Ground-based validation of CCI ozone profile Climate Research Data Package release 2015

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ABSTRACT

Validation is one of the cornerstones of ESA's Climate Change Initiative programme and of the Ozone_cci subproject in particular. Its objective is threefold: identification of the optimal retrieval algorithm for each instrument, characterisation of all products in the Climate Research Data Package, and assessment of their compliance with climate user requirements and specific research needs. We present the latest validation analyses and results of the ozone profile products (from limb- and nadir-viewing instruments) developed during the second phase of the Ozone_cci project: explorations of data content and information content, and comparisons of satellite data to ground-based reference observations. Ultimately, the validation conclusions are presented to data product users in the Product Validation and Intercomparison Report.

1. INTRODUCTION

The evolution of the vertical distribution of atmospheric ozone (O_3), an Essential Climate Variable (ECV), has been monitored over the past few decades by various instruments in space. Ozone research activities depend more and more on global, stable and consistent multi-decennial O_3 profile data records to make further progress in understanding the interactions between changes in O_3, ultraviolet radiation and climate. This need led to several international initiatives to improve the synergistic use of complementary data records by satellite missions. ESA's Climate Change Initiative project on O_3 (Ozone_cci) represents a significant contribution to this effort. It is aimed at collecting, improving and merging observations from instruments aboard the European platforms ERS-2 (GOME), Envisat (GOMOS, MIPAS and SCIAMACHY) and MetOp (GOME-2, IASI), and aboard Third Party Missions Odin (OSIRIS, SMR) and SCISAT (ACE-FTS). Several prototype data records were developed in the first phase of the project: (1) a homogenized Level-2 data set of screened O_3profiles from each individual sensor, and (2) temporally and zonally averaged (at various resolutions) Level-3 data sets for each sensor separately and for all sensors combined. In the current second phase of the project, the Climate Research Data Package (CRDP) is being improved and expanded with additional instruments (e.g. IASI on MetOp, SAGE II on ERBS, HALOE on UARS, SABER on TIMED, and MLS on EOS-Aura) and new data products (focusing on the troposphere, the UT/LS and the mesosphere). An overview of the CRDP is shown in Fig. 1.

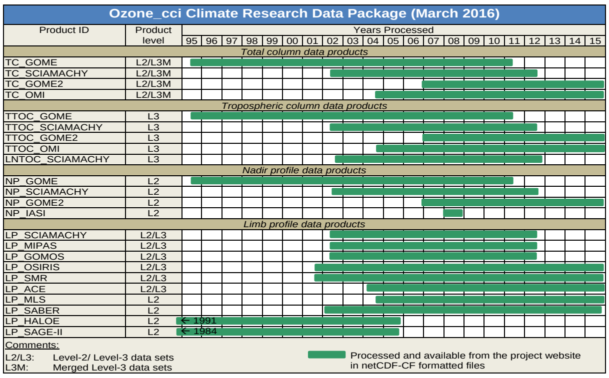

Figure 1. Overview of the data products in the Ozone_cci Climate Research Data Package (as of March 2016). Data is freely accessible at http://www.esa-ozone-cci.org/?q=node/160

2. VALIDATION AND INTERCOMPARISON ANALYSES

The Ozone_cci User Requirement Document (URD) [1] summarises observational requirements for O_3 ECV data products put forward by climate users, based on current needs and future targets of the Global Climate Observing System, the CCI Climate Modelling User Group (CMUG), the Integrated Global Atmospheric Chemistry Observation theme (IGACO) of the Integrated Global Observing Strategy (IGOS), and the WMO rolling requirements. The Ozone_cci validation team (VALT) translated these user requirements in validation requirements, which, ultimately, resulted in a framework for all activities related to the characterisation and the compliance assessment of

