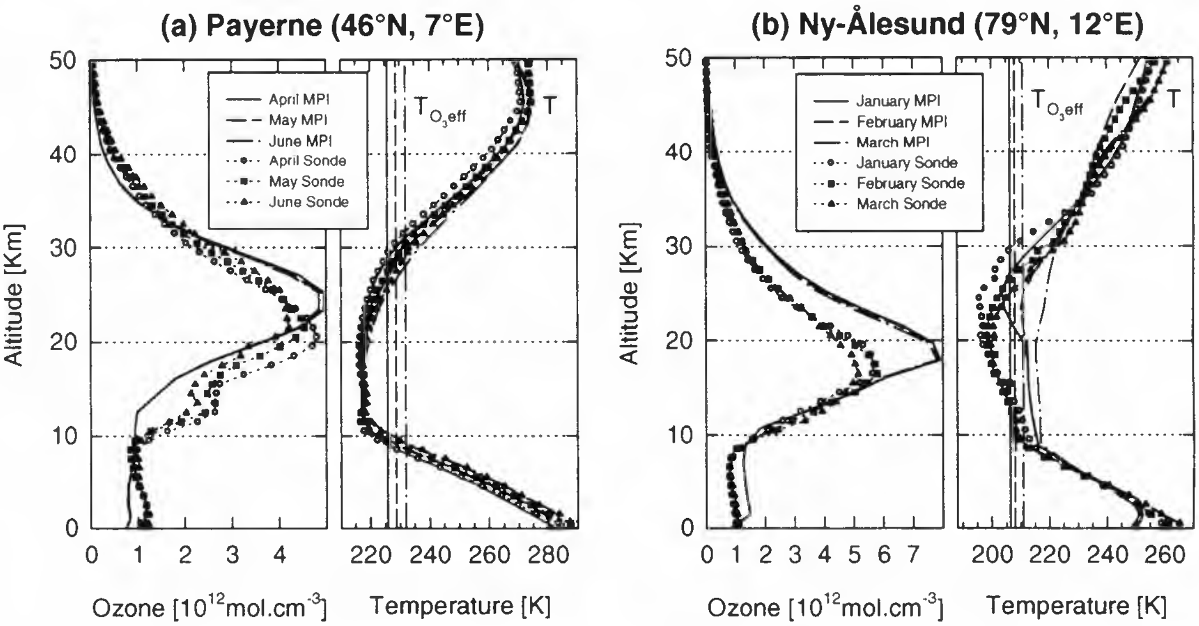


Figure 5-1. Climatological ozone and temperature profiles at Payerne (Swiss Alps) in springtime and at Ny-Ålesund (Spitsbergen) in wintertime, and corresponding profiles retrieved from the GDP database (MPI profiles). Effective ozone temperatures are also depicted for comparison with the temperature at the ozone density maximum.

5.2. Geophysical consistency of GDP air mass factors at middle latitudes

GOME AMFs have been calculated at IASB with the current GDP profile database and the ozonesonde data records. Figure 5-2 shows the comparison of GDP-based AMFs with AMFs based on 612 ozonesonde measurements at Payerne. While GDP AMFs and ozonesonde AMFs are in excellent agreement on a yearly average (better than 1%), striking shifts of about 5% and 3% occur on April 1 and October 1, respectively. Smaller shifts of less than 1% are also discernible on the first of January and of July. These shifts are obviously associated with each change of the reference ozone profile in GDP and demonstrate the need to improve the GDP profile database. They combine with those associated with other 3-month changes of reference parameters (e.g., multiple scattering correction of the AMF, or surface albedo) to generate the 3-month shifts observed in the GDP 2.4 total ozone data record. It is anticipated that the GDP 2.7 data record will be affected by a similar internal inconsistency.

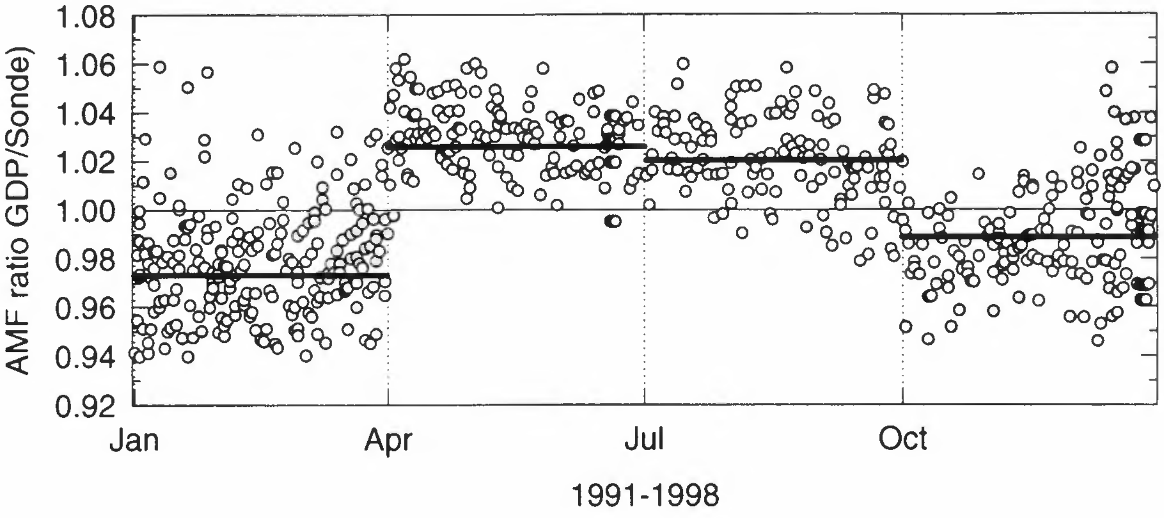


Figure 5-2. GOME ozone air mass factor at Payerne (Swiss Alps, 46°N): ratio of nadir AMFs calculated at 325 nm and at actual GOME solar zenith angle with: (i) atmospheric profiles used by GDP; and (ii) individual ozonesonde measurements from 1991 through 1998. Seasonal means of the ratio are depicted.

Shifts are inherent to the way seasonal changes of parameters are implemented in GDP. For parameters varying smoothly with time, geophysically consistent interpolation procedures are recommended instead of the current coarse substitutions.

Figure 5-2 addresses another issue related to the GDP retrieval design. The scatter around the mean behaviour of about 2% in the Alps – and more at higher latitudes and larger solar zenith angles (see next section) – points out a geophysical limitation of the static approach adopted in GDP for the calculation of GOME AMFs. Even with a profile database reflecting at best the seasonal and latitudinal variation of atmospheric constituents, the AMF evaluation based on single profiles can not account for day-to-day fluctuations of the actual profiles. Therefore an iterative approach using some profile information derived from GOME spectral data is recommended.

5.3. Seasonal variation of GDP air mass factors

Figure 5-3 compares the seasonal variation of the GOME AMF as deduced from the GDP atmospheric database and from the ozonesonde data records. The seasonal variation of the AMF combines the effect of changes in the ozone, pressure and temperature profiles with the seasonal variation of the GOME SZA. The AMF based on monthly mean ozonesonde data exhibits a seasonal variation of 3%-4% in the Alps and of a few percent more in the Arctic, with a maximum in summer-fall and a minimum in winter-spring. The seasonal variation of the AMF calculated with the monthly mean profiles used by GDP is much more pronounced, reaching 15% in the high Arctic. The phases are consistent in the Arctic but opposite in the Alps. Compared to climatological AMFs based on real profile measurements, AMFs based on the GDP profile database would introduce an erroneous seasonal signature in the GDP ozone vertical columns of about 5% of amplitude in the Alps and 8% in the Arctic.

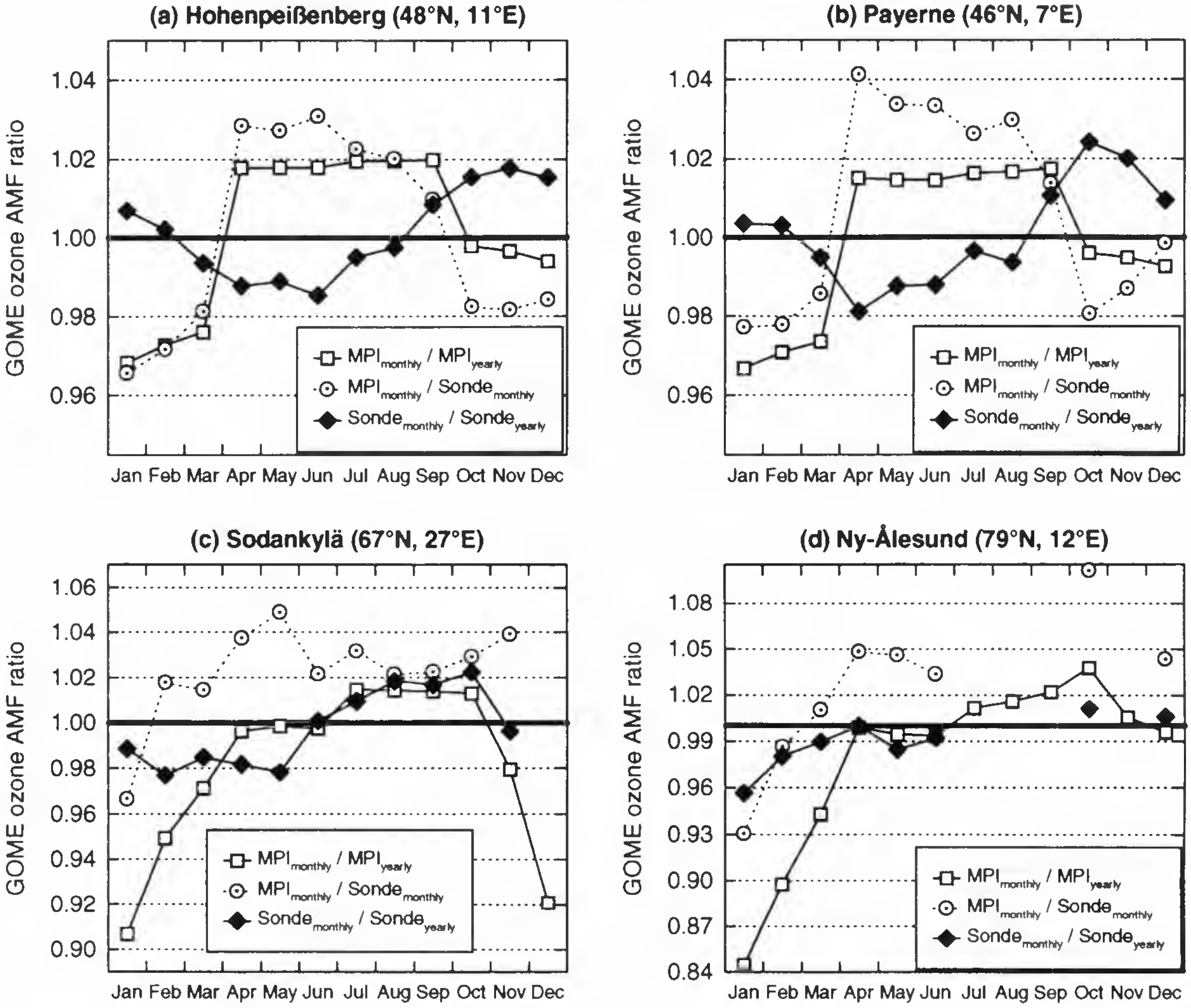


Figure 5-3. Seasonal variation of GOME ozone air mass factors at (a) Hohenpeißenberg, (b) Payerne, (c) Sodankylä, and (d) Ny-Ålesund: ratio of nadir AMFs calculated at 325 nm and at monthly mean mid-morning GOME solar zenith angle, with monthly mean and yearly mean atmospheric profiles derived from the MPI database used in GDP and from ozonesonde data.

5.4. Solar zenith angle dependence

In Figure 5-4, GDP ozone air mass factors are compared to GOME AMFs calculated at the Arctic Polar Circle station of Sodankylä using 274 individual ozonesonde profiles acquired from 1994 through 1998. The comparison is presented as a function of time and of the GOME solar zenith angle. At low and moderate SZA, GDP AMFs are found to overestimate ozonesonde AMFs by a few percent on average. Beyond 70°, this average overestimation increases with the SZA. The standard deviation of about 3% below 70° SZA increases rapidly beyond 70° due to the enhanced sensitivity of the AMF to the actual atmospheric profiles. Again, this scatter illustrates the limitation of the static AMF calculation approach adopted in GDP. A remarkable feature is the bias of about 8% appearing in spring and summer between AMF ratios at moderate (mid-morning) and high (midnight sun) SZA. This bias compares quite well with the systematic 8% bias reported between mid-morning and midnight sun GOME total ozone at all stations in the Arctic. This latter finding stress the need for refinement of the atmospheric database as a further improvement of GDP.

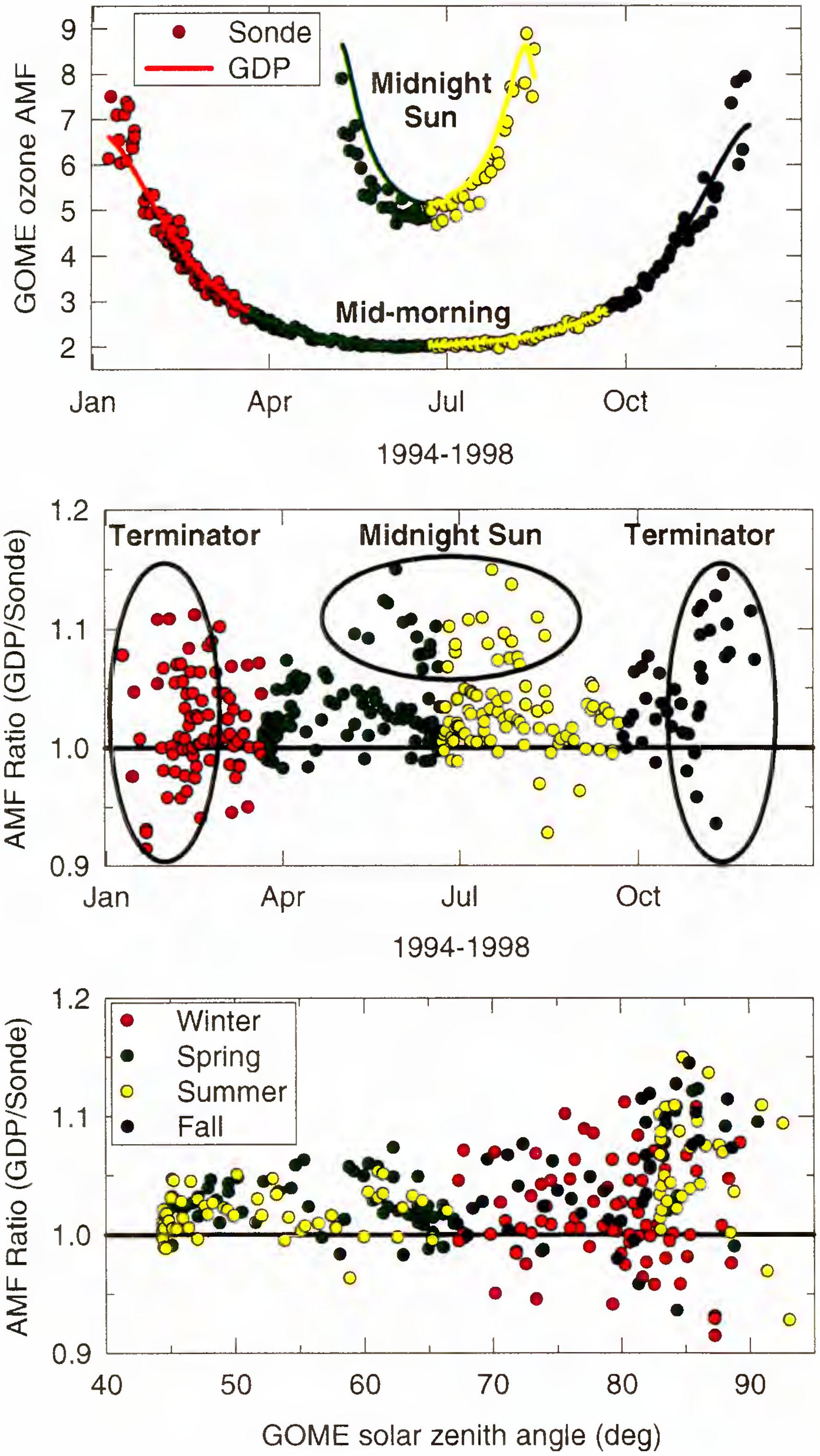


Figure 5-4. Comparison of GOME ozone air mass factors at Sodankylä on the Arctic Polar Circle, calculated with individual ozonesonde profiles and with the GDP database. Upper panel: seasonal variation of the AMF; middle panel: seasonal variation of the ratio of GDP AMFs to ozonesonde AMFs; lower panel: solar zenith angle dependence of the GDP/ozonesonde AMF ratio. Data points corresponding to high solar zenith angle (summer midnight sun and winter terminator) are identified in the middle panel.

6. Conclusions

6.1. Total ozone

Cross-correlation studies of GDP data and comparisons with NDSC measurements indicate that GDP upgrades from version 2.4 to 2.7 should not affect dramatically the total ozone data product. Except at the poles where somewhat larger differences can be observed, total ozone changes generally fall within a few percent and are mainly related to changes in the AMF calculation. The mean agreement with ground-based measurements seems to have barely changed. At several latitudes the deterioration of the agreement during one season is compensated by an improvement of similar amplitude during the other season. Major problems – such as the SZA/column/latitude dependence of the GDP total ozone – remain, for which possible solutions are known.

GDP AMF data exhibit unphysical features such as temporal shifts and peculiar latitudinal patterns. AMF aberrations propagate similar geophysical inconsistencies directly in the GDP total ozone data record. AMF shifts and patterns are inherent to the way seasonal and spatial changes of radiative parameters are implemented in GDP. For parameters varying smoothly with time and latitude, geophysically consistent interpolation procedures are recommended instead of the current coarse substitutions.

An AMF study based on extended ozonesonde data sets has demonstrated the urgent need to revisit the GDP atmospheric profile database. The current database might generate uncertainties in both the fitting of slant column amounts and their conversion to vertical columns. Among others, it might contribute significantly to the GOME SZA dependence at low sun elevation and to seasonally varying biases at all latitudes. The AMF study emphasises also the limits of the static approach adopted in GDP for the calculation of the GOME AMF.

6.2. Total nitrogen dioxide

Cross-correlation studies of GDP data and comparisons with NDSC and HALOE measurements indicate that GDP upgrades from version 2.4 to 2.7 yield more consistent slant and total NO_2 data sets. Negative and out-of-range values have mostly disappeared, except within the South Atlantic Anomaly. Although reduced, the pixel-to-pixel and day-to-day variations in total NO_2 remain higher than the variability observed from the ground. Changes in NO_2 AMFs are insignificant compared to changes in slant columns.

A general increase of GDP NO_2 slant columns is noted which improves considerably the agreement with ground-based and HALOE measurements especially in the Tropics. To a lesser extent, the improvement is also observed at higher southern latitudes and in the Arctic. The situation is less clear at northern middle latitudes where further investigation based on larger data sets is needed.

Despite the striking progress of the GDP NO_2 data product, it still needed to improve the GDP NO_2 database with seasonal/latitudinal stratospheric features and a consistent tropospheric background to get accurate AMFs under unpolluted conditions. Accurate AMF evaluation under polluted conditions remains a real matter of concern.

