A long-term total ozone climate data record based on European nadir UV-visible sensors

C. Lerot[1,✉], M. Van Roozendael[1], R. Spurr[2], D. Loyola[3], J. van Gent[1], J.-C. Lambert[1], D. Balis[4], M. Koukouli[4] and C. Zehner[5]

(1) BIRA-IASB, (2) RT Solutions, Inc., (3) DLR-IMF, (4) AUTH, (5) ESA/ESRIN, ✉: christl@oma.be

Ozone is one of the atmospheric Essential Climate Variables (ECVs) under focus as part of the ESA's Climate Change Initiative (CCI) programme. The Ozone_cci project aims at producing, from multiple satellite sensors, global long-term ozone data series of high quality in order to meet requirements from the climate change research community.

We present the total ozone retrieval algorithm GODFIT (GOME-type Direct FITting) that has been selected as the baseline for the production of the ESA CCI total ozone ECV. The algorithm uses a direct-fitting approach in which total ozone is derived from a non-linear least-squares adjustment of reflectances simulated in the Huggins bands. In this work, we focus on new algorithmic developments recently carried out in the context of the Ozone_cci project. These include improved treatment of the Ring effect and explicit corrections for polarization effects. A new reflectance correction scheme has been designed to minimize the impact of level-1 calibration errors and time-dependent degradation effects. Although significantly slower than the DOAS approach, the performance of the algorithm has been considerably enhanced using principal component analysis of the optical properties (see poster by Spurr et al. [Session 3Ea #5963]). It consequently facilitates the ingestion of Level-1 measurements from the European sensors GOME/ERS-2, SCIAMACHY/Envisat and GOME-2/Metop-A and offers the potential to generate a consistent data record over more than 17 years (see poster by Coldewey-Egbers et al. [Session 4C, #5861] and presentation by Van Roozendael et al. [Session 4C, #5990]).

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 **tropospheric part** of the profile is scaled in order to match tropospheric columns from the **OMI/MLS climatology** [3].
- Temperature-dependent O_3 absorption cross-sections from Brion, Malicet, Daumont et al. [4].
- 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; [4] Malicet et al, J. Atmos. Chem., 1995.

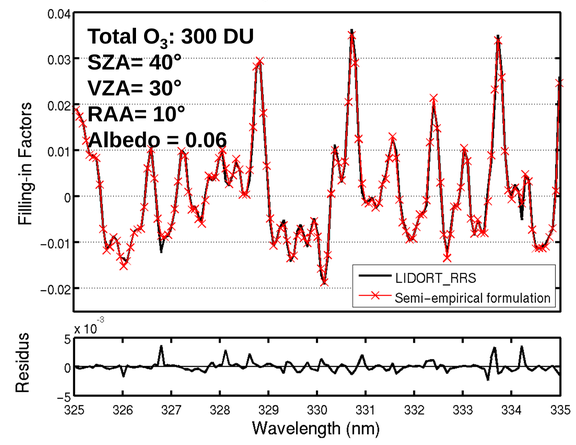
Semi-empirical Ring correction

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:

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

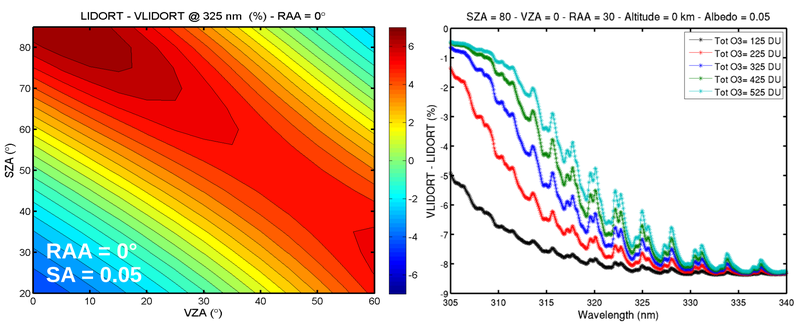
This formulation includes:

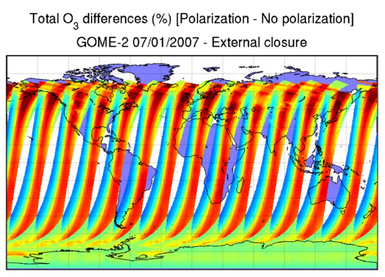
- Source and loss terms due to inelastic scattering.
- Absorption by ozone of the inelastic light.
- RRS-smoothing of the ozone absorption before inelastic scattering processes.
- A_{out} and A_{in} are pre-calculated in order to reproduce accurate filling-factors provided by LIDORT_RRS.

