Ozone_cci+

Algorithm Development Plan (ADP)

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Executive Summary

The Algorithm Development Plan (ADP, deliverable D2.1 in Ozone_cci+) describes the plans for algorithmic developments addressing total ozone columns, nadir-based ozone profiles, and limb-based ozone profiles.

A series of new algorithms will be developed with a focus on both level-2 and level-3 data products.

For total ozone, the following activities will be undertaken:

- Integration of Sentinel-5P and MetOp-C/GOME-2 in the GTO-ECV data record, based on the reference GODFIT level-2 algorithm
- Merging of GTO-ECV data record with historical NASA/SBUV/TOMS data records to create a 40-year CDR starting in 1979
- Tentative expansion of the MSR data record back to 1960 using ground-based total ozone measurements

For ozone profiles from nadir sensors:

- Integration of Sentinel-5P and MetOp-C/GOME-2 in CCI data sets based on the reference RAL level-2 retrieval algorithm
- Creation of a first European merged ozone profile and total ozone data record (GOP-ECV) starting with ERS-2/GOME in 1995 and consistent with the GTO-ECV total ozone data record
- Improvement of IASI level-2 retrieval algorithm (FORLI) to reduce uncertainties and systematic biases in the UTLS region
- Exploration of the potential to reduce uncertainties in nadir profile level-2 products in the lower troposphere and UTLS through exploitation of the synergy between UV, VIS and TIR retrievals

For ozone profiles from limb sensors:

- Integration of several new sensors (POAM-III on SPOT-4, SAGE-III on Meteor-3M, and SAGE-III on ISS) in the HARMOZ data record
- Intercomparison of different competing OMPS-LP level-2 retrieval algorithms. This activity might lead to the identification of a need for a dedicated round-robin exercise.
- Improvement of OMPS-LP level-2 algorithm in the UTLS and in polar regions
- Extension of the merged SAGE-II/CCI/OMPS long-term zonal mean data record with additional sensors to improve its accuracy, especially in lower stratosphere
- Improvement of latitude-longitude gridded level-3 data products based on limb-type sensors

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1 Purpose and scope

1.1 Purpose

This document summarises the plans of the Ozone_cci+ team for algorithmic developments addressing total ozone columns, nadir-based ozone profiles, and limb-based ozone profiles. This plan is expected to evolve and shall be updated as the definition of the ozone ECV product consolidates and the understanding of algorithmic issues improves.

1.2 Scope

The scope of the ADP is to establish through analysis of the trade-off between requirements and feasibility, a prioritisation of what R&D on ECV data product generation should be developed to maximise benefits to the users. The document also includes a specification of the ECV products planned for development in the project. The ADP is provided as an annex to the Project Management Plan (PMP).

1.3 Applicable documents

[AD-1] Data Standards Requirements for CCI Data Producers. Latest version at time of writing is v1.2: ref. CCI-PRGM-EOPS-TN-13-0009, 9 March 2015, available online at: http://cci.esa.int/sites/default/files/CCI_Data_Requirements_Iss1.2_Mar2015.pdf

[AD-2] CCI Data Policy v1.1. Available online at: https://earth.esa.int/documents/10174/1754357/RD-7_CCI_Data_Policy_v1.1.pdf

1.4 References documents

[RD-1] GCOS Climate Monitoring Principles, November 1999, reproduced in [RD-5], p48.

[RD-2] Guideline for the Generation of Satellite-based Datasets and Products meeting GCOS Requirements, GCOS Secretariat, GCOS-128, March 2009 (WMO/TD No. 1488). Available online at: http://library.wmo.int

[RD-3] Quality assurance framework for earth observation (QA4EO): http://qa4eo.org

[RD-4] EU Research Programmes on Space and Climate: Horizon 2020 (H2020), (http://ec.europa.eu/programmes/horizon2020/en/h2020-section/space, https://ec.europa.eu/programmes/horizon2020/en/h2020-section/climate-action-environment-resource-efficiency-and-raw-materials) and Copernicus (http://www.copernicus.eu/).

