

GOMOS level 2 processor Status - May 2004

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GOMOS level 2 algorithms

Historical background :

GOMOS ESL algorithms, approved at ESAMS'99 workshop

Users Recommendations - December 2002

Main lessons : bright limb/scintillation effects/
underestimation of errors/ Lack of knowledge about
model contribution/ More information about observations conditions.

Actions in 2003

1. Algorithms improvements
2. Error estimates
3. Products content

Resulting status May 2004

From Cal/val dataset to GOMOS 2002-2003 Reprocessing

Users recommendations - December 2002

Level 2 - Algorithms :

Short term - emergency (test and specifications within 6 months)

1. Experiment and qualify alternative spectral inversion schemes
2. Qualify and adapt smoothing in vertical inversion
3. Improve the error estimates and quality indicators (to be continued)

Medium term (within 12-18 months)

1. Specify modelling error
2. Experiment and qualify the full covariance matrix method
3. Compute averaging kernels and provide them in products

Long term

1. Experiment coupling of spectrometers
2. Other species retrieval (OCIO, ...)
3. Study aerosol model variations and the use of a priori information

Users recommendations - December 2002

Level 2 - Algorithm tuning :

Short term (2003)

1. Tuning of High resolution Temperature Profile and its error estimates
2. Check temperature effects in spectral inversion (p-loop)

Level 2 - Products updates :

Short term (2003)

1. New temperature/density products : GOMOS only (Rayleigh + O₂ + HRTP) and external ECMWF+MSIS profiles
2. Add HRTP product into the meteo product
3. Solar zenith angle at tangent point should be provided

Users recommendations - December 2002

Validation :

1. Validation must continue
2. Supply reprocessed data to validating teams
3. DDS antenna is absolutely required to pursue the ESL activity
4. Frequent reprocessings are required during the whole next year
5. OZVAL - AO160 (validation via assimilation) must continue

Data dissemination :

YES, after the **red** actions are implemented and validated in PDS

Users recommendations implementation status

Where are we today ?

Alternative spectral inversion schemes ☒

Smoothing in vertical inversion ☒

Error estimates improvements and quality indicators derivation ☒

Tuning of High resolution Temperature Profile and its error estimates (*on-going*)

Check temperature effects in spectral inversion (p-loop) ☒

New temperature/density products : GOMOS only (Rayleigh + O₂ HRTP) (*see disclaimer*)

New temperature/density products : external ECMWF+MSIS profiles ☒

HRTP product into the meteo product ☒

Solar zenith angle at tangent point is provided ☒

Processor improvements (level 2)

1. Spectral inversion (algorithm+parameters)

implementation of GDI method (Global DOAS iterative scheme) for NO₂ and NO₃, applied at all tangent point altitudes

2. Vertical inversion (algorithm+parameters)

Tikhonov regularisation with target vertical resolutions

Processor improvements (level 2)

3. Aerosol optical thickness model (algorithm)

set to a/λ

4. Error estimate (algorithm)

correction factor has been derived and applied to local species error bars to account for turbulence error (scintillation)

5. H RTP (algorithm)

weaknesses in the time handling of the photometers data has been fixed

Alternative spectral inversion schemes

GDI : Global-DOAS Iterative algorithm

Motivation :

Scintillation effects in transmission spectra induce strong perturbations in retrieved NO₂ and NO₃ line densities with the global algorithm

The GDI algorithm combines advantages of DOAS inversion (species selectivity) and global inversion (consistency between the inversion of the species)