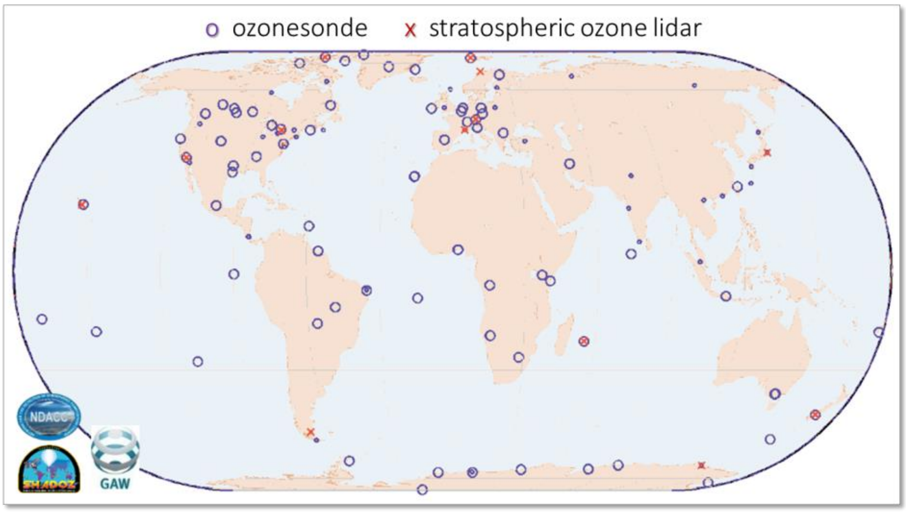

Figure 2. Geographic location of the NDACC/GAW/SHADOZ ozonesonde and NDACC stratospheric O_3 lidar instruments used in the validation analyses of O_3 profile products

product data quality, the Product Validation Plan [2].

The diversity in characteristics (nadir/limb geometry, Level-2/3/4, sampling properties, …) of the Ozone_cci CRDP necessitates a validation approach tailored to each product family. In the following, we consider the Level-2 vertical O_3 profile products from limb- and nadir-viewing instruments (see bottom half of Fig. 1). The assessment of other products, such as total O_3 column and tropospheric O_3 column data, is discussed elsewhere (e.g. [3–5]). A generic protocol for the validation of O_3 profile data products is established in [6]. VALT implemented a system that includes community-agreed quality assessment protocols and practices, as well as more advanced tools for most components in the analysis chain to address more specific demands.

The validation analyses typically include an exploration of the data content (i.e. spatio-temporal coverage and sampling) and of the information content (i.e. properties of the vertical averaging kernels (AK)), and a comparison of the satellite data to co-located reference observations collected by the ground-based networks of ozonesonde (NDACC/GAW/SHADOZ) and stratospheric O_3 lidar instruments (NDACC), see Fig. 2. The set of quality indicators that results from these analyses form the basis of the final step in the validation process: the assessment of the compliance of each data product with user requirements.

The VALT team is responsible for the Product Validation and Intercomparison Report (PVIR) [7], which assists the users of Ozone_cci data products in judging the fitness-for-purpose for their particular research needs. The PVIR contains a description of the validation methodology, a discussion of the validation results and the derived quality indicators, and the compliance assessment with user requirements. The PVIR is progressively updated with the release of new or updated products in the Ozone_cci CRDP. Updates are currently foreseen for summer 2016 and at the closure of the Ozone_cci project, around spring 2017.

3. VALIDATION OF LIMB OZONE PROFILE PRODUCTS

The Level-2 limb O_3 profile data package contains observations by ten European, Canadian and US satellite sounders, see Fig. 1 (tagged LP_XXX). Two of these contribute two data sets to the CRDP: SMR (501 GHz and 544 GHz retrievals) and GOMOS (stellar occultation and bright limb data). In total the CRDP contains twelve data products, together spanning the period 1984–2015, and covering the upper troposphere, the stratosphere and the mesosphere, on a global scale. The pre-screened O_3 profile data are stored in a user-friendly and harmonised netCDF format for all sounders. It can be accessed at http://www.esa-ozone-cci.org/?q=node/161.

