acve

→ ATMOSPHERIC COMPOSITION VALIDATION AND EVOLUTION

ABSTRACT BOOK

18–20 October 2016 | ESA-ESRIN | Frascati (Rome), Italy

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European Space Agency

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4 Abstracts

Day 1 : 18 October 2016

Calibration of Measured Radiances

New GOME Level-1 Product: In-Flight Calibration and Degradation Correction

Coldewey-Egbers M.[1], Aberle B.[1], Slijkhuis S.[1], Loyola D.[1], Dehn A.[2]

[1]German Aerospace Center, Germany; [2]European Space Agency, Italy

The Global Ozone Monitoring Experiment (GOME) was launched on-board the second European Remote Sensing satellite (ERS-2) in April 1995 and operated successfully for more than 16 years until the decommissioning of the spacecraft in July 2011. The objective of GOME was to measure solar radiation reflected or scattered in the Earth's atmosphere or from its surface in the ultraviolet, visible and near-infrared spectral range. A range of atmospheric trace constituents in the troposphere and stratosphere, such as ozone or nitrogen dioxide, as well as cloud information can be observed.

Within the framework of the European Space Agency's GOME Evolution project an improved and consistent Level-1 data product covering the entire mission has been created. The reprocessing took advantage of updated and improved calibration algorithms and a detailed in-flight calibration parameter characterization. The algorithm improvements comprise the polarization correction, the dark signal correction, and the wavelength calibration, and they lead to refined radiance and irradiance spectra of excellent long-term stability. The consistent off-line processing of in-flight calibration data optimized for the complete mission enables us to monitor the long-term performance of the instrument.

Special emphasis has been put on the GOME degradation monitoring and correction. By means of the daily solar irradiance measurements it was found that in channels 1 and 2 the intensity decreased during the 16 years mission by 80 to 95% and 40 to 80%, respectively. The degradation in channels 3 and 4 is lower and periods of enhanced transmission were observed. The main degradation is explained in terms of deposits on the scan mirror and damage in the instrument's optical path. The signals of the three Polarization Measurement Devices (PMDs) show qualitatively a similar degradation as the corresponding channel wavelengths. A correction scheme using measurements from the beginning of the mission as reference has been successfully applied to both solar irradiance and PMD data. A similar degradation correction approach has been developed and applied to reflectance spectra within the total ozone fitting window from 325 to 335 nm. This method is based on the long-term analysis of cloud-free reflectances – taking into account the dependence on wavelength and viewing angle – over four CEOS (Committee on Earth Observation Satellites) pseudo-invariant calibration test sites located in northern Africa.

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The GOME-2 level 1 instrument degradation model version 1b and the GOME-2 level-1 reprocessing campaign R3

Lang R., Huckle R., Retscher C., Polit G., Lindstrot R., Tschimmel M., Munro R.

EUMETSAT, Germany

GOME-2 on Metop-A and -B is suffering from signal degradation in the shorter wavelength regime below 420 nm, like many instruments measuring in the UV/VIS. After more than 9 years in orbit on Metop-A and more than 3 years on Metop-B, enough data has been acquired to setup a model to correct for most (but not all) signal degradation. The model is combining an empirical and instrument correction in one step.

We will present an updated first version of the degradation model for GOME-2 on Metop-A and Metop-B. The full spectral range between 240 and 790 nm is covered as well as corrections for the two polarisation measurement devices (PMDs). The individual degradation components and how they are accounted for will be discussed.

This updated version currently covers the time frame from launch to end of 2015 for each instrument. A forecast for the degradation correction is also included which will be of importance for a possible near real time implementation.

Results of the corrected spectra will be presented as well as the impact on level-2 retrieval for ozone and atmospheric composition quality.

In 2017 EUMETSAT plans to initiate the third reprocessing campaign R3 of the GOME-2 level 1b data record, based on a significant updated processor version 7. The updated version addresses aspects of solar diffuser in-flight calibration, improved spectral calibration and a better treatment of instrument key-data. We will also address various aspects on how to cope with a changing thermal environment both over the orbit and in the long term.

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Mirror Contamination in Space: In-flight (SCIAMACHY) Contaminant Modelling

Krijger M.[1,2], Snel R.[1]
[1]SRON Space Research Netherlands; [2]Earth Space Solutions, Netherlands

We present our generic model that can be employed to describe and correct for degradation of (scan) mirrors and diffusers in satellite instruments that suffer from changing optical Ultraviolet to Visible properties during their operational lifetime. Our hypothesis is that mirrors in flight suffer from the deposition of a thin absorbing layer of contaminant, which slowly builds up over time. Demonstration of application to different instruments will be shown, e.g. SCIAMACHY on ENVISAT and GOME on ERS-2.

