

DISCLAIMER FOR GOME LEVEL-1 AND LEVEL-2 DATA PRODUCTS

December 2004

1. Introduction

Operational GOME data products are generated by the GOME Data Processor (GDP) at the German Processing and Archiving Facility (D-PAF) at DLR on behalf of ESA. Quality assessment of these products is aimed at improving their accuracies, to the point of achieving theoretical minimum error values. The improvement of operational algorithms and their associated data products is a continuous activity, ongoing since the start of GOME operations in July 1995. This process has benefited from a number of validation campaigns, involving specialist groups in the atmospheric science community with expertise in the retrieval of trace constituents from ground-based and other instrumentation appropriate to GOME validation.

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 O₃ (Dobson Unit); Vertical Column amount of NO₂ (molecule cm⁻²); Cloud Fractional Coverage; Cloud-top Height (km); Cloud-top Albedo.

The first dedicated validation campaign for GOME products was conducted during the commissioning phase in the second half of 1995. As reported in an ESA publication (ESA WPP-108), studies carried out by more than 20 different groups highlighted a number of critical issues for prototype GDP data products. Recommendations were made for modifications to the developmental GDP, to data analysis and instrument operation procedures, and to data processing and distribution policies. Some of these recommendations were implemented during the first months of 1996, and the first public version (GDP 2.0) was released later in that year.

Since then, a number of additional recommendations have been made regarding GDP modifications, and most changes to GDP have been implemented in successive versions, from GDP 2.4 (operational in the 1998-2000 time frame), to GDP 2.7 (2000-2002), GDP 3.0 (2002-2004), and lastly to the current version GDP 4.0 (from December 2004 onwards).

Before implementation of major GDP changes in the operational processing chain and subsequent reprocessing of all historical data, it is essential not only to verify the accuracy and effectiveness of the proposed modifications but also to assess the quality of the new data product. This has been done by means of so-called 'delta' validation campaigns executed by a sub-group of the GOME validation group; such campaigns use a limited but representative subset of validation orbits selected to test expected changes. Results from delta validation campaigns were reported at dedicated meetings in May and June 1996, in January 1998, in May and July 1999, in January and April 2002, and most recently in November 2004 at ESRIN.

At the same time, detailed validation and algorithm improvement studies have been carried out by a wider segment of the atmospheric science community and reported on many occasions, both at international conferences and workshops and in the open literature.

The present disclaimer summarises the status of the current GDP data quality, with reference to version 2.2 for GDP level-0-to-1 processing, and version 4.0 for GDP level-1-to-2 algorithms.

2. Current Data Quality of GOME level 1-Product

GOME level-1 data products possess good wavelength stability, indicating a high instrument precision. Level-1 products are affected by spectral and radiometric distortions of instrumental origin. The solar irradiance measurements exhibit an anticipated slow degradation in the ultraviolet (channels 1 and 2); there is an option to correct for this degradation in the GDP extraction software. In addition, there is a seasonal variation of sensitivity depending on the solar azimuth at the sun diffuser. For retrievals of ozone column amounts using the DOAS technique, these degradation and instrumental errors are relatively minor in importance. 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 ultraviolet.

2.1 Solar spectral irradiance

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

Deviations at the beginning of the GOME Instrument lifetime:

Despite the relatively good agreement with SOLSTICE measurements, the GOME irradiance measurement in channel 1 is considerably lower, by 5 % to 10 %. In channel 2, the agreement is better, but etalon features limit the accuracy of GOME data with modulations of $\pm 2\%$.

The average deviations of GOME data from SOLSTICE data on 3 July 1996 and the rates of linear decay between 3 July 1995 and 14 January 1996 are given in the following table:

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

Deviations at mid 1999:

The average deviations of GOME data from SOLSTICE V12 data on 1 January 1999 and the rates of linear decay in 1998 are given in the following table:

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

The observed degradation in the ultraviolet was expected and is similar to that observed in other remote sensing instruments measuring solar irradiance in the ultraviolet (e.g. TOMS). It can be corrected by the extraction software. Note that the solar azimuth on the solar diffuser differs between January and July data; this 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.