[RD-5] The Global Observing System for Climate: Implementation Needs, GCOS-200, October 2016. Available online at: http://library.wmo.int

[RD-6] Status of the Global Observing System for Climate, GCOS-195, October 2015. Available online at: http://library.wmo.int

[RD-7] Hollmann, R., et al., The ESA climate change initiative: Satellite data records for essential climate variables. American Meteorological Society. Bulletin, Vol. 94, No. 10, 2013, p. 1541-1552.

[RD-8] Joint Committee for Guides in Metrology, 2008, Evaluation of measurement data — Guide to the expression of uncertainty in measurement (GUM), JGCM 100: 2008. Available online at http://www.bipm.org/en/publications/guides/gum.html.

[RD-9] Merchant, C., et al., 2017, Uncertainty information in climate data records from Earth observation, Earth Syst. Sci. Data Discuss., vol. 9, p511-527.

[RD-10] Ohring, G., 2007: Achieving Satellite Instrument Calibration for Climate Change. Eos, Transactions, American Geophysical Union, Vol. 88, Issue 11.

[RD-11] Copernicus Space Component: www.esa.int/Our_Activities/Observing_the_Earth/Copernicus/Space_Component

[RD-12] User requirements for monitoring the evolution of stratospheric ozone at high vertical resolution (Operoz), 2015, ESA Expro contract 4000112948/14/NL/JK. Available online at: http://projects.knmi.nl/capacity/Operoz/Operoz_final_report_with_exec_summary_1mar2015.pdf

1.5 Acronyms

ACE-FTS	Atmospheric Chemistry Experiment – Fourier Transform Spectrometer
BIRA-IASB	Belgian Institute for Space Aeronomy
CCI	Climate Change Initiative
CDR	Climate Data Record
C3S	Copernicus Climate Change Service
DLR	German Aerospace Centre
ECMWF	European Centre for Medium-range Weather Forecast
ECV	Essential Climate Variable
EVISAT	Environmental Satellite (ESA)
EO	Earth Observation
ESA	European Space Agency
EU	European Union
EUMETSAT	European Organisation for the Exploitation of Meteorological Satellites
FMI	Finnish Meteorological Institute
GAW	Global Atmosphere Watch
GCOS	Global Climate Observation System

GOME	Global Ozone Monitoring Experiment (aboard ERS-2)
GOME-2	Global Ozone Monitoring Experiment – 2 (aboard MetOp-A)
GOMOS	Global Ozone Monitoring by Occultation of Stars
GOP	GOME-type Ozone Profile
GTO	GOME-type Total Ozone
IASI	Infrared Atmospheric Sounding Interferometer
KNMI	Royal Netherlands Meteorological Institute
MetOp	Meteorological Operational Platform (EUMETSAT)
MIPAS	Michelson Interferometer for Passive Atmospheric Sounding
MLS	
NASA	National Aeronautics and Space Administration
NDACC	Network for the Detection of Atmospheric Composition Change
OMI	Ozone Monitoring Instrument (aboard EOS-Aura)
OSIRIS	Optical and Spectroscopic Remote Imaging System (aboard Odin)
RAL	Rutherford Appleton Laboratory
SCIAMACHY	Scanning Imaging Absorption Spectrometer for Atmospheric Cartography (aboard Envisat)
TOMS	Total Ozone Mapping Spectrometer
UV	Ultraviolet

2 Introduction

2.1 Summary of user requirements for ozone ECV data products

Data product and algorithm developments in Ozone_cci are driven by GCOS. The goal of the Global Climate Observing System (GCOS) is to provide continuous, reliable, comprehensive data and information on the state and behaviour of the global climate system. GCOS focuses on satellite and *in situ* observations for climate in the atmospheric domain. Long-term consolidated data sets based on different satellite instruments are the foundation for improved model quality evaluation, allowing a more detailed insight into individual dynamical and chemical processes.

Long-term consolidated data sets are mainly required for: (1) monitoring the Earth climate system on longer (decadal) time scales; (2) investigation of long-term changes as well as of short-term variability; (3) improved description of processes in numerical models for more robust assessment of future evolution.

Table 1 summarizes the requirements established within GCOS for the Ozone ECV.

