DUE GLOBVAPOUR

Algorithm Theoretical Basis Document
L3 GOME+SCIAMACHY+GOME-2

Issue 1 Revision 0

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1 Introduction

1.1 Purpose

This document describes the algorithms used in the generation of the GOME/SCIAMACHY/GOME-2 total column water vapour data for ESA's DUE GlobVapour project. The algorithms take Level 3 products of the respective instruments as input – these are monthly or weekly mean maps generated by DLR. The SCIAMACHY and GOME-2 data are aligned and merged with the GOME dataset, using the algorithms described in this ATBD.

1.2 Definitions, acronyms and abbreviations

AMF	Air Mass Factor
BRDF	Bi-directional Reflectance Distribution Function of the diffuser
DLR	German Aerospace Centre
DOAS	Differential Optical Absorption Spectroscopy
DUE	Data User Element - a programmatic component of ESA's Earth Observation Envelope Programme
ENVISAT	Environmental Satellite
ERS-2	European Remote Sensing Satellite -2
ESA	European Space Agency
EUMETSAT	European Organisation for the Exploitation of Meteorological Satellites
FOV	Field of View
GDP	GOME Data Processor
GOME	Global Ozone Monitoring Experiment on ERS-2
GOME-2	Global Ozone Monitoring Experiment on MetOp
IMF	Remote Sensing Technology Institute (DLR)
MetOp	METeorological OPerational Satellite (EUMETSAT)
O3M-SAF	Ozone and atmospheric trace gas Monitoring SAF
SCD	Slant Column Density (concentration integrated along the atmospheric light path)
SCIAMACHY	Scanning Imaging Absorption spectroMeter for Atmospheric CHartography
SSM/I	Special Sensor Microwave/Imager
SZA	Solar Zenith Angle
TCWV	Total Column of Water Vapour [kg/m^2]

UPAS	Universal Processor for UV/VIS Atmospheric Spectrometers
VCD	Vertical Column Density (vertically integrated concentration)

1.3 Applicable Documents

[AD-1]	DUE GLOBVAPOUR Requirements Baseline Document (RBD), issue 1, revision 0, dated 16 April 2010.
[AD-2]	DUE GLOBVAPOUR Technical Specification Document (TSD), issue 1, revision 0, dated 16 April 2010.
[AD-3]	DUE GLOBVAPOUR Software Development Plan (SDP), issue 1, revision 0, dated 16 April 2010.
[AD-4]	DUE GLOBVAPOUR Summary Report on Existing Algorithm Comparison and Validation Reports (SVR), issue 1, revision 0, dated 29 July 2010.
[AD-1]	ESRIN Statement of Work, EOEP-DUEP-EOPS-SW-09-0003, iss. 1 rev. 1, 13.05. 2009
[AD-2]	DUE GLOBVAPOUR Proposal, issue 1 revision 3, dated 9 July 2009

1.4 Reference Documents

RD-1	Loyola, D. G., N. Hao, M. Rix, S. Slijkhuis, P. Valks, 2010: Algorithm Theoretical Basis Document for GOME-2 Total Column Products of Ozone, Minor Trace Gases, and Cloud Properties. DLR/GOME-2/ATBD/01, Iss.2/C.
RD-2	Kalakoski, N., T. Wagner, K. Mies, S. Beirle, S.Slijkhuis, D. Loyola (2010) O3M SAF Validation Report, Offline Total Water Vapour, SAF/O3M/FMI/VR/H2O/I02 in preparation
RD-3	GlobVapour Technical Specification Document from February 2010
RD-4	Loyola, D. G., Coldewey-Egbers, R. M., Dameris, M., Garny, H., Stenke, A.,Van Roozendael, M., Lerot, C., Balis, D. and Koukouli, M., 2009: Global long-term monitoring of the ozone layer - a prerequisite for predictions. Int. J. Rem. Sens., 30(15), pp. 4295-4318.
RD-5	Wagner T., Heland J., Zoeger M., Platt U., 2003: A fast H2O total column density product from GOME-Validation with in-situ aircraft measurements, Atmos. Chem. Phys., 3, pp. 651-663
RD-6	Loyola, D. G., Thomas, W., Livschitz, Y, Ruppert, T., Albert, P. and Hollmann, R., 2007, Cloud properties derived from GOME/ERS-2 backscatter data for trace gas retrieval. IEEE Transactions on Geoscience and Remote Sensing, 45, pp. 2747-2758