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DELTA CHARACTERISATION OF GOME DATA PRODUCTS WITH THE RUSSIAN MONITORING NETWORK

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1. Introduction

Comparing satellite measurements of different atmospheric parameters with a data of independent observations provides a real estimation of satellite measurements quality. These investigations are the essential part of monitoring of atmosphere. Taking into account the high accuracy of total ozone and other trace gases measurements, required in atmospheric physics and chemistry, such comparisons play the great role in the development of satellite measurements' processing and improve remote sensing accuracy. Of special importance is the problem of validation with respect to the tasks of long-term monitoring of atmosphere. For that purposes it is necessary to perform an inter-calibration of different measuring systems (ground-based, sonde, airplane, and satellite), that makes possible to combine data from different sources e.g., for the trend analysis of different gases.

The accuracy of satellite atmospheric measurements depend on many factors. On account of that the comparisons between satellite data and independent measurements should be performed under different conditions (different seasons, latitude zones, Sun zenith angle, etc.). Such investigations may help to separate the influence of different factors and find the way to improve processing of measurements.

Numerous validation studies were performed within the GOME project on board the ERS-2 satellite, as well. The main goal of that experiment is to determine the global distributions of total ozone and NO_2 contents. The validation of GOME total ozone measurements over the

Russia was accomplished on the base of comparisons with observations from the ground-based ozonometric network; these studies were later expanded on the NO_2 total content measurements. Before presenting results of the new comparisons in the framework of WP 2000-3200 it is necessary to give a brief description of Russian ground-based system of atmospheric monitoring and the results of previous Russian validation studies.

2. Russian (and CIS) ground-based stations for measuring the atmospheric trace gases

The Network for the Detection of Stratospheric Change (NDSC) is the most perspective to validate satellite measurements of atmospheric composition. The NDSC is the international program joining the ground-based stations equipped with standardized set of the most recent devices for remote sensing of the atmosphere from the Earth surface which were mutually compared and calibrated.

None of the Russian observing stations has the instrumentation system necessary for the primary NDSC station. By the early 1997, the visible spectrometers placed at Zvenigorod Scientific Station (55.42°N, 36.47°E; 200 m above see level) of the Institute of Atmospheric Physics RAS (IAP RAS) and at Zhigansk station (67.42°N, 123.0°E) of the Central Aerological Observatory (CAO) were involved in the NDSC as the secondary means. In September 1997, a number of visible spectrometers participated in International Comparisons with primary spectrometer of the Lauder station (New Zealand) and will be used as the secondary means of the NDSC for measuring the NO_2 content. These spectrometers are placed at the following stations (Figure 1): Kislovodsk Mountain Scientific Station (43.73°N, 42.66°E, 2070 m), of the Institute of Atmospheric Physics RAS; Tomsk Station (56.47°N, 84.95°E, 280 m) of the Institute of Atmospheric Optics (IAO), Loparskaya (Lovozero) Station (68.6°N, 35.0°E, Murmansk Region) of the Polar Geophysical Institute RAS (PGI RAS), Issyk-Kul Station (42.63°N, 76.98°E, 1650 m) of Kyrgyzstan State University (KSU).

In Russia, there is a number of the stations equipped with instruments recommended for applying at NDSC but those were not compared with the primary standards. The most favorable conditions for carrying out the validation experiments are in the Central Russia where the concentration of instruments meant for remote sensing of atmospheric content is maximal (Figures 2 and 3). Several lidars, microwave radiometers, UV-, visible- and IR-spectrometers for measuring the O_3, NO_2 and aerosol profiles and the H_2O, CO, CO_2, CH_4, SO_2 total content are placed within about 500 kilometers. Therefore the validation of the O_3 measurements can be carried out taking into account the horizontal nonhomogeneity of the ozone distribution.

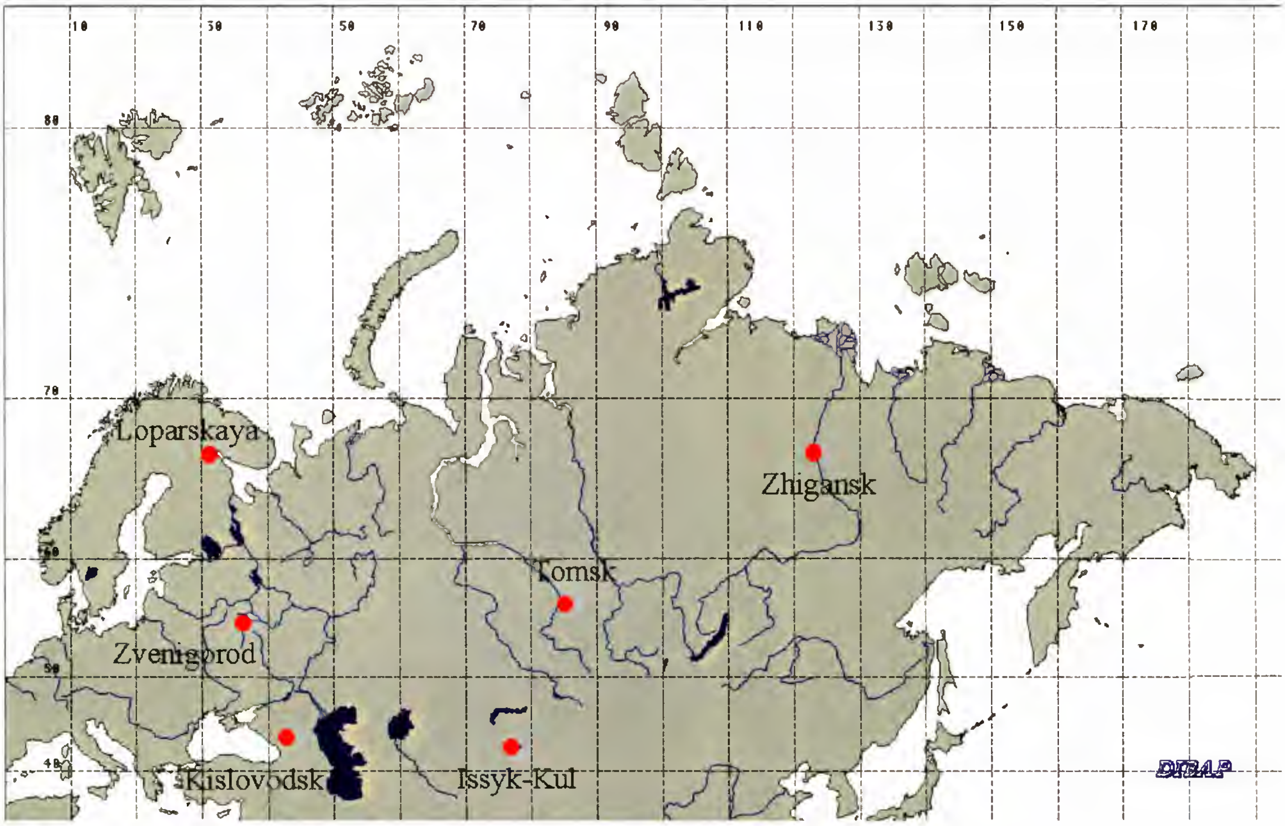


Figure 1. Russian (and CIS) ground-based stations for measuring the NO_2 content

2.1 Ground-based Ozonometric Network of Russia and CIS countries

The Russian and CIS countries' network of total ozone observations is equipped with filter ozonometers M-124 measuring the direct solar or diffused zenith radiation. Two spectral intervals with 302 and 326 nm maxima and half-width of about 20 nm are used for the observations. Total ozone is retrieved from direct sun light measurements at zenith angles 20-70° and blue or cloud zenith radiation measurements at zenith angles 20-85°.

All the M-124 ozonometers are calibrated against the standard (for Russian network) measurement instrument - the Dobson spectrophotometer No.108, which is regularly compared with the WMO standard. Comparisons in 1974, 1988, 1993 and 1997 showed that the measurement scale drift of the Dobson No.108 did not exceed 0.5% during this time period.

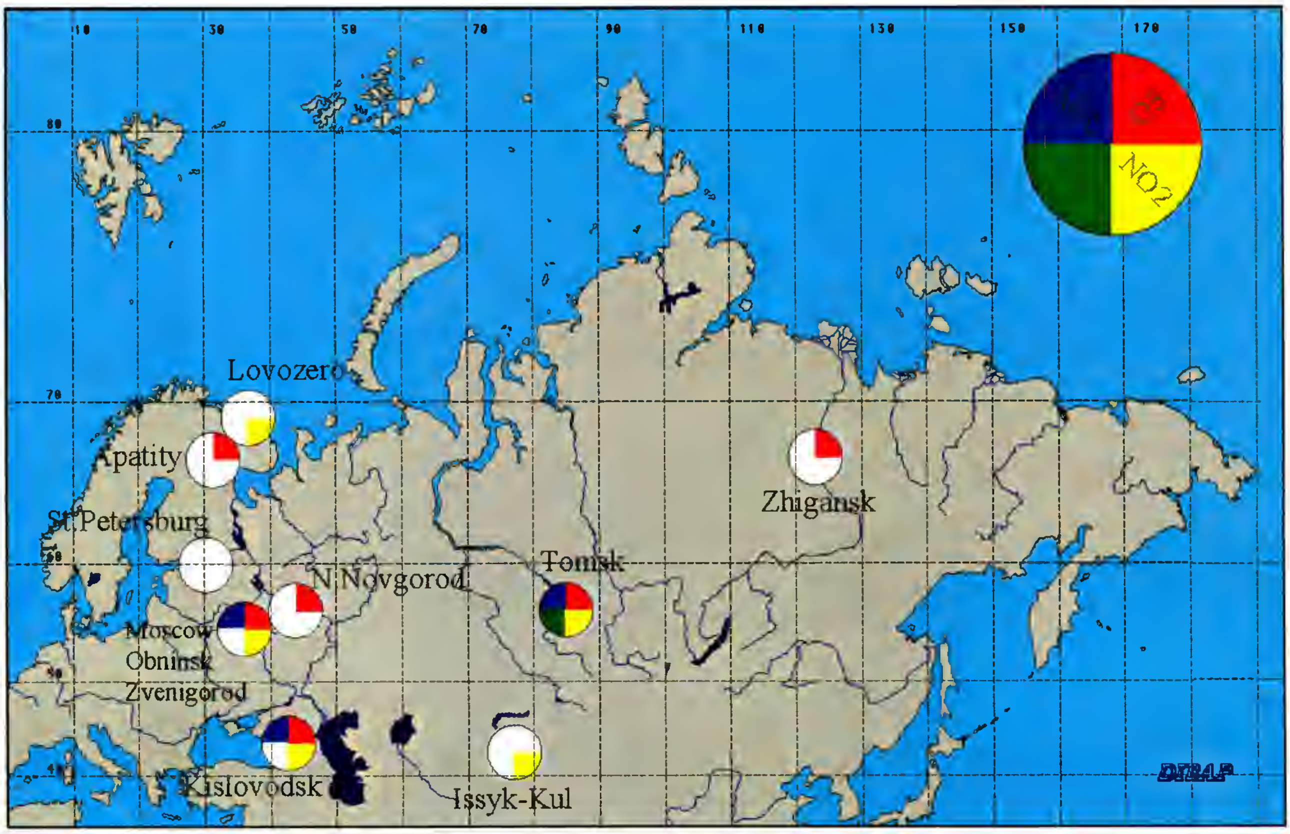


Figure 2. Stations of atmospheric remote sensing in Russia and CIS countries (profile measurements).

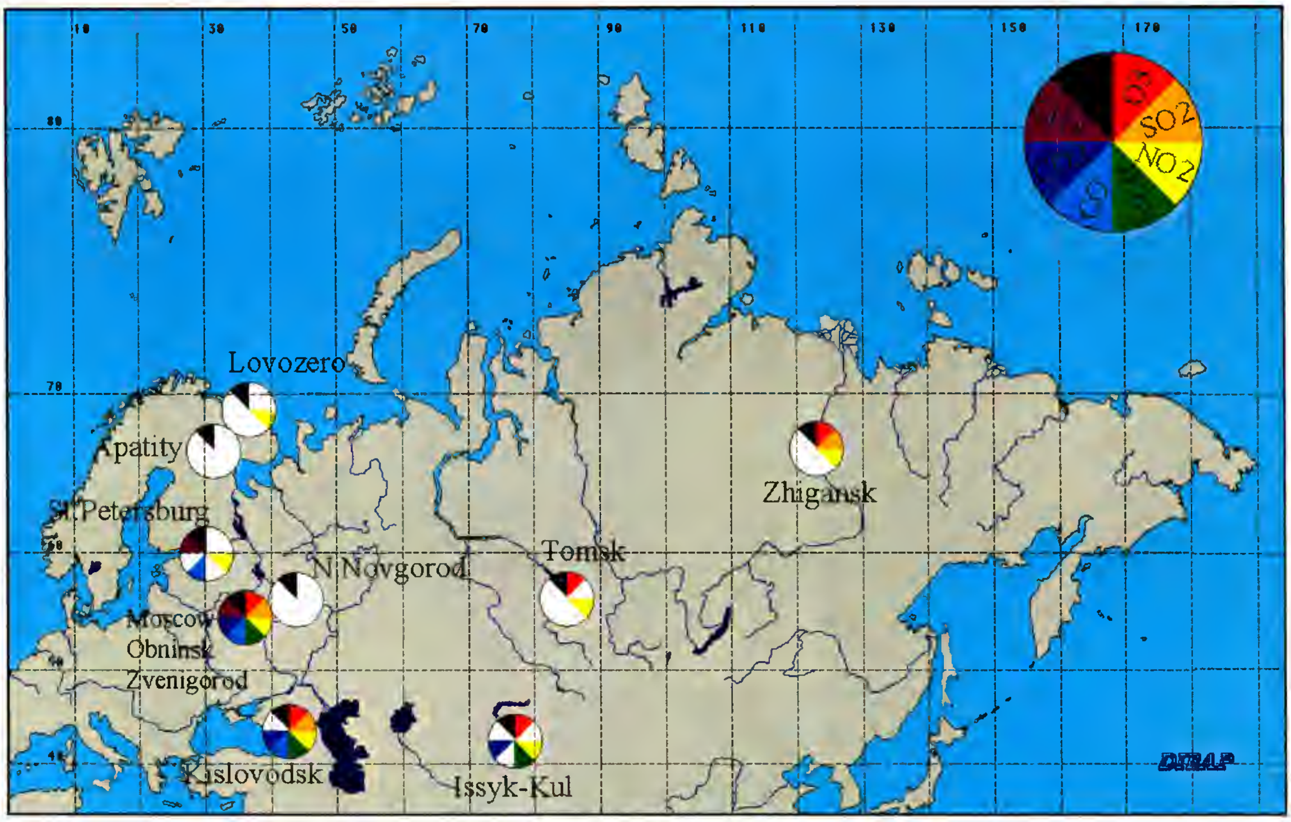


Figure 3. Stations of atmospheric remote sensing in Russia and CIS countries (total content measurements).

The error of single measurement by M-124 ozonometer is about 8%, but operational measurement procedure with obligatory analysis of results, provides a detection of systematical errors (which are about 90% of the total error) and the data correction.

As Russian stations are located, for the most part, northward of 60°, the zenith blue and cloud measurements dominate. Therefore a permanent control of measurement scale is the obligatory part of the instrument calibration and verification. The control of measurement quality is based on:

1. monthly comparison of two ozonometers (by which any station is equipped);
2. comparison of the direct sun light and zenith radiation measurements (difference between those can not exceed 1-3%);
3. the control on the presence of "false daily run" indicating on a change of instrument spectral characteristics;
4. and, finally, inter-station analysis of the observing results.

This analysis is performed at A.V. Voeikov Main Geophysical Observatory (MGO) and allows the measurement error to be reduced to 3-4%.

Regular calibration of M-124 ozonometers and routine control support the measurement scale on an international level. The errors of both the mean long-term (a scale level) and the mean monthly measurements for M-124 ozonometers are within the same limits as for Dobson spectrophotometers used by foreign ozone stations.

Locations of ozonometric network stations of Russia and CIS countries is given on Figure 4.

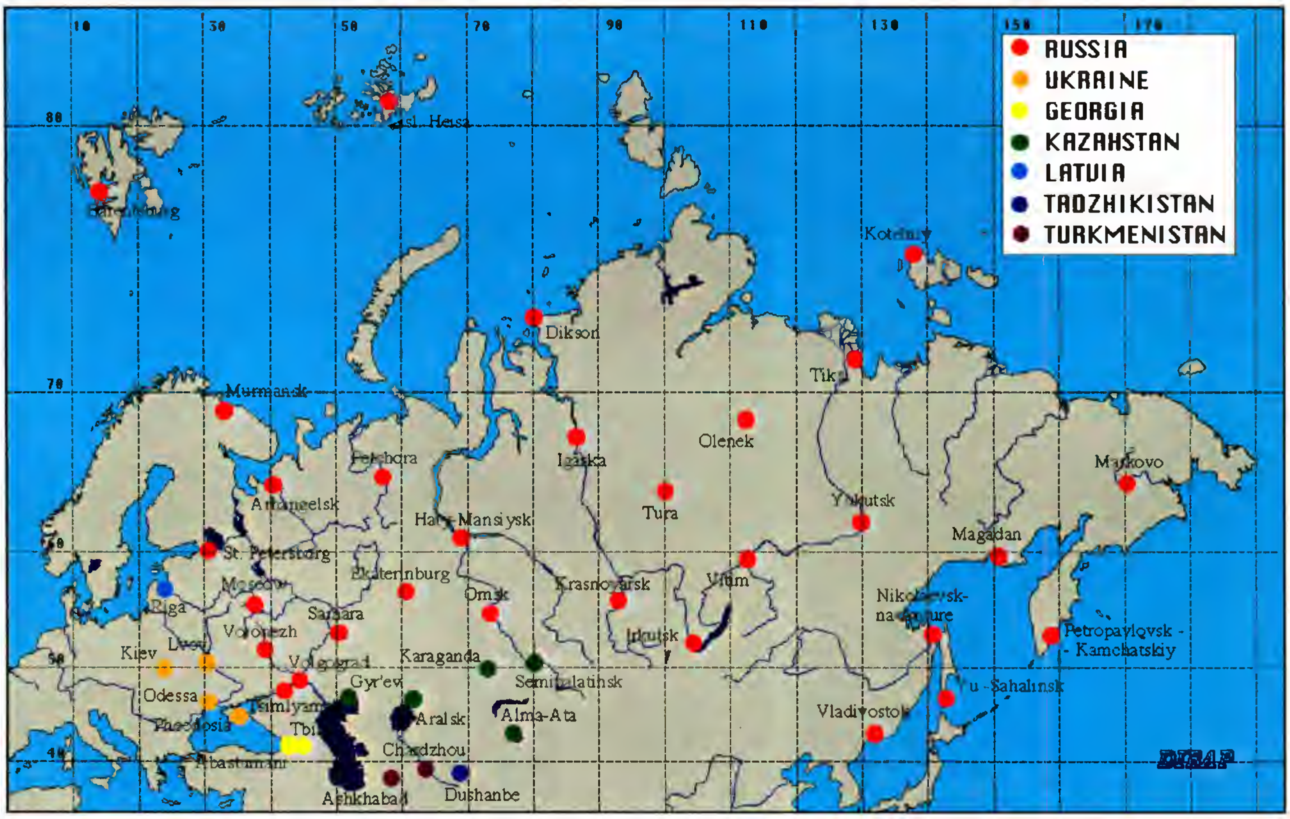


Figure 4. Ground-based Ozonometric Network of Russia and CIS countries.