Table 1: **GCOS Target Requirements for the Ozone ECV.**

GCOS			Current status		
	Troposphere	Stratosphere	Total Columns	Tropospheric Columns	Profiles
Accuracy	10%	5%	1-5%	25%	5-15%
Spatial resolution	5-50 km	5-100 km	5.5x3.5 km^2	5.5x3.5 km^2	10x160 km^2
Temporal resolution	3 hours	3 hours	1- 6 days	1- 6 days	1- 6 days
Vertical resolution	0.5 km	0.5-3 km	N/A	1.3 km	2-3 km
Stability	1%	0.6%	1-3%	15-20%	5-10%

The horizontal and vertical resolution and observation frequency are mainly justified on the commonly used (standard) resolution of currently available and used model systems. For the troposphere regional models are often used which have a much higher horizontal resolution. The required horizontal resolution (i.e. 50-100 km) is generally too high; for most climate applications it would be sufficient to have 100-300 km.

It should be noted that the GCOS target requirements also refer to requirements for future (operational) observations.

As part of the User Requirements Document (URD) produced during Ozone_cci Phase I & II, achievable user and data requirements have been specified for ozone ECV products derived from existing observations having known attributes and covering the past 30 years. Although they are likely to be revised in the course of the current project, the latter requirements have been used as a reference for prioritization in CCI+.

2.2 Priorities for new algorithm developments

As stated in the ESA SoW, CCI+ capitalizes on the success of the CCI programme element to date. The objective is therefore to continue the successful achievements of CCI on research, development and assessment of pre-operational ECV processing systems, with the goal of transferring them into operational production outside CCI.

CCI actively coordinates with other European initiatives (e.g. C3S or EUMETSAT) with the aim to ensure an optimal uptake of the R&D performed under CCI in the operational production of ECVs outside CCI, and to assess the R&D that is needed for the evolution of the climate services.

The scope of CCI+ covers four main themes:

(i) Development of new ECVs, not yet included in CCI
(ii) New R&D on ECVs that were already started in CCI between 2010 and 2015
(iii) Cross-ECV scientific exploitation
(iv) Supporting activities on Knowledge Exchange

The general criteria for new R&D on existing ECV are the following:

- Match GCOS requirements, cross-ECV consistency
- Difficult ECVs required by GCOS
- Extend ECV length, develop new corrections
- Add new sensors (e.g. Sentinels)
- Further develop multi-mission time-series to fill gaps
- Improve uncertainty estimates
- Develop better merged products
- Perform Round-Robins

Having these general criteria in mind, specific priorities were identified for new R&D activities on existing ozone data records:

- Generally speaking : maximize the impact of new developments on the C3S ozone portfolio

- Integrate new sensors into existing CDRs, with a focus on Copernicus mission, e.g. Sentinel-5 Precursor
- Integrate more historical data sets in to existing CDRs, with a focus on making a significant impact on the applicability of the resulting new data sets for climate analysis and trend studies
- Improve the accuracy and precision of the existing ozone data products at L2 and L3
- Improved the characterization of the uncertainties of the existing data products
- Strive to design new algorithms or approaches to maximize the information content of the observations in critical altitude ranges (e.g. troposphere and lower stratosphere), as well as in critical regions of the globe (e.g. in polar regions)

These criteria and the consideration of the available resources for new developments have guided us in performing a trade-off analysis leading to the selection of the activities outlined in the next sections.

3 Algorithm Development Plan

3.1 Overview

Algorithm developments planned in this project aim at improving and enhancing the current portfolio of ozone data products generated in the previous phases of the CCI programme. The emphasis has been put on enhancing data records suitable for inclusion in the C3S service delivery.

Efforts will concentrate on (1) adding new EO sensors, in particular Sentinel data, (2) extending existing data records in time both backward and forward, (3) reducing uncertainties in critical observational conditions, e.g. in the UTLS or in polar areas, (4) improving the characterization of the data sets, through improved error budget analysis and better identification of various sources of biases.

Table 2 presents a tentative overview of the planned distribution of efforts on algorithm developments during the 3 contractual phases of the projects. Detailed descriptions of the planned activities in each topic are given in the subsequent sub-sections.