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CIAMACHY: Spectral Calibration in the SWIR Channels

Lichtenberg G., Hamidouche M., Schreier F., Hochstaffl P., Meringer M.
DLR - Deutsches Zentrum für Luft- und Raumfahrt, Germany

SCIAMACHY (SCanning Imaging Absorption spectroMeter for Atmospheric CHartographY) is a scanning nadir and limb spectrometer covering the wavelength range from 212 nm to 2386 nm in 8 channels. It is a joint project of Germany, the Netherlands and Belgium and was launched in February 2002 on the ENVISAT platform. After the platform failure in April 2012, SCIAMACHY is now in the postprocessing phase F.

SCIAMACHY was designed to measure column densities and vertical profiles of trace gas species in the mesosphere, in the stratosphere and in the troposphere (Bovensmann et al., 1999). It can detect a large amount of atmospheric gases (e.g. O3, H2CO, CHOCHO, SO2, BrO, OClO, NO2, H2O, CO, CH4, among others) and can provide information about aerosols and clouds.

The standard spectral calibration of the SCIAMACHY detectors is done with an on-board Spectral Line Source (SLS) by comparing theoretical line positions with line positions retrieved during calibration measurements. However, the used PtCrNe lamp does not have enough strong lines in the SWIR range (channels 6 -8) upwards of 1000 nm. The retrieval of in-flight line positions is additionally hampered by many damaged detector pixels of the SWIR detectors. An analysis of the mission data showed that for channels 6-8 no in-flight correction of the on-ground spectral calibration can be done with the standard approach, even at the beginning of the mission with a significant lower number of damaged pixels.

We therefore started a study to investigate an alternative spectral calibration approach. In this approach a highly resolved reference spectrum is fitted with a DOAS like algorithm to retrieve the wavelength for each detector pixel. This approach was already tested by us for the Sentinel-4 UVN and the former Earth Explorer 8 candidate mission CarbonSat.

For the method to work it is essential to have a good knowledge of the *in-flight* spectral response function and its change over time. Preliminary results show that the shape of the response function deviates from the current assumption of a Gaussian. For a successful fit it is also necessary to handle the many outliers caused by the bad pixels in an appropriate way. In this paper we present the first results of our investigations, focussing on channel 6 and the methane retrieval window.

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MIPAS Level 1B Version 8 Radiometric Accuracy Assessment

Perron G.[1], Kleinert A.[2], Birk M.[3], Wagner G.[3]
[1]ABB Inc., Canada; [2]KIT-IMK, Germany; [3]DLR, Germany

The MIPAS mission is in its post-operational phase F. A final algorithm improvement will be done along with a full reprocessing of the entire data set covering a period of ten years from 2002 to 2012. The goal is to improve as much as possible the MIPAS data quality. The new data set will be referred as version 8.

The MIPAS instrument has measured Infra-Red (IR) emission spectra at the Earth's limb in the middle and upper atmosphere along the orbit during day and night. The spectral range covered is 685 to 2410 cm-1 with a spectral sampling of 0.025 cm-1 during Full Resolution (FR) period and 0.0625 cm-1 during Optimised Resolution (OR) period. The MIPAS level 1B processor transforms instrument raw data into spectra calibrated spectrally and radiometrically with geo-location determined over the earth geoid of the line of sight tangent point.

This paper presents an assessment of the radiometric accuracy budget. The main contributors to the error are the detector non-linearity, the gain calibration noise and variation along time. The detector non-linearity was re-characterized in-flight and related error estimated. A validation of the new characterization was done looking at overlaps with linear channels. This has led to an improvement of level 2 trending analyses and validation. The error due to the gain calibration noise was controlled and limited through the calibration scenario. The ice accumulation in the output optics and instrument temperature variation lead to a gain calibration variation along time. The effect of ice was monitored and controlled through periodic decontamination.

Compared to the requirements and the previous version, the MIPAS level 1B version 8 will have an improved radiometric accuracy.

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Methods and Instruments for Validation

Validating the NRT Total Ozone Retrieval Algorithm for TROPOMI/S5P based on GOME-2/Metop-A observations

Koukouli M.E[1], Balis D.[1], Hao N.[2], Gimeno Garcia S.[2], Loyola D.[2], Zimmer W.[2], Lerot C.[3], van Roozendael M.[3]

[1]Laboratory of Atmospheric Physics, Aristotle University of Thessaloniki, Greece.; [2]Institut für Methodik der Fernerkundung (IMF), Deutsches Zentrum für Luft- und Raumfahrt (DLR), Oberpfaffenhofen, Germany.; [3]Belgian Institute for Space Aeronomy, Brussels, Belgium.

The Tropospheric Monitoring Instrument, TROPOMI, is the payload instrument for the Sentinel 5 Precursor, S5P, Mission, due to be launched end of 2016. TROPOMI will extend the atmospheric composition record initiated with GOME/ERS-2 in 1996 and continued with the SCIAMACHY/ENVISAT, OMI/AURA and the two GOME-2/MetOp missions, until 2022 in the least. Total ozone will continue to be the main gas of interest due to the continuing efforts to understand and monitor the recovery of the ozone layer.