A comprehensive analysis framework to perform assessments of the mutual consistency of limb and occultation O_3 profilers was recently established in [8]. It is based on a harmonised and robust statistical analysis of the relative difference between co-located pairs of satellite and ground-based O_3 profiles. The demonstrated quality of the ozonesonde and stratospheric O_3 lidar networks (Fig. 2) allows us to investigate, from the ground up to the stratopause, the following main aspects of data quality: long-term stability, overall bias, and short-term variability, together with their dependence on geophysical parameters. Below, we restrict ourselves to the key results and conclusions of our validation studies of the database in its native profile representation (O_3 number

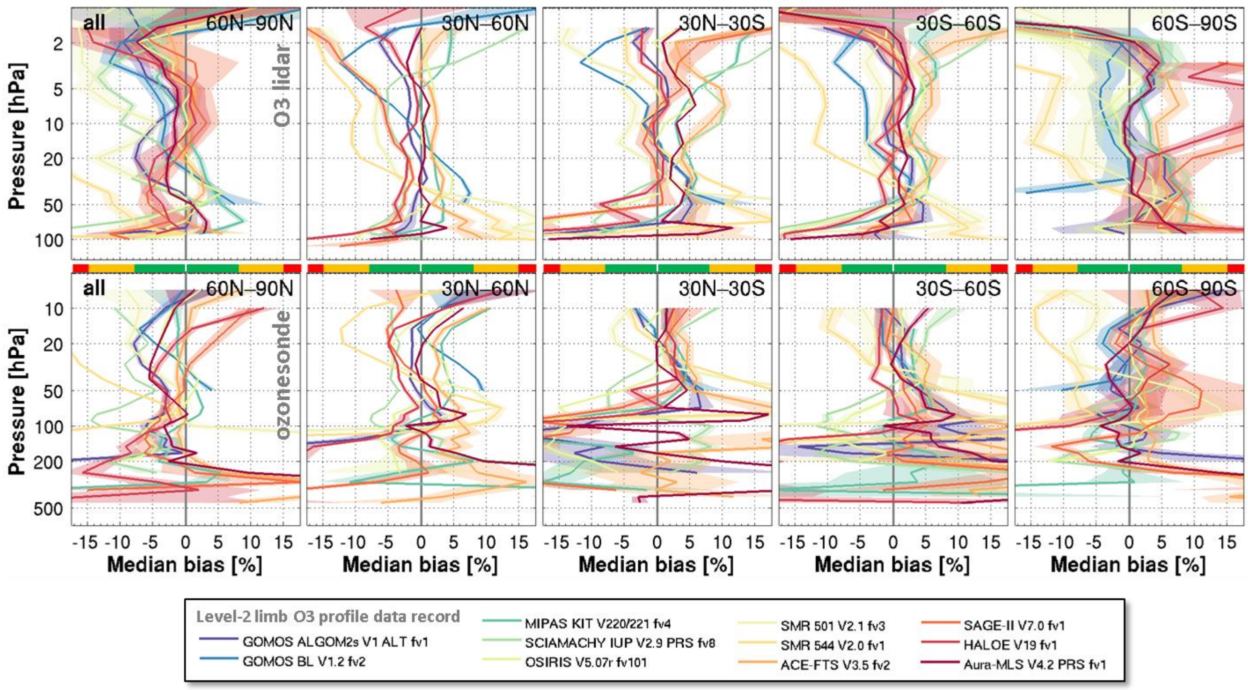

Figure 3. Vertical structure of median relative bias of limb/occultation O_3 profile data relative to ground-based observations by the lidar (top) and ozonesonde networks (bottom), in five latitude bands. The shaded area represents the 68% confidence interval around the bias estimates. The green/orange/red colour bar in the central part illustrates whether the satellite bias is fully/partially or not compliant with user requirements.