3.3 Ground-based NO_2 content measurements at Zvenigorod Scientific Station

Zvenigorod Scientific Station (ZSS) of the Oboukhov Institute of Atmospheric Physics (56°N, 38°E,) is located at a distance of 50 km to the west from Moscow. However, because of the westerly winds prevail in this region through out the year the influence of the polluted air from Moscow on the observations is not too important. In the region of station there are no sources of pollution the environment. The highways and main roads are far from the station.

The regular measurements of column abundances and vertical profiles of NO_2 at ZSS have been performed since March 1990. The station is a member of the International Network for Detection of Stratospheric Change (NDSC) as a station for complimentary measurements of column NO_2. Vertical NO_2 profiles are retrieved out of the framework of the NDSC activity.

Column amount NO_2 contents are obtained from zenith-scattered solar radiation measured by the grating spectrometer MDR-23 operating in the 435-450nm wavelength range with spectral resolution 0.7nm and time of scanning 40s. A photomultiplier optimized in the visual wavelength range is used as a detector. The measurements are taken at twilight in mornings and evenings at solar zenith angles 84°-96°, and during daytime , if necessary, to control NO_x pollution of the boundary layer. Detected spectrum is proposed to be the sum of the solar spectrum exponentially attenuated by NO_2 and O_3 absorption and by Rayleigh and aerosol scattering, and a constant. The constant is believed to include effects of detector dark current, spectrometer stray light leakage, and the Ring effect. The slant NO_2 contents are derived from the observed spectra with the use of differential NO_2 absorption.

To retrieve columnar NO_2 contents and NO_2 vertical distributions from the slant NO_2 contents, air mass factors for NO_2 are needed. They are computed using a spherical scattering model for solar radiation and a non-stationary one-dimensional photochemical model including the O_x and NO_x photochemistry. The spherical scattering model takes into account ozone and NO_2 absorption, single molecular and aerosol scattering, refraction and refraction divergence. Parameters of the models: ozone, temperature and air density vertical distributions are seasonally dependent and taken from simultaneous measurements, if available, or from empirical models specified for the latitude of observations.

The photochemical model provides the altitude-dependent diurnal variation of NO_2, which is the input parameter in the scattering model. Taking into account photochemical processes is very important as NO and NO_2 undergo rapid changes at sunrise and sunset. Given calculated air mass factors for NO_2, the NO_2 contents in 5-km thick layers and in the thin near-surface layer are then obtained as a solution of the inverse mathematical problem, with the use of modified method (Chahine method). The modification is concerned with introducing into consideration the thin near-surface layer where NO_2 concentration can be large during pollution episodes. The NO_2 content in the 0-5 km layer does not include NO_2 in the near-surface layer. Derived quantities are (1) NO_2 contents within 5 km thick layers in the stratosphere and the troposphere (0-50 km), (2) NO_2 content in the thin atmospheric surface layer, and (3) columnar NO_2 contents in the troposphere (0-10 km) and the stratosphere (10-50 km) as integrals over appropriate layers. Comparison of the NO_2 profiles retrieved from ground-based and SAGE-2 measurements demonstrated a good agreement of the data.

The accuracy of NO_2 slant abundances determination with a step 0.5° of solar zenith angle is better than $1 \cdot 10^{15}$ mol/cm^2, under the good measuring conditions.

3. The main results of comparisons between GOME level-2 data and Russian ground-based measurements

3.1 Validation of GOME total ozone data

Validation of GOME total ozone measurements has been performed by comparing with data of ground-based, ozonosonde and satellite experiments by many scientists. Comparison of GOME total ozone measurements with the data of Russian ozonometric network, performed previously for 7 stations of the north-west and central Russian regions (Figure 5) and two months (summer and autumn), has shown that satellite measurements underestimate total ozone in comparison with ground-based measurements. These results together with some additional investigations allowed to make the following conclusions:

1. Ground-based total ozone measurements by the M-124 ozonometer (both direct solar and zenith scatted observations) carried out in North-West and Central Russia during 1996-1998 are in a good agreement with the TOMS satellite data. Mean deviations between zenith M-124 and TOMS data are 2.3 % (1996), 2.2 % (1997) and -0.1 % (1998), RMS deviations - 4.2 %, 2.7 % and 2.2 %, respectively. These results demonstrate possibilities of applying the Russian (and CIS) ozonometric network for validation of different satellite measurements. Such comparisons have been made possible after developing the specialized methods of measurements, calibration, data processing and quality control;
2. Comparison of ground-based (M-124) and satellite (GOME) total ozone measurements over the northern-west and central regions of Russia in July and September-October of 1996 revealed that satellite measurements systematically underestimate the total ozone in comparison with ground-based measurements - by 6-12 % depending on comparison conditions;
3. GOME measurements over the White Sea region in summer of 1997-1998 underestimate total ozone in comparison with both ground-based M-124 and satellite TOMS data. In the region of ground-based observations, these mean and RMS deviations varied in the ranges of 5.4 - 8.6 % and 6.0 - 8.8 %, respectively;
4. In 1998, the total ozone underestimation by the GOME was some smaller then in 1997. This result is likely to be associated with applying the improved code of the GOME data processing (GDP 2.4).

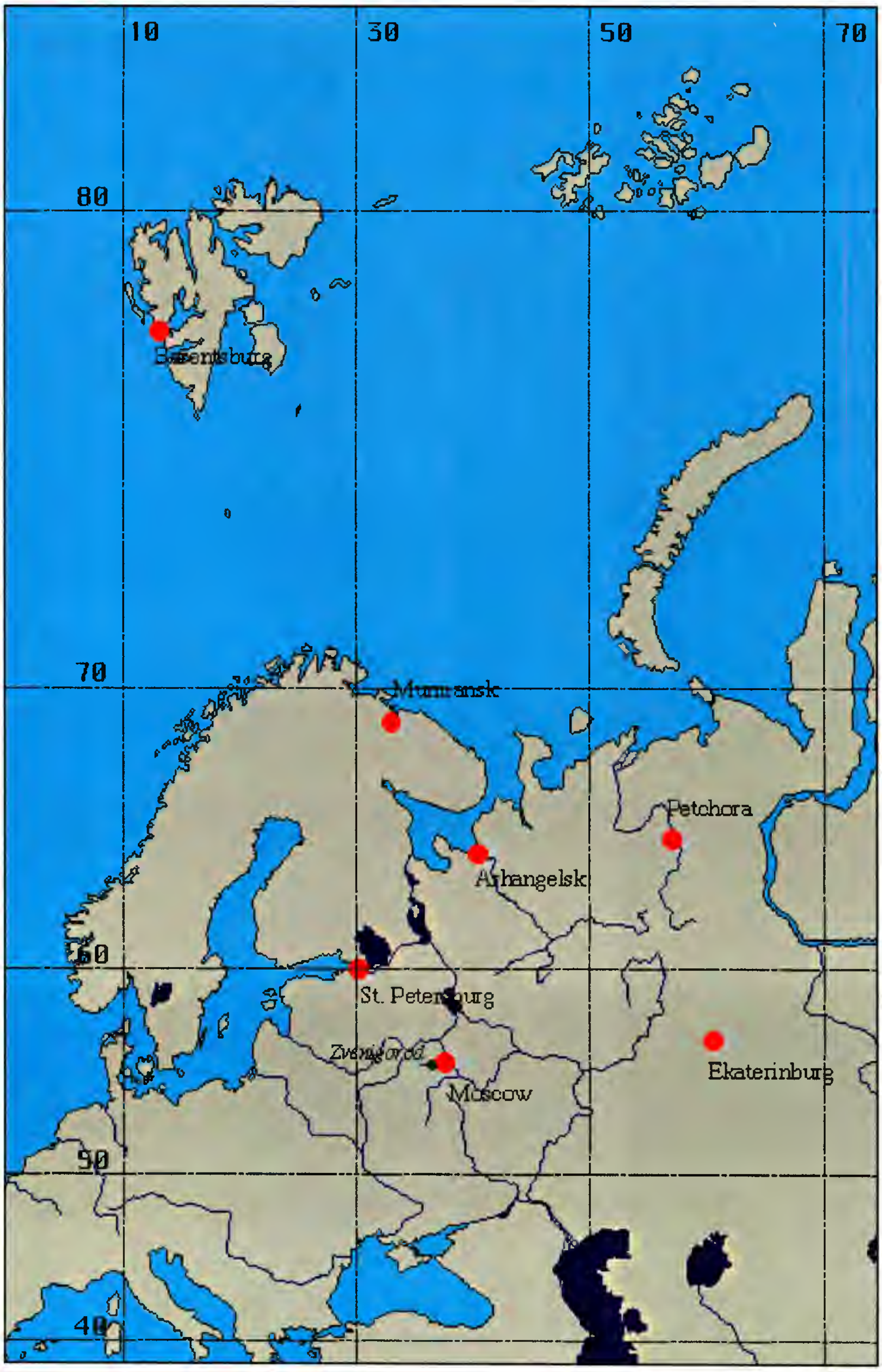


Figure 5. Locations of seven Russian ground-based ozonometric stations.

3.2 Comparison of the GOME and ground-based NO_2 column amount measurements

In these studies the GOME data on NO_2 total content was compared with ground-based measurements at Zvenigorod Scientific Station (1996, 1998). The simplest approximation was used to consider the diurnal variation of total NO_2 - the GOME measurements were compared with a half-sum of corresponding sunrise and sunset ground-based observations. The reason for such approach is that the GOME measurements occur near the local noon time, as the ERS-2 satellite has a sun-synchronized orbit. The results of these investigations allowed to make the following conclusions:

1. Results of comparison between GOME and ground based NO_2 column amount measurements in 1996 (ZSS, Russia; 56°N, 38°E) (331 GOME measurements, 280 sunrise and 286 sunset ground-based observations) demonstrate a very poor agreement between satellite and ground-based measurement systems. The mean deviation $\Delta_{S\text{-}g}$ between the GOME measurements and a half-sum of ground-based observations is 176 %, standard deviation $\sigma_{S\text{-}g}$ is 549 %, the coefficient of correlation R is - 0.04±0.05. It is clear that the GOME significantly overestimates the value of total NO_2 in comparison with ground-based observations;
2. The similar comparison for the limited data set of satellite and ground-based observations in the time period from 1 of January to the 26 of July 1996 demonstrates much better agreement between satellite and ground-based data. The mean deviation $\Delta_{S\text{-}g}$ for the comparison of GOME measurements with a half-sum of ground-based observations is 33.2 %, with standard deviation $\sigma_{S\text{-}g}$ = 67.3 %. Although the absolute values of satellite and ground-based measurements agree rather well, correlation of these data sets is still very poor - R = 0.00±0.12;
3. Comparison of the GOME NO_2 total content data and ground-based observations over Zvenigorod station in March 1998 shows that satellite measurements give, on the average, 30.5 % higher the total NO_2 values than ground-based system, with corresponding standard deviation $\sigma_{S\text{-}g}$ = 60.0 %. GOME measurements performed on March 26 and 29 are nearly 2 times higher than the ground-based ones. Elimination of these data from the comparison reduces the average discrepancy between satellite and ground-based systems to 8.9 %, with corresponding standard deviation $\sigma_{S\text{-}g}$ = 20.2 %. Our preliminary conclusion is that the GOME data of March 1998 has the better quality than data of 1996.

4. Delta characterisation of GOME data products

4.1 Comparisons of GDP 2.8 level-2 data with GDP 2.0, GDP 2.4 and ground-based measurements

Comparisons performed in the framework of WP 2000-3200 include an analysis of validation set with level-2 GOME data that was used in the previous investigations to verificate GDP 2.4 processing. These data was compared with corresponding set of GOME data processed with the new GDP 2.8, as well as with data of GDP 2.0 and Russian ground-based total ozone and NO_2 measurements. Data used in investigation cover the year of 1996

with total NO_2 measurements over Zvenigorod and total ozone measurements over the 7 stations (Arhangelsk, Barentsburg, Ekaterinburg, Moscow, Murmansk, Petchora and St.Petersburg).

The spatial coverage of GOME orbits involved in quick validation allowed to get a limited set of comparisons, especially for NO_2 measurements validation. Those satellite measurements with pixels overlapping in space with locations of ground-based stations were used in comparison. Only 93 orbits out of the whole set matched that criteria for 7 ozone and 1 NO_2 measuring stations. The average of GOME measurements that occur over the station during the day were compared with corresponding ground-based observations. In case of total NO_2 measurements, a half-sum of sunrise and sunset twilight observations was compared with GOME data.

4.2 Delta characterisation of total ozone measurements

The data set used in comparisons consisted of about 400 satellite and more than 100 ground-based measurements, covering almost the whole year of 1996 (12th of February - 13th of December). Comparisons of GOME data with corresponding ground-based measurements over the 7 stations are presented in Figure 6. Statistical characteristics of observed discrepancies between the data compared, are given in Table 1. The number of comparisons is different for different stations and vary from 10 (Moscow) to 28 (Barentsburg).

As can be seen from the plot, GOME ozone vertical columns are noticeably lower than ground-based measurements of all of GDP versions. The average deviation Δ_{s-g} of GDP 2.0 from ground-based data is -8.0%. The data of GDP 2.4 is slightly closer to ground-based measurements - Δ_{s-g}=-7.0%.

The overall deviation of GOME total ozone (TO) values from ground-based measurements (7 stations), provided with the last GDP 2.8 (June release), is about 6% on the average (see the Table). This is also few % less than for GDP 2.0 (Δ_{s-g}=-8%) and for GDP 2.4 (Δ_{s-g}=-7%) as well.

The relative difference of GOME total ozone (TO) data from ground-based measurements as a function of TO value is presented in Figure 7. GOME mostly underestimates TO, in comparison with ground-based measurements, except the case of relatively low TO content (<300 DU).

The seasonal dependence of relative difference between GOME and ground-based TO measurements is given in Figure 8. For the most part of the year GOME TO measurements provide lower values than ground-based ones. The opposite effect is observed in winter-spring months, when GOME overestimate TO in some cases.

The relative difference between GOME and ground-based TO measurements as a function of Sun zenith angle (SZA) and cloud fraction is presented in Figure 9 and Figure 10, respectively. The deviation of GOME total ozone from ground-based data increases at high SZA and cloud fraction values.

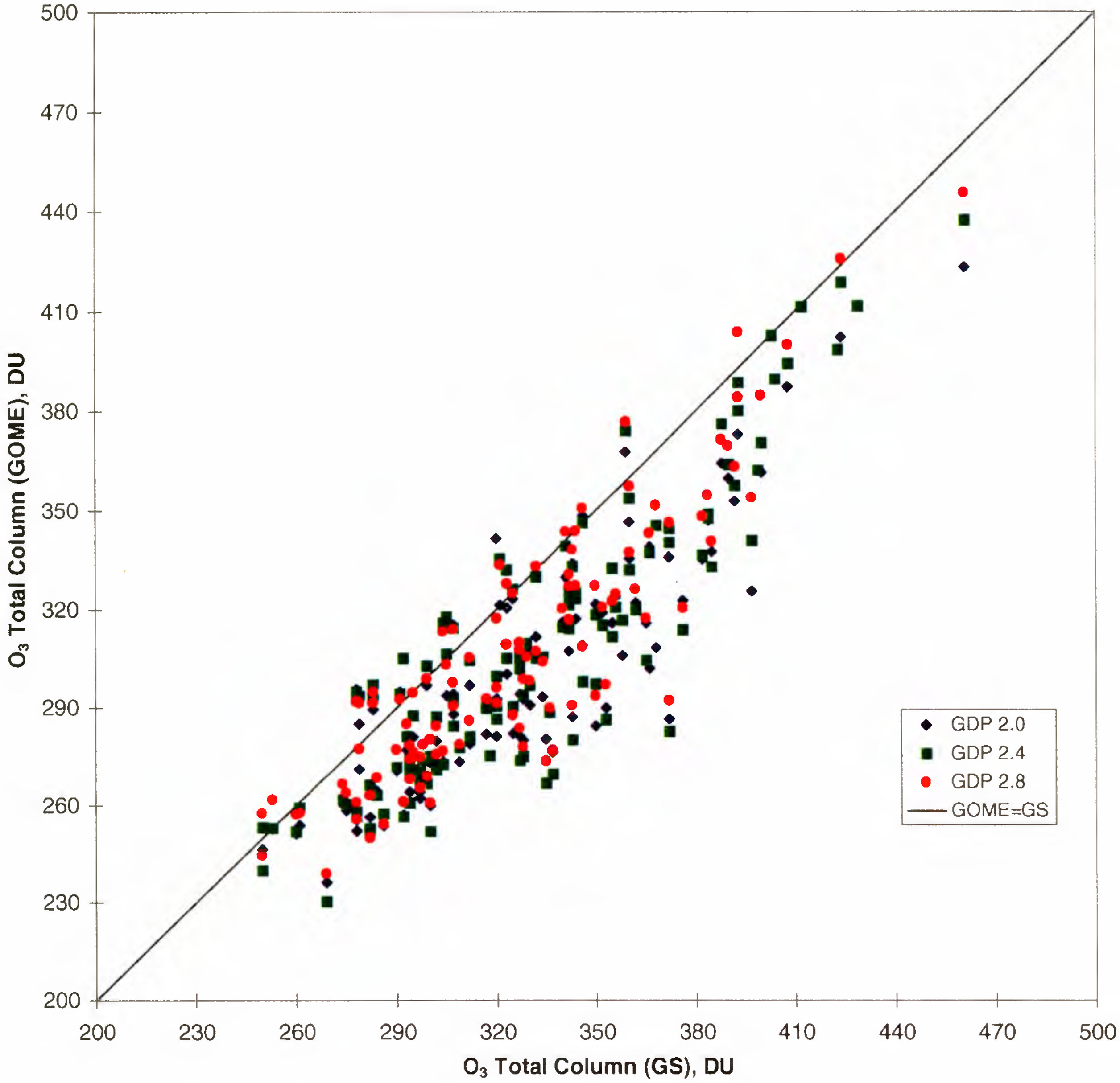


Figure 6. Comparison of satellite (GOME) and ground-based (GS) total ozone measurements over 7 Russian ozonometric stations in 1996

GDP version number:		***2.0***		***2.4***		***2.8***	
Station	**N**	**Δ**	**σ**	**Δ**	**σ**	**Δ**	**σ**
Arhangelsk	11	-10.1	12.3	-9.5	12.3	-8.4	11.0
Barentsburg	28	-7.4	9.1	-6.7	8.6	-5.2	7.8
Ekaterinburg	16	-8.8	9.1	-7.4	7.9	-7.0	7.4
Moscow	10	-8.5	10.1	-7.0	8.2	-6.6	8.2
Murmansk	20	-8.1	10.7	-7.8	11.3	-6.4	9.5
Petchora	23	-6.8	9.2	-5.5	8.9	-5.0	7.9
St.Petersburg	13	-7.6	10.5	-6.1	7.4	-3.3	4.7
overall:	121	-8.0	10.0	-7.0	9.3	-5.9	8.2

Table 1. Mean (Δ) and RMS (σ) deviations (%) of GOME total ozone data from ground-based measurements (N - number of comparisons).

