10-Years Operational GOME/ERS-2 Total Column Products: The GDP 4.0 Algorithm

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Diego Loyola et al.
Outline

➤ GOME Ground Segment

➤ GDP 4.0 Algorithm

➤ Perspectives for GOME-2

➤ Conclusions
GOME Data Processor (GDP) – Overview

Level 0
Raw Data

GDP Level 0-to-1
Calibrated and Geolocated Radiances

O_3, NO_2, BrO, …

GDP Level 1-to-2
Atmospheric Trace Gases

Level 3 & 4
Global Maps
GOME Off-line Ground Segment

ERS-2
GOME

Low-bit Rate (15 MB/s)

Communication Satellite

BDDN Link

ESA Receiving Stations

Kiruna
Maspalomas
Gatineau (Prince Albert)

D-PAF

DMS
Archive
GOME Data Processor
GDP QA

Exabyte

CD-R

Internet

http://wdc.dlr.de/sensors/gome
GOME Off-line Ground Segment (2)

- A total of 57475 are being processed since July 1995
- Level 0 data
  - \( \approx 1.5 \text{ TB} \) (32 Mbyte per orbit)
- Level 1 off-line data
  - \( \approx 750 \text{ GB} \) (14 MB per orbit)
  - Products of around 2.5 days are bundled in one CD
  - 28 institutes order the products regularly (initially 9)
  - 41852 CDs delivered since 1995
- Level 2 off-line data
  - \( \approx 30 \text{ GB} \) (0.7 MB per orbit)
  - Products of one month are bundled in one CD
  - 30 institutes order the products regularly (initially 15)
  - 9081 CDs delivered since 1996
- Level 1 to Level 4 products are additionally distributed via internet
The GOME NRT service was initiated in January 1997 as a collaboration between IUP, ESA and DLR.

The GDP system was installed at the main ERS-2 receiving stations.

GOME level 2 products were initially transmitted via ISDN.

The service has been continuously updated and extended.

NNORSY ozone profiles (ZSW) available since 2002.

EGOC (level 0) data is now transmitted via internet.

Automatic NRT processing takes place at DLR.
GOME NRT – ERS-2 Receiving Stations

GOME/ERS-2 station coverage (courtesy W. Lengert, ESRIN).
GOME NRT – Coverage

ERS2 GOME
Ozone Vertical Column Densities

Oct 03, 2005

ERS2 GOME
NO2 Vertical Column Densities

May 01, 2006

Composite
Level2 Version 4.0 / ESA
http://wdc.dlr.de

Composite
Level2 Version 4.0
http://wdc.dlr.de

Dobson Units

150 200 250 300 350 400 450

10^15 molecules cm^-2

0 1 2 3 4 5 6 7

DLR
Deutsches Zentrum für Luft- und Raumfahrt e.V.
in der Helmholtz-Gemeinschaft
**GOME NRT – Chemical Data Assimilation**

**Assimilated Total Ozone Column**
- Oct, 15, 2005
- Dobson Units

**Analysed Ozone Loss at 20 km**
- Oct, 15, 2005
- Parts per Billion per Day

**Polar Stratospheric Clouds at 20 km**
- Oct, 15, 2005
- Temp. °K
- Surface Density
- Based on UK Met Office Analysis

**Analysed Chlorine Activation at 20 km**
- Oct, 15, 2005
- Parts per Billion

[http://wdc.dlr.de](http://wdc.dlr.de)
**GDP Milestones**

- **GDP Level 0-to-1**
  - 1996/07 GDP L01 1.0
  - 1999/07 GDP L01 2.1 (Rep. L1)
  - 2002/04 GDP L01 2.2 (Rep. L1)
  - 2006/10 GDP L01 3.0 (Rep. L1 and L2)
    - S. Slijkhuis, et al.
    - M. Coldewey-Egbers, et al.

