Towards an improved total ozone climate data record from GOME, SCIAMACHY and GOME-2 as part of the ESA Climate Change Initiative

C. Lerot(1), M. Van Roozendael(1), R. Spurr(2), S. Kochenova(1), D. Loyola(3), Vijay Natraj(4), J. van Gent(1), J.-C. Lambert(1), D. Balis(5), M. Koukouli(5) and C. Zehner(6)

aeronomie.be

(1) BIRA-IASB, (2) RT Solutions, Inc., (3) DLR-IMF, (4) JPL, (5) AUTH, (6) ESA/ESRIN

The ESA's Ozone Climate Change Initiative project (Ozone_cci) aims at producing and characterizing a number of high quality ozone data products generated from multiple satellite sensors. To facilitate the merging of data from different sensors while minimizing error sources and biases, it is essential to work on improving and harmonizing the data sets from individual sensors. One way to facilitate such a harmonisation is to apply common retrieval algorithms to all level-1 data sets.

In this study, we concentrate on total ozone retrieval from the European sensors GOME, SCIAMACHY and GOME-2 using the GOME-type Direct FITting (GODFIT) algorithm, selected as the baseline for total ozone ECV production. GODFIT forms the basis of the current operational GOME Data processor version 5 and provides an improved GOME total ozone product (see poster of Koukouli et al.). The latest algorithmic developments realized within the Ozone_cci project are presented here. To speed up the algorithm and make it suitable for processing large data sets, radiative transport calculations have been accelerated by about one order of magnitude without significant loss of accuracy using a new 2-stream model coupled to a principal component analysis correction scheme. In addition, a new reflectance correction approach has been designed that minimizes the impact of instrument degradation and inter-sensor level-1 inconsistencies on total ozone retrievals in the Huggins bands.

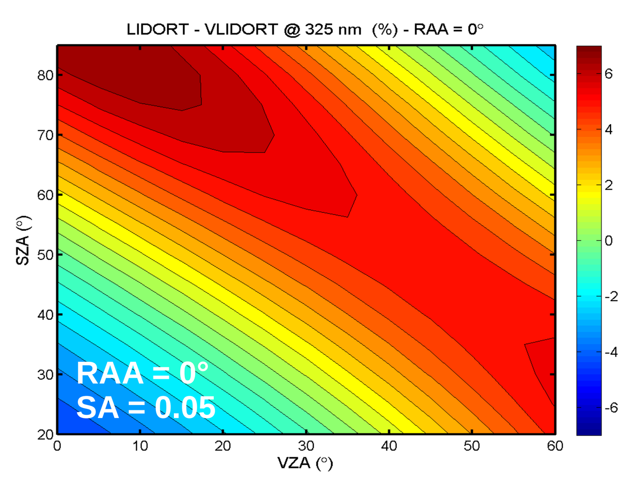
The GODFIT algorithm[1]

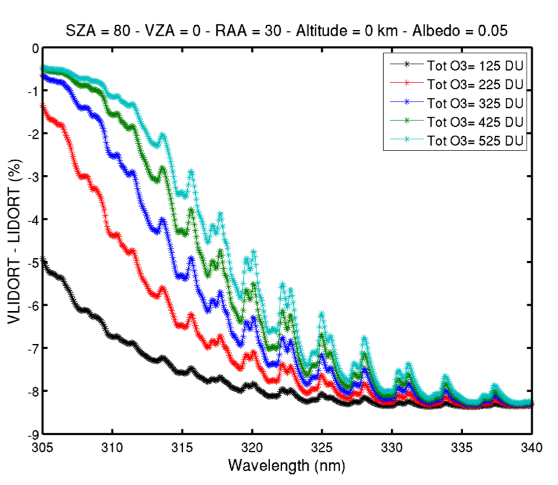
- **Direct fitting** of measured back-scattered radiances from nadir UV satellite instruments (GOME, SCIAMACHY, GOME-2) using on-line spectral simulations.
- Simulated radiances and total ozone, temperature and albedo weighting functions calculated «on-the-fly» with **LIDORT** radiative transfer (RT) models at all wavelengths.
- **T-shift procedure:** the a priori T° profile is allowed to be uniformly shifted in the retrieval.
- **A priori O_3 profiles** prescribed using the total column-classified climatology **TOMSv8**[2]. The **troposheric part** of the profile is scaled in order to match tropospheric columns from the **OMI/MLS climatology** [3].
- Fitting window: **325.0 - 335.0 nm**
- Clouds treated in the **independent pixel approximation.** Cloud parameters externally provided (FRESCO v6 or OCRA/ROCINN).