In the following we present the validation of the operational algorithm to be used for the near-real-time retrieval of TROPOMI/S5P total ozone applied to GOME2/Metop data. Wide swath GOME2/MetopA observations, from July 2012 to July 2014, and reduced swatch observations from August 2013 to July 2014, provide two years of observations on which to base these comparisons.

With respect to the operational GOME-2 GDP-4.8 algorithm, a number of improvements were developed for TROPOMI: an optimized choice of wavelength at 328.125nm instead of 325.50nm for the AMF calculation was performed; a correction for polarization was applied to the AMFs instead of an East-West pixel post-correction; a combined MLS/TOMSv8 climatology was introduced instead of the "pure" TOMSv8 climatology. Furthermore, the *Clouds As Layers,* CAL, cloud treatment is employed instead of the *Clouds as Reflecting Boundaries CRB.* The CAL model is more precise than the CRB model and it does not require ghost column and intra-cloud corrections typical for the CRB model.

Using total ozone measurements by ground-based Brewer and Dobson spectrophotometers deployed globally as the background truth, the behaviour of the new algorithm with respect to cloud fraction, cloud top pressure, slant column density, solar zenith and viewing angles, among others, is examined and first results are presented in this work.

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Investigating the effect of horizontal gradients of trace gases, aerosols and clouds on satellite validation of tropospheric trace species using multi-azimuth MAX-DOAS observations

Wagner T., Remmers J., Wang Y., Donner S., Beirle S.

MPIC, Germany

We investigate a fundamental problem for the analysis of tropospheric data products from satellite observations: the effect of vertical and horizontal gradients of trace gases (here we focus on NO_2 and HCHO), aerosols and clouds within a satellite ground pixel. For that purpose we analyse MAX-DOAS measurements performed in 4 azimuth directions at the Max-Planck-Institute for Chemistry in Mainz, Germany. From these observations horizontal gradients of trace gases and aerosols around the measurement site can be determined. Such gradients can be expected, because the MAX-DOAS instrument is located close to the city of Mainz and the surrounding industrial areas. The horizontal sensitivity area of our measurements is typically of the order of 10 to 20 km and thus covers the ground pixel size of the upcommig TROPOMI instrument. In addition, also information on the cloud cover can be derived. We use the information derived from our MAX-DOAS observations to investigate the effect of horizontal gradients on the satellite validation of HCHO and NO_2. We also suggest a method for the improvement of the satellite observations in the presence of horizontal gradients.

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A Missing Term In Ground-based Satellite Validation: Spatiotemporal Mismatch Quantified

Verhoelst T., Compernolle S., Granville J., Hendrick F., Hubert D., Keppens A., Lambert JC

Royal Belgian Institute for Space Aeronomy (BIRA-IASB), Belgium

Significant effort is currently being invested in tailoring the ground-based validation infrastructure for satellite atmospheric composition data, to the stringent requirements of the upcoming Sentinel-5p/4/5 missions and in support to the Copernicus services on climate change (C3S) and atmospheric monitoring (CAMS): e.g., within EC-funded projects QA4ECV (FP7) and GAIA-CLIM (H2020) and ESA's CCI and FRM programs. This includes work on the availability and traceability of the ground-based measurements, and on the definition and implementation of the validation protocols to be integrated in an operational environment. A key concept in these endeavors is the uncertainty budget, both for a single measurement and for the comparison of two different measurements. In principle, differences between satellite and ground-based reference measurements ought to be mostly smaller than the combined measurement uncertainty, and this is the test performed in most validation studies. However, in reality the equation defining acceptable agreement should actually contain additional terms representing the impact of spatial and temporal mismatches in smoothing and sampling of the inhomogeneous and variable atmosphere. The mean and spread of the measured differences should not be interpreted as proxies of data quality without an assessment of the mismatch terms. While sophisticated co-location criteria can be adopted to minimize sampling mismatches, the relatively sparse sampling of most atmospheric composition measurement systems and the large differences in smoothing properties (e.g., between remote sensing and in situ measurements), often impose a non-negligible, irreducible lower limit on mismatch terms.

In this paper, we report on our ongoing effort to quantify those additional mismatch terms in the uncertainty budget of a data comparison. To this end, we have developed the Observing System of Systems Simulator for Multi-missiOn SynErgies OSSSMOSE, which provides an explicit description of multi-dimensional effects impacting the error budget of an atmospheric composition measurement and of data comparisons. It is shown for real world and topical case studies on columns and profiles of ozone, methane and nitrous oxide, that mismatch errors and the resulting uncertainties are most often not negligible and sometimes of complex nature, exhibiting cycles and long-term systematics. Detailed results are shown for comparisons between observations by instruments on Envisat and MetOP-A/B, and ground-based UV-Vis, ozone sonde, and FTIR measurements. We conclude with a discussion on implications for the validation of the upcoming Sentinel-5p TROPOMI data sets.