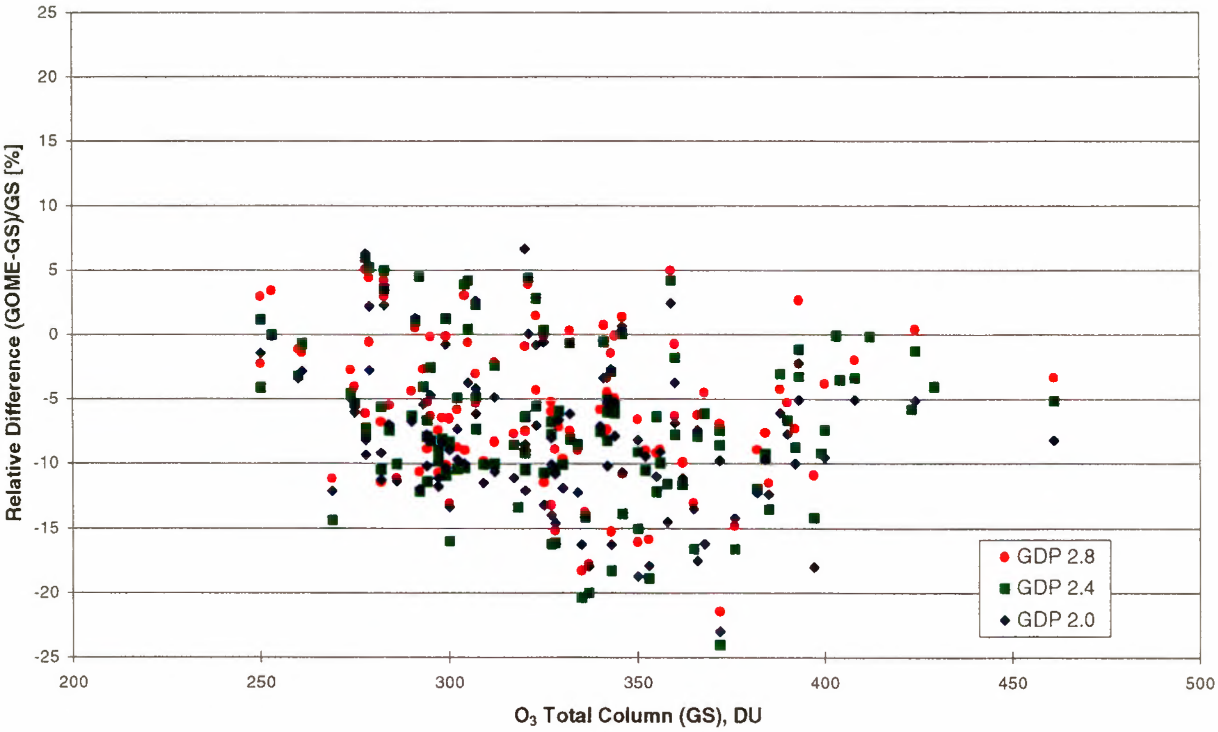


Figure 7. The relative difference of satellite (GOME) total ozone data from ground-based (GS) measurements over 7 Russian ozonometric stations in 1996, as a function of ground-based total ozone data

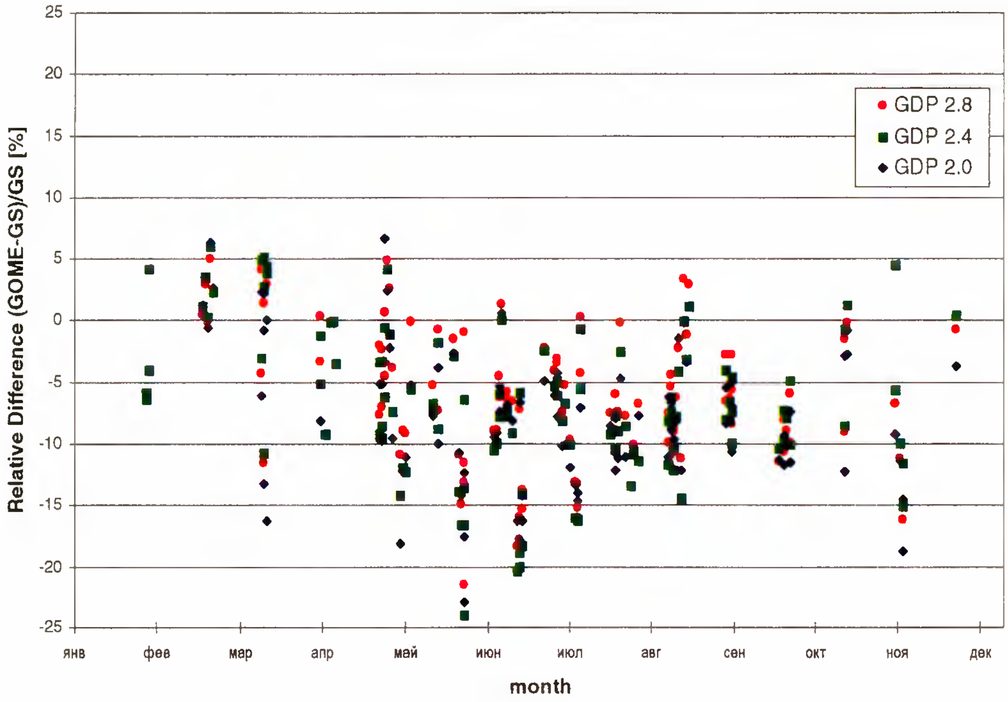


Figure 8. The relative difference of satellite (GOME) total ozone data from ground-based (GS) measurements over 7 Russian ozonometric stations in 1996, as a function of season.

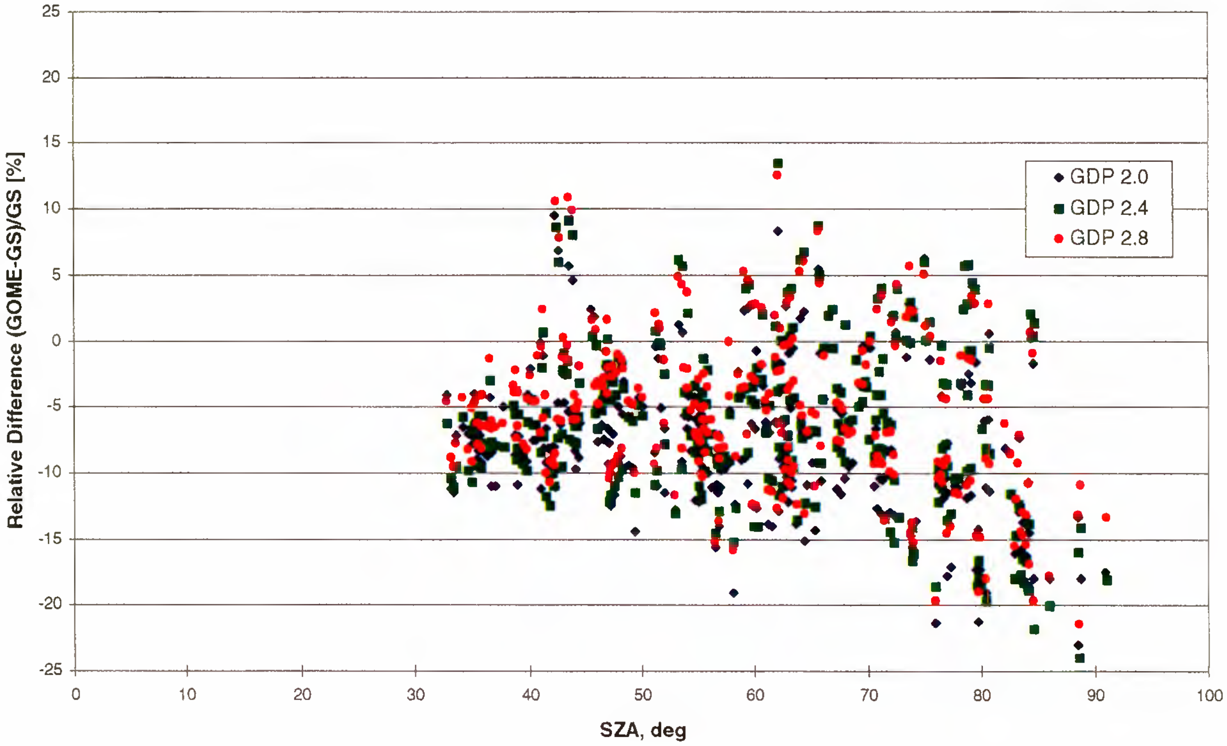


Figure 9. The relative difference of satellite (GOME) total ozone data from ground-based (GS) measurements over 7 Russian ozonometric stations in 1996, as a function of Sun zentih angle (SZA).

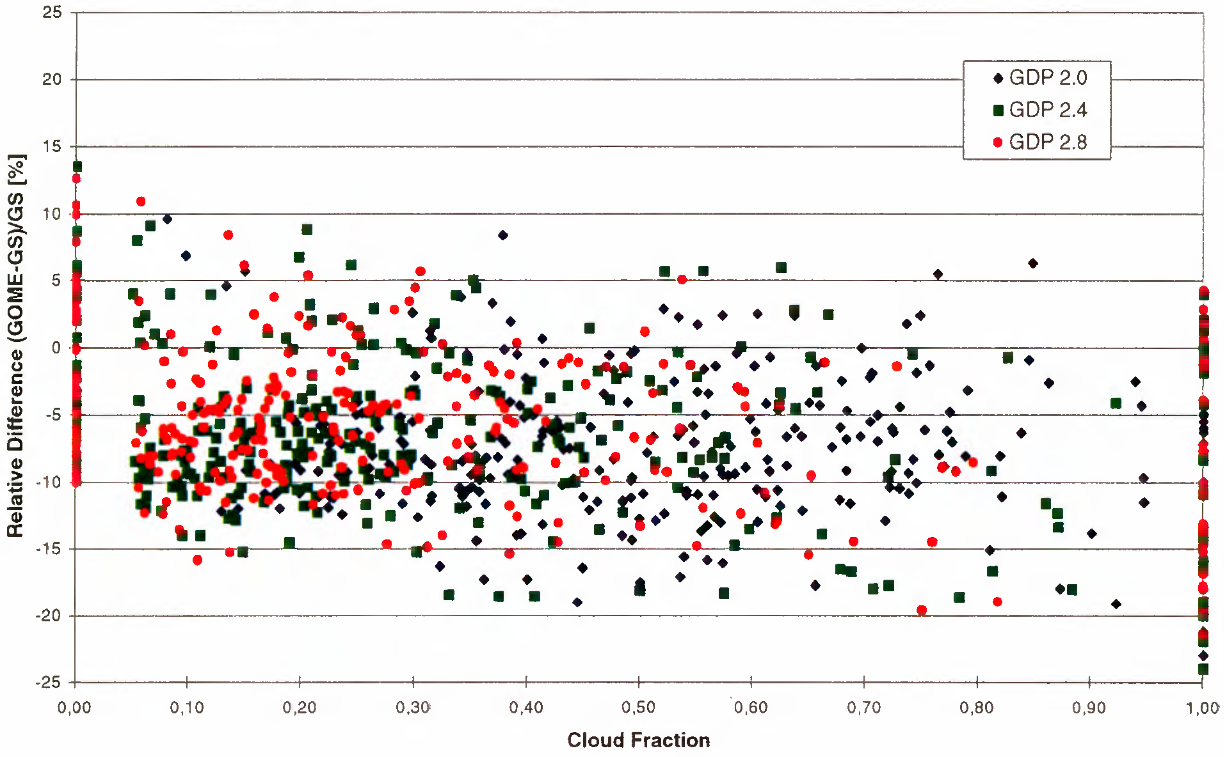
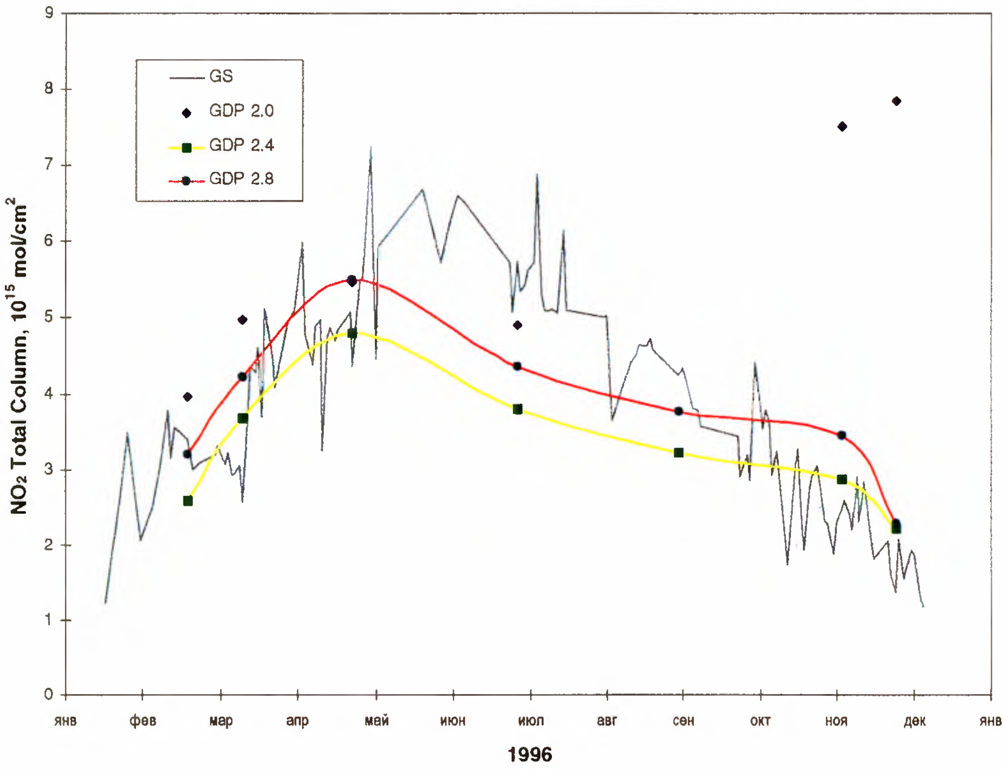


Figure 10. The relative difference of satellite (GOME) total ozone data from ground-based (GS) measurements over 7 Russian ozonometric stations in 1996, as a function of cloud fraction.

4.3 Delta characterisation of total NO_2 measurements

Data set used in validation involves 7 comparisons of GOME total NO_2 data processed by GDP 2.0, 2.4 and 2.8 algorithms with corresponding ground-based measurements over Zvenigorod for the different dates of 1996. Only these measurements out of the whole set of GOME orbits coincide with each other. Results of the comparison are presented in Figure 11. As it seen from the plot, the data of GDP 2.4 is much closer to ground-based values than the data of previous processing (GDP 2.0) - the jumps in GOME total NO_2 values that exist in GDP 2.0 data disappeared or reduced significantly in GDP 2.4 data. The standard (RMS) deviation between ground-based and GOME GDP 2.4 total NO_2 data is 30%. Although statistical significance of available comparisons is questionable, it is possible to note, the data of GOME total NO_2 measurements, processed with GDP 2.8 is slightly closer to ground-based measurements: the mean deviation is about 11% now.



DATE	GS	GDP 2.0	GDP 2.4	GDP 2.8
05-Mar-96	3.40	3.96	2.60	3.20
27-Mar-96	2.57	4.97	3.67	4.22
10-May-96	4.36	5.47	4.79	5.50
15-Jul-96	5.74	4.91	3.81	4.35
18-Sep-96	4.23	36.47	3.21	3.77
23-Nov-96	2.47	7.51	2.88	3.45
15-Dec-96	1.37	7.85	2.22	2.29

average and standard (RMS) deviations:

GDP 2.0: $\Delta_{s\text{-}g}=74\%$, $\sigma_{s\text{-}g}=106\%$ (*)

GDP 2.4: $\Delta_{s\text{-}g}=-4\%$, $\sigma_{s\text{-}g}=30\%$

GDP 2.8: $\Delta_{s\text{-}g}=11\%$, $\sigma_{s\text{-}g}=31\%$

• - date of 18-Sep-96 is eliminated from analysis of GDP 2.0 data

Figure 11. Comparison of satellite (GOME) and ground-based (GS) total NO_2 measurements over Zvenigorod station in 1996 (total NO_2 values in 10^{15} mol/cm^2; GS - half-sum of sunset and sunrise ground-based observations).

4.4 Conclusions

In this study the data of GOME total ozone and NO_2 measurements, processed with different GDP versions (2.0, 2.4 and 2.8), were compared with corresponding ground-based total NO_2 observations over Zvenigorod and total ozone observations over the 7 Russian stations. The main results of these investigations are:

1. The agreement between ground-based measurements and GOME total ozone data is slightly better with GDP 2.8 data processing (Δ_{s-g}=-5.9%) than with GDP 2.4 (Δ_{s-g}=-7.0%) and GDP 2.0 as well (Δ_{s-g}=-8.0%);
2. The systematical underestimation of total ozone from GOME measurements in comparison with Russian ground-based observations, was revealed in GDP 2.0 validation, and it still remains in the data of GDP 2.4 and GDP 2.8 processing;
3. The large jumps in total NO_2 data removed in GDP 2.4 than compared with GDP 2.0; the same is true for GDP 2.8 data, too;
4. GOME GDP 2.8 total NO_2 values appear to be a little bit higher than GDP 2.4 data that slightly increases the deviation of GOME measurements from ground based ones.

In general, the overall agreement with ground-based measurements has not improved significantly from GDP 2.4 to GDP 2.8. For total ozone data, agreement of GDP 2.8 with ground-based measurements has become a little bit better than for GDP 2.4. A very limited set of comparisons with total NO_2 measurements has not shown any improvements in GDP 2.8 total NO_2 data, when compared with previous GDP version (2.4).

Our limited studies of the new GOME total NO_2 validation dataset do not provide any arguments to recommend proceeding to the new GDP version. On the other hand, we may state, that the implementation of operational processing with GDP 2.8 will improve the agreement of GOME total ozone data with ground-based measurements.

DELTA CHARACTERISATION OF GOME DATA PRODUCTS DETAILED VERIFICATION REPORT

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1. Introduction

The main objective of the Global Ozone Monitoring Experiment (GOME) is the provision of global maps of high precision ozone vertical columns. Since the start of GOME on the European ERS-2 satellite on April 1995 and the first operational data products, the GOME Data Processor GDP operated by DLR/DFD has been updated several times to improve the quality of the derived ozone columns. For most situations, the GDP ozone columns now have a high degree of accuracy, but problems remain at high latitudes and under low ozone conditions. Unfortunately, these scenarios are those with the highest scientific interest.

In addition to ozone, global NO_2 fields are provided in the GDP. Mainly due to airmass factor problems related to the uncertainty in the tropospheric contribution, NO_2 columns were not very useful in the first versions of the data product. This has been significantly improved with the current GDP 2.4 version, but calibration problems and uncertainties in the airmass factor still are an issue.

With the new GDP version 2.7, several minor bug fixes and a number of software updates were introduced as well as major improvements to the wavelength calibration in channel 3. Significant changes were expected for the NO_2 columns, but ozone columns should not have been affected strongly. As shown below, the new data version meets the expectations. However, with the limited amount of data and the short time period available all results and conclusions are necessarily preliminary and have to be confirmed by more detailed analyses.

1.1 Data problems in the GDP 2.4 level-2 data

In past validation and characterisation exercises, a number of problems have been identified for both O_3 and NO_2 vertical columns in GDP 2.4:

O_3:

1. Too low values at northern mid-latitudes when compared to ground-based and TOMS measurements;
2. Too high values at large solar zenith angles and low ozone (high latitudes in winter/spring under ozone loss conditions) when compared to other ground-based and satellite sensors.

NO_2:

1. Large scatter of values during some time periods due to wavelength calibration problems. This problem mainly arises in the equatorial regions but to a lesser degree also at other latitudes;
2. Too low values when compared to ground-based measurements, in particular in the southern hemisphere;
3. Larger pixel-to-pixel variability than expected from ground-based measurements;
4. Larger day-to-day variability than expected from ground-based measurements. GOME GDP 2.4 NO_2 columns are subject to oscillations with frequencies of several days or weeks that are not seen in the ground-based measurements.