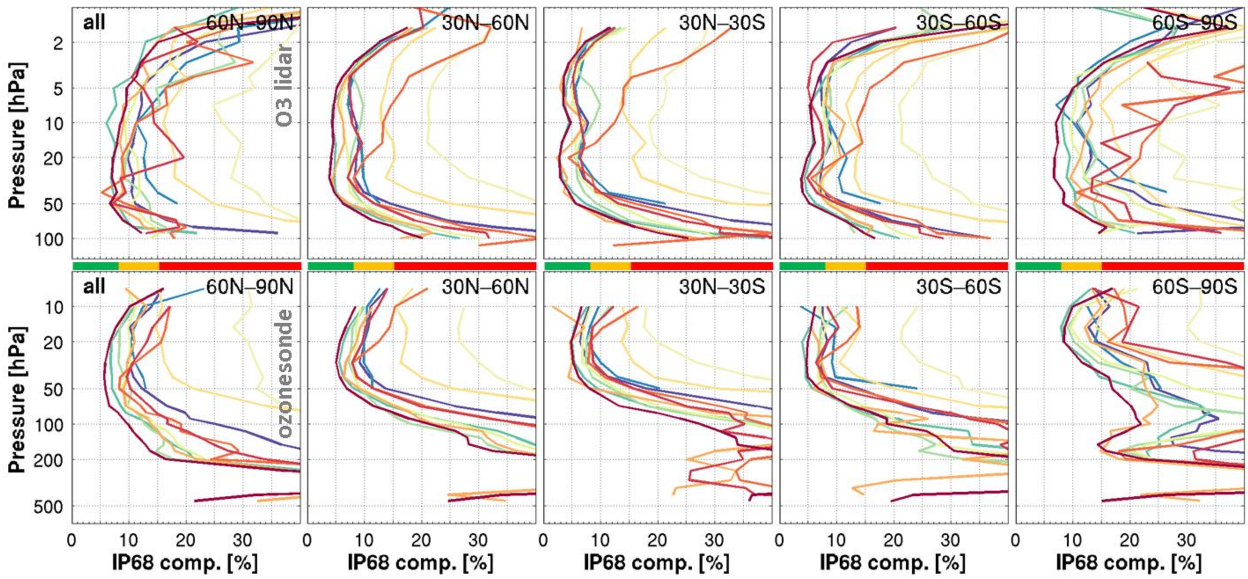

Figure 4. Similar as Fig. 3, but for the spread (1σ) observed in the comparisons. The legend can be found in Fig. 3.

density on fixed pressure levels). More details can be found in the PVIR document [7].

An important indicator of data quality is *bias*, i.e. the median difference between satellite and reference measurement. Fig. 3 shows the vertical dependence of the satellite bias in five latitude bands for eleven data records. The bias relative to ground-based data is generally less than about 5-10% in the middle and upper stratosphere, compliant with user requirements. But towards the stratopause and especially the tropopause the consistency between satellite records appears to deteriorate. This may appear as a result of lower O_3 abundances at these altitudes, but also due to larger systematic uncertainties in the lidar measurements (stratopause) or due to the increased inference by clouds and aerosol (tropopause). In latter part of the atmosphere the requirements by climate users are not