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Dealing With The Influence Of Differences In Measurement Time, Space and Addressed Air Volume Of Satellite and Reference Measurements On Validation Results: Development And Presentation Of An Internet-Based Tool

Wüst S.[1], Wendt V.[2], Bittner M.[1,3], Yee JH[4], Mlynczak M.G[5], Russell J.M III[6]

[1]DLR Oberpfaffenhofen, Germany; [2]Hochschule Ostwestfalen-Lippe, Institut für industrielle Informationstechnik, Ostwestfalen-Lippe, Germany; [3]Universität Augsburg, Institut für Physik, Augsburg, Germany; [4]Applied Physics Laboratory, The Johns Hopkins University, Laurel, Maryland; [5]NASA Langley Research Center, Hampton, USA; [6]Center for Atmospheric Sciences, Hampton, USA

In most cases, satellite validation is based on statistical comparison with reference data. However, satellite and reference measurements do neither exactly match in time and space (mistime and misdistance) nor address the same volume of air (misintegration). Therefore, the natural atmospheric variability leads to differences between both data sets. These differences must not be interpreted in terms of a satellite's malfunction.

Based on ECMWF ERA-40 temperature data, the expected differences due to mistime and misdistance are quantified depending on location, height and season. The results are compared to TIMED-SABER and radiosonde based results. Regions of lower atmospheric variability which are optimal for satellite validation are identified.

The misintegration effect is shown for stratospheric gravity waves which are extracted from TIMED-SABER and radiosonde based temperature measurements over Europe. We point out how this effect can be used for the extraction of additional information about the horizontal orientation of gravity waves.

At least, an internet based tool is presented which allows the user to retrieve information about the mean differences due to mistime and misdistance for his specific location. This tool is integrated in the Alpine Data Analysis Centre (AlpenDAC) which is currently under construction and will be available via the environmental station Schneefernerhaus (UFS, www.schneefernerhaus.de), Germany.

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Versatile QA/validation System For The Evaluation Of Atmospheric Ozone Data Retrievals, From GOME To The Copernicus Sentinels Era

Keppens A., Granville J., Hubert D., Verhoelst T., Compernolle S., Lambert JC

Royal Belgian Institute for Space Aeronomy, Belgium

Informed decisions about air quality, the stratospheric ozone layer, and climate change require global and long-term monitoring of the vertical distribution of atmospheric ozone at ever-improving resolution and accuracy. Over the past decades, global tropospheric and stratospheric ozone profile measurement capabilities from space have therefore improved substantially, including new generation hyperspectral instruments measuring limb, occultation, and backscattered (nadir) UV-visible sunlight and thermal emission. Enhanced versions of existing nadir instruments are now being developed within EU's Copernicus Earth Observation programme: the UV-VIS-NIR instrument TROPOMI on board of the upcoming polar orbiting Sentinel-5 Precursor (S-5p), and both UV-VIS and infrared instruments on board of the future geostationary Sentinel-4 and polar orbiting Sentinel-5 series, to be launched by the end of the decade.

Before being used in scientific research and operational applications, the fitness-for-purpose of ozone data products must be warily verified and documented by means of in-depth QA/validation studies of the satellite data and associated retrieval algorithms. To that purpose, an extensive satellite validation system has been developed at BIRA-IASB on the heritage of various validation activities, starting in the 1990s with SUBV/2 and the first GOME ozone profile validations, and progressively extending up to the current ESA's Multi-TASTE Envisat Phase F data evolution and Ozone_cci production of multi-mission climate data records.

Currently this validation system is being further consolidated with metrological traceability practices and with generic QA guidelines established within the EU FP7 QA4ECV project, and with error propagation and uncertainty characterisation within the EU H2020 GAIA-CLIM project. The end-to-end approach of this system combines preliminary QA/QC procedures, data content studies, information content studies, information-content based co-location procedures, and data harmonization, to conclude with the more traditional data comparisons with respect to reference measurements acquired by ground-based networks of ozonesonde and lidar stations (NDACC, SHADOZ, WMO GAW GO_3OS). The in-house observing systems simulator OSSSMOSE – providing detailed metrology of remote sensing data – is thereby used to assess the propagation of errors associated with differences in smoothing and space-time sampling between the various measurements.

In this work we describe the principles and practical implementation of this versatile QA/validation system, with atmospheric ozone as an illustrative focus. Through evaluation activities that were performed on 14 limb and occultation data products and on 4 nadir datasets (mostly within ESA's Ozone_cci project and SI2N context), we demonstrate its broad applicability to virtually all ozone (tropospheric) column and profile retrievals. We conclude with a perspective on current developments of the system addressing the specific challenges of the upcoming Sentinel-5p TROPOMI ozone data validation and our specific contribution to the S-5p Validation Team (S5PVT) and the S-5p Mission Performance Centre/Validation Data Analysis Facility (MPC/VDAF).