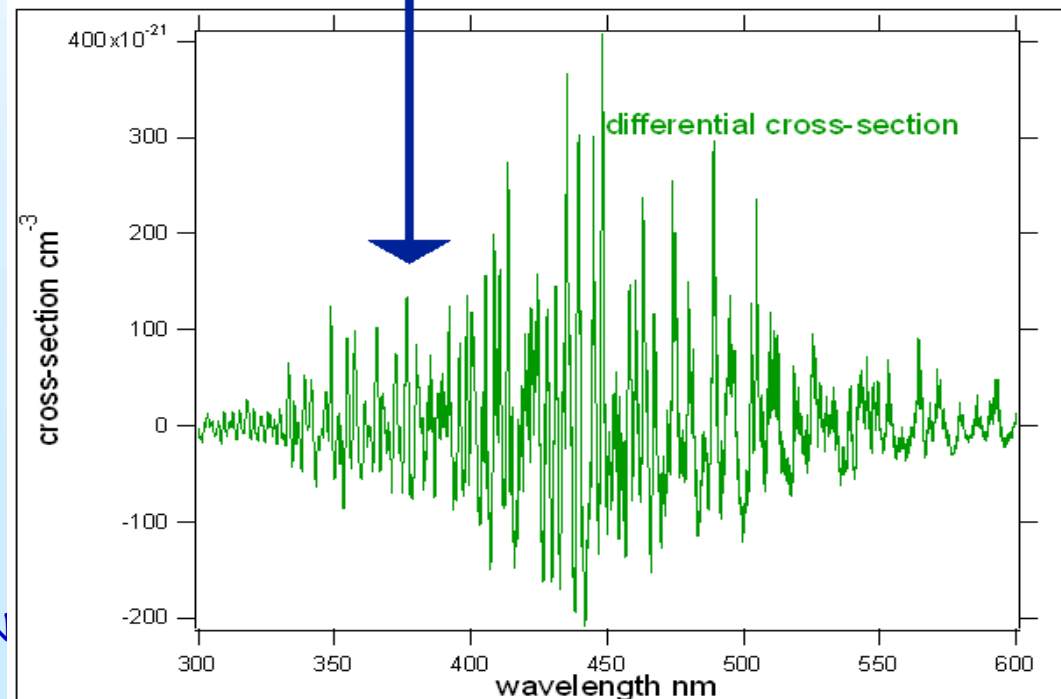
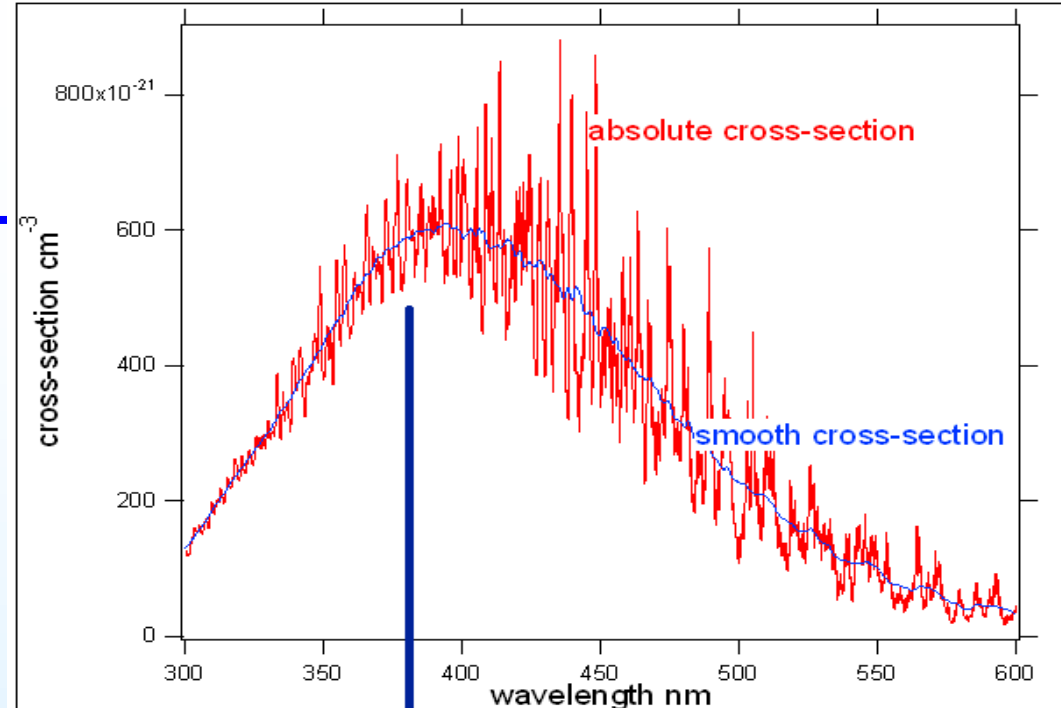
DOAS technique

Differential absorption spectroscopy

In GPR V6.0 :

NO₂ : smoothing over 15 nm

NO₃ : smoothing over 30 nm



GDI : Global-DOAS Iterative algorithm

- NO₂ and NO₃ divided in 2 species : a *smoothed* NO₂ and a *DOAS* NO₂ with respectively smoothed and DOAS cross-sections
- Step 1 : Levenberg-Marquard fit made with a fixed a-priori value of *smoothed* NO₂ and a free value of *DOAS* NO₂
- Step 2 : New Levenberg-Marquardt fit made with *smoothed* NO₂ set to the previous value of *DOAS* NO₂
- After 3 iterations of step 2, convergence between *smoothed* and *DOAS* NO₂ better than 10⁻³