Table 2: Overview of ozone algorithm developments planned over the 3 contractual phases (CP-1, CP-2, CP-3)

Algorithm development	Responsible team	CP-1				CP-2				CP-3			
		Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Total ozone developments													
Inclusion of Sentinel-5 Precursor	BIRA-DLR												
Inclusion of GOME-2 on MetOp-C	BIRA-DLR												
GTO-ECV extension with S-5p and GOME-2C	DLR												
GTO-ECV extension with SBUV/TOMS data sets	DLR												
MSR extension backward in time	KNMI												
Nadir profile developments													
Inclusion of Sentinel-5 Precursor	RAL												
Inclusion of GOME-2 on MetOp-C	RAL												
Generation of GOP-ECV from nadir profiles constrained by GTO-ECV total columns	DLR												
Inclusion of IASI on MetOp-C	ULB												
Intercomparison of UV/VIS/TIR retrieval scheme for information content and accuracy improvement	RAL												
IASI retrieval scheme investigation for accuracy improvement in UTLS	ULB												
Limb profile developments													
HARMOZ extension	UBR												
OMPS algorithm development for accuracy improvement in polar regions	UBR												
OMPS algorithm intercomparison	UBR												
Extension of SAGE-CCI-OMPS merged data set with more sensors	FMI												
Improvement of ozone profile level-3 gridded data products	FMI												

3.2 Total ozone developments

3.2.1 Inclusion of Sentinel-5 Precursor

The direct-fitting algorithm developed as part of the CCI Phases I & II (GODFIT-3) has been successfully transferred for operational off-line processing of Sentinel-5 Precursor. We will investigate the consistency of the corresponding S-5p off-line operational product with the current CCI GODFIT-3 data record available from the GOME, SCIAMACHY, GOME-2 (A & B) and OMI sensors. As a result, the suitability of the new S-5p product for integration in the CCI Climate Data Record will be assessed. These activities will take place during CP-1.

3.2.2 Inclusion of GOME-2 on MetOp-C

As part of the activities planned in the Third Continuous Development and Operations Phase (CDOP-3) of the Satellite Application Facility on Atmospheric Composition Monitoring (AC SAF), the CCI direct-fitting algorithm (GODFIT-3) will be implemented for operational processing of the off-line total ozone product from GOME-2 on the three MetOp platforms using the DLR UPAS-2 processor. During CP-2, we will investigate the consistency of the AC SAF off-line operational product with the current CCI GODFIT-3 data record available from the GOME, SCIAMACHY, GOME-2 (A & B) and OMI sensors, and assess its suitability for integration in the CCI Climate Data Record. The actual implementation of the AC SAF product into the C3S processing line will depend on the timing of the AC SAF for reprocessing of the complete GOME-2 A, B, C data series using UPAS-2. Until then, the GOME-2 processing (including MetOp-C) will be performed at BIRA using the CCI GODFIT algorithm.

3.2.3 GTO-ECV extension with S-5p and GOME-2 on MetOp-C

After a successful integration of the new S-5p (Sect. 3.2.1) and GOME-2C (Sect. 3.2.2) level-2 products in the CCI Climate Data Record, the existing level-3 total ozone merging algorithm will be adapted and extended to ingest the data from the additional sensors and to expand the GTO-ECV data record. Possible biases among S-5p and GOME-2C and the selected GTO-ECV reference data base will be reduced by applying an inter-sensor calibration approach. Finally, the adjusted total columns from both sensors will be integrated in GTO-ECV; the reprocessing is planned for CP-2.

3.2.4 GTO-ECV extension with SBUV/TOMS data sets

In CP-1 the existing level-3 total ozone merging algorithm will be adapted and extended to ingest SBUV/TOMS total ozone data from NASA and to expand the GTO-ECV data record backward in time to the period 1979-1995. An extensive comparison of the TOMS/SBUV data with GTO-ECV will be performed in advance in order to find optimum settings for the adjustment and to remove possible biases. Finally, the adjusted SBUV/TOMS data will be integrated in GTO-ECV. The reprocessing of GTO-ECV is planned for the end of CP-1.