1.5 Structure of the document

Section 2 of the document provides background information to the GOME-family of instruments and their Total Column of Water Vapour (TCWV) products (Level 2).

Section 3 describes the algorithms to perform the alignment of the TCWV of GOME-2 and SCIAMACHY onto the standard taken from GOME, in order to come to a merged GOME/ SCIAMACHY/ GOME-2 TCWV time series

2 Algorithm overview

2.1 Background: the GOME family of Instruments

The GOME/SCIAMACHY/GOME-2 family of instruments are nadir-looking spectrometers operating in the UV/VIS/near-IR wavelength region (SCIAMACHY has more extended capabilities as well, which are not considered here). For the retrieval of H_2O, a spectral window around the H_2O absorption lines near 630 nm is used. The retrieval can be employed both over ocean and over land surfaces. The properties of the various instruments are summarised in Table 1.

Table 1: Satellite instrument properties.

Parameter	GOME	SCIAMACHY	GOME-2
Data Availability	06/1995 – today [1)]	07/2002 - today	01/2007 - today
Spectral resolution at 630 nm	0.35 nm	0.4 nm	0.5 nm
Ground Pixel size	320 x 40 km^2	60 x 30 km^2	40 x 80 km^2
Swath Width	960 km	960 km	1920 km
Equator crossing local time	10:30 a.m.	10:00 a.m.	9:30 a.m.
Global Coverage	3 days [1)]	6 days	almost daily

[1)] no global coverage since June 2003

2.2 TCWV (Level 2) from GOME-type instruments

Total H_2O from GOME and SCIAMACHY is processed at DLR using the GDP 4.4 algorithm in DLR's UPAS processing environment. The algorithm is based on the work of Wagner et al. 2003 [RD-5]. The UPAS system also provides Cloud information (fractional cover, cloud-top height and cloud-top albedo), using the Optical Cloud Recognition Algorithm (OCRA) and the Retrieval Of Cloud

Information by Neural Networks (ROCINN) algorithm (Loyola et al., 2007) [RD-6]. As the same algorithms are used in the O3M-SAF for operational processing of GOME-2 data, this ensures consistent H_2O and cloud information from all three instruments.

The GDP algorithm has two major steps: a Differential Optical Absorption Spectroscopy (DOAS) least-squares fitting for the trace gas slant column, followed by the computation of a suitable Air Mass Factor (AMF) to make the conversion to the vertical column density. The AMF algorithm used here is optimised for generating self-consistent long-term climatological data, by minimising external inputs. The algorithm is not tuned to achieve maximum accuracy for each individual measurement.

The baseline of the current algorithm is to use as little external, a priori information as possible. The calculation of slant columns of water vapour, as derived by the DOAS method, is practically free from a priori assumptions on the state of the atmosphere. However, to convert measured slant columns to vertical columns (by means of AMF), a certain amount of a priori information is needed. The atmospheric profile of H_2O, which is an important parameter in the AMF calculation, is assumed the same everywhere on Earth. The influence of variable aerosol loading is neglected. Only the surface albedo for each pixel is taken from a (seasonally dependent) database. These assumptions may cause higher errors in TCWV for each individual measurement, but provide on climatologically relevant time scales a result which is independent of external input.

Detailed information on the Level 2 algorithms can be found in [RD-1].