In this report, the quality of the new GDP versions will be judged by assessing which of the above mentioned problems have been solved and by checking, if there have been introduced new data problems.

2. Methodology

The quality of the new GDP 2.7 GOME level-2 data has been assessed using the three complimentary methods described below.

2.1 Comparison with the GDP 2.4 level-2 data

Level-2 data from the new and the current GDP versions have been compared for randomly selected orbits. The intention is to get an impression of the magnitude of the changes between the two product versions, to determine which quantities have changed and to check the consistency of the files. In addition, zonal averages have been computed for selected latitude bands and the seasonal variation of these averages compared for the different data versions.

2.2 Comparison with ground-based measurements

The Institute of Environmental Physics at the University of Bremen is currently operating two zenith-sky viewing DOAS instruments, one at the NDSC station in Ny-Ålesund (79°N, 12°E) and one in Bremen (53°N, 9°E). Both instruments have been operational throughout 1996 and 1997 with the exception of short maintenance breaks and the polar night in Ny-Ålesund. During summer in Ny-Ålesund the sun is over the horizon for several months making the standard operation mode of the instrument (twilight measurements) impossible. For these time periods, trace gas columns are measured at higher sun and therefore have larger uncertainties than in spring and fall.

For the comparison with the ground-based measurements, all GOME measurements having centre pixel co-ordinates within 200 km of the station have been extracted from the validation data-set. From these data, daily averages have been derived and compared to the corresponding zenith-sky measurements. Validation of NO_2 columns is complicated by the diurnal variation of the stratospheric column and the uncertainty in the tropospheric column at mid-latitudes. As GOME is crossing the equator at about 10:30 local time, the morning values of the ground-based instruments have been used for the validation. Due to the daytime photolysis of the NO_2 reservoir gases (mainly N_2O_5), GOME NO_2 columns are expected to be higher than these values by less than 10 % depending on season and latitude.

2.3 Comparison with columns derived at the IUP Bremen using GDP V1.35 level-1 data and the DOAS algorithm of the IUP (for NO_2 only)

For NO_2, GOME GDP 1.35 level-1 data have been used to determine columns with the DOAS algorithm developed at the Institute of Environmental Physics at the University of Bremen. All calibration steps with the exception of leakage current correction have been switched off as problems with the wavelength calibration corrupt a large part of the spectra in channel 3. To compensate for the lack of calibration, both the radiance response and the polarisation dependence of the instrument have been corrected in an empirical way. A detailed summary of the parameters used for the fit is given in Table 1.

Parameter	Value
Wavelength interval	425 - 450 nm
Wavelength calibration	Correlation with Kurucz Fraunhofer atlas
Shift & stretch	earth-shine only
Degree of Polynomial	4
O_3 cross-section	GOME 221 K (Burrows et al., 1999)
NO_2 cross-section	GOME 241 K (Burrows et al., 1999)
O_4 cross-section	Greenblatt et al., wavelength corrected
H_2O cross-section	HITRAN (Rothmann et al., 1992)
Ring	Synthetic (Vountas et al., 1998)
Undersampling correction	Chance et al., 1998
Smoothing	none

Table 1. Fit parameters used for the IUP Bremen NO_2 fit.

Vertical columns have been derived using airmass factors calculated with the radiative transfer program GOMETRAN using the vertical NO_2 profile from the US-Standard atmosphere. The airmass factors have been determined for the nadir viewing geometry only, ignoring the dependence on line of sight and relative azimuth. The resulting errors are in the order of 2-5 % for individual pixels and much smaller than the differences discussed below.

3. Results

3.1 Comparison with the GDP 2.4 level-2 data

As an example, some key quantities from orbit 61217112 are compared in Figure 1. As can be seen from the figure, for this particular orbit ozone vertical columns are within 2% of the values from GDP 2.4, the main differences coming from the airmass factors and not the slant columns. It has however to be pointed out, that ozone slant columns have changed significantly (4%) for large solar zenith angles. NO_2 changes are much larger (up to 100% and more) and mainly due to changes in the slant columns. For most zenith angles, the NO_2 airmass factors have changed little. ICFA values in GDP 2.7 data are different from GDP 2.4 cloud cover by up to 10%, generally giving lower values in the new data version.

In Figure 2, the global change in ozone vertical column is shown for 4 months.

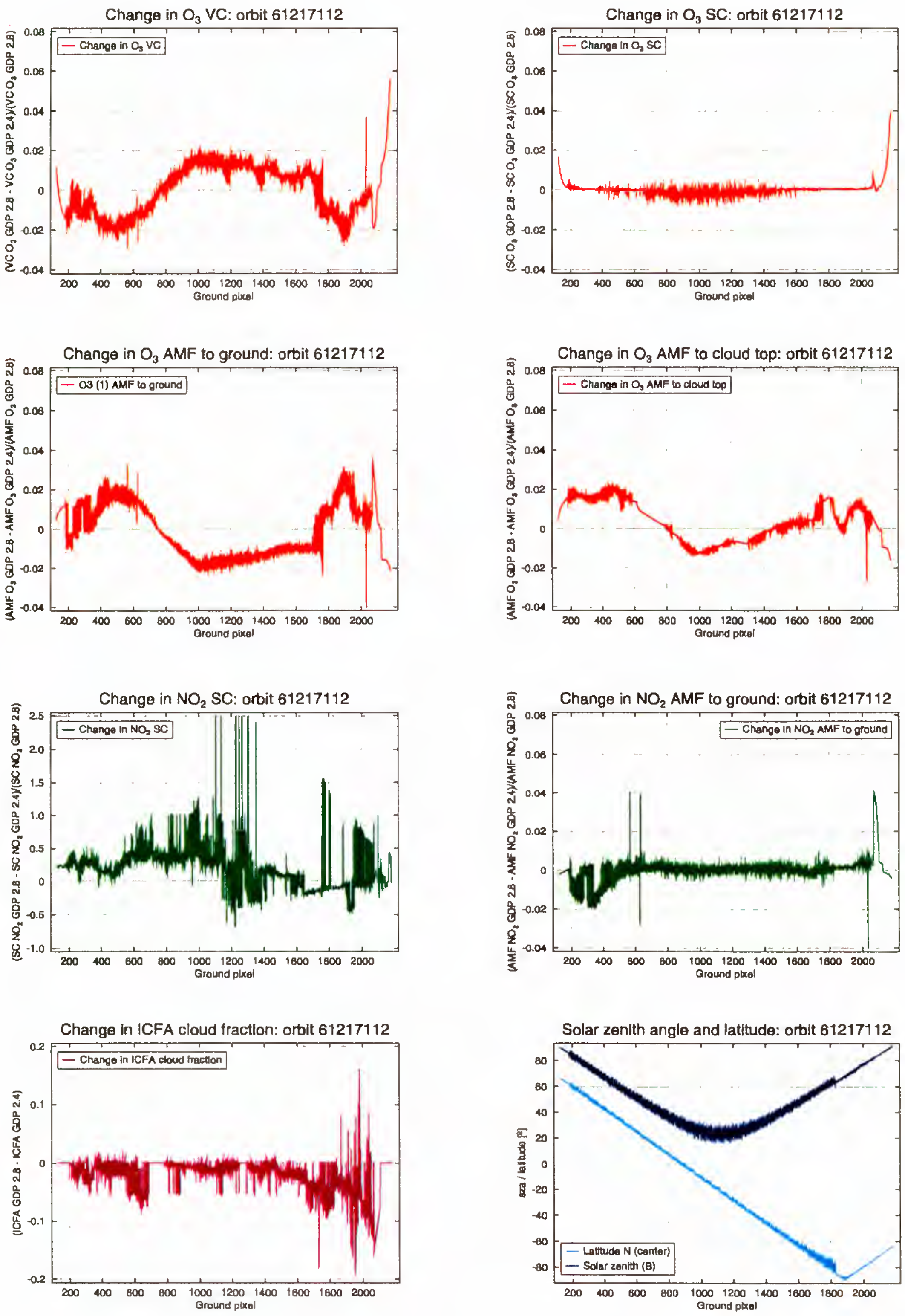

Figure 1. Differences between GDP 2.7 and GDP 2.4 (orbit 61217112) for O_3 slant column, O_3 airmass factor to ground, O_3 airmass factor to cloud top, NO_2 slant column, NO_2 airmass factor to ground and ICFA.

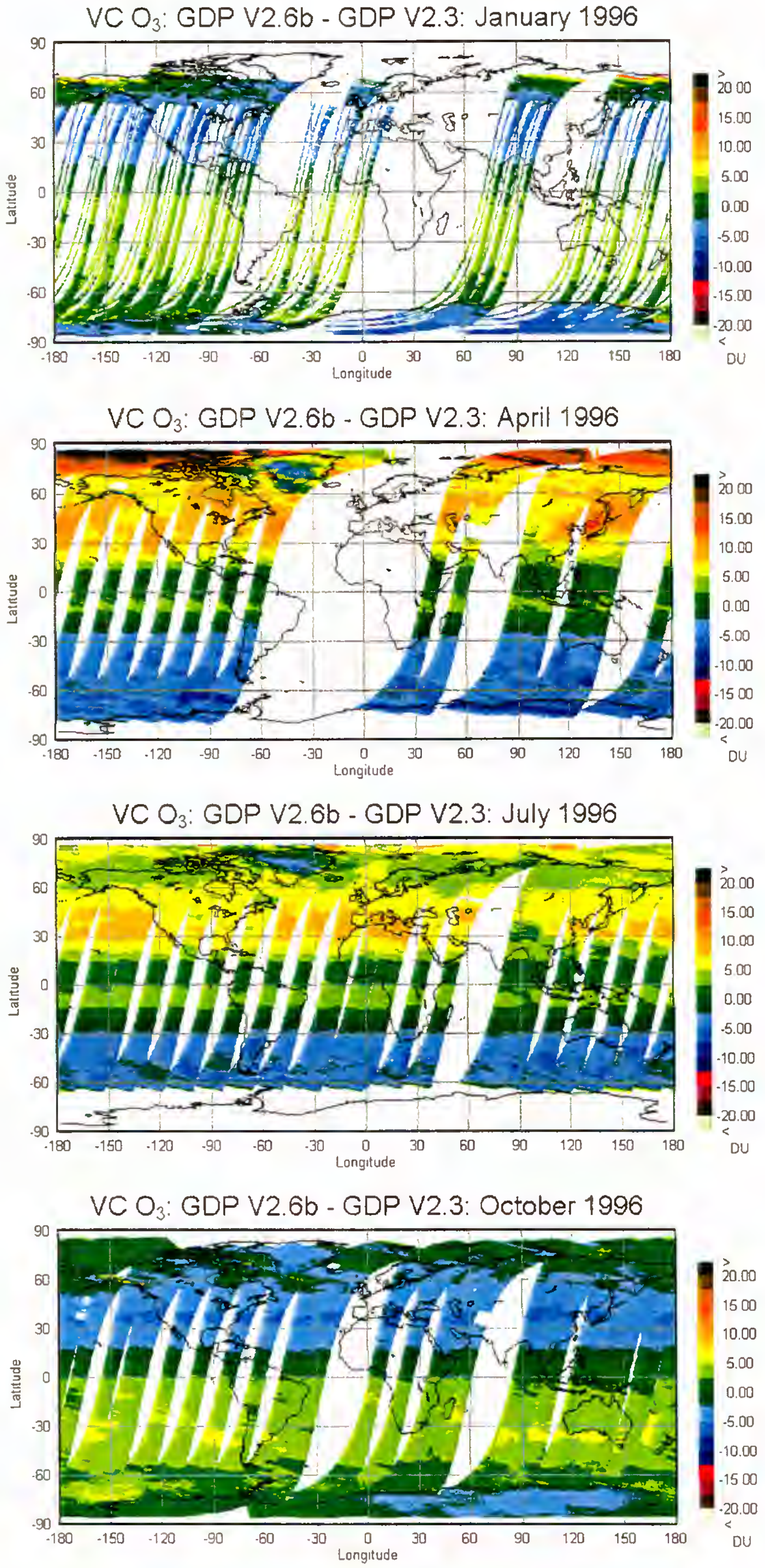

Figure 2. The difference in ozone vertical column between GDP 2.4 and GDP 2.7. The values are averages over all available validation orbits for the particular month.

In most situations, the differences between ozone columns from GDP 2.4 and GDP 2.7 are smaller than 10 DU. Ozone in GDP 2.7 is lower in the winter hemisphere and over Antarctica

and Greenland. Ozone columns are clearly higher over the north pole in April, a somewhat surprising result. The observed changes are mainly due to the change in multiple scattering correction to the O_3 airmass factors and to a smaller degree also to the change in snow albedo. From the figure is is clear, that for most situations the ozone column in the GDP 2.7 version is not significantly different from that in the previous version 2.4.

3.2 Comparison with ground-based measurements

GOME ozone and NO_2 vertical columns have been compared to the ground-based measurements performed by the University of Bremen in Ny-Ålesund and Bremen. In Figure 3, the results of this comparison is shown for ozone.

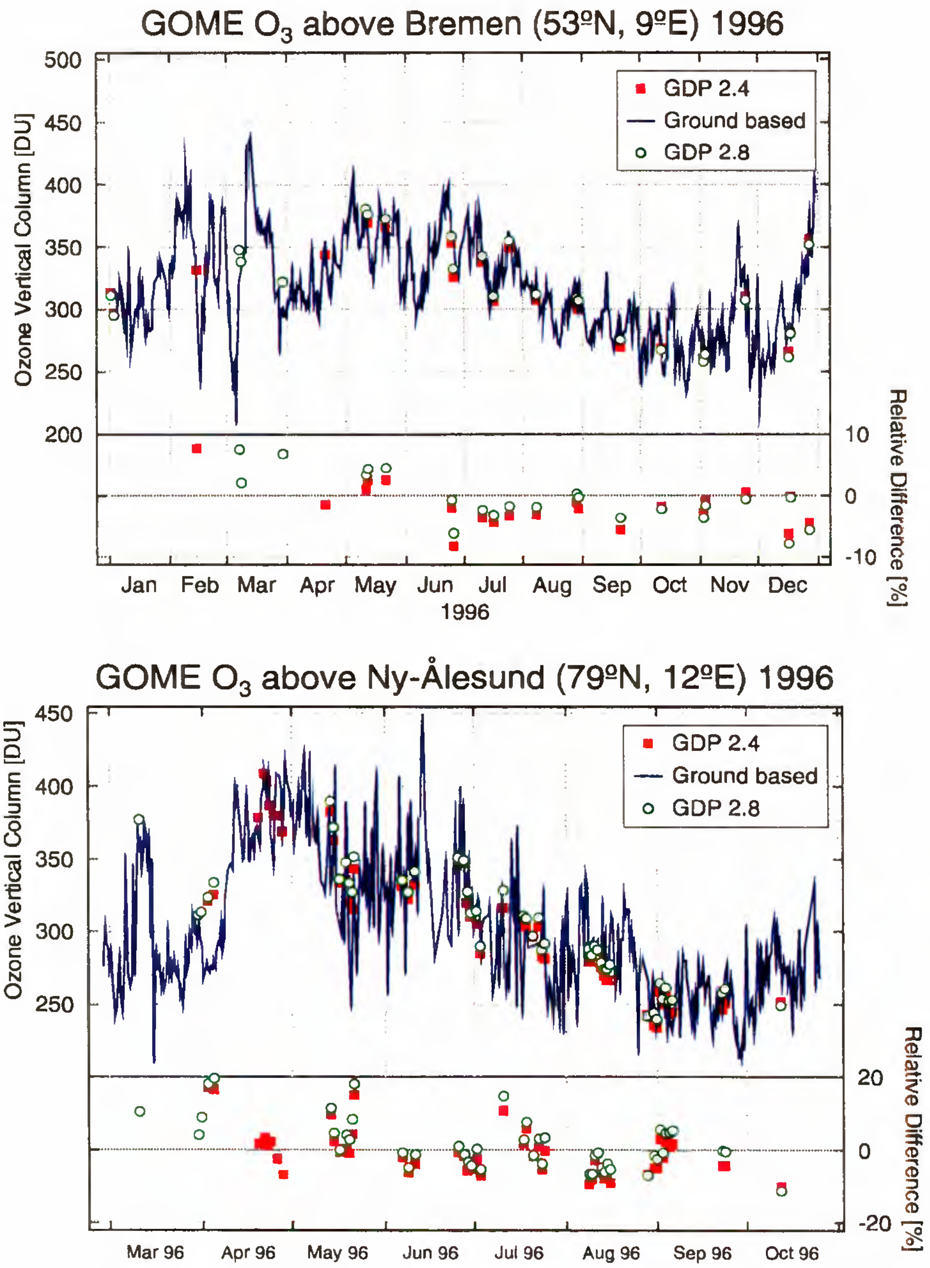

Figure 3. GOME GDP 2.4 and GDP 2.7 ozone vertical columns compared to ground-based measurements in Bremen and Ny-Ålesund 1996.

As can be seen from the plots, GOME ozone vertical columns for both stations have not changed significantly in the new GDP version. At the mid-latitude station Bremen, the GDP 2.7 data generally are in good agreement with the ground-based results although they tend to be low in fall and winter. In Ny-Ålesund, the results are similar but the scatter is larger due to larger errors in both the ground-based and satellite data. This is in agreement with the results of previous validation studies and the results shown in Fig 2.The same type of comparison is shown for NO_2 in Figure 4.

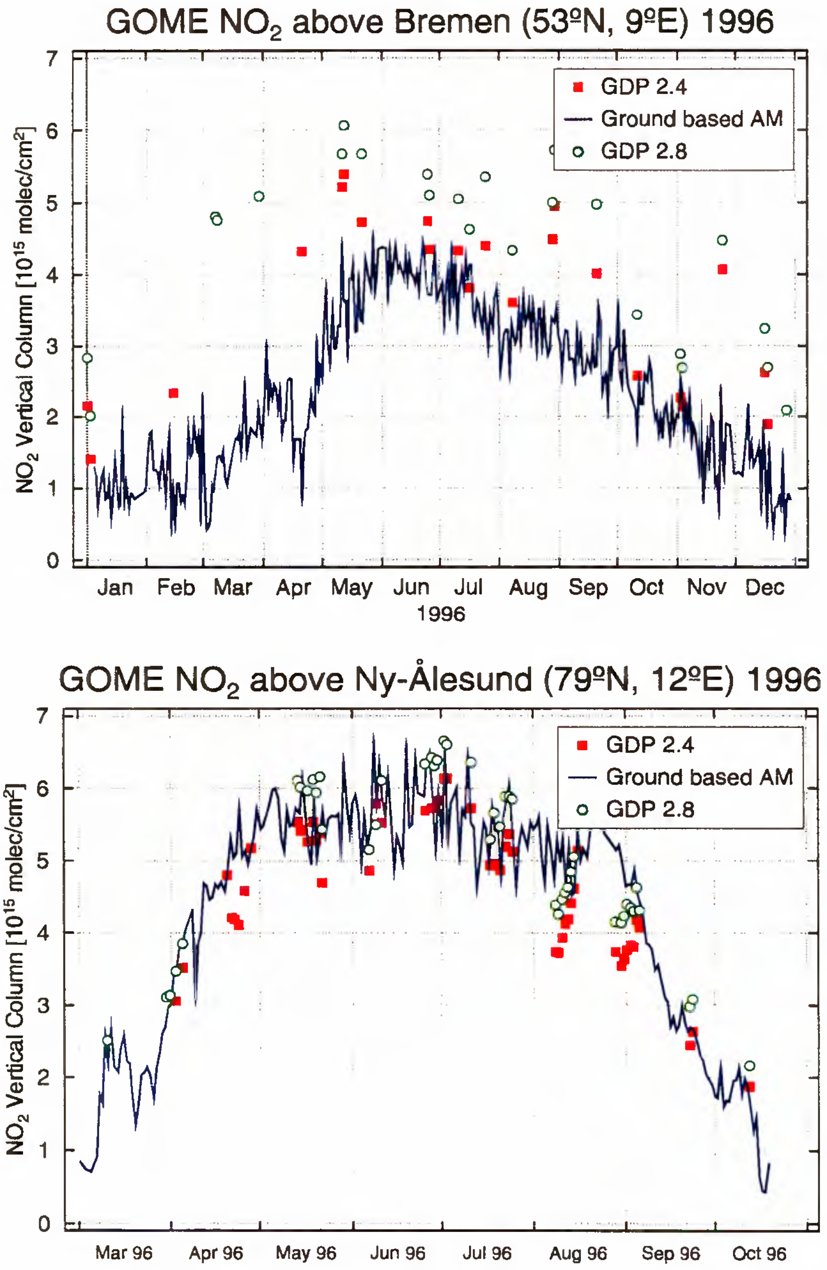

Figure 4. GOME GDP 2.4 and GDP 2.7 NO_2 vertical columns compared to ground-based measurements in Bremen and Ny-Ålesund 1996.