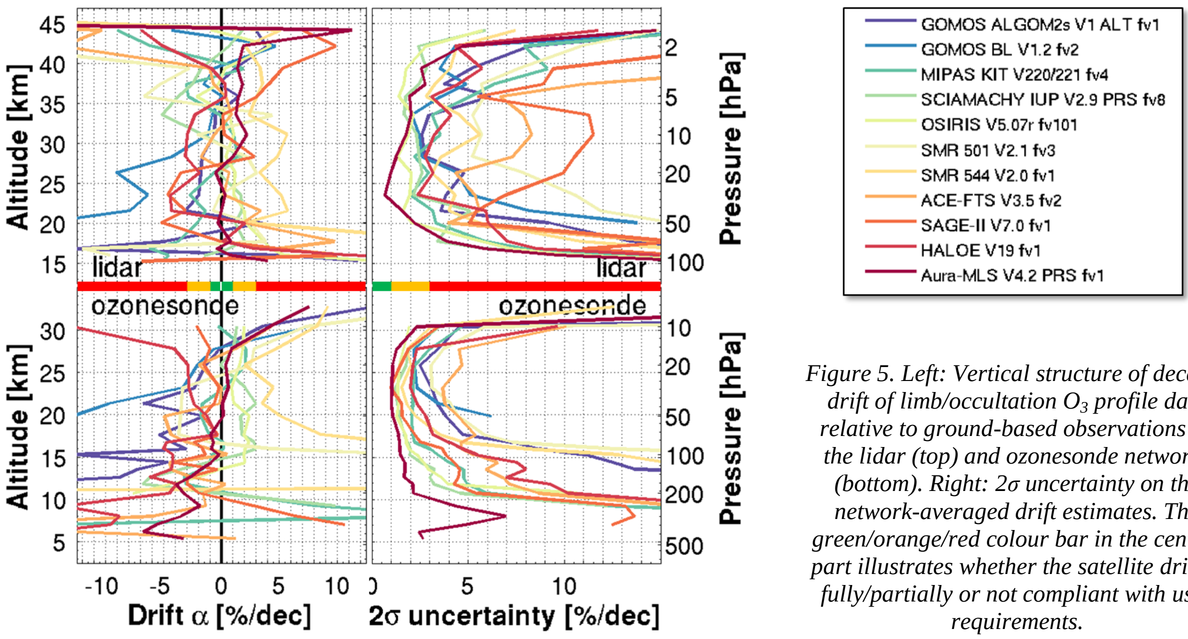

Figure 5. Left: Vertical structure of decadal drift of limb/occultation O_3 profile data relative to ground-based observations by the lidar (top) and ozonesonde networks (bottom). Right: 2σ uncertainty on the network-averaged drift estimates. The green/orange/red colour bar in the central part illustrates whether the satellite drift is fully/partially or not compliant with user requirements.

always fulfilled.

Fig. 4 shows a similar vertical behaviour for the second quality indicator, the half-width of the 68% inter-percentile in the relative difference distributions. It is a measure of short-term variability of the satellite record, although the indicator also receives non-negligible contributions from natural variability due to an imperfect co-location and a difference in horizontal smoothing of the compared airmasses. The *comparison spread* is hence an upper limit to the precision of the satellite record. It ranges generally between 5-12% and increases towards the stratopause (15-20%) and tropopause (>40%). This makes most data sets compliant with user requirements in a large part of the stratosphere. The exception is SMR 501 GHz (v2.1) data that is clearly much more noisy (>25%) than other data records, as a result of the weak emission line. The 544 GHz retrievals are more precise.

A third quality indicator is *decadal drift*, derived from a linear, robust regression analysis of the comparison timeseries. Fig. 5 shows the ground network-averaged estimates of satellite drift (left) and its 2σ uncertainty (right). For most records no significant instabilities are found, drift estimates are below ±5% per decade in the middle and upper stratosphere. The significance of GOMOS (ALGOM2s V1) and SMR 501 GHz (V2.1) drift estimates are located right at the detection threshold in, respectively, the UT/LS and upper stratosphere. But a few records drift significantly: SCIAMACHY around 35 km, GOMOS bright limb data below ~25 km, HALOE around 25 km, and SMR 544 GHz between 20-30 km. Users of latter data sets should be careful with the interpretation of trend results in the respective part of the atmosphere.

Fig. 5 (right) also shows that it is not possible to detect satellite drift below 1-2% per decade. For dense samplers (Aura MLS, SCIAMACHY, MIPAS, OSIRIS) or long timeseries (SAGE II) 2-3% per decade is accessible over the middle and part of the upper stratosphere. But for other data records we can probe at best down to 3-5% per decade, and worse in the lower stratosphere. This limits our ability to assess the compliance with user requirements, which are set at 1-3% per decade. To improve the compliance assessment we rely critically on longer timeseries and, especially, on improvements in the homogeneity of ground-based network data.

Another crucial characteristic of data records, not shown here, is the quality of the auxiliary data needed to convert between O_3 profile representations (pressure ↔ altitude, O_3 number density ↔ O_3 volume mixing ratio). More details can be found in the PVIR document [7].

4. VALIDATION OF NADIR OZONE PROFILE PRODUCTS

The Level-2 nadir O_3 profile data package contains observations by four types of European nadir sounders, see Fig. 1 (tagged NP_XXX). Two instruments (GOME-2 and IASI) are flown on two platforms (MetOp–A and –B). In total, the CRDP contains six data products, together spanning the period 1995–2015, and covering the troposphere, the stratosphere and lower mesosphere, on a global scale. The O_3 profile data are stored in a user-friendly and harmonised netCDF format for the GOME-SCIAMACHY-GOME-2 series. These can be accessed at http://www.esa-ozone-cci.org/?q=node/164.