The TCWV from instruments operating in the visible/near-infrared wavelength region is by principle limited to clear sky conditions. Especially in the case of GOME, with its big pixel size, the number of truly cloud-free pixels is very small, and a limited amount of cloud contamination may have to be accepted. Furthermore, there is an issue with cloud detection above snow/ice surfaces, as the GOME sensors do not have infrared channel

Global total column water vapour from GOME/SCIAMACHY/GOME-2, over land and over ocean, is considered mature enough to be used as climate data series, as demonstrated in a number of publications. However, the absolute accuracy estimate on the water vapour columns needs further investigation. Validation studies show acceptable bias against radio-sondes and the SSM/I instruments [RD-2].

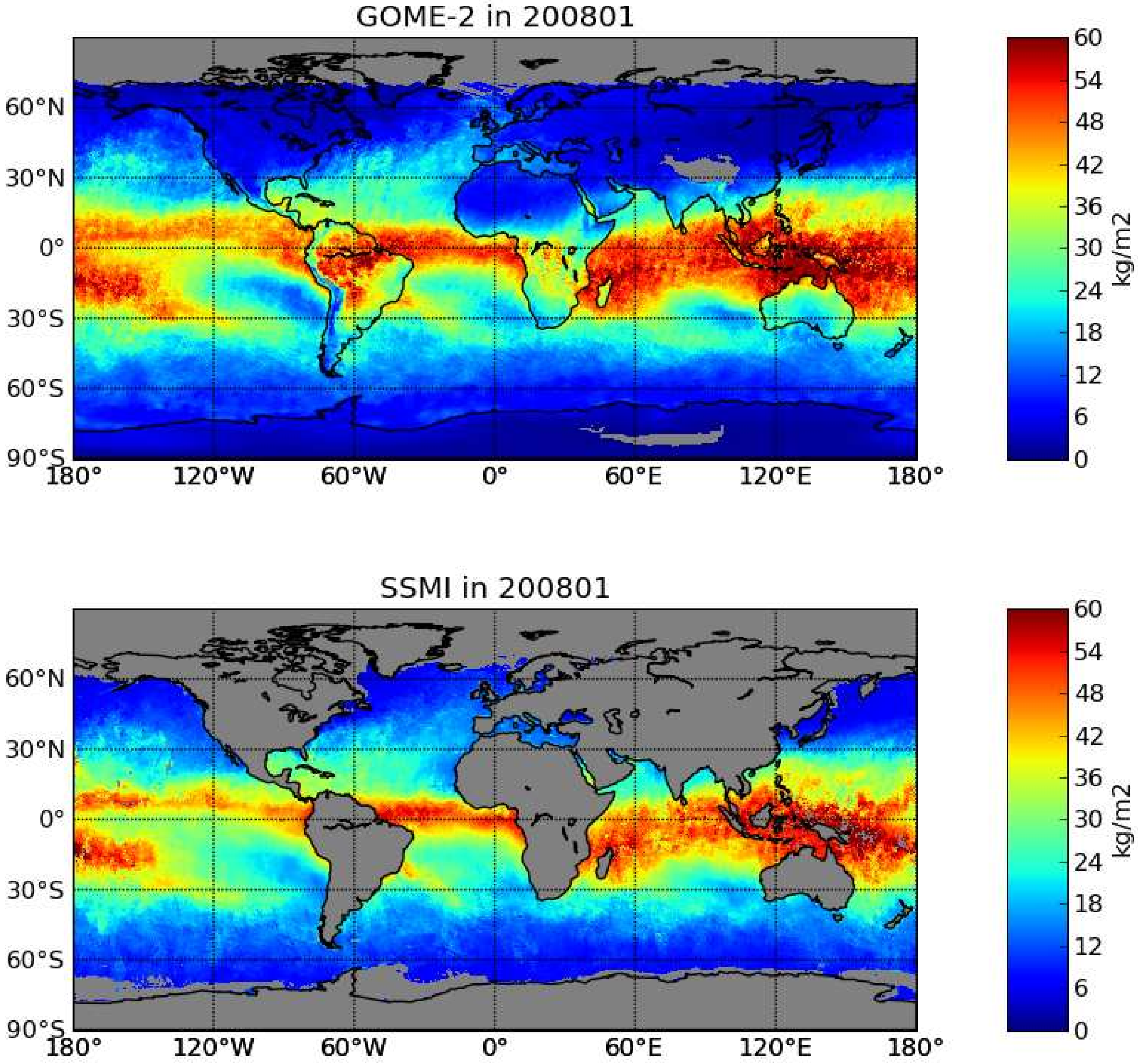

Figure 1: Monthly mean maps of TCWV from GOME-2 (top) and SSM/I F14 (bottom) for January 2008; used are only data within 5 hours of collocated overpass, applying the GOME-2 cloud mask to both datasets. The mean time difference of sounding is 3.5 hours (GOME-2 around 9:30h, SSM/I earlier).

3 Algorithm description

3.1 Theoretical description

The harmonisation of the TCWV time series from the various instruments is done following the method described in [RD-4] for the harmonisation of ozone time series. Input to the harmonisation process are monthly means of TCWV for each instrument, using a grid of 0.5^o x 0.5^o. The satellite measurements have been projected on to this regular grid using the Lambert Azimuthal equal-area projection with area-weighting (see [RD-4]), and contain forward scan measurements only (the backward scan measurements cover the same area as the forward scans, but with bigger ground pixel size). A cloud screening, mainly based on the oxygen column derived from the O_2-A band, is applied to remove cloud contaminated measurements.