3.2.5 MSR extension backward in time

We intend to extend the Multi Sensor Reanalysis (MSR) of total ozone columns back in time to the period 1960-1979, bearing in mind however that the quality of the resulting data will be low for some regions and in some time periods.

This task will involve the following steps:

1. Evaluation of available satellite total ozone column measurements for their use in the MSR.
2. Evaluation of available ground-based total ozone column measurements for their use in the MSR.
3. Improving the Cariolle parametrisation of the heterogeneous chemistry in the chemical-transport model by including a dependency on the chlorine content. The latest Cariolle parametrisation has a fixed Chlorine dependency based on the year 2000, which is not valid in the years before 1979 but is also questionable for the most recent years.
4. Extension of the MSR reanalysis during the 1970s using ground-based total ozone column measurement data. Establish the benefit of assimilation of ground-based data as well as the robustness of the assimilation results.
5. Extension of the reanalysis back to 1960 using ground-based data.
6. Quality control by (a) Evaluation of daily total ozone columns, analysis of long term changes in the respective seasonal and annual probability distributions; (b) Comparison of the analysis of model results and of the reanalysis data for consistency.

In parallel we will check the feasibility of including new satellite missions in the MSR total ozone data set. These new missions are the Chinese FengYun missions (FY-3A, FY-3B) and the NPP-OMPS instrument of NASA.

3.3 Nadir profile developments

3.3.1 Inclusion of Sentinel-5 Precursor and GOME-2 on MetOp-C

Through ESA CCI Phases I and II RAL's ozone profile retrieval scheme for UV sounders, was developed and applied to process GOME-1, SCIAMACHY, GOME-2A, GOME-2B and OMI. Subsequent to CCI Phase II, the scheme has recently been further developed (through UK national funding) to generate improved full mission datasets from these sensors for C3S.

In CP-1 of CCI+, the improved UV sounder scheme will be adapted to Sentinel-5P and GOME-2C. Tests will be performed to demonstrate their performances in comparison to GOME-2A, -2B and/or OMI flying concurrently and an ozone sonde ensemble and CAMS analyses. A sample 1 year dataset will be produced from each sensor and provided for independent validation and assessment within CCI+. Towards the end of CP-2, potential algorithm improvements for GOME-2C and S5P will be identified, taking into account results from the independent validation and assessment. The sample 1 year of data will then be re-processed and delivered in CP-3 for final validation and assessment.

3.3.2 Generation of a GOME-type Ozone Profile Essential Climate Variable (GOP-ECV) data record from nadir sensors constrained by GTO-ECV total columns

From the level-2 nadir ozone profile data products retrieved with the RAL scheme level-3 total ozone and ozone profile averages will be generated in CP-2 for each individual sensor. A thorough investigation of the spatial and temporal coverage will be performed in advance in order to optimize the representativeness of the level-3 products. The total ozone values from the integrated profiles will be compared with the existing GTO-ECV total columns. According to this analysis the ozone profiles will be adjusted in order to match the GTO-ECV total columns. An altitude-dependent scaling will be applied using novel machine learning techniques. Finally, in CP-3 the objective is to generate and deliver a homogeneous merged nadir ozone profile level-3 product which covers more than 20 years of measurements.

3.3.3 Inclusion of IASI on MetOp-C

The FORLI-O3 data production will be extended to IASI/MetOp-C using the operational version of the FORLI-O3 software (v20151001; provided to EUMETSAT in the frame of the ACSAF activities) after commissioning. The FORLI-O3 products (profiles and tropospheric/total columns) from IASI-C will be verified against those of IASI-A and -B to check the stability of the three IASI instruments and the consistency between the full available IASI datasets. If required from the comparison between the three IASI O_3 records, minor algorithm developments will be considered and investigated for IASI-C compliance purpose.