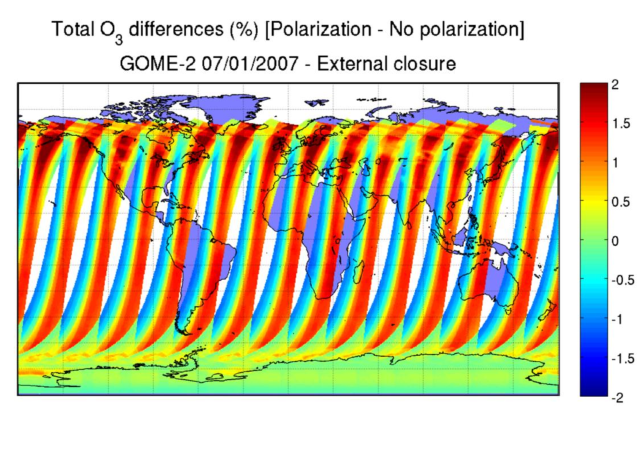
[1] Van Roozendael et al., JGR, 2012; [2] Mc Peters et al., JGR, 2007; [3] Ziemke et al., ACP, 2011.

Polarization correction factors

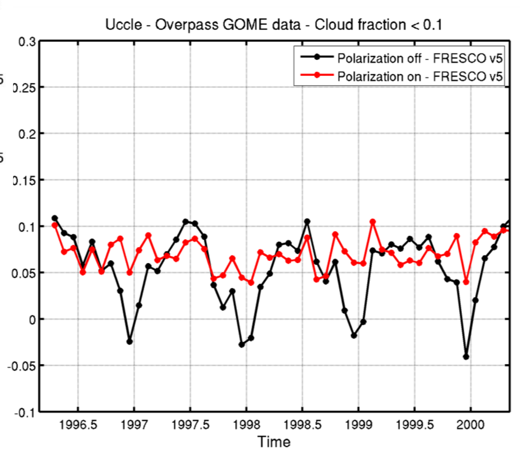
- Polarization has a significant impact on radiance intensity in specific observation geometries (up to ±7%).
- For large ozone optical depth, the impact of polarization correlates with ozone absorption structures, leading to errors in ozone retrievals if neglected.
- Polarization correction factors are applied to radiances simulated using a scalar code. These factors are calculated from the differences between simulations carried out by VLIDORT 2.5 in vector and scalar modes, and tabulated as a function of the SZA, VZA, RAA, O_3 column, surface albedo and height. The impact on GODFIT retrieved total ozone and surface albedo is illustrated in the figures beside.







Retrieved surface albedo



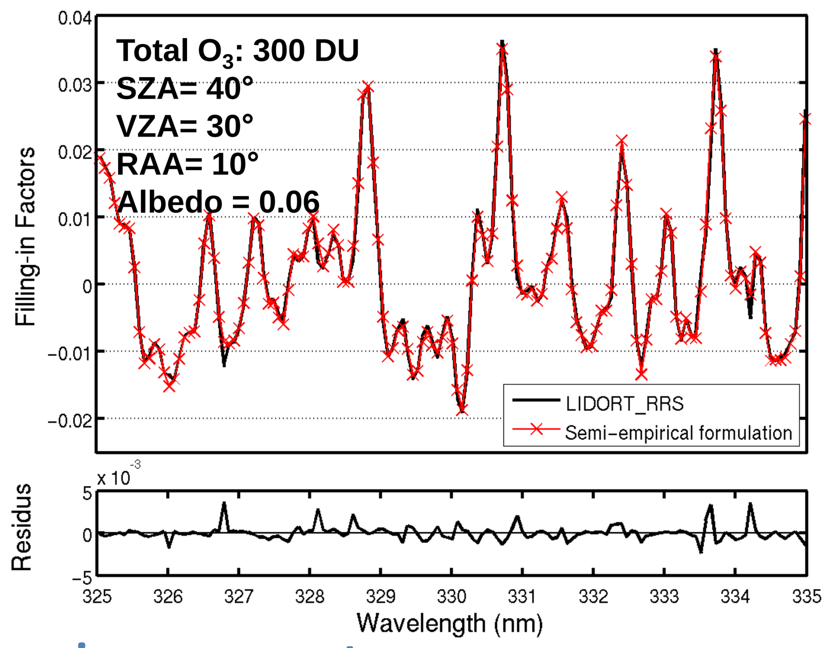
Semi-empirical Ring correction

Inelastic scattering (RRS) leads to filling-in of solar and molecular lines in measured spectra. The filling-factors, which perturb the elastic radiance, are expressed as:

$$FF(\lambda)=\rho_0\left\{\sigma_r \exp\left(\tau_{O3}\left(A_{tot}(\lambda)-A_{out}\right)-\tau_{O3}^{RRS}A_{in}(\lambda)\right)-1\right\}$$