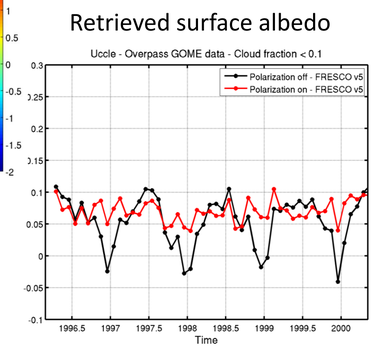


Polarization correction factors

- 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.

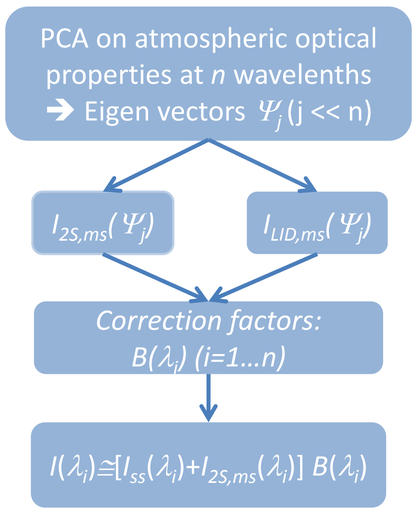




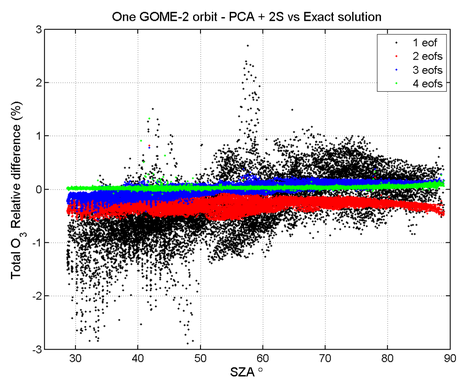


Computing performance improvement

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 provides a performance enhancement by a factor of about 3.5. 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. More details are given in the poster of Spurr et al. [Session 3Ea #5963].

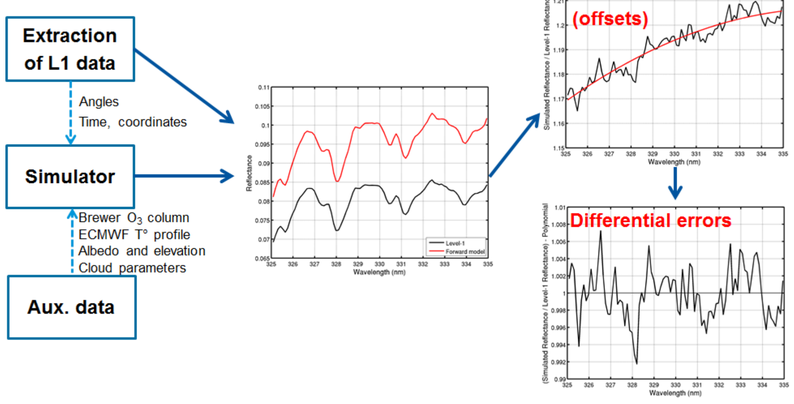


Accuracy of the method as a function of the number of eigen vectors.



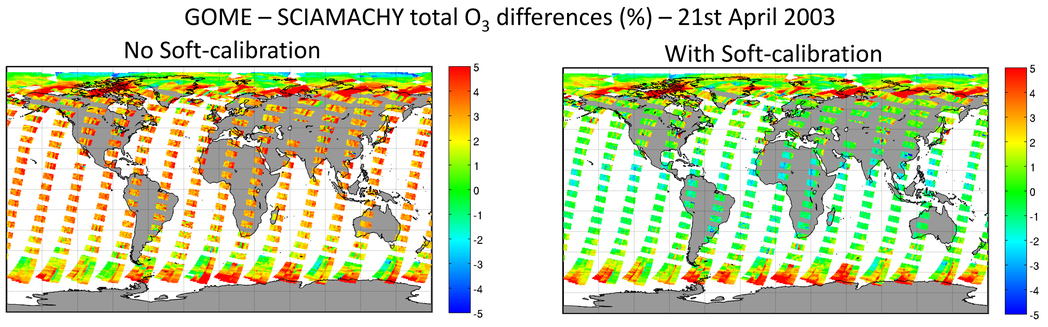
Soft calibration of measured reflectances

- 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.