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Validation of aerosols, reactive gases and greenhouse gases of the Copernicus Atmosphere Monitoring Service

Eskes H.[1], Basart S.[2], Blechschmidt A.[3], Chabrillat S.[4], Clark H.[5], Cuevas E.[6], Engelen R.[7], Kapsomenakis J.[8], Katragkou E.[9], Mantzius Hansen K.[10], Niemeijer S.[11], Ramonet M.[12], Schulz M.[13], Sudarchikova N.[14], Wagner A.[14], Warneke T.[15]

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The Atmosphere Monitoring Service of the European Copernicus Programme (CAMS) is an operational service providing analyses, reanalyses and daily forecasts of aerosols, reactive gases and greenhouse gases on a global scale, and air quality forecasts and reanalyses on a regional scale. CAMS is based on the systems developed during the European MACC I-II-III (Monitoring Atmospheric Composition and Climate) research projects. In CAMS data assimilation techniques are applied to combine in-situ and remote sensing observations with global and European-scale models of atmospheric reactive gases, aerosols and greenhouse gases. The global component is based on the Integrated Forecast System of the ECMWF, and the regional component on an ensemble of 7 European air quality models. CAMS is implemented by ECMWF, and the transition from MACC to CAMS is currently being implemented (2015-2016).

CAMS has a dedicated validation activity, a partnership of 14 institutes co-ordinated by KNMI, to document the quality of the atmospheric composition products. In our contribution we discuss this validation activity, including the measurement data sets, validation requirements, the operational aspects, the upgrade procedure, the validation reports and scoring methods, and the model configurations and assimilation systems validated. Of special concern are the forecasts of high pollution concentration events (fires, dust storms, air pollution events, volcano ash and SO2). A few recent validation results will be shown.

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The Boundary Layer Air Quality Using Network Of Instruments (BAQUNIN) Super Site For Satellite Atmospheric Chemistry Products Validation

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In the context of the IDEAS+ support contract (ESA/ESRIN SPPA) and in the framework of the PANDONIA project (ESA), the Physics Department of Sapienza University of Rome and ESA/ESRIN EOP-GMQ section have set-up a joint instrumental suite for atmospheric chemistry (satellite) validation activities and Planetary Boundary Layer (PBL) studies.

Ground based active and passive remote sensing instruments are operating in synergy, in both an urban context (University of Rome) and in a rural environment (ESA/ESRIN). This instrumental set-up composes a so called "Super Site", offering quantitative and qualitative information for a wide range of atmospheric parameters for polluted areas such as the Rome city centre.

The list of the BAQUNIN Super Site instrumentation comprises: Raman and elastic LIDAR systems operating day and night (aerosols, H2O, clouds), SODAR (wind profiles in PBL), MFRSR radiometer (aerosols, O3 ,H2O), POM 01 L Prede sun-sky radiometer (aerosols, precipitable water content), Brewer spectrophotometer (O3, SO2, NO2), Pandora Spectrometers (O3, NO2, H2O, aerosols), CIMEL photometer (aerosols, H2O), YES broad-band UV radiometer, and meteorological sensors (for air temperature and relative humidity measurements).

The atmospheric data acquired during BAQUNIN lifetime will be made available to the scientific community, and will contribute to the validation of the aerosol and tropospheric trace gases products produced by the Copernicus Sentinel-5p, Sentinel 4 and Sentinel 5 and by the ESA Third Party Missions (TPM), such as the ozone Monitoring Experiment (OMI).

In this work, the BAQUNIN Super Site structure and operation strategies will be described in details.

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Validation of GOMOS High Resolution Temperature Profiles using Wavelet Analysis - Comparison with Thule Lidar Observations

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In support of the ESA EO Sensor Performance, Products and Algorithm activities (https://earth.esa.int/web/sppa/home), we propose a new approach for analysing the effects of small-scale structures on the GOMOS (Global Ozone Monitoring by Occultation of Stars) High Resolution Temperature Profiles (HRTP).

In the present work, a wavelet technique is applied to temperature and density vertical (stratospheric) profiles from Envisat GOMOS-HRTP occultations and from co-located Rayleigh Lidar measurements at Thule, Greenland (76.5°N, 68.8°W, operated by ENEA and the University of Rome "La Sapienza"). The lidar profiles are analysed in the height interval overlapping with GOMOS data (18-37 km), and the density and temperature profiles are obtained with 250 m vertical resolution. Data are relative to the winter and early spring period of years 2003-2012.

We first discuss the results of our approach based on the use of a Morlet wavelet transform, which captures the amplitude of the dominant waves. This analysis allows the subtraction of a background from the temperature profiles. The remaining perturbations are therefore assumed to be small-scale fluctuations. The Arctic winter and spring middle atmosphere is characterized by a high variability, and a specific strategy for the selection of the profiles was implemented. This strategy is based on the variability of dynamical indicators (potential vorticity, geopotential height, and temperature) in meteorological analyses at Thule and the GOMOS sounding location.