Spectro B algorithm

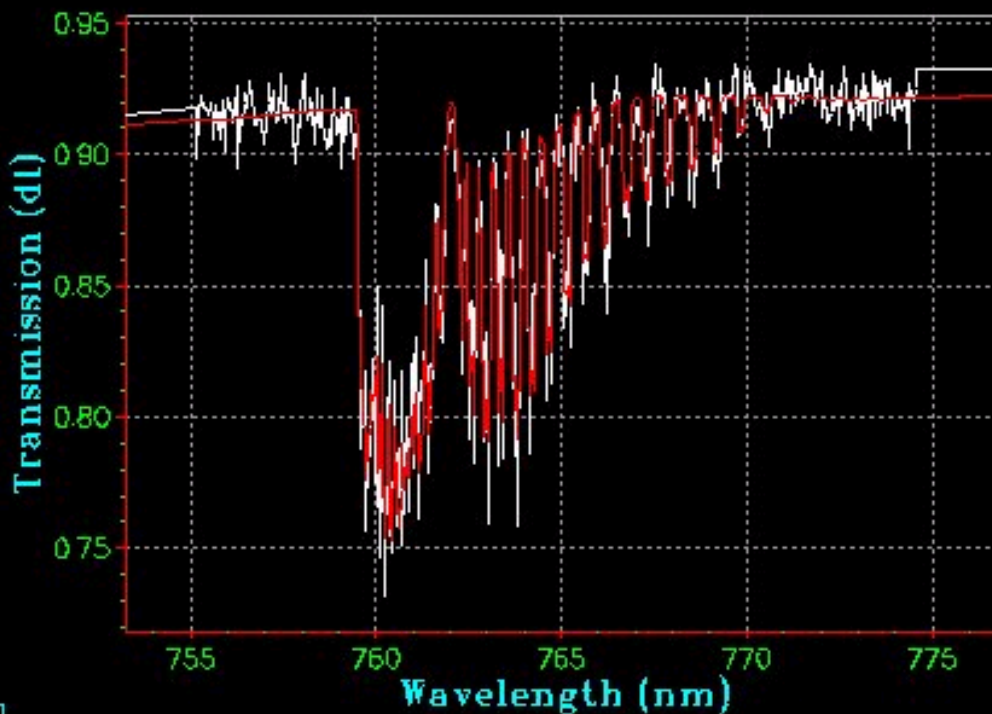
Retrieval of H₂O, O₂ by linear fit with LUT for transmissions after correction of the measured transmission by the retrieval of Rayleigh, Aerosols and O₃ (Spectro A).

Some problems still exist for the spectrometer B2 in the comparison between the transmission LUT of H₂O and the measured transmission, probably due to level 1b calibration.

R02945/todel
Tmodel vs T Fri 20 Feb 16:27:23 by gb

Transmission model versus Corrected Transmission
for spectrometers A and B
Time = (595 , 60.0) s
Tangent point altitude = 31.7 km

— T model
— Corrected T

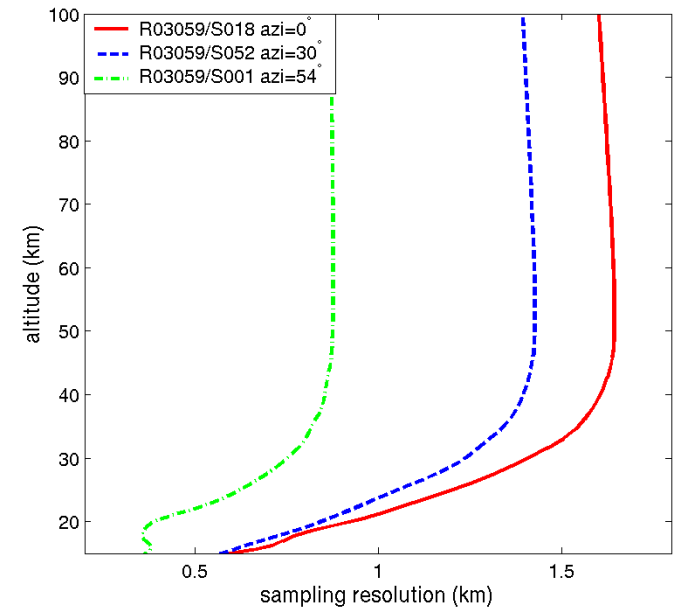


Smoothing in vertical inversion

Characteristics of GOMOS vertical inversion

- Simple linear inversion ($N = Kr$)
- Varying accuracy depending on stars
- Varying sampling resolution depending on occultation geometry (0.5 -1.7 km)
- Impact of scintillation largest when sampling resolution is best
- Regularization achieved by discretization is not sufficient: oscillating profiles