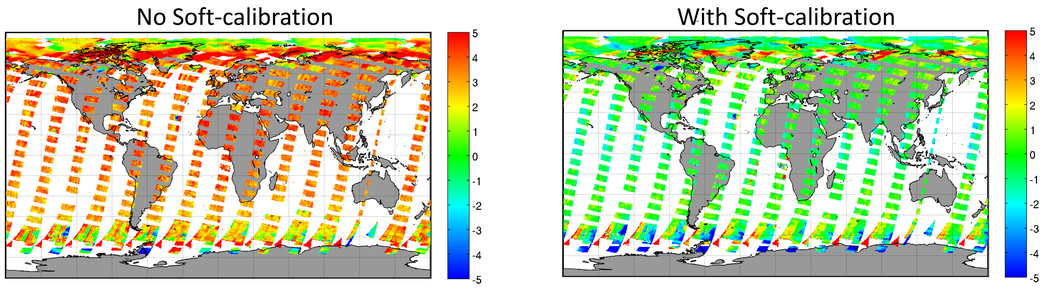


Impact of the soft calibration on total ozone retrievals at the global scale

GOME – SCIAMACHY total O_3 differences (%) – 21st April 2003

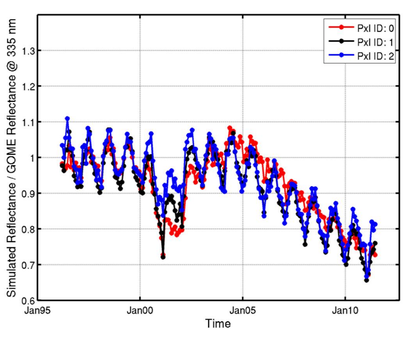


GOME-2 – SCIAMACHY total O_3 differences (%) – 23rd August 2007

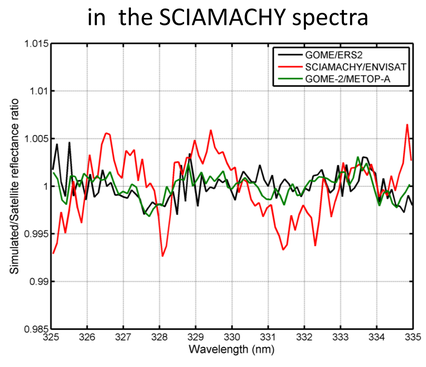


Examples of detected absolute and differential errors

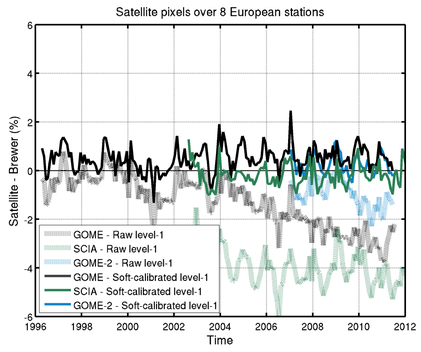
GOME degradation



Artificial structures in the SCIAMACHY spectra

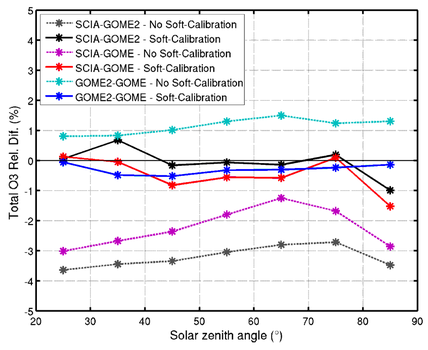


Satellite – Brewer differences at the reference mid-latitudes stations

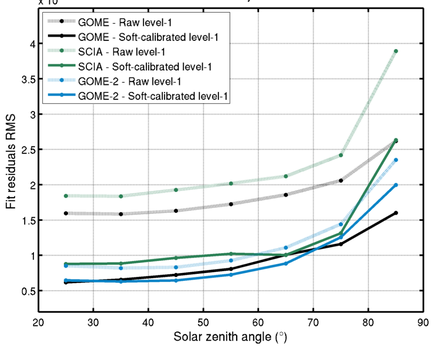


Solar zenith angle dependence – Data from 12 days in 2007

Inter-sensor consistency



Fit quality



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, especially since they lead to a significantly improved inter-sensor consistency. A prototype data set from these three sensors covering the 1996-2011 period is scheduled to be made available in early 2013.