Beside the extension of the IASI datasets with MetOp-C to cover ~20 years of measurements, the objective is also to build a homogeneous and improved O_3 record from IASI for climate study. To that end, a new version of FORLI will be developed and tested. The changes that will be considered in FORLI include:

- New input parameters for the temperature and humidity profiles from ERA-5 reanalysis
- Time-varying CO_2 concentration profile instead of the constant one considered until now.
- A new set of a priori profile/covariance matrix built from harmonized CCI datasets or from ERA-5 or MERRA-2 O_3 profile climatology with a consistent discretization of the atmosphere for possibly improving the inversion process in the UTLS (if required, based on results in Section 3.3.6 below).
- Possible new other input parameters (e.g. IR surface emissivity atlas, cloud flag)

Statistical comparisons with the operational version of FORLI (delivered by EUMETSAT) will be done on a limited IASI Level 1C dataset (e.g. a few days global or time series around ozonesonde stations) to assess the differences in terms of (1) retrieval error, (2) vertical sensitivity and bias with a special focus in the UTLS, and (3) drifts against ozone sondes, especially in the troposphere and in the mid-upper stratosphere.

If found necessary after the statistical comparison performed in (2) and possibly the outcome of the UTLS improvement analysis to be carried out (see 3.3.6), the back-processing of the IASI Level-1C (from MetOp-A, -B & -C) with the new FORLI version will be initiated. This is expected to be done on the CICLAD-IPSL computing facility. Pending on complexity of implementation and computing resources, only a small part of the dataset will be reprocessed within this CCI+.

3.3.4 Intercomparison of UV/VIS/TIR retrieval scheme for information content and accuracy improvement

Through research in the UK National Centre for Earth Observation (NCEO), RAL has developed a scheme to retrieve ozone profiles from the combination of UV measurements from GOME-2 and thermal IR measurements by IASI. This can improve vertical resolution and accuracy, particularly in the UT/LS region, compared to the UV only scheme (see Figure 1). RAL will also be further developing a scheme to exploit the visible Chappuis band of GOME-2 to improve sensitivity and resolution of lower tropospheric ozone. Within CCI+, these combined wavelength schemes will be applied to generate a 1 year subset of GOME-2 and IASI data which will be compared to results from GOME-2 (UV only) and IASI (IR only) schemes. Diagnostics will be examined to assess retrieval vertical resolution and precision (averaging kernels and retrieval covariance matrices) and retrieved ozone distributions from the combined scheme and single-sensor schemes will be assessed through statistical comparison of profiles with an ozone sonde ensemble and comparison of global distributions with CAMS analyses. The assessment will include comparisons to both RAL and FORLI IASI-only ozone profiles, with a view to identifying improvements to the combined GOME-2+IASI scheme.

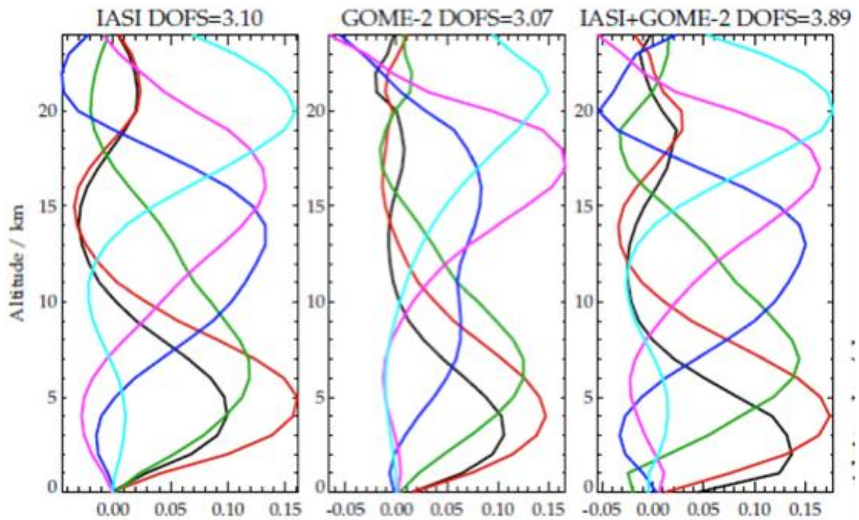

Figure 1: Illustration of the gain in information that can potentially be obtained as a result of combining UV and TIR retrievals based on the IASI and GOME-2 sensors.