→ Smoothness requirement



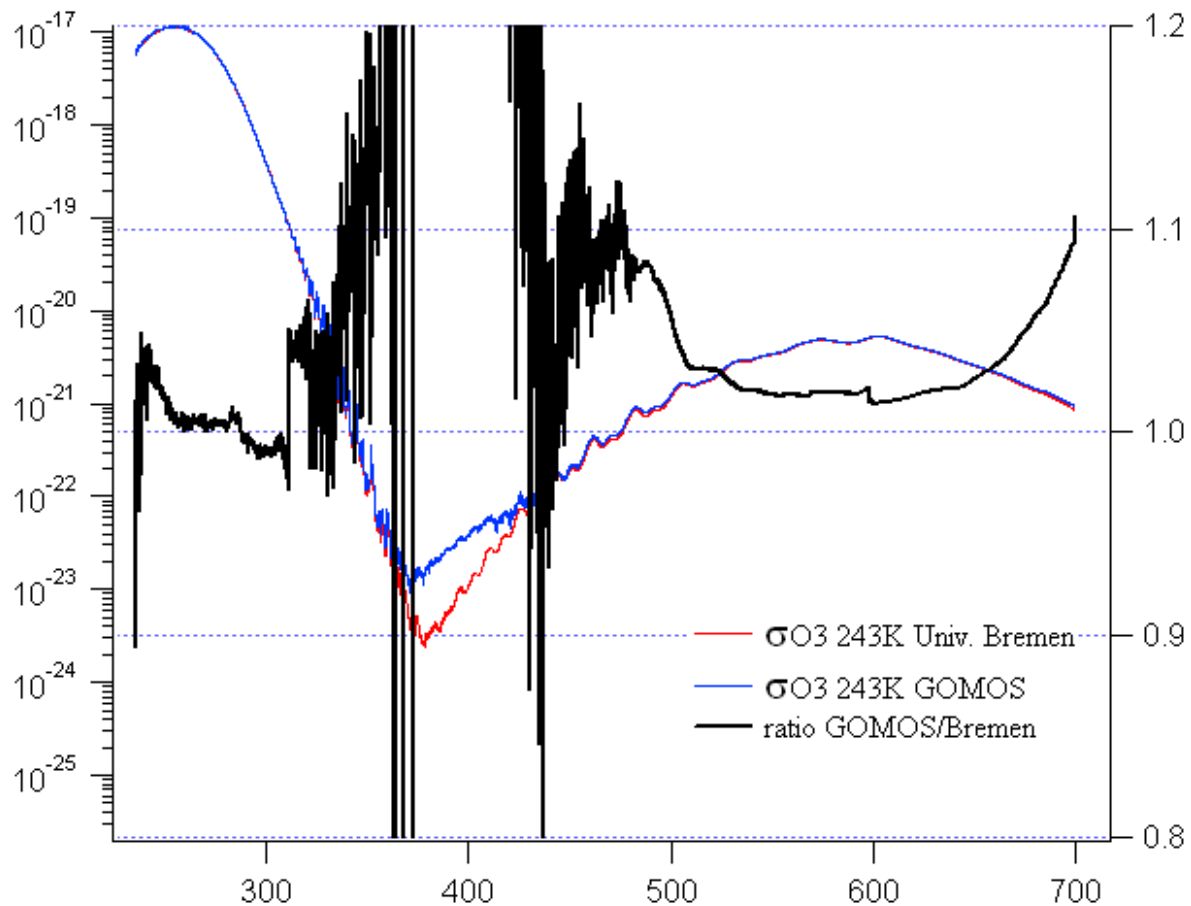
Tikhonov regularization

- Additional smoothing obtained by introducing Tikhonov regularization
- Amount of smoothing is designed according to target resolution
- Altitude dependent smoothing:

	< 30 km	30-40 km	> 40 km
O3	2 km	2-3 km	3 km
Air	3 km	3-5 km	5 km
O2	3 km	3-5 km	5 km
NO3	4 km		
Aerosols	4 km		
H2O	4 km		
NO2	4 km		

Error estimates improvements and quality indicators derivation

- Modelling errors (e.g. due to cross sections uncertainties) are not yet taken into account in the fit.
- Ozone cross-sections are not the same as the ones used by other missions (SCIA, GOME)
- An empirical random error estimates has been added to the error bar of line densities after inversion to account for uncorrected scintillation. This "patch" is not reflected in the χ^2 and off-diagonal elements of the covariance matrix.



... could provoke up to 3 % of difference for the line densities

Check temperature effects in spectral inversion (p-loop)

A loop is performed over spectral and vertical inversions to correct for:

- Chromatic refraction effect (< 0,1 % on O₃, <0,5% on NO₂)
- Time integration of the measurement (0,5 to 1% on O₃, small on NO₂, 2-3 % on NO₃)
- Temperature of the cross-sections along the ray path (0.5 to 1% on O₃, Bias of 15% on NO₂)

Updated products

1. Illumination (in both lv1b and lv2 products)

- . sun zenith angles at satellite and tangent point*
- . sun azimuth angle at the tangent point*
- . sun coordinates*
- . illumination condition (PCD_{illum}) dark, twilight/straylight, daylight*

2. Geometrical information (lv2 product)

- . occultation obliquity*

3. Limb signal in the central band (lv1b and lv2 products)

- . ratio U/C indicates the percentage of limb light mixed to the star signal (lv1b product)*
- . lower altitude where this ratio is lower than 25% (lv2 product)*

Updated products

4. HRTP (lv2 product)

error bars have been added to the air density profile derived from the High Resolution Temperature Profile algorithm

5. Transmission model for SPB (residual ext. product)

transmission model has been added to the product as well as a new transmission model flag array

Updated products

6- New temperature/density products : GOMOS only (Rayleigh + O2 HRTP) (*see disclaimer*)

GAP products are not released.