As can be seen from the plot, GOME NO_2 has increased from GDP 2.4 to GDP 2.7 both in mid and high-latitudes. In Ny-Ålesund, the values now are in excellent agreement with the ground-based data. However, in Bremen the GDP values now are clearly larger than the columns derived from the zenith-sky measurements. The difference may in part be explained by the diurnal variation in stratospheric NO_2 and a larger contribution of tropospheric pollution

to the NO_2 column measured in the nadir viewing geometry, but still the values are larger than expected. In summary, the agreement between GOME and ground-based measurements has improved for NO_2 in Ny-Ålesund but not in Bremen.

3.3 Comparison with columns derived at the IUP Bremen using GDP V1.35 level-1 data and the DOAS algorithm of the IUP (for NO_2 only)

In addition to the 1996 validation data set, 79 orbits from 1997 have been provided by DLR to check the improvements in the GDP 2.7 NO_2 columns. For this data set, NO_2 vertical columns have been determined using the DOAS software developed at the IUP Bremen and a simple airmass factor for the nadir viewing geometry. As for ozone, the data have been zonally averaged and the seasonal variation computed for selected latitude bands. In Figure 5, the results are compared for the GDP 2.7 data and the IUP evaluation.

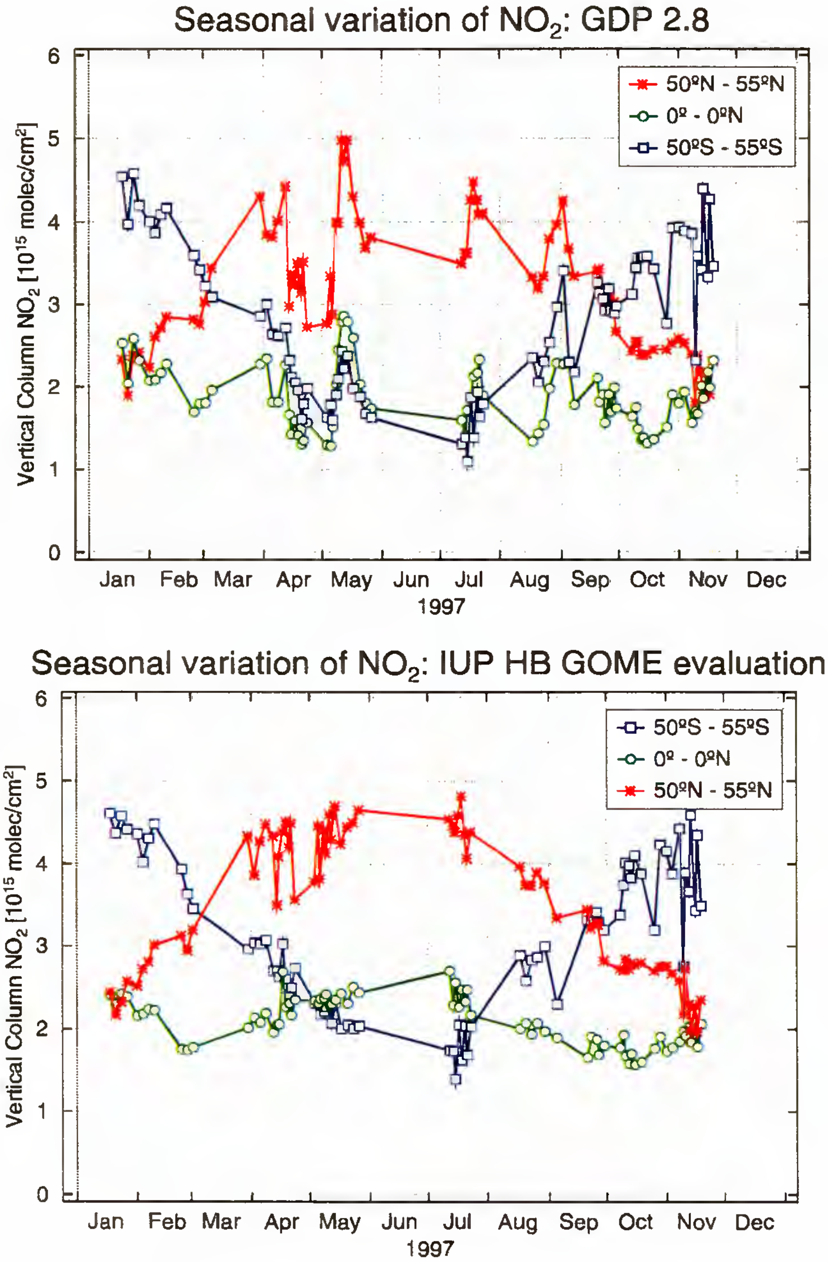

Figure 5. Zonal means of NO_2 vertical columns for selected latitude bands. In the upper panel, GDP 2.7 data are shown, in the lower panel, the IUP-Bremen evaluation is plotted.

In general, the results of both evaluations agree very well in both the absolute values and the seasonal and latitudinal variation. However, the IUP analysis gives a "smoother" variation of the NO_2 columns with time.

In conclusion, the GDP 2.7 and the IUP Bremen evaluation give very similar results for NO_2. The smaller day to day variation in the IUP Bremen data shows, that there still is potential for further improvements in the GDP NO_2 analysis.

3.4 Comparison of IUP fit results using lv1-data from different GDP versions

A limited set of lv1-data calibrated with the new GDP has been delivered after the kick-off meeting. On these orbits, the NO_2 analysis with the IUP Bremen algorithm (see last section) has been repeated. In general, the results of the two analyses are nearly identical, with the exception of those pixels, where the wavelength calibration was off in the old lv1-data. For these pixels, the new lv1-data give more realistic results for NO_2. The degree of improvement in the wavelength calibration is illustrated in Figure 6.

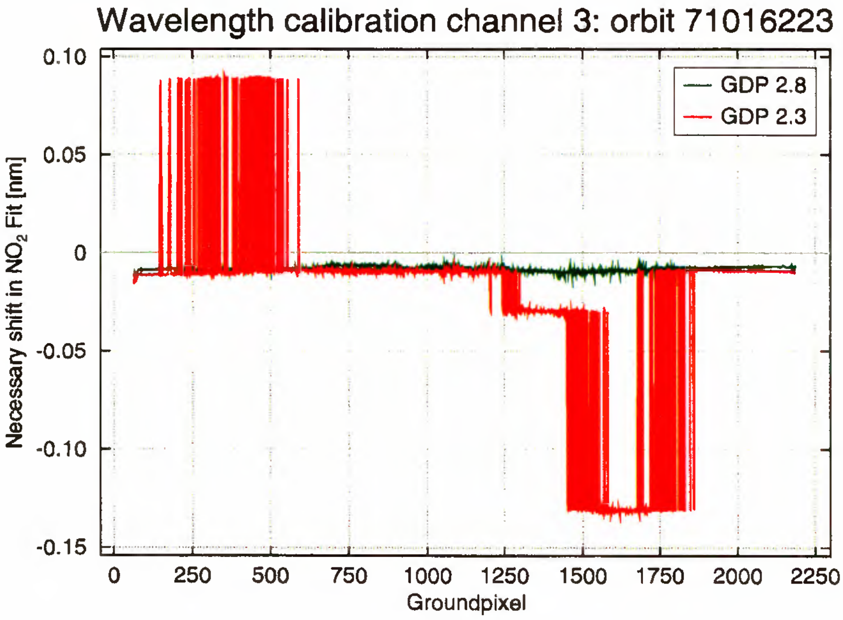

Figure 6. Spectral shift derived for the GOME earth shine spectra in the NO_2 fitting region for both the new and old lv1-data.

4. Conclusions

In this study, a GDP 2.7 validation data set has been compared to GDP 2.4 data, ground-based measurements and the IUP Bremen DOAS evaluation of GOME lv1-data. The main results of this validation are summarised below.

In GDP 2.7, several bug fixes and algorithm improvements have been implemented in the data processor. As a result,

1. total ozone in GDP 2.7 has not changed significantly compared to GDP 2.4;

2. the agreement between ground-based measurements and GOME ozone columns has not changed significantly;
3. in GDP 2.7, the large scatter in NO_2 columns has been removed;
4. the agreement with ground-based NO_2 measurements has improved with GDP 2.7 in high and low latitudes, but not in mid-latitudes;
5. IUP Bremen NO_2 columns are "smoother" than GDP 2.7 columns.

In summary, for most situations the ozone columns in GDP 2.7 have not changed significantly from those of GDP 2.4. The overall consistency of the NO_2 columns has been improved significantly, and for some orbits NO_2 now agrees better with ground-based measurements in Ny-Ålesund and at low-latitudes than with version 2.4. It is mainly this improvement in consistency that leads to the recommendation to replace GDP 2.4 by GDP 2.7 as the operational GDP version.

5. Outlook

For NO_2, the new GDP version 2.7 represents a clear improvement. However, it should be borne in mind that there still are several known problems with the GOME data products that have to be addressed in future GDP versions. The most important of these problems are:

1. GOME O_3 vertical columns are too large for low ozone conditions at large solar zenith angles. The most probable reason is the column dependence of the airmass factors, which up to now is only taken into account in an climatological approach;
2. GOME O_3 vertical columns depend critically on surface albedo. Up to now, the latter is not derived from the measurements themselves, but from climatological assumptions, leading to large errors over snow covered land;
3. GOME airmass factors are not including multiple scattering in an "ab initio" way, but instead consist of a mixture of single scattering airmass factors and a multiple scattering correction factor. This is both error prone and confusing for the data users;
4. In the GOME O_3 fit, the wavelength dependence of the airmass factor is not taken into account. While the effect is treated in the airmass factor calculation itself, neglecting it still introduces an unnecessary error in the fit;
5. In the GOME O_3 fit, the temperature of the ozone cross-section is selected from the climatological temperature in the height of the ozone concentration maximum. Instead, ozone cross-sections at two temperatures should be used to determine the "right" temperature from the data themselves;
6. GOME NO_2 airmass factors use the US standard atmosphere for all times and locations. This necessarily introduces errors in the NO_2 vertical columns;
7. GOME NO_2 vertical columns show much larger day to day variations than expected from ground-based measurements. This probably is due to a calibration problem;
8. GOME NO_2 vertical columns are unreasonably large at large solar zenith angles in polar summer on both hemispheres.

GOME NO_2 VALIDATION STUDIES

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1. Overview

The main contribution of the Institute für Umweltphysik (IUP) at the University of Heidelberg, Germany is the comparison of the Level-2 NO_2 data with the results of the IUP DOAS algorithm. The results of this comparison are presented in section 5.

Further activities included the selection of the wavelength range for the NO_2-DOAS algorithm (section 3) and the recommendation of the use of a H_2O reference spectrum in the fitting procedure (section 4).

In section 2 we start with an overview over the IUP-NO_2 algorithm; in section 6 we give a summary and recommendations.

2. IUP NO_2 analysis

The IUP NO_2 analysis for GOME data was developed in 1997 [Wagner, 1999] and used so far for several studies [Leue et al., 1999; Leue, 1999].

The NO_2 absorption is analysed using a spectral range from 431 to 452 nm (see Figure 1). The measured spectra and the cross sections are smoothed by convoluting with a Gaussian function with a FWHM of about 2.5 pixel. Included in the fitting procedure are the reference spectra listed in Table 1 and a polynomial of degree 2.

Reference spectrum	temperature	Source
O_3	221 K	GOME [Burrows et al., 1999]
NO_2	221 K	GOME [Burrows et al., 1998]
H_2O	293 K	Rothman et al. [1992]
Calculated Ring spectrum	250 K	MFC, Bussemer [1993]
Fraunhofer spectrum	-	GOME direct sun light

Table 1. Reference spectra used for the GOME NO_2 analysis [Wagner, 1999].

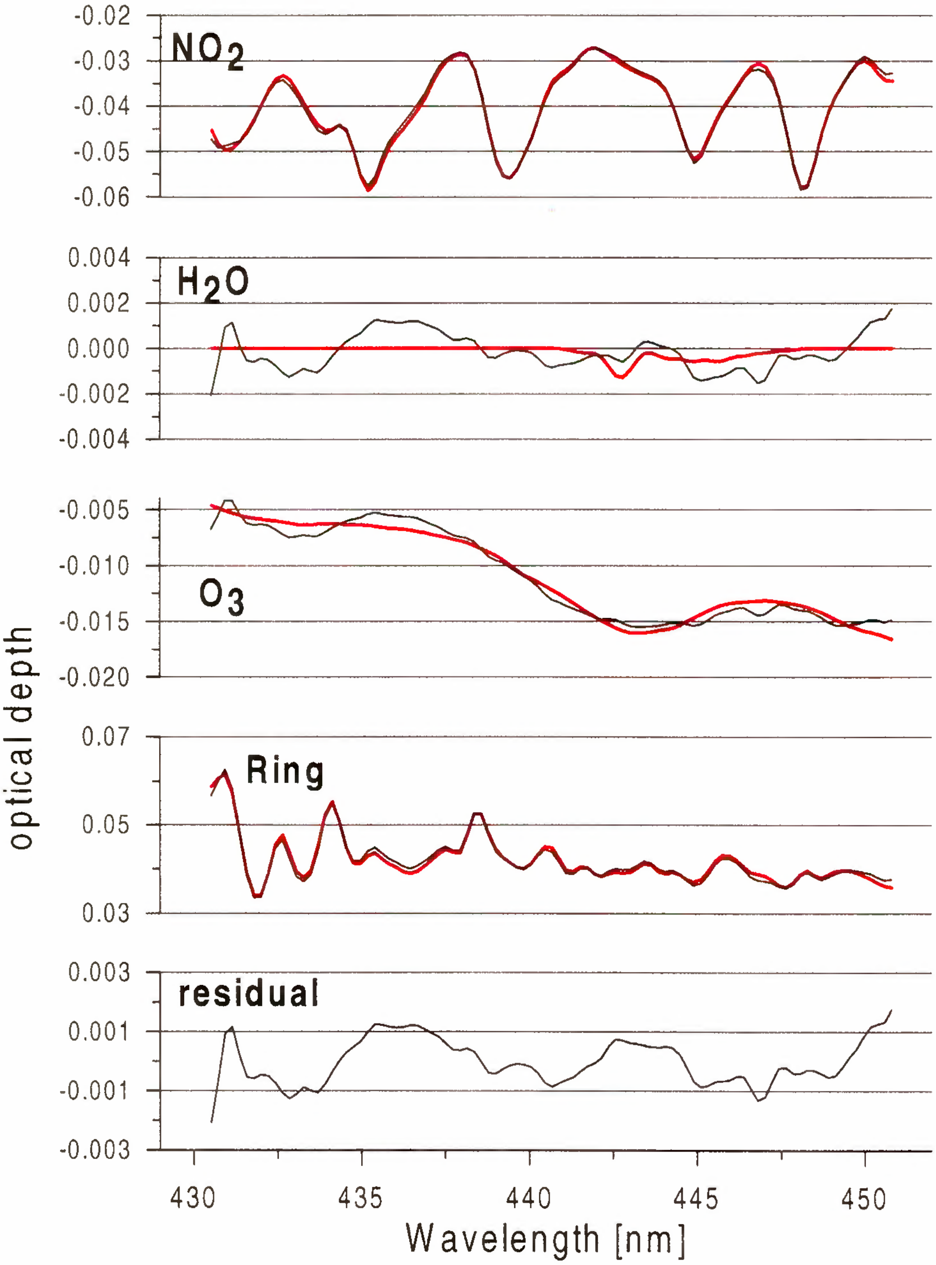


Figure 1. Example for the NO_2 evaluation of an atmospheric GOME spectrum (GOME orbit 71127003, 01:27:50, SZA: 88.9°). The thick lines indicate the trace gas absorption spectra scaled to the respective absorptions retrieved from the GOME spectrum (thin lines).

3. Selection of the wavelength range

The NO_2 molecule shows characteristic absorption features over a wide wavelength range in the UV/vis spectral region. The most pronounced differential spectral structures show up around 440 nm and consequently this spectral range has been used for many analysis procedures so far.

However, in the case of the GOME measurements the spectral region in channel 3 for wavelengths above 400 nm is subject to several problems due to a changing Fabry-Perot-etalon effect and the changing optical properties of the Dichroic filter [ESA, 1996]. Thus it seemed worth investigating the quality of the NO_2 results derived also from other spectral regions, in particular in the UV around 350 nm (BrO analysis) and the visible spectral range around 550 nm (O_3 analysis).

The reference spectra used for both analysis are shown in Table 2 and Table 3.

Reference spectrum	temperature	Source
O_3	221 K	GOME [Burrows et al., 1999]
O_3	241 K	GOME [Burrows et al., 1999]
NO_2	227 K	GOME [Burrows et al., 1998]
OClO	203 K	Wahner et al. [1987]
BrO	227 K	Wahner et al. [1988]
O_4	296 K	Greenblatt et al. [1991]
Calculated Ring spectrum	250 K	MFC, Bussemer [1993]
Fraunhofer spectrum	-	GOME direct sun light

Table 2. Reference spectra used for the GOME BrO analysis (344 and 359 nm) [Wagner et al., 1998, 1999; Wagner, 1999].

Reference spectrum	Temperature	Source
O_3	248 K	GOME [Burrows et al., 1999]
NO_2	241 K	GOME [Burrows et al., 1998]
H_2O	293 K	Rothman et al. [1992]
O_4	296 K	Greenblatt et al. [1991]
Calculated Ring spectrum	250 K	MFC, Bussemer [1993]
Fraunhofer spectrum	-	GOME direct sun light

Table 3. Reference spectra used for the GOME O_3 analysis (500 to 578 nm) [Wagner 1999].

The Comparison of the NO_2 results derived in the different spectral regions are shown in Figures 2 and 3. The most important finding is that the scatter of the NO_2 SCDs for small SZAs and thus small absorptions is much weaker in the 'standard IUP NO_2 analysis' compared to the other spectral ranges (Figure 2). This indicates that the spectral range of the 'standard' NO_2 analysis seems to be best suited for the evaluation of the NO_2 absorption in GOME spectra.

In Figure 3 it can be seen that the NO_2 SCD for large SZA differs depending on the spectral range used for the evaluation. This is an expected effect and results from the different atmospheric radiative transport in the different spectral ranges.