Finally, we describe the validation methodology demonstrating that the wavelet transform therefore provides new perspectives in data analysis, particularly minimising the impact of atmospheric fluctuations in the framework of validation exercises.

The results will be discussed in detail, along with case studies.

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Tools and Methods for Validation

The Sentinel 5 Precursor Mission Performance Centre

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The Sentinel 5 Precursor (S5P) is the first of the Copernicus Sentinel missions dedicated to observations of the atmospheric composition and is expected to be launched by the end of 2016. The payload of S5P is the TROPOspheric Monitoring Instrument (TROPOMI), which has been developed by The Netherlands in cooperation with ESA. In preparation for the routine operations phase, the development of the S5P Mission Performance Centre (MPC) has started in May of this year.

The MPC is the element within the Ground Segment in charge of covering the following functionalities:

- Calibration: the objective of which is to update on-board and on-ground configuration data in order to meet product quality requirements.
- Geophysical Validation: the objective of which is to assess, by independent means with respect to the methods and tools used for calibration, the quality of the generated data products. Validation functions provide feedback to calibration and data processors corrective and perfective maintenance activities.
- Quality Control: the objective of which is to routinely monitor the health of the instrument, the detection of instrument degradation and to check if the derived products meet the quality requirements along mission lifetime.
- Data processors and tools maintenance: the objective of which is to manage the updates of the processors, quality control tools, calibration tools and all auxiliary files in order to meet the product data quality requirements.
- Communication: the objective of which is to provide ESA and other stakeholders -including end users- with relevant information on the status, data usage and data quality of the Sentinel 5 Precursor mission.

In this contribution the design of the MPC is presented, with a special focus on the information that will be provided to the end users.

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Day 2 : 19 October 2016

Fiducial Reference Measurements (FRM)

Recent developments and ongoing efforts within the NDACC network towards FRM

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In several EU H2020 projects and within the Copernicus Atmospheric Monitoring Service (CAMS), efforts have been put in ameliorating the consistency, quality and characterization of the data available in the Network for the Detection of Atmospheric Composition Change (NDACC) data archive in order to improve the applicability of NDACC as a more operational reference network for both model and satellite data validation. More specifically, during the NORS project a CAMS NDACC validation server (nors-server.aeronomie.be) was created where NDACC FTIR, Microwave Radiometer (MWR), LIDAR and UVVIS DOAS measurements are used to validate the CAMS operational model osuite in a systematic and fully automated way. The EU QA4ECV project has enhanced the network consistency concerning the reported measurement uncertainties for FTIR CO and UVVIS DOAS OFFAXIS NO2 and H2CO products. Similarly, in the EU GAIA-CLIM project, uncertainty harmonization for UVVIS DOAS zenith O3 and FTIR CH4 and O3 are primary goals. These harmonized time series will be used in the S5-P Mission Performance Center for operational validation of S5-P L2 data. In this talk we present an overview of the NDACC instruments and archive and show recent results of NDACC data and their characterization used for satellite and model validation and in the CAMS NRT validation reports.

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How Homogeneous Are Ozonesonde Network Data?

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Balloon-borne ozonesondes measure the abundance of atmospheric ozone in situ from the surface up to the middle stratosphere at about 100-200m vertical resolution. Soundings started around the 1960s, first at a few sites but this gradually evolved into an operational pseudo-global network under the auspices of WMO's Global Atmospheric Watch (GAW) and its main contributors, the Network for the Detection of Atmospheric Composition Change (NDACC) and the Southern Hemisphere ADditional OZonesonde programme (SHADOZ). The measurement techniques evolved over the past decades with improvements in sensing technique, sensor types, buffer solutions, pre-flight preparation procedures and post-flight processing schemes. Laboratory and field experiments like JOSIE and BESOS showed that such changes have a non-negligible impact on the derived ozone concentration, which results in temporal inhomogeneities in the ozonesonde record of individual sounding stations. Moreover, different techniques are used at different sites, so the networks exhibit inhomogeneities in the spatial domain as well. For numerous applications it is crucial to quantify these inhomogeneities. A prime example is the role of the networks as a reference standard for the long-term, global validation of satellite ozone profile records. In addition, sonde profile data are used routinely in trend assessments of the vertical distribution of ozone.

The ozonesonde community has therefore initiated the WMO-endorsed OzoneSonde Data Quality Assessment (O3S-DQA), aimed at documenting any changes in the measurement process, at correcting the time series where feasible and at quantifying the uncertainties. We present a study of the homogeneity of the currently available ozonesonde network data from the past decade and in the 20-30 km altitude range, as a contribution to the O3S-DQA initiative. Fully validated satellite data by limb and occultation instruments (ERBS SAGE-II, Odin OSIRIS, Envisat GOMOS and MIPAS, and Aura MLS) were selected as a transfer standard to characterize the vertical structure of the bias of the ozonesonde record at each ground site. The bias curves clearly depend on the type of sensor and are consistent with findings from sonde intercomparison campaigns and laboratory studies. We probed the spatial homogeneity by comparing the site-specific bias profiles across the network. The station-to-station scatter remains below ~3 % between 22 and 27 km, and somewhat worse at lower and higher altitudes. We conclude with a status update of the O3S-DQA initiative and what can be expected for the upcoming release of a homogenized ozonesonde data set.