The vertical smoothing properties of nadir O_3 profile retrievals are much more complex than those of limb/occultation retrievals. The nadir analyses therefore include a thorough study of the vertical AK, leading to various measures of information content (e.g. degrees of freedom of signal, vertical sensitivity, vertical resolution, …) and their dependence on geophysical parameters (latitude, solar zenith angle, season, …).

Fig. 6 shows the long-term evolution of DFS and vertical sensitivity at a mid-latitude site in the Northern hemisphere. GOME profiles lose about 1 DFS over 15 years, GOME-2A profiles about 0.5 DFS over 6 years. This shows the success of the RAL v2.14 algorithm in correcting for the faster degradation of the GOME-2A instrument compared to its predecessor. Shorter-term variations in DFS are correlated with variations in SZA.

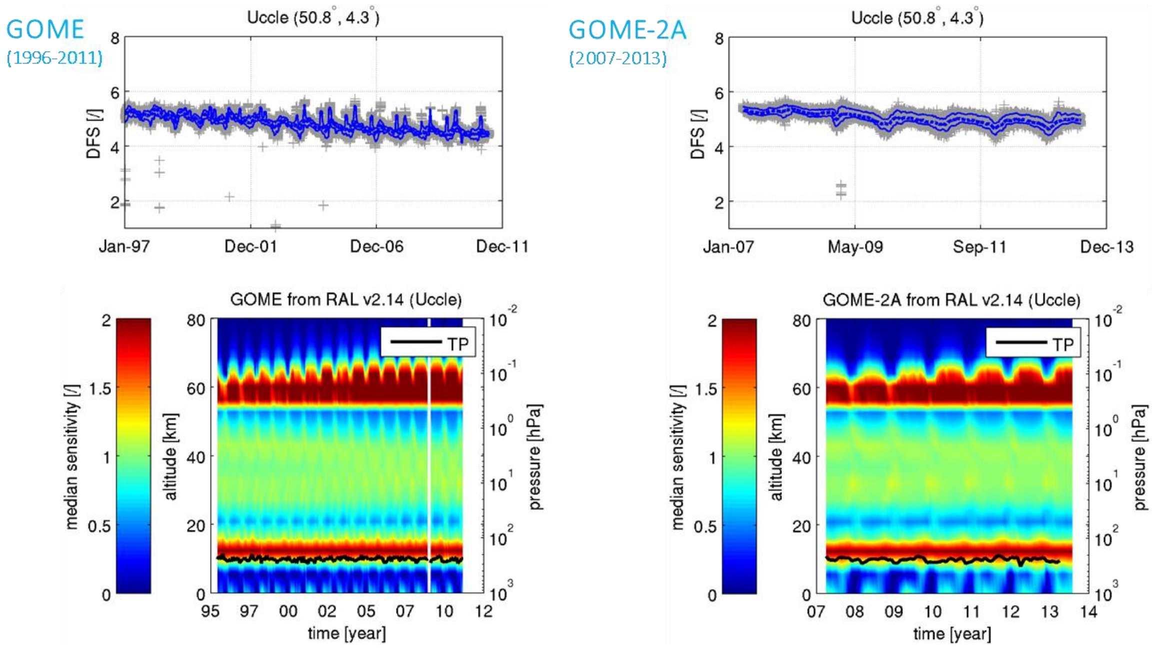

Figure 6. Timeseries of two measures of information content of the GOME (left) and GOME-2A (right) nadir O3 profiles around the Uccle ground station. Top: degrees of freedom of signal (blue curve shows monthly running averages and 1σ spread); bottom: vertical structure of median sensitivity (black curve shows tropopause).