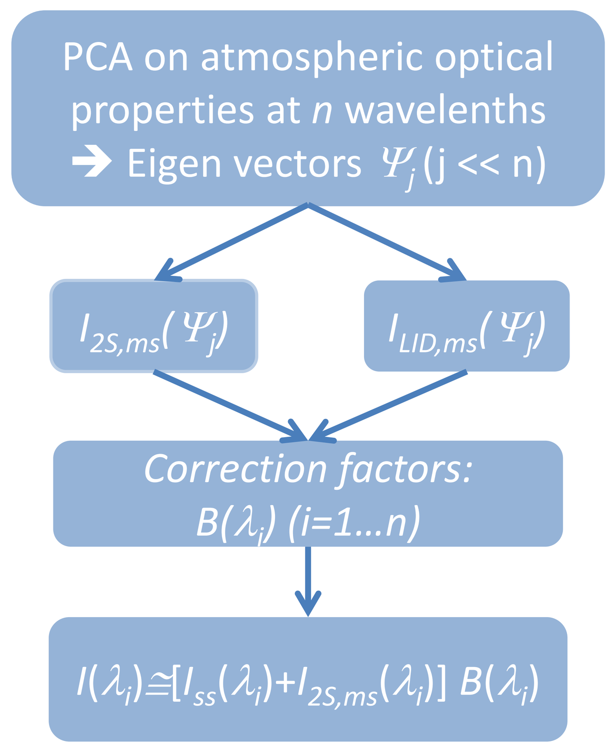
This formulation includes:

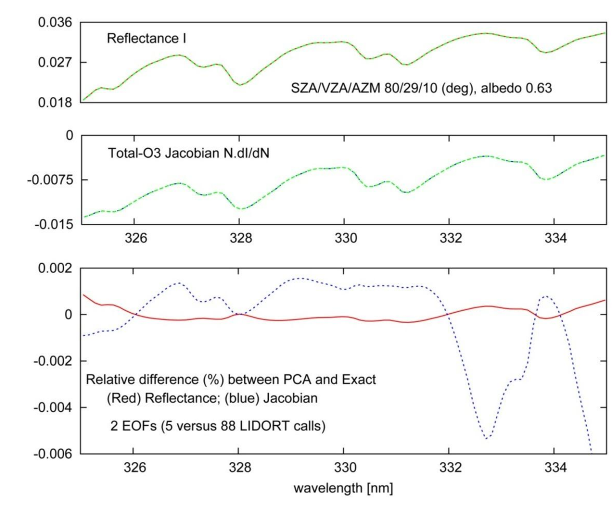
- Source and loss terms due to inelastic scattering.
- Absorption by ozone of the inelastic light.
- RRS-smoothing of the ozone absorption before inelastic scattering processes.
- A_{out} and A_{in} are pre-calculated in order to reproduce accurate filling-factors provided by LIDORT_RRS.



Computing performance improvement

Direct fitting requires much more computing resource than the DOAS technique since radiances and Jacobians are calculated at every wavelength of the fitting interval. RT Solutions, Inc. has developed a suite of RT tools, which provide a one-order-of-magnitude acceleration of the simulations when combined together. It includes single-scattering (*ss*) and accurate (*LID,ms*) and approximate 2-streams (*2S,ms*) multiple-scattering RT models, as well principal component analysis (*PCA*) tools.