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An Integrated Approach for the Validation and Exploitation of Atmospheric Missions

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Current advances in atmospheric composition measurements from space require access to independent, high-quality, global atmospheric composition ground-based data for the validation of the upcoming European EO missions and payloads S3, S5p, ADM-Aeolus, EarthCARE, S4, S5, MERLIN, GOME-2c, 3MI. To address the societal benefits and scientific objectives set forth by the missions, the downstream services and GEOSS, coordinated development of synergistic ground-based measurements techniques and algorithms are needed, for example the combination of air chemistry and aerosol measurements or the combination of aerosol profile and speciation information.

DIVA project is setting up a pilot hub to collect, handle, archive, and exploit in a synergetic way observational data, as provided by the future integrated atmospheric composition ground-based network infrastructure, for the validation of ESA and Copernicus missions. In Europe, mature and coordinated networks collecting data on atmospheric composition and structure are ACTRIS (Aerosol, Clouds and Trace gases Research InfraStructure) and Pandonia. DIVA targets a better exploitation of these data in preparation of Cal/Vals for S3, S5p, ADM-Aeolus, EarthCARE. In order to do so, the pilot will integrate ground-based (lidar, sun/lunar photometer and spectrometer), satellite and model data, stand-alone and synergetic algorithms for advanced data products, using combined data from

different platforms and sensors, as well as innovative data mining and data visualization tools.

One of the main initiatives in the recent years has been focused to develop data assimilation systems based on an integrated approach including observations from space-borne, in-situ or ground-based platforms in one modeling framework. The data assimilation system development in the EU GEMS (Hollingsworth et al., 2008) and MACC (http://www.gmes-atmosphere.eu/) projects, the current pre-operational atmospheric service of the European GMES programme (http://www.gmes.info/) are very good examples for this issue.

Recently, several efforts were undertaken for applying GRASP for operational processing of observations by satellite sensors such as PARASOL/POLDER, Envisat/MERIS, Sentiel-3/OLCI, Sentinel-4, etc. However, there was no dedicated attempts for applying GRASP on operational processing ground-based observations such as those by AERONET sun-photometers or EARLINET lidars in spite of several highly promising GRASP retrieval features proposed for improving the aerosol retrieval and synergizing complimentary observation.

DIVA will provide unique opportunity for demonstrating the operational performance of GRASP, and advancing the routines to process ground-based and satellite observations in a synergetic way. The preparation of observational data to be fed into the GRASP includes: a) coordination of the LIDAR, photometer and spectrometer network operations, and centralized archiving and processing; b) development of standard procedures (best practice and schedules) for calibration and operation of the instruments; c) development of algorithms for retrieving advanced data products in a “single instrument” approach. However, DIVA goes one step further, and focus on the development of a data aggregation and processing system providing advance environment for applying cutting-edge algorithms, such as combining multiple measurement techniques, and tackling the challenges of isolated locations with slow/broken connections, providing fail-over, and adding extended data analysis and data mining functionality.

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ACTRIS Research Infrastructure For Satellite Validation Activities

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ACTRIS, the Aerosol, Clouds, and Trace gases Research Infrastructure, is the European Research Infrastructure for the observation of Aerosol, Clouds, and Trace gases. ACTRIS is composed of observing stations, exploratory platforms, instruments calibration centres, and a data centre. ACTRIS serves a vast community working on models and forecast systems by offering high quality data for atmospheric gases, clouds, and trace gases. ACTRIS capitalizes from already existing networks aiming to develop and disseminate integration tools to fully exploit the use of multiple atmospheric techniques at ground-based stations. Calibration facilities and on site checks are put in place for the most of observing components (others are in developing phase) for assuring always the best possible quality of data and for the quality assurance traceability in data provision.

ACTRIS is providing systematic and timely collection, processing and distribution of data and results for use in modeling and cal/val activities, in particular towards implementation of atmospheric and climate services. Nowadays ACTRIS and its components provides more than 15 years of aerosol, clouds and trace gases data. ACTRIS is now on the ESFRI roadmap envisioning the long-term sustenance of the observations on next 20-year plan.