Yearly deviations up to and including 2004:

The following table shows the yearly mean percentage degradations of GOME channels (starting point on 3 July 1995 for reference) from 1996 to 2004.

Wavelength (nm)	240-250	250-300	300-350	350-400	400-600	600-790
1996	-0.2 %	-0.1 %	0 %	0 %	0 %	0 %
1997	-9.4 %	-3.0 %	-1.6 %	-0.5 %	-0.6 %	-0.1 %
1998	-22.8 %	-7.6 %	-3.5 %	-1.4 %	-1.3 %	-1 %
1999	-48.8 %	-16.9 %	-5.3 %	-1.8 %	-0.7 %	-2.2 %
2000	-60.6 %	-35.7 %	-9.1 %	-2.3 %	+1.2 %	-1.4 %
2001	-55.6 %	-47.8 %	-25.1 %	-7.7 %	+1.7 %	+2.3 %
2002	-77.9 %	-53.0 %	-36.9 %	-21.7 %	-1.6 %	+3.5 %
2003	-82.0 %	-63.1 %	-37.3 %	-26.7 %	-4.9 %	+7.1 %
2004	-86.3 %	-71.7 %	-42.9 %	-31.8 %	-11.5 %	+4.1 %

2.2 Earthshine spectral radiance

The Level-1 Earthshine radiance product suffers from the same instrument degradation as the Solar Irradiance product.

A correction for the GOME instrumental response to polarisation is required for the radiance products. This polarisation correction (PC) of the up-welling radiation from the atmosphere is determined as follows:

- i. For wavelengths below 300 nm, it is assumed that the Rayleigh single scattering determines the degree of polarisation.
- ii. For wavelengths larger than 300 nm, three instrument-derived values for the degree of polarisation have been deduced from integrated detector array measurements in channels 2, 3 and 4 and the corresponding broad-band measurements from the three Polarisation Monitoring Devices (PMDs).
- iii. To estimate individual values of the degree of polarisation at all channel wavelengths, a polynomial is then fitted to these four determinations of the degree of polarisation; the fitting includes a parameterisation based on model calculations between 300 and 325 nm.

Allowing for degradation corrections 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 ultraviolet, where it is limited to 5% because of additional pre-flight calibration uncertainties and to remaining uncertainties of atmospheric polarisation. Below 350 nm the Earth's radiance has not yet been fully validated.

A significant source of radiance error arises from inadequacies in the polarisation-correction procedure implemented in the level-1 extractor software. Interpolation of polarisation values between 350 nm (PMD1 polarisation value) and 300 nm (single scatter polarisation value) is problematic due to the paucity of polarisation information.

Discontinuities in the absolute radiance values are observed between channels. This is caused by the serial read-out 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 that for the 1024th detector pixel. This aliasing effect is pronounced for earthshine scenes having significant albedo changes in the field of view between the first and last detector pixel. 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

Geophysical validation is a vital tool to assess the quality of Level 2 products and to direct the maturation of Level 1-to-2 GDP retrieval algorithms. GOME total ozone data and related algorithms have been validated from pole to pole (a) through comparisons with ground-based measurements from SAOZ/DOAS UV-visible spectrometers, Brewer and Dobson ultraviolet spectrophotometers, and ultraviolet filter radiometers; and (b) with global data from the TOMS satellite sensor (both V7 and V8) and from modelling/assimilation tools. In-depth validation of the GDP retrieval algorithms has also been carried out using independent DOAS-type algorithms, a novel algorithm based on the direct fitting approach, and the TOMS v7 algorithm.