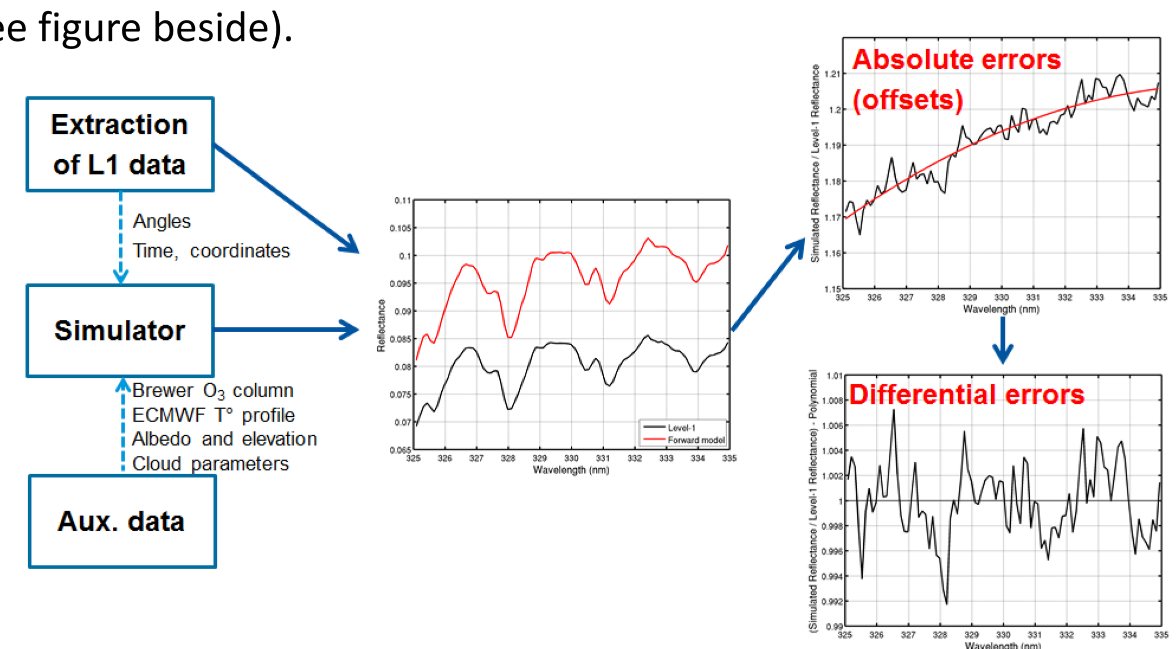


Computing time for 100 simulations

	2S + PCA	LIDORT	Time savings
Radiance	6.8 s	70.2 s	10.4
Radiance + 3 Jacobians	12.8 s	162.4 s	12.7

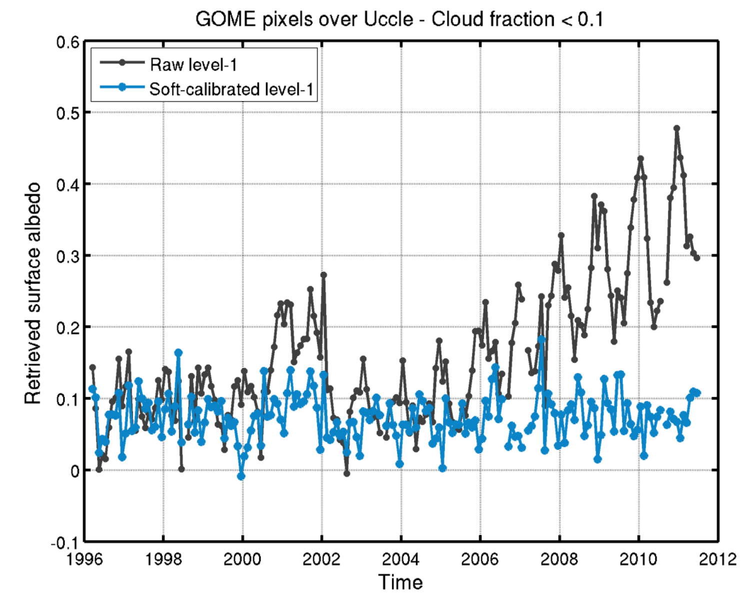
Soft calibration of measured reflectances

- Inconsistencies between different level-2 total O_3 data sets partly originate from calibration limitations (including instrumental degradation).
- Goal of the work: identification of the artificial structures present in the measured spectra, characterization of their main dependences (Time, SZA, VZA, …) and soft correction of the level-1 data at the sub-percent level to improve the consistency of the individual level-2 data sets.
- Method: Comparison of simulated reflectances with measured reflectances extracted over reference ground-based stations (see figure beside).
- Input for the simulations:
  - Total ozone column from Brewer measurements in 8 European stations.
  - ECMWF T° profiles (ERA-INTERIM).
  - Surface albedo from Kleipool et al. (JGR, 2008)
  - Surface height from ETOP02.
  - FRESCO v6 parameters for cloudy scenes.