The GAP (GOMOS Atmospheric Profile) information is not provided in the geolocation ADS products as the results are somehow and sometimes unrealistic. The products are replaced by 0 values and error is set to 65535.

7- New temperature/density products : external ECMWF+MSIS profiles

8- HRTP product into the meteo product

High Resolution Temperature Profile (H RTP)

Caution: The results are currently not considered as valid. This product is currently thoroughly examined in the frame of a dedicated activity. The activity will most probably lead to recommend updates of the processing chain.

Repeated values are signature of exception handling in the algorithm (will be improved in the future).

Error bars for H RTP are largely overestimated.

Products assessment

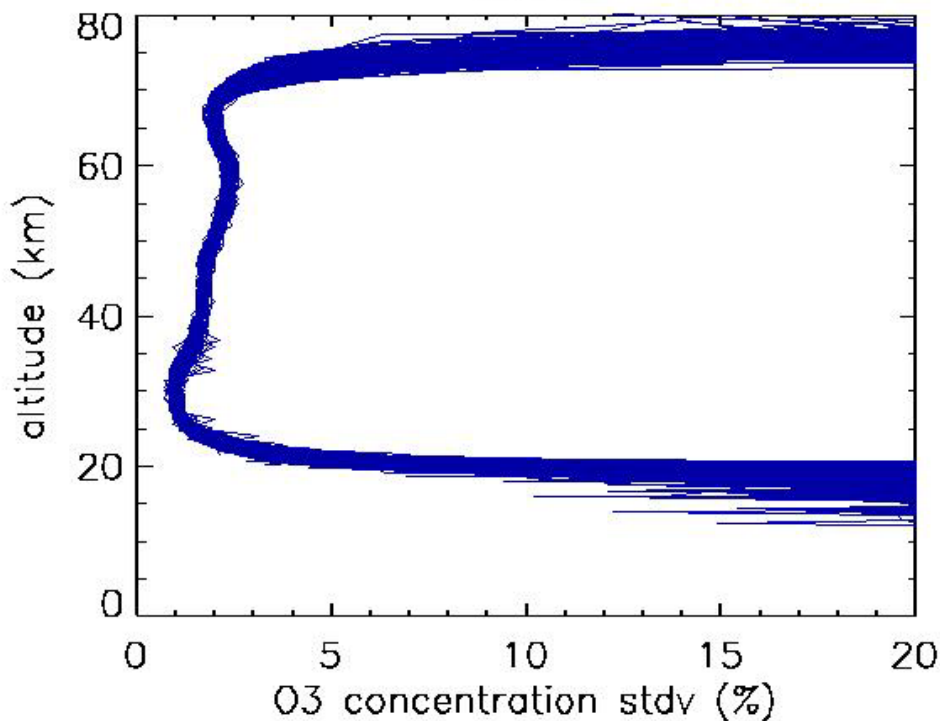
Ozone

- ✓ Error bars are not fully validated although the errors bars have been increased and better reflect the true errors.
- ✓ The current limitations of the processing chain should hardly impact the performance of O₃ (remaining errors can reach at most several percent at some altitudes)
- ✓ A large number of unrealistic wavy profiles have been improved.
- ✓ Accuracy is degraded below the altitude where the ratio U/C is greater than 25%