The DOAS approach adopted in GDP to ultraviolet-visible level 1-to-2 retrievals of total column amounts consists of the spectral fitting of the apparent slant column amount, followed by its conversion into vertical column amount using a calculated Air Mass Factor (AMF). The latter determination is based in part on cloud information inferred from GOME measurements. The spectral fitting of ozone slant columns in the 325 to 335 nm works well. Compared to GDP 2.7, GDP 3.0 included a new determination of effective absorption temperature derived by spectral analysis, better atmospheric databases, and AMFs determined iteratively using a neural network trained on column- and latitude-classified atmospheric profiles and measurement parameters. GDP 3.0 upgrades resulted in a reduction by about 30-50% of the amplitude of the GOME total ozone dependence on the SZA, the latitude, the season, and the ozone column amount. Compared to GDP 3.0, the current version GDP 4.0 includes an improved correction for ozone absorption distortion due to inelastic rotational Raman scattering by air molecules, a new cloud treatment for the retrieval of three auxiliary pieces cloud information, and further improvements to the AMF calculation using on-the-fly radiative transfer modelling. The main achievement with GDP 4.0 is the drastic reduction of nearly all remaining dependencies on latitude, season, SZA and ozone column persisting with GDP 3.0.

In general, the average agreement of GDP 4.0 with correlative ozone column measurements is now at the “percent level”, that is, within the precision level of ground-based sensors when the latter are corrected for their own dependencies on the season, solar elevation, temperature etc. At polar latitudes, and at GOME solar zenith angles larger than 80°, preliminary validation indicates that the agreement is slightly worse; however, average differences at low solar elevation usually do not exceed 5%. A remarkable feature of the reprocessed GOME GDP 4.0 data record is that, despite the anticipated degradation of the instrument with time, the total column products do not suffer from any long-term drift of quality. This is the case even in late 2004, when the degradation of the UV ozone channel has reached 42.9%. More qualitatively, GOME gives a consistent picture of the global ozone field with temporal signals and spatial structures similar to those observed by other high-quality sensors.

3.2 Vertical column amount of nitrogen dioxide

The GOME GDP total nitrogen dioxide product has also been validated from pole to pole, with comparisons to ground-based measurements of the NDSC network of SAOZ/DOAS UV-visible spectrometers and Fourier Transform Infrared spectrometers, and to global data from the HALOE and POAM satellite sensors and tropospheric and stratospheric modelling tools. GDP retrievals have also been compared with GOME NO₂ retrievals performed with independent DOAS-type algorithms.

NO₂ absorption in the usual fitting window (425-450 nm) is optically thin, and retrieval using the two-step DOAS approach is suitable for total column retrieval of this species. The DOAS fit

includes amplitudes for interfering absorptions by O₄ and H₂O. GOME total nitrogen dioxide is in reasonable agreement with ground-based and other satellite measurements: within $\pm 5 \cdot 10^{14}$ molec.cm⁻² in areas of low tropospheric NO₂ and within $\pm 8 \cdot 10^{14}$ molec.cm⁻² in areas of very low slant column of NO₂. Atmospheric parameters currently in use in the NO₂ AMF calculation introduce a fictitious latitudinal/seasonal variation of a few percent superimposed on the geophysical variations in NO₂. Although it is difficult to make a precise evaluation of the NO₂ total column accuracy (due to various problems such as the photochemical diurnal cycle of NO₂), the overall accuracy is estimated to fall within the 5% to 10% range, provided that the contribution of tropospheric NO₂ to the vertical column remains low. GDP total NO₂ has larger errors under certain circumstances, e.g., in the South Atlantic Anomaly and over polluted areas. In the latter case, current NO₂ AMF values and effective absorption temperatures calculated for pure stratospheric scenarios do not account for variations in the tropospheric burden of NO₂ and are consequently subject to systematic errors. For scenarios of extreme pollution, modelling results suggest that AMF errors can lead to an underestimation of the actual NO₂ vertical column amount by a factor of two.