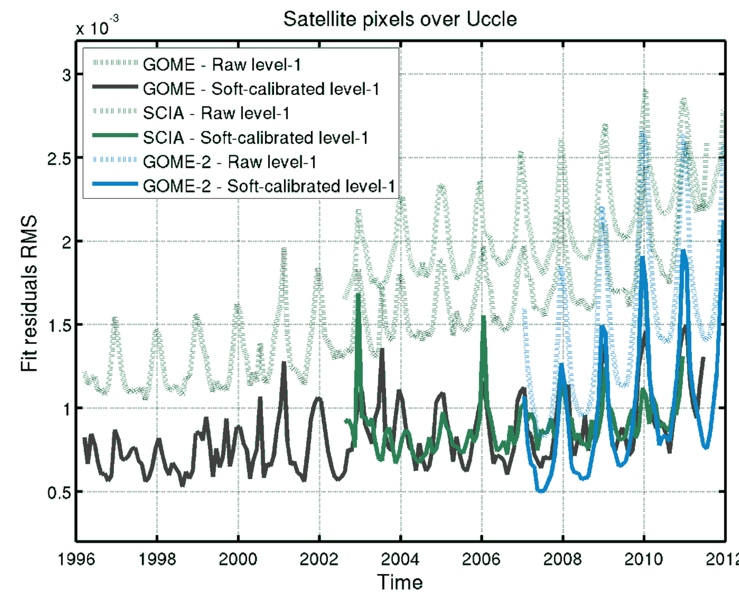


Examples of the impact of the soft calibration on total ozone retrievals

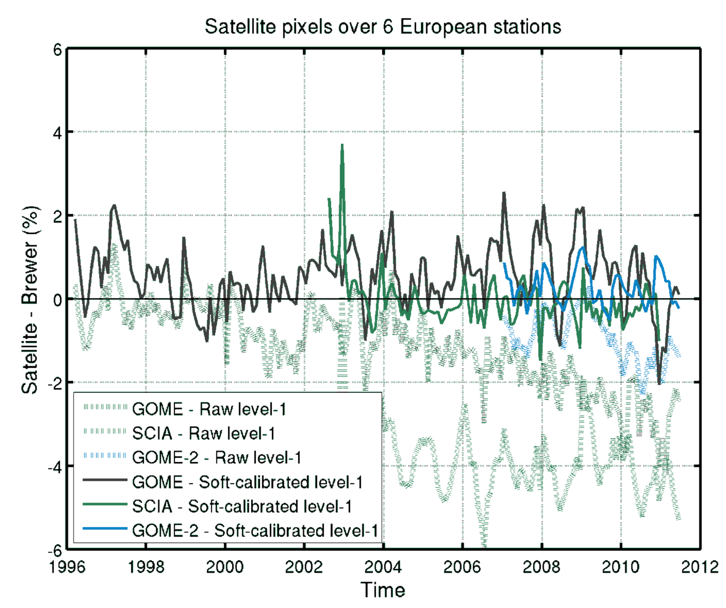
GOME surface albedo



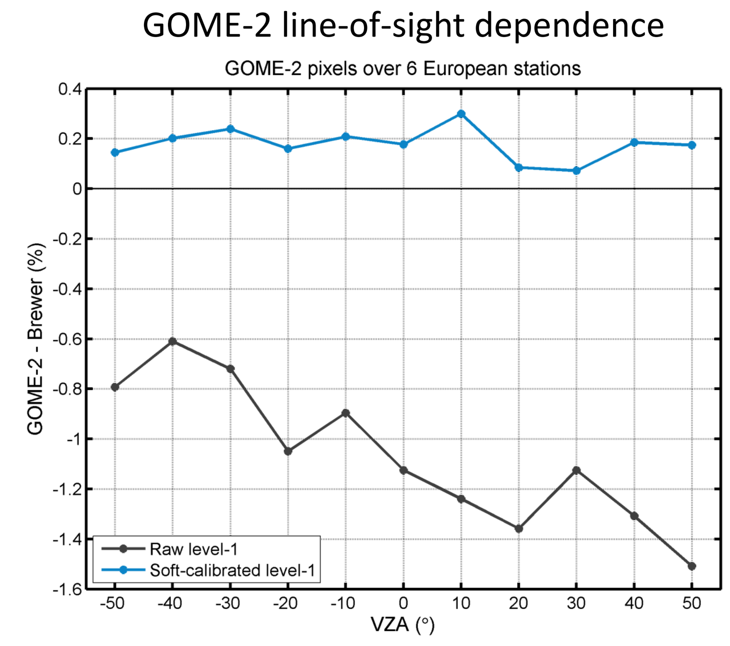
Fit quality



Satellite – Brewer difference time series

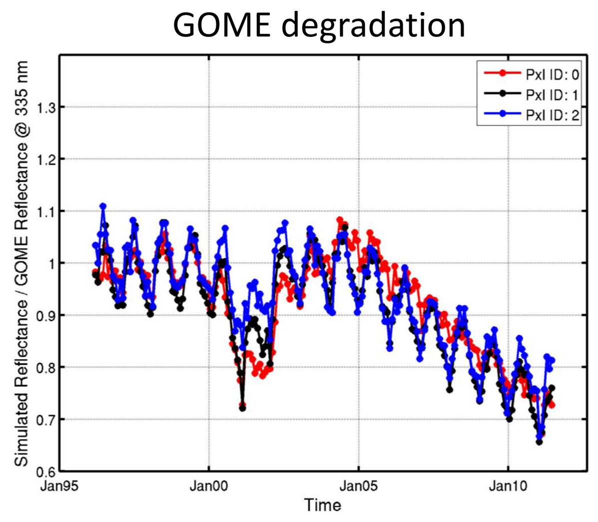


GOME-2 line-of-sight dependence

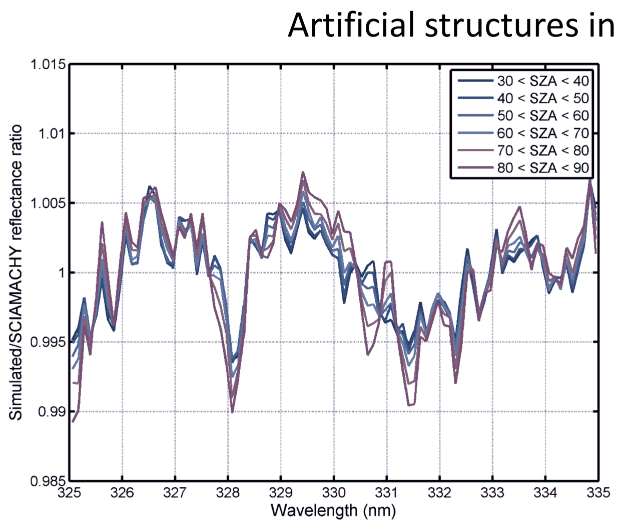


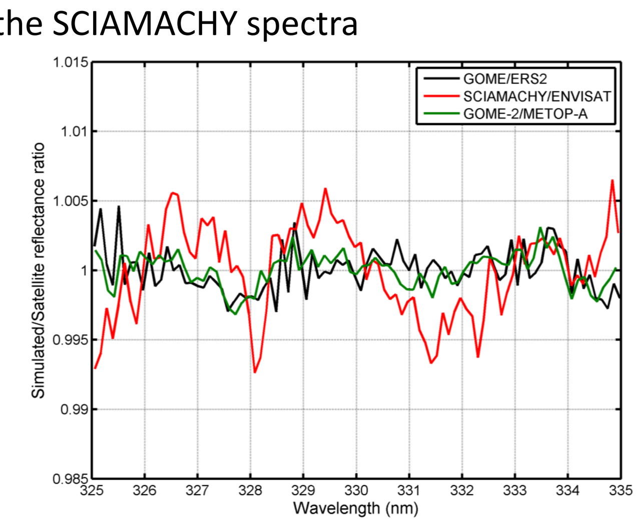
Examples of detected absolute and differential errors

GOME degradation



Artificial structures in the SCIAMACHY spectra





Outlook: Owing to these recent developments and their implementation in GODFIT, we expect to deliver total ozone products of very high quality for GOME, SCIAMACHY and GOME-2. In particular, the first results obtained on the basis of soft-calibrated level-1 reflectances are very promising. Once extended at the global sale, it should strongly enhance the consistency between the individual data sets. The generation of a prototype data set from these three sensors covering the 1996-2011 period is scheduled for Autumn 2012.