- **GDP Level 1-to-2**
  - 1996/07 GDP L12 2.0
  - 2000/12 GDP L12 2.7 (Rep. L2)
  - 2002/07 GDP L12 3.0 (Rep. L2)
  - 2004/12 GDP L12 4.0 (Rep. L2)
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GDP 4.0 – Historical Overview

- GOME Data Processor version 3.0 (GDP 3.0) issued in 2002
  - Iterative DOAS/AMF algorithm with NNs for AMF parameterization
  - Details explained in an *Applied Optics* paper
- Despite significant improvements w.r.t. GDP 2.7, discrepancies remain when comparing GOME total ozone to ground-based measurements
  - Limitation for trend studies.
- Summer 2002: ESA-ESRIN ITT for improved total ozone algorithms for GOME; 3 consortia participate: GODFIT/GDOAS (BIRA/SAO), TOGOMI (KNMI) and GOTOCORD (Bremen).
- **February 2004**: Review at ESRIN, GDOAS selected for fast reprocessing of 9-year GOME total ozone record.
- **May 2004**: ESA-DLR project initiated to implement and validate GDOAS within the UPAS operational system.
The GDP 4.0 Algorithm – Overview

- GDOAS Inheritance: “iterative” two steps DOAS approach as in GDP 3.0
  - slant column fitting then AMF computation.

- UPAS/GDOAS Cloud pre-processing:
  - Improved cloud algorithms: OCRA&ROCINN (D. Loyola)

- UPAS/GDOAS O₃ retrieval:
  - Improved slant column settings (M. van Roozendael)
  - New Molecular Ring correction (M. van Roozendael)
  - New on-the-fly iterative AMF scheme using LIDORT V2.2+ (R. Spurr)
  - Improved error budget calculation

- UPAS/GDOAS NO₂ retrieval:
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Iterative DOAS/AMF for Ozone

\[
V^{(n+1)} = \frac{E^{(n)} + \phi G^{(n)} A^{(n)}_{\text{cloud}}}{(1 - \phi) A^{(n)}_{\text{clear}} + \phi A^{(n)}_{\text{cloud}}}
\]

where

- \( V^{(n+1)} \) is the **Vertical Column** at the \( n+1 \)th iteration
- \( E^{(n)} \) is the Molecular Ring corrected **Slant Column** at the \( n \)th iteration
- \( \phi \) is the intensity-weighted **Cloud Fraction**
- \( G^{(n)} \) is the associated **Ghost Column** (below the cloud-top pressure level)
- \( A^{(n)} \) (cloud and clear) is the **Air Mass Factor** at the \( n \)th iteration based on guess \( V^{(n)} \).
**OCRA & ROCINN © D. Loyola**

GOME

O$_2$ A-Band

PMD

ROCINN

Cloud-top height

Cloud-top albedo

OCRA

Cloud fraction

$c_j = \sqrt{\sum_{\lambda=k,j} \max(\rho(\lambda) - \rho_{\text{ref}}(\lambda))^2 - \beta(\lambda_i))}$
OCRA&ROCINN – Errors Induced in Ozone

Cloud-top Albedo

Cloud-top Height

Total Ozone

Histograms for Increased CF

Histograms for Decreased CF

Error [%]
The DOAS Ozone Algorithm

- Pre-processing: optimized wavelength calibration
  - Wavelength grid of solar spectrum is the reference
  - Cross-correlation done at start of orbit in ozone fitting interval (325-335 nm)
  - GOME FM98 O₃ cross-sections, I₀-corrected, optimized pre-shift 0.016 nm
  - GOME FM98 NO₂ cross-sections, pre-shift 0.016 nm
Molecular Ring Correction © M. van Roozendael

- New simplified DOAS formulation including Raman scattering, adequate for stratospheric absorbers.
- Ring correction definition requires knowledge of AMFs.
- The DOAS fitting is essentially unchanged; effective slant column for ozone is adjusted iteratively after the fit through the relation below.

\[ E'_{O3} \approx E_{O3} \left\{ 1 + E_{Ring} \cdot \bar{\sigma}_{Ring} \cdot \left( 1 - \frac{\sec(\theta_0)}{A^{(n)}_{total}} \right) \right\} \]
**Molecular Ring Correction - example**

![Graph showing molecular ring correction example]
AMF calculation with LIDORT V2.2+ © R. Spurr

- On-the-fly iterative AMF scheme using LIDORT V2.2+.
- LIDORT is a generic discrete ordinate radiative transfer tool that computes simultaneously intensities and weighting functions.
- LIDORT 2.2+ has approximately-spherical capabilities.
  - Important for polar view orbits
- TOMS V8 ozone profile climatology used. Around 1500 profiles classified as function of
  - 18 latitude bands
  - 12 months
  - total columns
The DOAS NO$_2$ Algorithm

- Pre-processing: optimized wavelength calibration
  - Wavelength grid of solar spectrum is the reference
  - Cross-correlation done at start of orbit in ozone fitting interval (425-450 nm)
  - GOME FM98 NO$_2$ cross-sections, pre-shift -0.016 nm
  - Improved Fraunhofer Ring spectrum (SAO)
  - Two undersampling cross-sections (BIRA)
  - New H$_2$O cross-sections (HITRAN 2000)
The AMF NO\textsubscript{2} Algorithm