For several trace gases, and in particular for ozone, it has been observed that the time series from GOME show more stable results than those of the other instruments. Therefore, we will take the GOME TCWV measurements as reference. SCIAMACHY and GOME-2 data will be adjusted to GOME in periods of instrument overlap.

In the following we describe the adjustment for SCIAMACHY. For GOME-2, the algorithms are exactly the same.

The adjustment applied to SCIAMACHY data comprises of two parts

1. a basic latitudinal correction for each month of the year,
2. a time-dependent correction for each individual month from July 2002 to present, which is then an offset averaged over latitude from 60° N to 60° S.

For the latitudinal correction, monthly averages of the differences between SCIAMACHY (denoted SCIA) and GOME are calculated first, as a function of latitude ϕ, as:

$$mean\_diff(m,\phi) = \frac{1}{7}\sum_{y=2002}^{2010} \frac{GOME(m,y,\phi)}{SCIA(m,y,\phi)} \qquad (1)$$

with month *m* from January to December (starting in July for 2002), and year *y* from 2002 to 2010.

For each of the 12 monthly differences, the latitudinal correction is then obtained as a third-order polynomial fit over latitude:

$$lat\_corr(m,\phi) = poly\_fit\_order\_3\_in\_\phi(mean\_diff(m,\phi)) \qquad (2)$$

Since the GOME dataset seems to be the more stable one, the adjustment also requires a time-dependent component. This time-dependence is taken as independent of latitude.

For this temporal contribution to the overall correction, the mean difference between GOME and SCIAMACHY over all available N_{Φ} latitudes from 60_N to 60_S is computed for each month (*m*,*y*) as:

$$diff\_60(m,y) = \frac{1}{N_{\phi}} \sum_{\phi=-60}^{60} \frac{GOME(m,y,\phi)}{SCIA(m,y,\phi)} \tag{3}$$

This difference is compared to the monthly mean difference over all years for the same latitude range:

$$mean\_diff\_60(m) = \frac{1}{7} \sum_{y=2002}^{2010} \frac{1}{N_{\phi}} \sum_{\phi=-60}^{60} \frac{GOME(m,y,\phi)}{SCIA(m,y,\phi)} \tag{4}$$