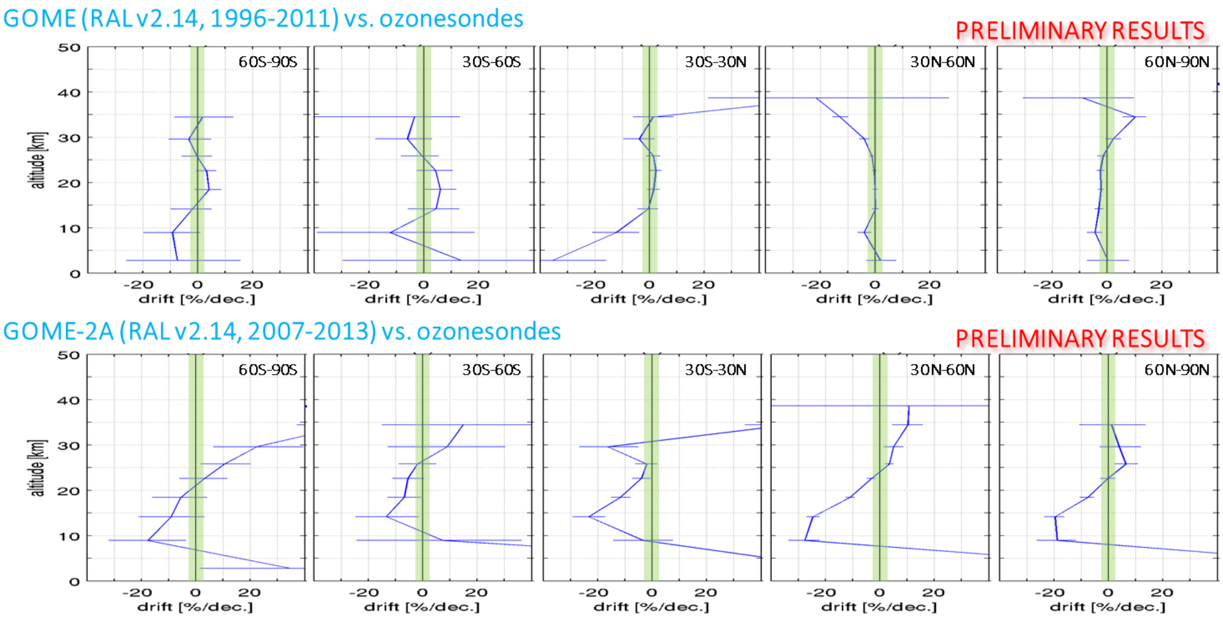

Figure 7. Vertical structure of the decadal drift of GOME (top) and GOME-2A (bottom) relative to ozonesonde observations in five latitude bands. The results are preliminary, especially the estimates above 30 km and below 10 km need to be confirmed. Error bars indicate the 95% confidence interval, the green shaded area represents the loose user requirements (3% per decade).