- On-the-fly AMF scheme using LIDORT V2+
  - Composite stratospheric NO\textsubscript{2} profile climatology (BIRA)
    - Based on HALOE, POAM III and NDSC NO\textsubscript{2} data
    - 16 latitude bands, time dependent
  - Combined TOMS (NASA) and GOME (KNMI) spectral surface reflectivity database
  - GTOPO 30 Surface height database
GDP 4.0 – NO$_2$ Algorithm

NO$_2$ vertical column: GDPv 4 vs GDPv3

Orbit: 5606

Latitude (degree) vs GDPv 4 - GDPv3 (molec cm$^{-2}$)
UPAS – Overview

UPAS (Universal Processor for UV/VIS Atmospheric Spectrometers) is the new generation of level 2 processing systems for operational NRT and off-line trace gas retrieval.
GDP Level 2 - Performance

- **GDP 2.0**
  - F77 core, C client/server architecture
  - Sun Cluster, 40 CPU’s @ 0.3GHz
  - Reprocessing 1 year in 4 months

- **GDP 3.0**
  - F77 core, C client/server architecture
  - PC Linux, 18 AMD CPU’s @ 2GHz
  - Reprocessing 7 years in 1 month

- **GDP 4.0**
  - C++ core, F77 RTM and Orbit_Propagator
  - PC Linux, 20 Intel CPU’s @ 2.8GHz
  - Reprocessing 9 years in 10 days
**GDP Level 2 - Accuracy**

- **GDP 2.0**
  - 2-5% for SZA<70°
  - 10-15% otherwise

- **GDP 3.0**
  - ±2-4% for SZA<70°
  - -8% to +5% otherwise
  - 50% less seasonal dependencies

- **GDP 4.0**
  - “percent level” for SZA<80°
  - below 5% otherwise
  - Drastically reduction of dependencies

GDP 4.0 Validation © D. Balis

**Format:**

- GDP Level 2: Accuracy
- GDP 2.0: 2-5% for SZA<70°, 10-15% otherwise
- GDP 3.0: ±2-4% for SZA<70°, -8% to +5% otherwise, 50% less seasonal dependencies
- GDP 4.0: “percent level” for SZA<80°, below 5% otherwise, Drastically reduction of dependencies

**Graphs:**

- Scatter plots for GDP levels 2, 3, and 4, with data points and trend lines indicating accuracy improvements.

**Note:**

- GDP Level 2 accuracy improvements are noted across different solar zenith angles, with significant reductions in seasonal dependencies for higher levels.
GDP 4.0 Long-Term Stability – GOME Degradation
GDP 4.0 Validation © J-C. Lambert
Differences between GOME and Hohenpeissenberg monthly mean ozone:

- Mean Bias 0.3%
- Amplitude of 0.5%
GDP Data Dissemination – Level 1 and Level 2

- NRT Products:
  - Level 1 & 2 via FTP
- Off-Line Products:
  - Level 1 & 2 via CDs
  - Level (1 & ) 2 via FTP
- GDP 4.0 Search Engine

http://wdc.dlr.de/sensors/gome
GDP Data Dissemination – Level 3 and Level 4
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Interactively coupled Climate-Chemistry Model E39/C

NO\textsubscript{x} Emissions [Tg N/a]
Surface, aircraft, lightning

Photolysis

Chemistry (CHEM)
Methane oxidation
Heterogeneous Cl reactions
PSC I, II, aerosols
Dry/wet deposition

Feedback
O\textsubscript{3}, H\textsubscript{2}O, CH\textsubscript{4}, N\textsubscript{2}O, CFCs

Dynamics (ECHAM)
T30, 39 layers, top layer centred at 10 hPa
Prognostic variables
(vorticity, divergence, temperature, specific humidity, log-surface pressure, cloud water),
hydrological cycle, diffusion,
gravity wave drag, transport of tracers,
soil model, boundary layer;
sea surface temperatures.