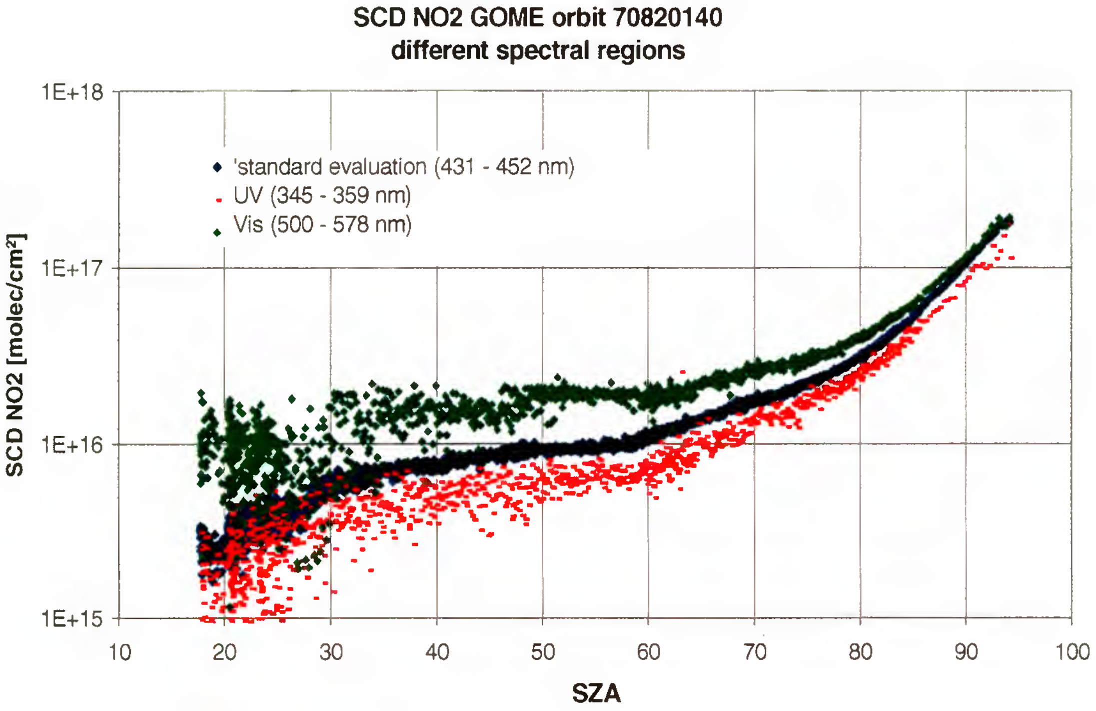


Figure 2. NO$_2$ SCD for the GOME orbit 70820140 derived in different spectral ranges. For small SZAs the weakest scatter of the results is belongs to the wavelength range 341-352 nm.

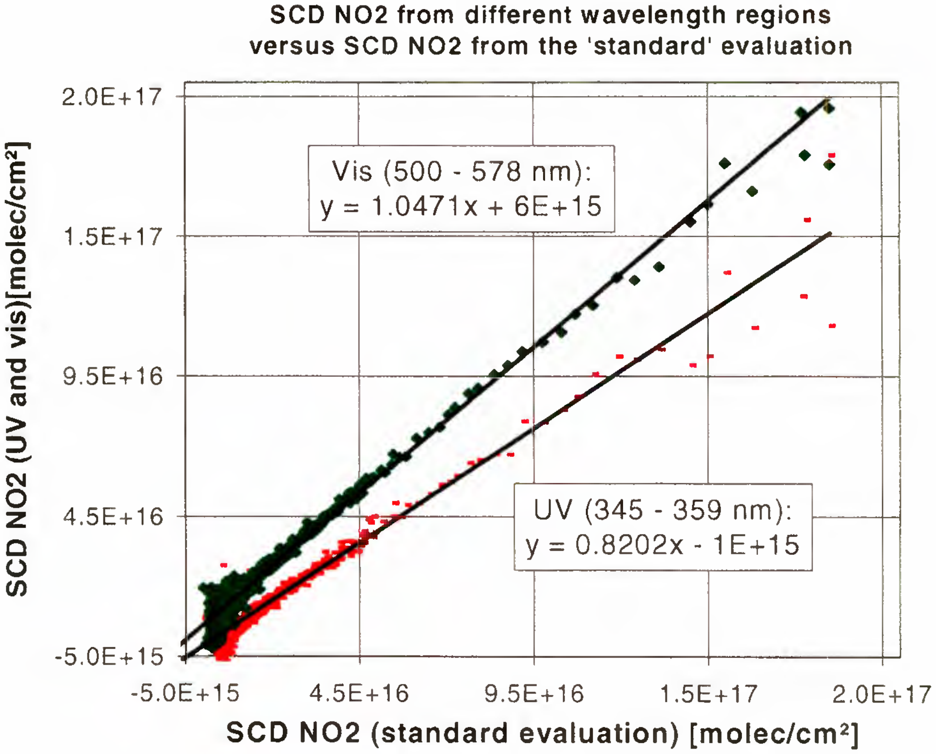


Figure 3. NO$_2$ SCD for the GOME orbit 70820140 derived in the two 'non standard' wavelength ranges plotted as a function of the NO$_2$ SCD derived in the standard wavelength range.

4. Importance of the H_2O reference spectrum

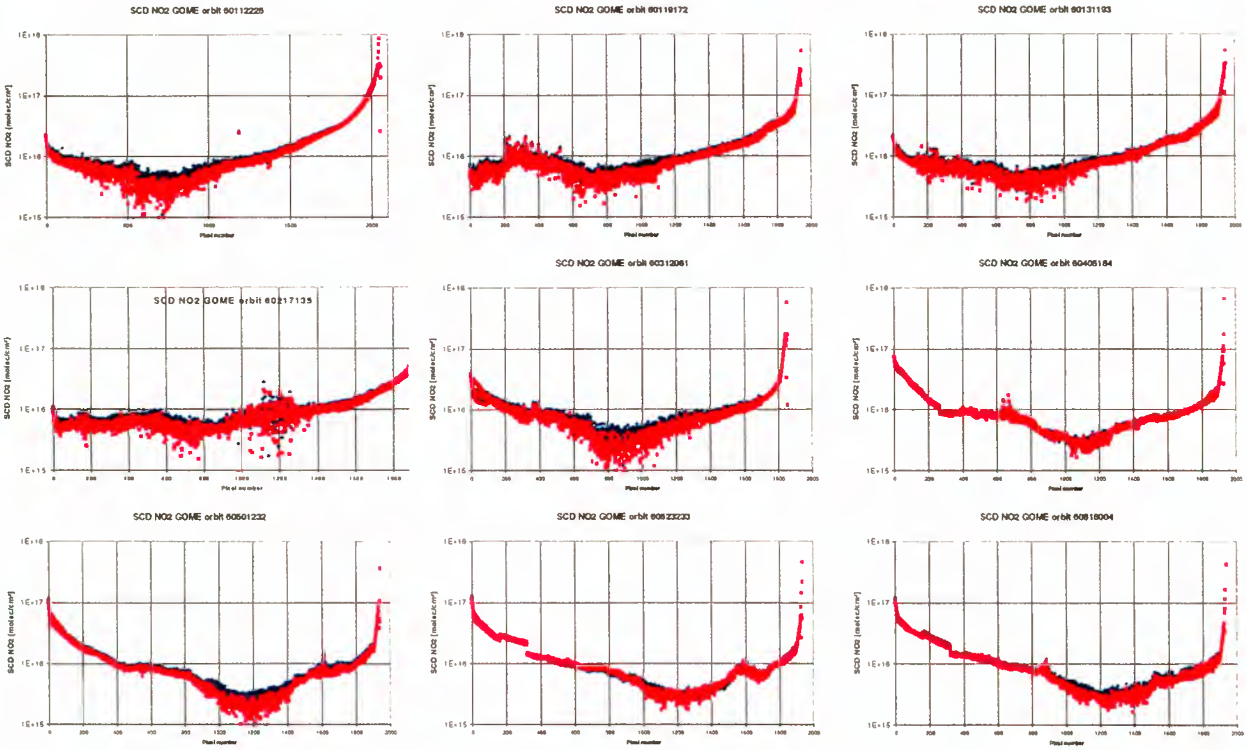
Water vapour shows characteristic absorption features around 442 nm. These absorptions are relatively weak compared to those at larger wavelengths. However, for specific atmospheric conditions, e.g. in the tropics where the atmospheric water vapour content is high, the H_2O absorption around 442 nm can reach up to about 1 %. Thus it can be **much** larger than the simultaneous NO_2 absorption. Especially in the tropics the SZA and thus the air mass factor is small and consequently the NO_2 absorption can be by about one order of magnitude smaller compared to the H_2O absorption.

To minimise the influence of atmospheric H_2O absorptions a H_2O reference spectrum has to be taken into account in the DOAS fitting procedure.

5. Comparison study

In contrast to previous versions the new GOME level 1 to 2 processing (version 2.7) includes a reference spectrum for H_2O. The wavelength region is again extended to a relative broad region (425-450 nm). Thus, the main features of the official DLR/ESA (version 2.7) level 2 NO_2 processing are similar to those of the IUP NO_2 evaluation.

Figure 4 gives an overview of the comparison between the DLR/ESA (version 2.7) and the IUP NO_2 evaluation of several orbits during 1996 and 1997.



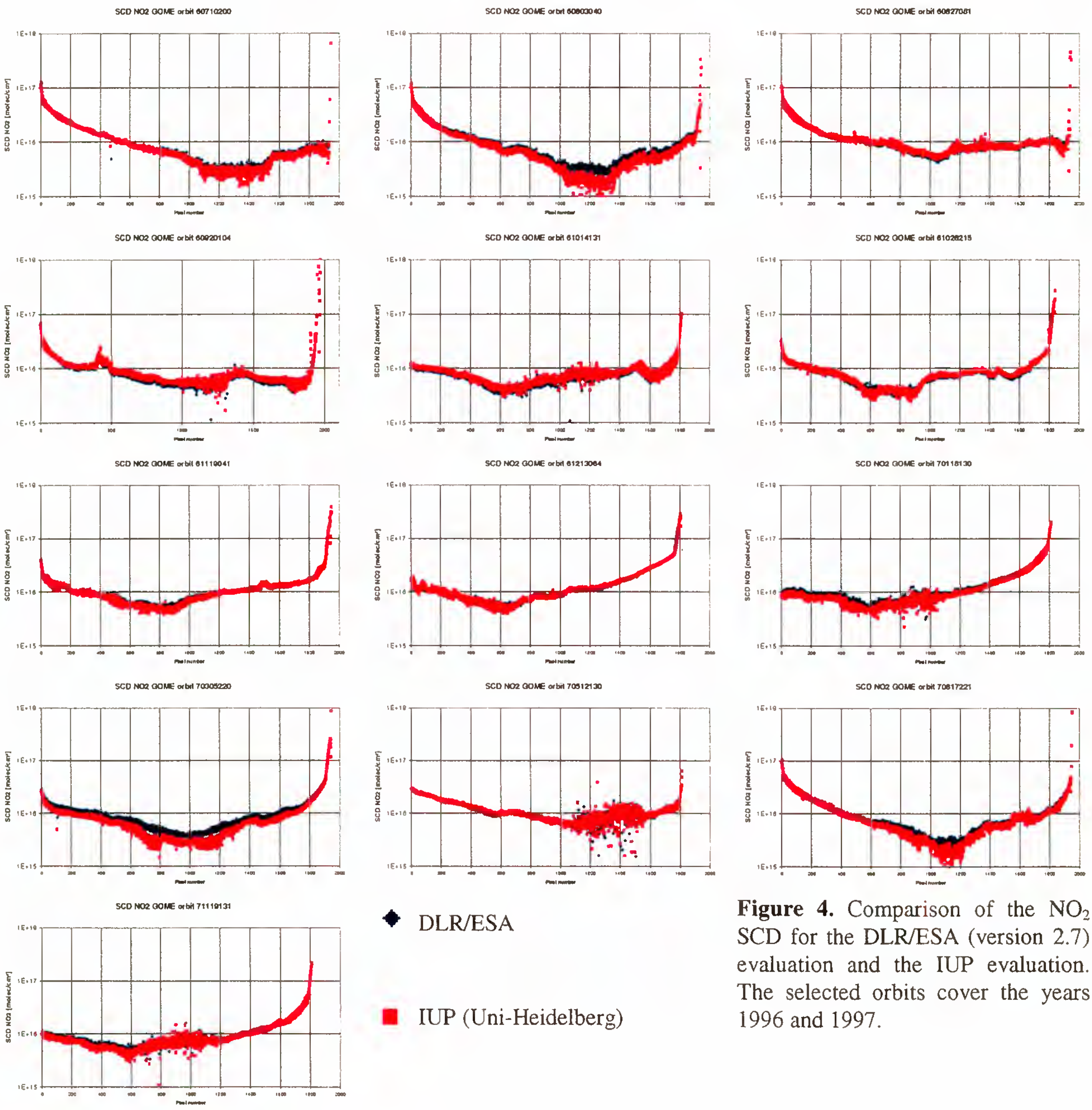


Figure 4. Comparison of the NO_2 SCD for the DLR/ESA (version 2.7) evaluation and the IUP evaluation. The selected orbits cover the years 1996 and 1997.

In general, the agreement of both data sets is very good for high SZAs and thus large NO_2 absorptions (better than about 5 %). In many cases a good agreement is also found for small SZAs. However, in some cases very large deviations (> 100 %) occur. The reason for these large deviations is investigated in the following. Three orbits representing different cases are selected (see Figure 5):

First an orbit with a large deviation and large scatter of the results (60803040), second an orbit with a small deviation and a small scatter (61119041), and third an orbit with a small deviation but a large scatter (70512130).

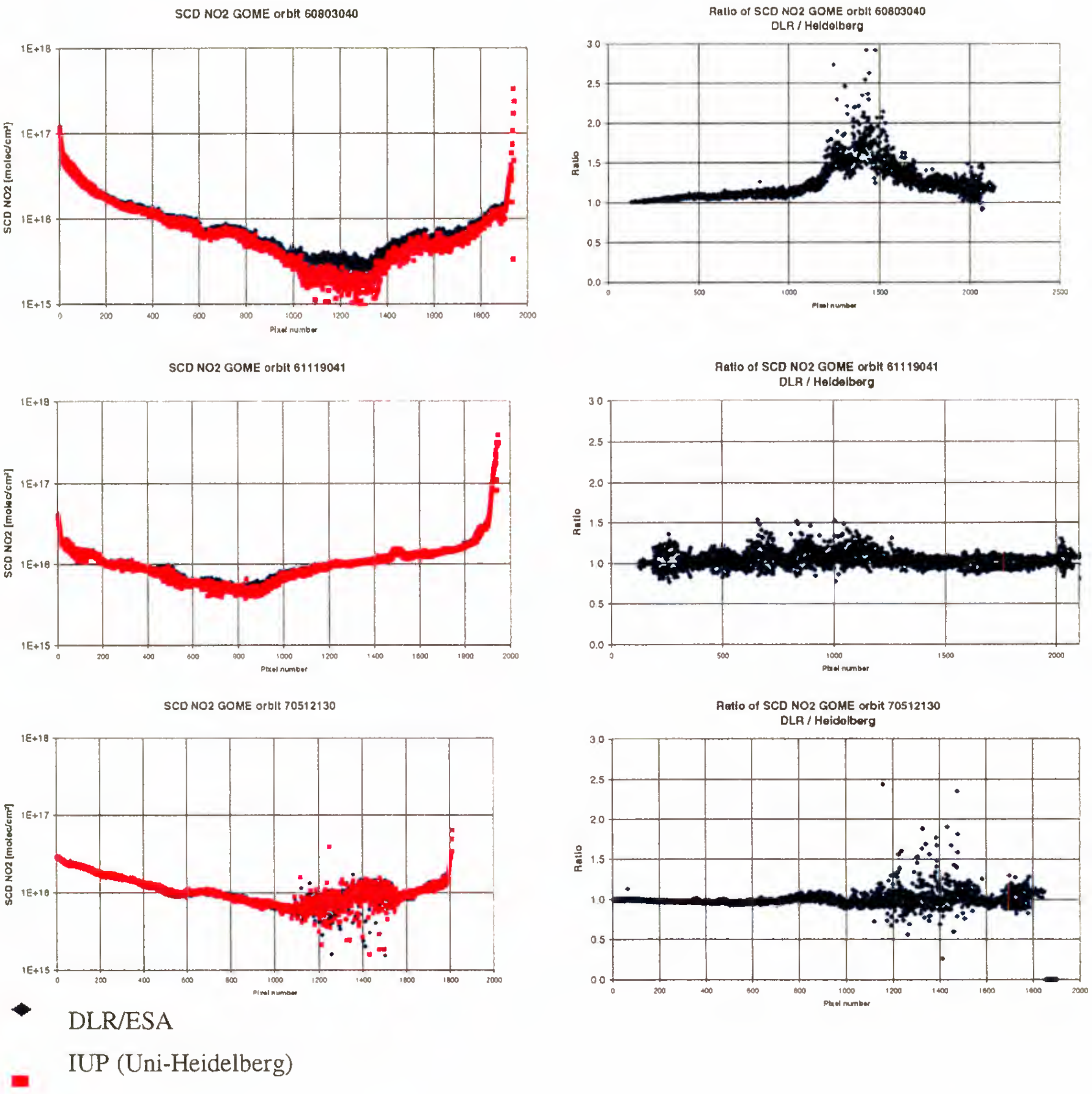


Figure 5. Left: NO_2 results of the DLR/ESA and the IUP evaluation for three GOME orbits. Right: Difference between both evaluations.