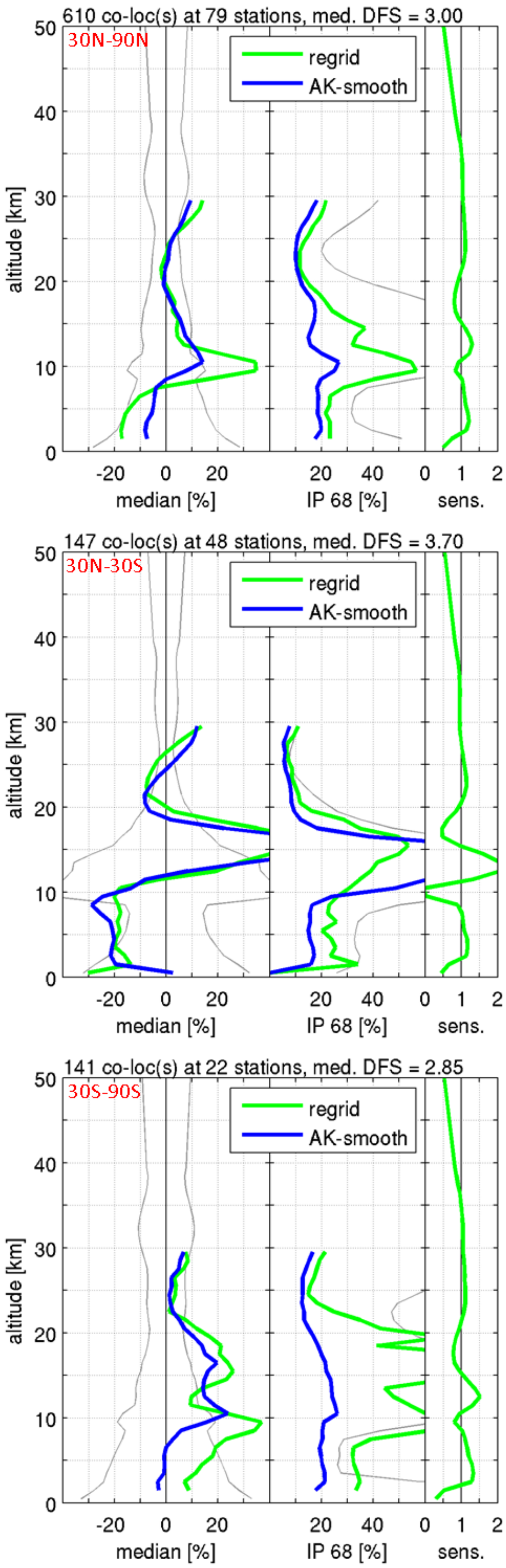

Figure 8. Structure of median bias (left), comparison spread (centre) and vertical sensitivity (right) of IASI 2008 nadir profile data (FORLI v20140922) relative to ozonesondes in 3 latitude bands. Correlative profiles are either regridded (green) or smoothed using IASI's vertical AK (blue).

Changes in vertical sensitivity are noted as well around the stratopause and lower mesosphere, resulting from the larger degradation of the short UV wavelengths.

Fig. 7 presents preliminary results of the long-term stability of the nadir O_3 profile records. No significant drift is found for the GOME data record. Estimates are less than ±5% per decade and the vertical structure is similar for the different latitude bands. The latter is also true for the GOME-2A drift results. However, the GOME-2A record does seem to drift to lower O_3 by 10-20% per decade compared to the sonde measurements in the lower stratosphere and to higher O_3 values at altitudes above 25-30 km. These results are preliminary and are subject of further investigation. Consolidated results will be provided in the PVIR document [7].

At the moment, only part of the IASI timeseries have been processed with the latest Level-2 processor. Fig. 8 shows bias, comparison spread and vertical sensitivity results for the comparisons of ozonesonde to IASI data from 2008, as a function of altitude and in three latitude bands. Around the tropopause, IASI overestimates O_3 by 10-20% and more. This is largely due to the fluctuation and misattribution (retrieval barycentre offset) of FORLI retrieval's vertical sensitivity, as can be seen by the often strong improvement of the bias results upon averaging kernel smoothing (blue instead of green lines). In the Tropics however this feature is strongest and hardly affected by smoothing, which is a known issue of the current version of the FORLI-algorithm [9]. The oversensitivity around the tropopause is somewhat compensated by an undersensitivity below, leading to negative biases in the troposphere. Yet again, this effect is much stronger in the Tropics, up to -20%.

5. CONCLUSIONS AND PERSPECTIVES

In the second phase of Ozone_cci the ozone profile Climate Research Data Package has been significantly upgraded: more instruments, more products, improved data quality, larger temporal and spatial coverage… Accordingly, the VALT team updated and tailored its validation and intercomparison analyses to the specific needs of each data product, giving special care to QA frameworks like QA4EO. Many Ozone_cci profile products are compliant with the requirements on total uncertainty and decadal stability put forward by climate users. The few products that are not or partially compliant are currently being improved by the retrieval teams. The quality of all O_3 products in the CRDP is characterised in the Product Validation and Intercomparison Report [7]. Users of Ozone_cci products are strongly encouraged to read this document prior to working with the data since it contains key information on the fitness-for-purpose for their intended application.

The requirements expressed by users, the algorithm descriptions and error characterization established by data producers, and the data validation performed by independent validation experts, form a coherent and necessary suite in the overall quality assurance of ECV product generation. Quality assessments including data validation by external means is a cornerstone of any climate data service. The coordination and harmonisation of QA, validation methods, activities and reporting by an identified team (e.g. VALT in Ozone_cci) is crucial: at product and project level, but also across the CCI programme, across the Copernicus programme and across agencies. Initiatives like CCI, SI2N, QA4ECV, GAIA-CLIM, Fiduceo, … are hence essential in the context of the production of high quality ECV data records.

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