Standard deviation of the vertical profiles

v5.4b

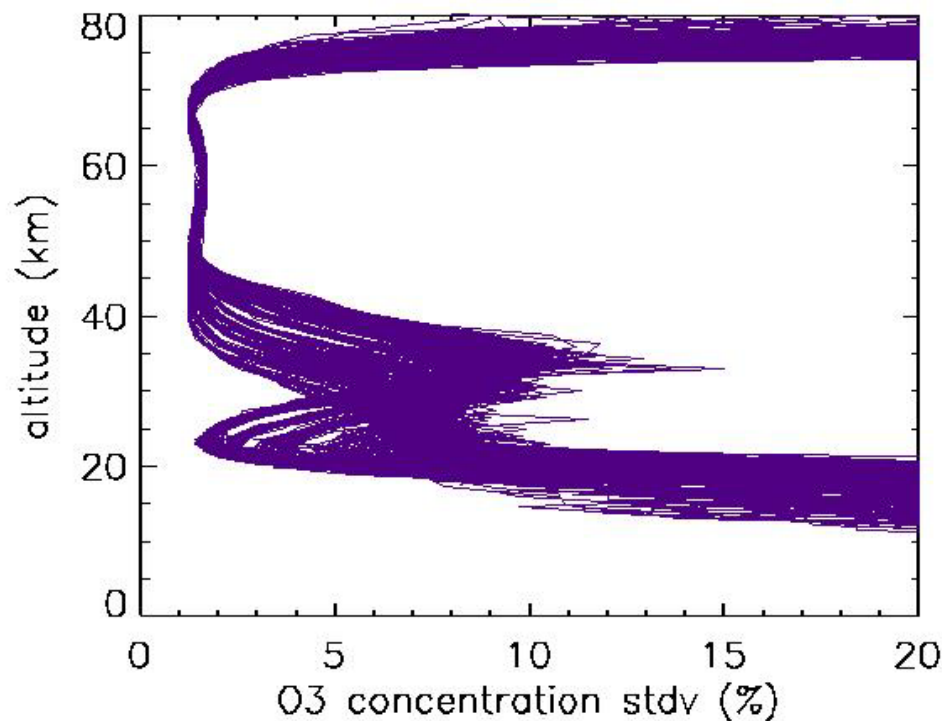
S029



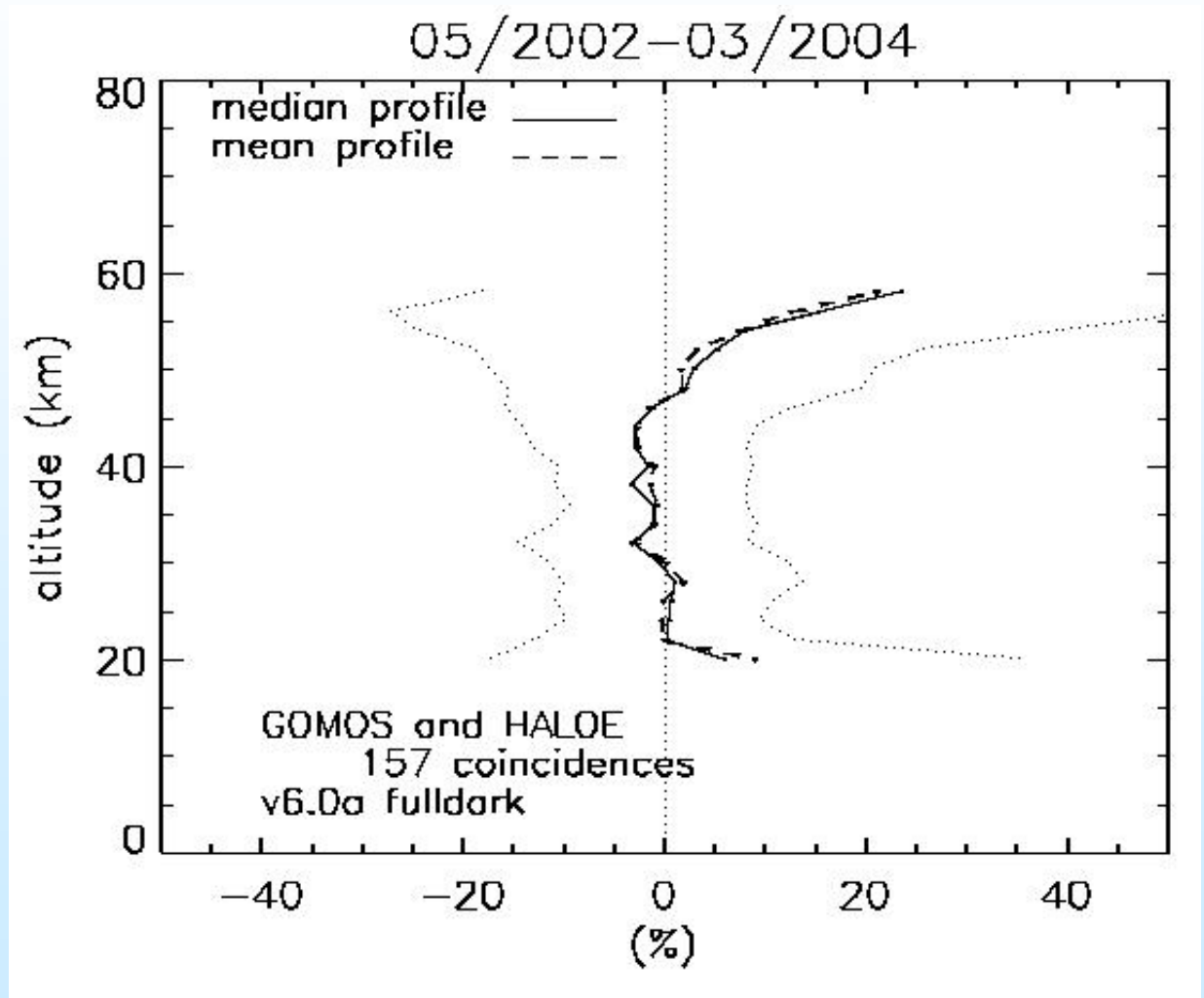
O₃

v6.0a

S029



Comparisons
with HALOE

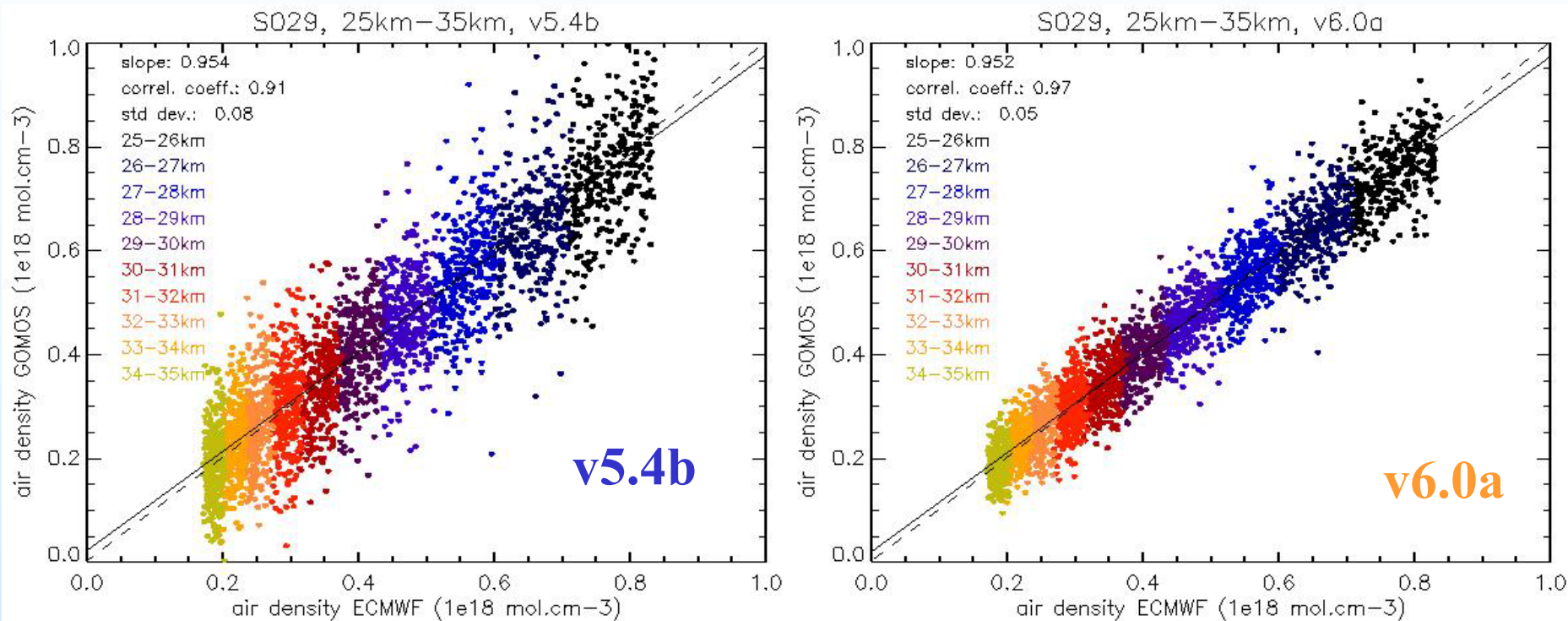


Products assessment

Air

Below 25 km and above 45 km, strong deviation from ECMWF is observed. Part of this deviation is explained by the aerosol model used under the form of a polynomial of degree 1, function of the wavelength.

Correlations air GOMOS/ECMWF



S029	slope	correlation coefficient	standard deviation
v5.4b	0.954	0.91	0.08
v6.0a	0.952	0.97	0.05

Products assessment

Aerosol

- ✓ As the current atmosphere is extremely transparent, the capability to retrieve individual profiles is often at the edge of the instrument sensitivity.
- ✓ Polar stratospheric clouds can be detected although there is currently no dedicated flag raised.
- ✓ Aerosols spectral dependence is very sensitive to residual scintillation.
- ✓ Data should be considered with caution above 35 km.

Products assessment

NO₂

✓NO₂ is sensitive to residual scintillation. Impact reduced thanks to the DOAS inversion and regularisation.

✓Validity range : 20-50 km. At other altitude ranges, data should be considered with caution.

NO₃

✓Validity range : 25-45 km.

✓At other altitude ranges, data should be considered with caution.

✓Retrieval is still noisy within the validity range.

Products assessment

O2

- ✓ No more bias (with respect to ECMWF) is observed in the altitude range 25-35 km.
- ✓ Still some noise on some profiles.