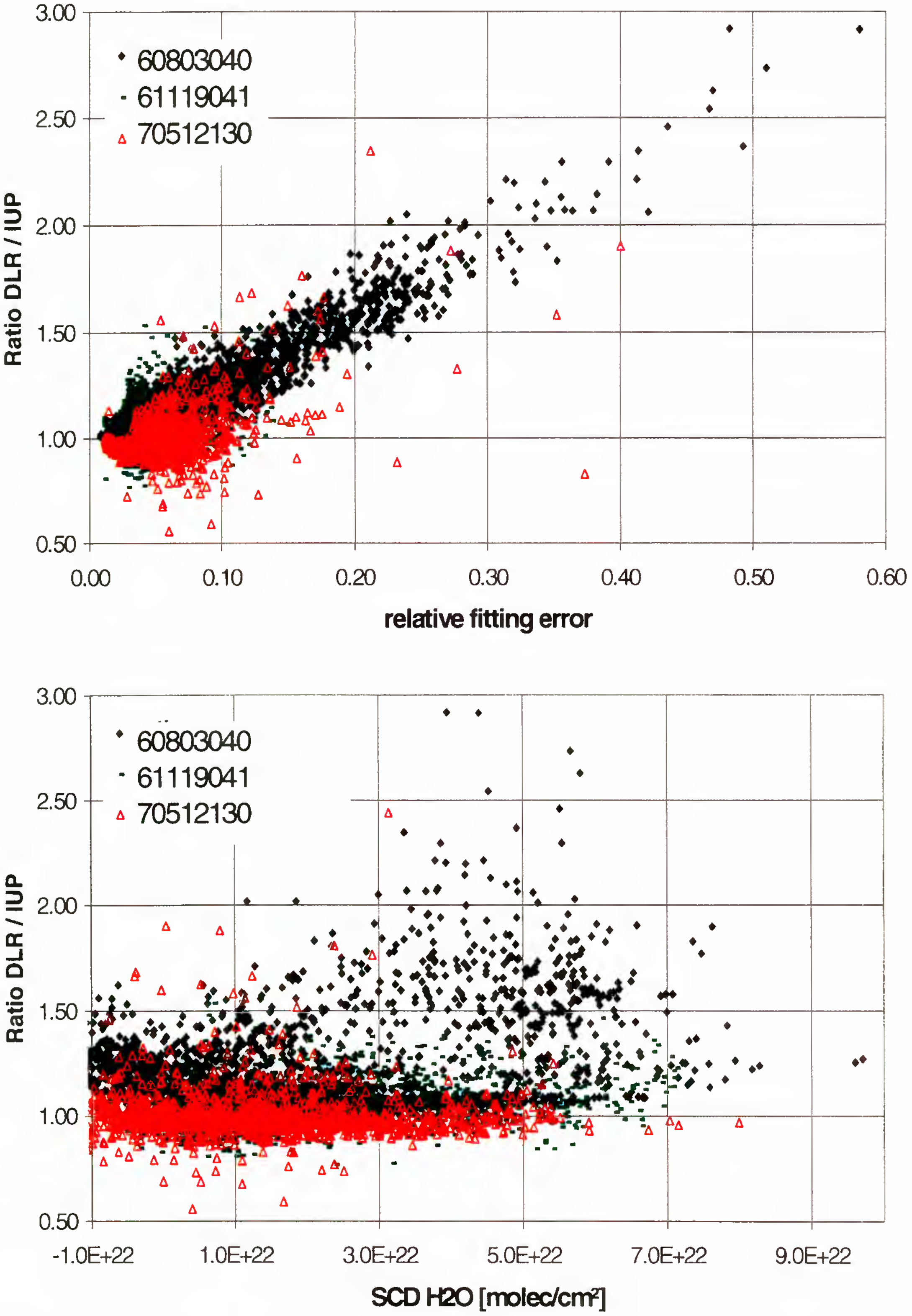


Figure 6. Relative deviation between the DLR/ESA and the IUP NO$_2$ evaluation as a function of the relative fitting error (top) and of the SCD H$_2$O (bottom).

In the top of Figure 6 the deviation between the NO_2 results of the DLR/ESA and the IUP evaluation is plotted as a function of the relative NO_2 fitting error. The good correlation indicates that the uncertainty of the GOME NO_2 results is well represented by the error given by the DOAS fitting procedure.

In contrast, nearly no correlation is found between the deviation of the NO_2 results of the DLR/ESA and the IUP evaluation and the H_2O SCD (bottom of Figure 6). Thus we conclude that the difference in the NO_2 results of both evaluations is not caused by possible spectral interferences with the atmospheric H_2O absorptions.

6. Conclusions and Recommendations

From our studies we draw the following conclusions:

General remarks

- The DOAS fitting window in the 'standard' spectral range (431 - 452 nm) is best suited for the GOME evaluation of NO_2 (compared to UV or green spectral range). The scatter of the NO_2 results in the 'standard' spectral range is significantly smaller compared to fitting windows in the UV or green spectral range;
- A broad spectral range should be used for the DOAS fitting to use the maximum spectral information. In the case of the GOME NO_2 evaluation we recommed a fitting window between about 425 and 450 nm;
- The H_2O absorption has to be taken into account (for the 'standard spectral range').

Comparison between DLR and IUP NO_2 evaluation:

- A good agreement (better than about 5 %) was found for strong NO_2 absorptions (SCD $NO_2 > 5 \cdot 10^{16}$ molec/cm²);
- In several cases large systematic deviations were found for weak NO_2 absorptions: up to 100% for SCD $NO_2 < 2 \cdot 10^{15}$ molec/cm². As a general feature the DLR/ESA (version 2.7) values are systematically larger than the IUP values;
- The deviations between both evaluations are only weakly correlated with the strength of the H_2O absorption. This indicates that the differences in the NO_2 results of both evaluations are not caused by possible spectral interferences with the atmospheric H_2O absorptions;
- In contrast we found a strong correlation of the deviation with the relative error given by the DOAS fitting procedure. Thus the uncertainty of the GOME NO_2 results seems to be well represented by the error given from the DOAS fitting procedure;
- The largest deviations occur for small SZA over tropical and subtropical regions. To further investigate the quality of the GOME NO_2 evaluation validation sources in that regions is required.

7. References

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7. CONCLUSIONS

The correctness of upgrades of GOME Data Processor level-0-to-1 to version 2.0 and level-1-to-2 to version 2.7, as well as their effect on GOME data products, has been investigated using different methods based on auto-correlation studies, on comparisons with high-quality correlative data, and on independent retrieval software tools.

The following data products and auxiliary information have been verified:

- spectral solar irradiance;
- spectral earthshine radiance;
- fractional polarisation (as measured by the Polarisation Monitoring Devices, PMD);
- clouds data (as determined by the Initial Cloud Fitting Algorithm, ICFA);
- nitrogen dioxide data: slant and vertical columns;
- ozone data: slant and vertical columns, air mass factors.

Modifications implemented in GDP 2.7 produce expected changes in the data products. New degradation corrections of channels 1-2 and PMD measurements improve solar irradiance and fractional polarisation data. The bias in ICFA cloud fraction has been largely removed. Changes in the ozone data product are generally small.

The main objective of GDP upgrades has been met: the geophysical consistency of NO_2 vertical columns has improved significantly at all latitudes, except at northern middle latitudes where it is difficult to conclude.

Accordingly, the existing documentation on the quality of GDP data products has been updated.

Despite the general improvement of most GOME data products studied here, it must be kept in mind that several major issues remain to be addressed.

As a result of the general improvement of GOME data products, the new version of the level-0-to-1 and level-1-to-2 segments of GDP has been implemented in the operational processing chain. Reprocessing of the whole GOME data record will be completed by the end of 1999. Reprocessed products can be used within the limitations outlined in the existing literature and updated in the present report.

A-1. GOME DATA PRODUCTS QUALITY STATUS : JUNE 1999

In the first half of 1999 the GOME Data Processor (GDP) was upgraded to versions 2.0 (level-0-to-1) and 2.7 (level-1-to-2). Before implementation of the changes in the operational processing chain, a delta validation study was conducted on a limited but representative set of orbits to verify the geophysical consistency and to identify and quantify improvements of the upgraded GOME data products. The present document provides a short summary about the current GDP products quality status.

GOME level-1 products are affected by spectral and radiometric distortions of instrumental origin, which change with time. The solar irradiance measurements exhibit an anticipated and in this sense normal, slow degradation in the UV (channels 1 and 2), which can optionally be corrected by the extraction software. The errors impact the retrieval of ozone and other constituents in a relatively minor way, thanks to the use of the DOAS retrieval technique. The accuracy of the Earth's reflectivity (i.e., the ratio between Earth radiance and solar irradiance) is considered to be about 3% except in the UV where it is limited due to pre-flight calibration uncertainties and to the remaining effects of atmospheric polarisation.

The version 2.8 of GOME level-2 products has been validated from pole to pole against well documented and controlled ground-based measurements. GDP retrievals have also been compared with retrievals from independent DOAS algorithms.

The accuracy of the GOME ozone vertical column amount varies with the solar zenith angle (SZA) and, in many cases, with the ozone column or profile. For SZA lower than 70 degree, the accuracy is in the range 2%-5%, and at larger SZA it is 10% or better. Under particular conditions, such as in wintertime polar regions, low ozone values can be overestimated by more than 15%. The SZA and column dependencies originate mainly from the enhanced sensitivity of the current retrieval algorithm approach to the actual atmospheric profiles.

The data quality and geophysical consistency of the GOME nitrogen dioxide vertical column amount have been improved in the latest version of the data products. Although difficult to evaluate, the overall accuracy is estimated to vary from 5% to 20%, outside of the Tropics. GOME total NO_2 is affected by larger errors under certain circumstances, e.g. over polluted areas or during midnight sun. Atmospheric parameters currently in use in GDP introduce a fictitious latitudinal/seasonal variation of a few percent superimposed on the geophysical variations in NO_2.

Since validation is an on-going activity, this report presents only an overview of the current situation. For more information, please refer to the Operational GOME Data Products Delta Validation Report 1999 or to the GOME Web page (http://earth1.esrin.esa.it:81/eeo2.600), or contact the ERS Help & Order Desk (eohelp@esrin.esa.it).

A-2. DATA DISCLAIMER FOR GOME LEVEL-1 AND LEVEL-2 DATA PRODUCTS : JUNE 1999

1. Introduction

Since the beginning of GOME operation aboard ERS-2 in 1995, the assessment of the quality of products generated by the GOME Data Processor (GDP), established at the German Processing and Archiving Facility (D-PAF), has been a continuing activity aimed at achieving data products having their theoretically achievable errors. This process and the algorithm improvement have benefited from the validation exercises involving the scientific community. The involved scientific groups have expertise in the development of retrieval algorithms and the measurement of trace constituents from other relevant instrumentation.

The operational products produced by the GDP are defined as:

- Level-1 data: Earthshine spectral radiance at the Top of the Atmosphere at the GOME viewing solid angle; Extra-terrestrial solar spectral irradiance.
- Level-2 data: Vertical Column amount of O_3 (Dobson Unit); Vertical Column amount of NO_2 (molecule cm-2); Cloud Coverage.

An intensive validation campaign for GOME products was conducted during the commissioning phase. Reported in an ESA publication (ESA WPP-108), studies carried out by more than 20 different groups highlighted a number of critical aspects of the GDP data products. As a result, recommendations were made for modifications to the GDP, data analysis, instrument operations, data processing, and data distribution. Some of these recommendations were implemented during the first months of 1996. Since then, several other important issues have been identified. Consequently further GDP modifications have been recommended and some of them implemented.

Before proceeding to the implementation of any major GDP changes in the operational processing chain, it is essential to verify the accuracy and effectiveness of the modification and to assess the quality of the new data product. Such 'delta' validation campaigns have been executed by a sub-group of the GOME validation group, with a limited but representative validation data set. Results were discussed during dedicated meetings in May and June 1996 and in January 1998 at the D-PAF and in May and July 1999 at ESRIN.

Complementarily, detailed validation and algorithm improvement studies have been carried out by a wider community and reported on many occasions during conferences and workshops as well as in the open literature.

Based on the results of the above-mentioned studies, the present disclaimer summarises the status of the current GDP data quality, referring to version 2.0 for GDP level-0-to-1 and version 2.7 for GDP level-1-to-2.

2. Current Data Quality of GOME level 1-Product

The level-1 data products exhibit good wavelength stability indicating a high instrument precision.

GOME level-1 products are affected by spectral and radiometric distortions of instrumental origin, which change with time. The solar irradiance measurements exhibit an anticipated and in this sense normal, slow degradation in the UV (channels 1 and 2), which can optionally be corrected by the GDP extraction software. In addition, the degradation is superimposed by a seasonal variation of sensitivity depending on the solar azimuth at the sun diffuser. The errors impact the retrieval of ozone and other constituents in a relatively minor way, thanks to the use of the DOAS retrieval technique. The accuracy of the Earth's reflectivity (i.e., the ratio between Earth radiance and solar irradiance) is considered to be about 3% except in the UV.

2.1 Solar Irradiance

The validation of GOME solar irradiance data is based on comparisons with SOLSTICE and SSBUV measurements in the 240-400 nm spectral range, on auto-correlation studies of GOME data, and on comparisons with high-resolution solar spectrum atlas data.

Deviations at the beginning of the GOME Instrument lifetime:

Despite the better agreement with SOLSTICE measurements, the GOME irradiance measurement in its channel 1 is considerably lower, by 5 % to 10 %. In channel 2, the agreement is better but the accuracy of GOME data is limited by etalon features (modulation of ± 2 %).

The average deviation of GOME data from the SOLSTICE data on 3-Jul-1996 and the rate of linear decay between 3-Jul-1995 and 14-Jan-1996 are given in the following table:

Spectral range	Average deviation	Linear decay / 100 days
240 - 250 nm	5.8 %	3.5%
250 - 300 nm	5.1 %	1.5%
300 - 370 nm	0.8 %	0.5%
370 - 400 nm	2.4 %	0%

Deviations at mid 1999:

The average deviation of GOME data from the SOLSTICE V12 data on 1-Jan-1999 and the rate of linear decay in 1998 are given in the following table:

Spectral range	Average deviation	Linear decay / 100 days
240 - 250 nm	-51 %	4.7 %
250 - 300 nm	-25 %	1.7 %
300 - 350 nm	-9 %	0.7 %
350 - 400 nm	-4 %	0.3 %

The observed degradation in the UV was expected and is similar to the degradation observed in other relevant instruments. It can optionally be corrected by the extraction software.

Note that the solar azimuth on the solar diffuser is different for January and July data, which affects the sensitivity in the spectral region below 260nm by about 6%. Therefore, the linear decay presented in the tables above must be considered as an upper limit.

2.2 Earthshine Radiance

The Earthshine radiance product suffers from the same instrument degradation as the Solar Irradiance product.

A correction for the GOME instrumental response to polarisation (PC) is required for the radiance products. This PC has been determined assuming that single scattering is dominant below 300 nm. The polarisation of the up-welling radiation from the atmosphere has been determined as follows:

i) for wavelengths below 300 nm, it is assumed that the Rayleigh scattering determines the degree of polarisation;

ii) for wavelengths greater than 300 nm, experimental values for the degree of polarisation have been determined from the detector arrays in channels 2, 3 and 4 and their corresponding polarisation monitoring device (PMD);

iii) a polynomial is then fitted to the four "measurements" of the degree of polarisation, with a parameterisation based on model calculations between 300 and 350 nm, providing individual values of the degree of polarisation.

After the degradation correction of the polarisation measurements, the accuracy of the radiometric calibration of GOME between 350 and 790 nm is considered to be about 3% except in the UV where it is limited to 5 % due to pre-flight calibration uncertainties and to the remaining effects of atmospheric polarisation. Below 350 nm the Earth's radiance has not yet been fully validated.

One aspect of the radiance error results from inadequacies in the polarisation-correction procedure implemented in the level-1 extractor software. The interpolation of the small p values in the region between 350 nm (measured PMD1 polarisation value) and 300 nm (theoretical polarisation value) is not fully satisfactorily.

Discontinuities in the absolute radiance values are observed between channels and are real. This is caused by the serial readout of the detectors, which means that although all array pixel detectors have the same integration time, the read-out of the first array detector pixel is 93 ms shifted in time compared with the 1024th array detector pixel. This effect occurs in a pronounced fashion for earthshine scenes having significant albedo changes in the field of view of the first and of the last pixel of the detector. An option in the extraction software is available to create an effective average scene for the four channels.

3. Current Data Quality of GOME level-2 products

3.1 Vertical column amount of ozone

GDP total ozone has been validated from pole to pole by comparison with well understood, controlled and documented ground-based measurements from SAOZ/DOAS UV-visible spectrometers, Brewer and Dobson spectrophotometers, and UV filter radiometers, and with global data from the TOMS satellite sensor and from modelling/assimilation tools. GDP retrievals have also been compared with retrievals from independent DOAS algorithms and from the TOMS V7 algorithm.

The spectral fitting of ozone slant columns in the UV region from 325 to 335 nm works well. GOME gives a consistent global picture of the total ozone field and results in temporal and spatial structures similar to those from other sensors. The studies do not reveal any long-term drift of quality.

The agreement of GDP level-2 total O_3 data product with the other sources of O_3 data is found to vary with both latitude and season. At Northern middle latitudes, the average agreement is within ±2-4%. At higher latitudes, a solar zenith angle (SZA) dependent difference appears. In addition a dependence of the GDP data product on the ozone column values has been identified. These two effects are coupled in the final data product.

The deviation of GOME from ground-based data does not exceed ±5% for SZA below 70°. Above SZA values of 70°, the error ranges from –10% to +10% depending on the season. Lowest total ozone values are overestimated by GOME by 15% and even more during ozone hole conditions.

The SZA/latitudinal/column dependence of GOME total ozone is attributed to two effects: the inaccurate treatment of the atmospheric profile shape effect in GDP, and the partial unsuitability of the particular spectral analysis when the atmosphere becomes optically thick.

The two-step DOAS approach adopted in GDP consists of the spectral fitting of slant column amount, followed by its conversion into vertical column amount using a calculated Air Mass Factor (AMF). Satellite ozone AMFs in the UV are sensitive to the shape of atmospheric profiles. GDP AMFs are determined using monthly and seasonal atmospheric profiles, which therefore may differ from the actual, highly variable atmospheric profiles. The two-step approach of GDP is well suited for relatively small absorptions which have a constant AMF across a selected spectral window. This assumption breaks down for ozone in the UV. As a result the difference between GOME vertical column ozone data and ground-based measurements exhibits a monotone solar zenith angle dependence when the air mass factor is calculated at the centre wavelength of the DOAS fit window (330 nm). Model calculations have shown that this latter effect is minimised by using the AMF at 325 nm.

Confidence levels for GOME total ozone values as derived from the GDP comparison with ground based measurements can be summarised as follows:

Solar zenith angle range	**Average difference (1 sigma)**	**Standard deviation (1 sigma)**
< 70 degree	< 5%	5%
< 90 degree	< 10%	10%

3.2 Vertical column amount of nitrogen dioxide

GDP total nitrogen dioxide has been validated from pole to pole by comparison with well-understood, controlled and documented data retrieved from ground-based measurements from a network of SAOZ/DOAS UV-visible spectrometers and from Fourier Transform Infrared spectrometers. GDP retrievals have also been compared with GOME NO_2 DOAS retrievals performed by members of the validation sub-group.

The inclusion in the fitting NO2 window (425-450 nm) of the absorptions of O_4 and H_2O, coupled with a number of software improvements, results in the GOME total nitrogen dioxide now being in reasonable agreement with ground-based measurements. Although it is difficult to evaluate precisely the accuracy of this product due to various problems such as the diurnal variation of NO_2, the overall accuracy in areas of low tropospheric NO_2 is estimated to fall within the 5% to 20% range. GOME total NO_2 is affected by larger errors under particular circumstances, e.g., over polluted areas or during midnight sun.

The relatively small NO_2 absorption in its selected fitting window implies that retrieval using the two-steps DOAS approach of GDP is well suited to generate accurate data products. However, the AMF calculation is strongly affected by variations in tropospheric burden of NO_2 especially for high pollution conditions in the boundary layer. In addition atmospheric parameters currently in use in GDP introduce a fictitious latitudinal/seasonal variation of a few percent superimposed on the geophysical variations in NO_2.

4. Conclusions

As a consequence of the anticipated degradation of the instrument and resultant changes of in-flight calibration parameters, a dynamic or temporally dependent database has been developed to provide the optimal calibration of the level-1 data. The database describes the temporal behaviour of GOME calibration parameters and was validated before implementation.

The present errors in the level-1 product have a negligible impact on the quality of the total column of ozone and nitrogen dioxide density derived by the DOAS in level-1-to-2 processing. This is because the DOAS algorithm uses the irradiance divided by the radiance spectra as its input. Thus many errors arising from the changes in calibration parameters cancel.

Future reprocessing of the complete data set is anticipated by the end of 1999.

The present understanding of the GOME data quality is based on the validation results presented in Frascati (January 1996, May and July 1999), Florence (March 1997), Noordwijk (January 1999) and during GOME science & algorithms workshops, on the existing literature, and on the findings of a sub-group of the GOME validation group, which investigated the quality of the GOME data after the successive implementations of major changes in GDP.

The improvement of GDP and the consequent validation work are still going on. This report presents only an overview of the current situation. Further improvement and detailed validation results based on an extended data set are expected in the future.