Radiation
Long-wave
Short-wave

Chemical Boundary Conditions
Atmosphere: CFCs, at 10 hPa: ClX, NO\textsubscript{y}
Surface: CH\textsubscript{4}, CO

Dameris et al., 2005
The transient model simulation - boundary conditions

Boundary conditions 1960-2020

QBO

Solar activity and volcanoes

Global sea surface temperatures and sea ice covering

Dameris et al., 2005
Total ozone deviations wrt time average for 1964-1980

Dameris et al., ACP, 5, 2121-2145, 2005

- Prescribed sea surface temperatures, the 11-year solar activity cycle, and the QBO play an important role for the variability of the (model-) atmosphere; large volcanic eruptions influence the atmosphere only for a few years.
- Lowest ozone values are expected until the end of the present decade. Onset of ozone recovery after next solar minimum.
GOME and E39C – Monthly Mean Ozone

Latitudinal Monthly Mean Ozone from 60N to 60S
GOME and E39C – Standard Deviation

![GOME and E39C Standard Deviation Diagrams](image)
GOME and E39C – Anomalies

Latitudinal Monthly Mean Ozone Anomaly from 60N to 60S
Further Applications of GDP 4.0

[Graph showing ozone changes over time with labels GOME, SCIA, and GOME-2]
Application of GDP 4.0 to SCIAMACHY

GDP 4.0 is being transferred to the SCIAMACHY ground segment SGPL12

Ch. Lerot et al., "Intercomparison of Global Total Ozone Measurements retrieved from ENVISAT/SCIAMACHY Using Different State-of-the-art Algorithms"
Application of GDP 4.0 to GOME-2

- GOME/ERS-2 paved the way for the a number of GMES atmospheric research applications.

- GOME-2/MetOp-A is moving atmospheric remote sensing from research to operational applications.

- GDP 4.0 is the baseline for total trace gases retrievals for GOME-2
- Operational Level 2 Products produced by EUMETSAT’s Ozone and Atmospheric Chemistry Monitoring SAF (O3M-SAF)
  - “Chemical Weather Forecasting” and Air Quality
  - Climate Monitoring
O3M-SAF – Ground Segment at DLR

GOME-2 product generated by DLR:
- Near-Real-Time: O3, (NO2)
- Off-line: O3, NO2, BrO, (H2O)
- Experimental: SO2, HCHO, OCIO

Hot Bird

EPS Station Spitzbergen

GOME-2 L0 Data

L1b nrt

L2 search, order

L2 offline

Scientific and Meteo Users

DIMS

L2 nrt

L1b => L2 processing

L1b nrt

L1b ordering & delivery

L2 validation

DLR

GTS

National Weather Services

Upward Absorption in the Polar Stratosphere (UPAS)

UV processing

EPS G/S

UMARF

EUMETSAT

Raw => L1b processing

Metop

GOME-2 product generated by DLR:
- Near-Real-Time: O3, (NO2)
- Off-line: O3, NO2, BrO, (H2O)
- Experimental: SO2, HCHO, OCIO
O3M-SAF – User Workshop

User Workshop
  ➤ Place: Thesaloniki area
  ➤ Date: October 31\textsuperscript{st}, November 1\textsuperscript{st} and 2\textsuperscript{nd}, 2006

Algorithm Forum
  ➤ November 2\textsuperscript{nd} and 3\textsuperscript{rd}, 2006
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GDP provide over 10 years $O_3$, $NO_2$ and Clouds
**GDP 4.0 – Conclusions**

- GDP 4.0 data being used in the WMO ozone assessment
- Key Contribution to GMES Pilot Atmospheric Service
- Details: JGR Papers in press
  - Ten years of GOME/ERS-2 Total Ozone Data: the new GOME Data Processor (GDP) Version 4.0: I. Algorithm Description
  - Ten years of GOME/ERS-2 Total Ozone Data: the new GOME Data Processor (GDP) Version 4.0: II. Ground-based validation and comparison with TOMS V7/V8
GDP – Acknowledgements

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- SRON
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- Uni. Heidelberg
- ESA (ESTEC/ESRIN)
- EUMETSAT
GDP 4.0 – Acknowledgements

The GDP 4.0 project was finished in Dec 2004 after only 8 months!
- New algorithms (GDOAS, LIDORT, OCRA&ROCINN)
- New operational system (UPAS)
- Geophysical validation
- Complete set of documents (ATBD, PSD, Validation, Disclaimer)
- 9 years GOME data reprocessed

GDP 4.0 Team
- ESA C. Zehner, R. Leone
- BIRA M. Van Roozendael, J-C. Lambert, C. Fayt
- SAO/RTS R. Spurr
- AUTH D. Balis
- S&T P. Kenter
- DLR D. Loyola, Y. Livshitz, P. Valks, T. Ruppert
Chemical Data Assimilation of GOME total ozone