As indicated in Table 2, this development and analysis work will take place in CP-1 and CP-2. A sample 1-year data will be produced for independent validation and assessment during CP-2. This dataset will, as a minimum combine UV and IR measurements[1].

On the basis of the above intercomparisons, and subsequent independent validation/assessment, potential improvements to the combined wavelength scheme will be tentatively identified. These would be implemented in CP-3 and a 2nd (final) version of the 1 year dataset would then be generated.

3.3.5 IASI retrieval scheme investigation for accuracy improvement in UTLS

The UTLS columns measured by IASI are known to display a large positive bias (10-15%) against ozone sondes. While it does not strongly affect the total O_3 column measurements that show excellent agreement with Dobson and Brewer spectrophotometers as well as with UV-vis instruments (~1-2% on average), identifying the causes of the bias in the UTLS region is capital for the profile climatology. One possible cause could be the poor representativeness of the a priori information in the UTLS that is characterized by low O_3 levels and large variability. UTLS also show the lowest sensitivity and the largest total retrieval errors. To investigate this, we will develop and test new sets of a priori profile/covariance matrix built from the available Ozone_cci datasets (e.g. the harmonized limb O_3 profile (Sofieva et al., 2017), the GOME-2 and the OMI datasets) or

[1] Incorporation of visible Chappuis measurements is to be confirmed, as subject to the outcome of research to be conducted under the remit of the UK NCEO.

from the homogenised ERA-5 or MERRA-2 (Yang et al., 2019) reanalysis. The potential improvement of the new set of a priori information will be evaluated on a restricted number of IASI spectra co-located with ozone sonde stations for validation purpose. The impact of the change in prior information on vertical sensitivity, retrieval errors and accuracy will be quantified over the entire profile as well as on the tropospheric and total O_3 columns.

Besides this, the impact of the discretization of the atmosphere in the inversion process will be investigated in terms of vertical sensitivity, retrieval errors and accuracy, with a focus on UTLS. The current FORLI-O3 retrievals are performed on 1-km thick layers between surface and 40 km with an extra layer from 40 km to TOA. Thinner or variable thick layers consistent with the new set of a priori profile/covariance matrix will be tested to explore the potential gain of vertical sensitivity especially to UTLS.

As mentioned in Section 3.3.4, a new version of FORLI will be developed for providing homogeneous IASI-O3 record by using ERA-5 reanalysis as new input parameters for the temperature and humidity profiles. This change might also improve the poor retrieval in the UTLS that could originate from large uncertainty on Level2 temperature or humidity profiles in that region. That impact will be verified as well.

3.4 Limb profile developments

3.4.1 HARMOZ extension

To facilitate the work of the users with satellite data sets and increase the redundancy and sampling of the data as well as the spatial and temporal coverage, Level-2 profile data from additional satellite instruments will be converted to the HARMOZ data format. This includes POAM III on SPOT-4, SAGE III on Meteor-3M, and SAGE III on ISS. In addition, some preparation to include data from the upcoming ALTIUS mission will be made, however, it is not expected that any ALTIUS data will be available before the end of this project. Furthermore, the data sets from the satellite instruments already included in HARMOZ and still operating (OSIRIS, Aura MLS, ACE-FTS, OMPS-LP) will be successively extended until the end of this project. Beside the format conversion, the activity includes data flagging in accordance with the recommendations given by the data providers.