H2O

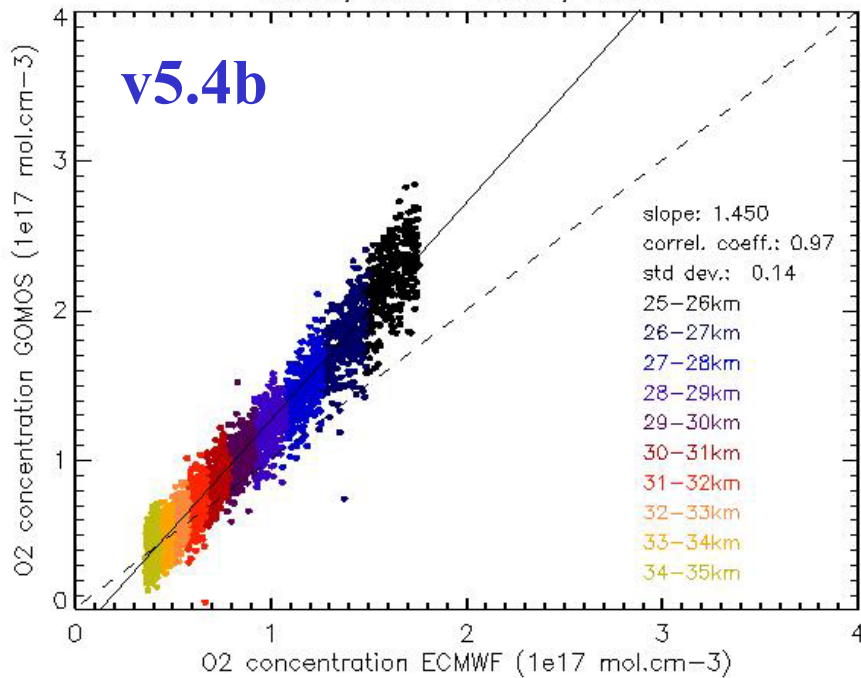
- ✓ Not retrieved above 50 km
- ✓ Results degraded probably due to non uniformity characterisation

OCIO

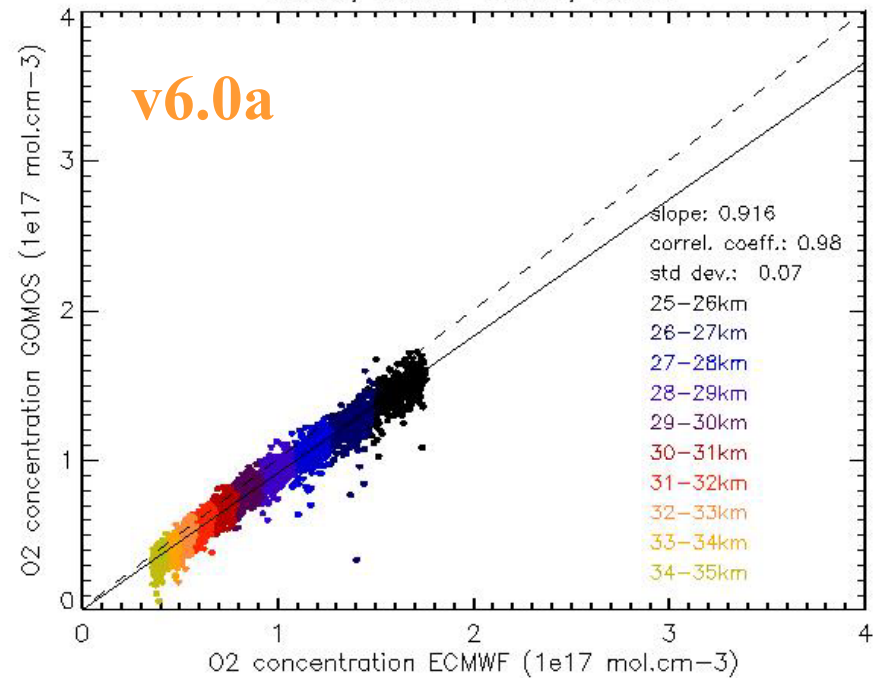
Not retrieved in current version of processing

Correlations O₂ GOMOS/ECMWF

S029, 25km–35km, v5.4b



S029, 25km–35km, v6.0a



S029	slope	correlation coefficient	standard deviation
v5.4b	1.450	0.97	0.14
v6.0a	0.916	0.98	0.07

From CALVAL to reprocessing configuration

CALVAL

- Aerosols spectral dependency is expressed under the form of a first order polynom of the wavelength.
- The non application of Global Iterative DOAS above 50 km introduces a bias on NO₂, and NO₃.

Reprocessing

- Aerosols spectral dependency is under the form of λ^{-1}
- Global Iterative DOAS is applied at all altitudes