The time-dependent correction (or offset) is then given by:

$$time\_corr(m) = diff\_60(m,y) - mean\_diff\_60(m) \tag{5}$$

Finally the overall adjustment for SCIAMACHY data is the sum of the latitudinal correction and the time-dependent offset:

$$corr(m,y,\phi) = lat\_corr(m,\phi) + time\_corr(m) \tag{6}$$

3.2 Practical application

The implementation of the algorithm, as described in Section 3.1, is straightforward. Output of applying the algorithm will be monthly correction factors, as function of latitude (see Eq. 6). Maps for GOME-2 and SCIAMACHY, where the TCWV values have been adjusted to the level of GOME, may then be generated by applying these correction factors to the values in the regular (i.e. before adjustment) monthly maps of the respective instruments.

The “Merged GOME, SCIAMACHY and GOME-2 TCWV product” is obtained by averaging the adjusted 0.5°x0.5° grid entries of each instrument into a single dataset.

4 Assumptions and limitations

When merging the datasets of GOME, SCIAMACHY and GOME-2 it is tacitly assumed that differences in monthly averages of TCWV from these instruments arise from instrument-related differences in TCWV retrieval for each observation. However, another contributor to differences in monthly means may be differences in spatial sampling, in combination with cloud shielding. The merging of the GOME/SCIAMACHY/GOME-2 datasets has first been applied to ozone, which is predominantly found in the stratosphere, where cloud shielding is insignificant. For trace gases which are predominantly found in the troposphere, such as H_2O, this issue becomes more important, especially if a high temporal variation is present. Especially the large pixel size of GOME may result in more cloudy pixels, and hence more rejected values in the monthly means. For a given location, the GOME monthly mean may then be based on less (sufficiently cloud-free) observations than the

GOME-2 of SCIAMACHY monthly mean, which in case of high temporal variation may result in a larger scattering between the various instruments, possibly also a dry bias for GOME. Considering the fact that the average cloudiness varies with latitude (e.g. more cloud cover in the tropical belts), there is a possibility of such a dry bias (if existent) to be aliased into the dependence on latitude in the correction factors – this needs to be carefully analysed.

Another effect which has currently been neglected, is that over ocean in the tropical regions sunglint may occur. The present retrieval method of TCWV does not correct for sunglint. Especially GOME-2, with its broad swath width, experiences more sunglint than the other instruments do. sunglint has the same effect as a high albedo and would cause an overestimation of the GOME-2 TCWV.

In general, two important systematic errors of the GOME data set are evident.

a) over surfaces with high albedo, the newly introduced albedo correction 'over-corrects' the originally too high values over such areas. This is mainly related to the assumption of a simplified standard H_2O profile and a simplified correction of the saturation effect (narrow absorption lines of H_2O and O_2). Both effects cannot be easily improved further, because this would require very extensive radiative transfer simulations. It should also be noted that the deviations after the albedo correction are smaller compared to the original GOME H_2O product.

b) over regions with low lying clouds (e.g. at the west coasts of the continents in the southern hemisphere), the GOME H_2O product underestimates the true H_2O VCD, because such clouds hardly affect the measured O_2 SCD, while the H_2O SCD is largely reduced. Since the H_2O VCD is determined from the ratio H_2O SCD / O_2 SCD, the resulting H_2O VCD is underestimated.

Like for effect a) it is not foreseen to apply a correction for effect b), because it also would require extensive radiative transfer efforts. In addition, and maybe more important, a detailed correction had to use additional information (like e.g. cloud properties or a-priori H_2O profiles), which would affect the suitability of the GOME-2 product for climate applications (e.g. trend analyses).

5 Conclusions

In this ATBD we have described a method to produce a merged dataset of TCWV from the series of GOME, SCIAMACHY and GOME-2 instruments. These instruments together will have a projected lifetime of over 25 years, which is valuable prerequisite for climatological studies.