3.4.2 OMPS algorithm development for accuracy improvement in the UTLS range and in polar regions

Despite a high scientific importance of the tropical UTLS altitude range and polar regions in ozone-climate research, ozone data sets from recent space-borne instruments have rather high uncertainties in these regions and the results from different sensors might differ significantly. In this study improvements of the OMPS ozone retrieval (University of Bremen) in these challenging regions are put in focus. Main issues limiting the quality of limb-scatter retrievals in the ULTS altitude region are saturation effects, interfering absorption features of atmospheric constituents other than ozone (e.g., O_4, H_2O), uncertainties in the determination of the surface albedo as well as uncertainties of the profile retrieval in the altitude range of the ozone number density peak. In the framework of this project we will investigate the influence of these factors on the uncertainty of the UTLS ozone retrieval. Possible ways to mitigate the influence of the identified issues will be elaborated and the retrieval algorithm developed at the University of Bremen will be adapted appropriately to improve the retrieval quality. With respect to the polar regions, the data sampling of the limb scatter instruments is limited in the presence of the Noctilucent Clouds (NLCs) in the summer season. For most of the instruments and retrieval algorithms, the retrievals in the presence of NLCs either fail completely or their results must be filtered out because of poor retrieval quality. Within the Ozone_cci Phase-II project this problem has been solved for SCIAMACHY observations by retrieving first the parameters of NLCs and then taking into account scattering by NLCs during the ozone retrieval. In the framework of this project, the SCIAMACHY algorithm will be adapted for the observations by the OMPS-LP instrument.

3.4.3 Intercomparison of OMPS-LP retrievals

Although the ozone data set retrieved from OMPS-LP measurements by the University of Saskatchewan research group have been used to create the merged data series within the Ozone_cci Phase-II project, neither a thorough validation of this product nor a comparison with other data sets from the same instrument (NASA, University of Bremen) have been published so far. In this project, an intercomparison of three OMPS-LP retrievals (University of Saskatchewan, University of Bremen, NASA) will be performed to assess the overall agreement between the different data sets. The overall judgement on the quality of different OMPS retrievals will be done using MLS and ground-based data sets as a reference.

3.4.4 Extension of SAGE-CCI-OMPS merged data set with more sensors

In the framework of the Ozone_cci project, a merged dataset of ozone profiles from several satellite instruments - SAGE II on ERBS, GOMOS, SCIAMACHY and MIPAS on Envisat, OSIRIS on Odin, ACE-FTS on SCISAT, and OMPS-LP on Suomi-NPP - has been created, with the aim of analyzing stratospheric ozone trends. All these instruments provide ozone profiles on a geometric altitude grid. For the merged dataset, we used the latest versions of the original ozone datasets. The datasets from the individual instruments have been extensively validated and inter-compared; only the datasets that are in good agreement and do not exhibit significant drifts with respect to collocated ground-based observations and with respect to each other, are used for merging.

The merged SAGE-CCI-OMPS dataset consists of deseasonalized anomalies of ozone in 10° latitude bands from 90°S to 90°N and from 10 to 50 km in steps of 1 km covering the period from October 1984 to July 2016. The SAGE-CCI-OMPS dataset is used in several studies evaluating ozone trends (Steinbrecht et al., 2017; Sofieva et al., 2017, Ball et al., 2018; the SPARC LOTUS report; WMO/UNEP Ozone Assessment, 2018).

The extension of the dataset by including recent OMPS-LP data is straightforward, and it is performed operationally in the C3S project. The possibility to exchange the currently used OMPS-LP product from U. Saskatchewan with another more suitable product (based on the outcome of 3.4.3) will be considered. Also as a new development, we plan to include also new ozone profile data from SAGE III on ISS. In addition, we will investigate the possibility of creating specialized datasets (limited in altitude or in latitude) with a special focus on the UTLS (Upper Troposphere and Lower Stratosphere) and polar regions. For these regions, we will investigate possibility of inclusion of ozone profiles from Aura MLS and POAM III.

3.4.5 Improvement of ozone profile level-3 gridded data products

The Level-3 merged dataset of ozone profiles with resolved longitudinal structure (Merged_LATLON), which has been created in the Ozone_cci Phase-II project, includes the ozone profiles from four satellite instruments: GOMOS, SCIAMACHY and MIPAS on Envisat, and OSIRIS on Odin. It covers the time period from late 2001 until now. The monthly mean gridded ozone profile dataset is provided in the altitude range from 10 km to 50 km, in bins of 10° latitude x 20° longitude.

In order to improve data coverage after 2012 we intend to include the data from OMPS-LP. This work will require some changes in the merging algorithm. We will also investigate the possibility of including Aura MLS into the Merged_LATLON dataset.

As a part of validation/intercomparison, climate data records from ground-based and satellite measurements will be compared.