4. Concluding Remarks

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

The present errors in the level-1 product have a negligible impact on the quality of the total ozone column density derived by DOAS in the level-1-to-2 processing. The reason is that many errors arising from the changes in calibration parameters cancel because the DOAS algorithm uses reflectances (irradiances divided by the radiances) as the basic measurement input, and intensity calibration errors, which have a polynomial dependence on wavelength, are subsumed in the DOAS polynomial closure term.

Present quality of level-2 data products makes them suitable for a wide variety of geophysical research applications, including ozone trend monitoring and polar process studies. The complete GOME data record from July 1995 onwards has been reprocessed with GDP 4.0 and is available to the public via the ERS Help & Order desk (see Contact Point below in Section 6).

The present level of understanding for GOME data quality is based on a series of validation results presented at GDP upgrade meetings held in November 2004, January and April 2002, January, May and July 1999, January 1998, March 1997, and January, May and June 1996; at a series of GOME science & algorithms workshops; in the existing literature; and on the findings of a GOME validation team responsible for the investigation of data product quality throughout the mission lifetime.

GDP improvement is an ongoing task. This report gives an overview of the current situation as at December 2004, based on a limited set of validation orbits. Further improvements and more validation results based on an extended data set are expected in the future.

5. Documentation

The available ESA documentation for the GOME system comprises:

- GOME WWW site: http://earth.esa.int/esa_doc/doc_gom.html
- GOME Interim Science Report (ESA-SP 1151, 1993)
- GOME Users manual (ESA-SP 1182, 1995)
- Product Specification Document of the GOME Data Processor (ER-PS-DLR-GO-0016, issue 4B, December 15th, 2004)
- GOME Level 0-to-1 Algorithms Description (ER-TN-DLR-GO-0022, issue 5B, April 10th, 2002)
- GOME Level 1-to-2 Algorithms Theoretical Basis Document (ER-TN-DLR-GO-0025, issue 4A, December 15th, 2004)
- Proceedings of GOME Geophysical Validation Campaign Final Results Workshop, ESA-ESRIN, Frascati, 24-26 January 1996 (ESA WPP-108, 1996).
- Proceedings of 3rd ERS Scientific Symposium, Florence, Italy, 17-20 March 1997 (ESA SP-414, Vol. 2, 1997).
- GOME Data Improvement Validation Report (Ed. B. Greco, ESA/ESRIN APP/AEF/17/GB, 1998).
- Proceedings of European Symposium on Atmospheric Measurements from Space, ESA-ESTEC, Noordwijk, The Netherlands, 18-22 January 1999 (ESA WPP-161, 2 Vol., 1999).
- Update Report for GDP 0-to-1 Version 1.5 and GDP 1-to-2 Version 2.4 (ER-TN-DLR-GO-0043, 1999).
- ERS-2 GOME Data Products Delta Characterisation Report 1999 (Ed. J.-C. Lambert and P. Skarlas, IASB, Brussels, Issue 1.0, November 1999).
- ERS-2 GOME GDP 3.0 Implementation and Delta Validation Report, ESA Technical Note ERSE-DTEX-EOAD-TN-02-0006, (Ed. by J.-C. Lambert, IASB, Brussels, Issue 1.0, November 2002)
- ERS-2 GOME GD 4.0 Algorithm Theoretical Basis Document, ESA Technical Note ERSE-DTEX-EOPG-TN-04-0007, 2004.
- Delta validation report for ERS-2 GOME Data Processor upgrade to version 4.0, ESA Technical Note ERSE-CLVL-EOPG-TN-04-0001 (Ed. by J.-C. Lambert, IASB, Brussels, Issue 1.0, December 2004)

In addition a growing scientific literature is available at the GOME WWW site, at the GDP WWW site (<http://wdc.dlr.de/sensors/gome/index.html>), and at the GOME Validation WWW site (<http://www.oma.be/GOME>). Links to other relevant GOME sites are provided.

6. Contact point

To order GOME products, or for further information, please contact the ERS Help & Order desk:

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