Particularly interesting in view of the Sentinel and Earth Explorer (EarthCARE and ADM-Aeolus) operations are the aerosol vertical profile measurements provided by EARLINET, the European Aerosol Research LIdar NETwork. EARLINET is actually playing a leading role at global scale for developing standards for lidar measurements, analysis and data archiving. EARLINET is mainly based on Raman lidar systems, able to provide vertical profiles of aerosol extinction and backscatter coefficients without significant assumptions. Most of the stations provide these quantities at different wavelengths and in some cases this information is coupled to measurements of the linear particle depolarization ratio allowing the aerosol type identification and the particle microphysical properties retrieval. EARLINET and ESA already collaborated through different research projects as VALID-1, ACE FTS, ESA-CALIPSO project for aerosol and clouds study through CALIPSO satellite data and LIVAS for providing a global and extensive aerosol and cloud optical database. At present, EARLINET is continuing correlative measurements for CALIPSO. EARLINET will provide their top-level expertise in aerosol vertical profiling for the validation and verification of Sentinel-5 Precursor level 2 products for aerosol and clouds (in conjunction with Cloudnet). Moreover, EARLINET will also contribute to future satellite missions with lidar instrumentation on board, such as the ADM-Aeolus and EarthCARE. Various members of the EARLINET community have been involved in the ESA EarthCare Mission Advisory Group and Aeolus studies.

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Campaigns / Fiducial Reference Measurements

First Results from CINDI-2 - the Cabauw Intercomparison of Nitrogen Dioxide Measuring Instruments 2

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As a follow-up to the successful CINDI project that took plance in 2009, CINDI-2 (Cabauw Intercomparison of Nitrogen Dioxide Measuring Instruments 2) was held at the Cabauw Experimental Site for Atmospheric Research (CESAR) site in September 2016.

The activity aims at characterising the differences between the measurement approaches and systems used within the overall DOAS community and to progress towards harmonisation of settings and methods for data acquisition and retrieval from similar but not identical systems of MAXDOAS type. Such an activity is essential to enable harmonised global validation of satellite missions focusing on air quality, such as the ESA Sentinel 4, 5 and 5P, and the future TEMPO and GEMS missions planned in the US and Korea respectively.

Furthermore, CINDI-2 aims to prepare for S5P/TROPOMI validation (scheduled to launch in Fall 2016) and to initialize the suite of instruments that will be used to create the European Fiducial Reference Measurements for Ground-Based DOAS Air-Quality Observations (FRM4DOAS) network of MAX-DOAS instruments.

Along with the nitrogen dioxide measuring instruments, use is made of the suite of instrumentation operated at CESAR to characterise the state of the atmosphere. In particular, in-situ and profile observations of aerosol observations, column integrated observations and extensive cloud information along with meteorological parameters.

The major science objectives of CINDI-2 can be summarised as follows:

1: to assess the consistency of slant column measurements of several key target species (NO_2, O_3, O4 and HCHO) of relevance for the validation of S5P and the future ESA atmospheric Sentinels, through coordinated operation of a large number of DOAS and MAXDOAS instruments from all over the world.

2: to study the relationship between remote-sensing column and profile measurements of NO_2, HCHO and O_3 and reference in-situ concentration measurements of the same species.

3: to study the relationship between column and profile measurements of NO_2, HCHO and O_3 and from MAXDOAS and the state of the atmosphere, inparticular the aerosol vertical distribution.

4: to investigate the horizontal representativeness of MAXDOAS measuring systems in view of their use for the validation of satellite tropospheric measurements featuring ground pixel sizes in the range of 25-50 km^2.

In the presentation, an overview of the campaign will be given, as well as initial results.

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Intercomparison of Three Airborne Imaging DOAS Systems for Mapping of Tropospheric NO2 (AROMAPEX Campaign, Berlin, April 2016)

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The *AROMAPEX*campaign took place in Berlin in April, 2016, co-funded by the EU (EUFAR) and ESA[AM1] . Its primary objective is the intercomparison of different airborne atmospheric imagers dedicated to the mapping of the spatial distribution of tropospheric NO_2. AROMAPEX is also a preparatory step for forthcoming intercomparison/validation campaigns of satellite air quality sensors. The instruments were operated from two planes, performing synchronized flights: APEX (VITO) was operated from DLR's DO-228 D-CFFU plane at 6.1 km altitude and both AirMAP (IUP Bremen) and SWING (BIRA-IASB) were operated from the FUB Cessna EAFU at 3 km. In addition, the Cessna also carried a demonstrator of the TROPOLite instrument

(TNO). The experiment took place on one cloud-free day on April 21, 2016 from 09:34 to 12:01 LT and from 14:24 to 16:39 LT.

Both imagers have a comparable swath width of 3 km and a spatial resolution of 60 by 80 m for APEX and AirMAP (pushbroom scanning), and 300 m for SWING (whiskbroom scanning). During the overpass of the imagers, simultaneous car mobile-DOAS observations were performed with three systems covering transects from north to south and west to east. The ground-based instrumental set-up was completed by 2 DOAS instruments and a ceilometer installed at FUB. The AROMAPEX experiment builds on the experience gained during the AROMAT campaigns held in September, 2014 and August, 2015 in Romania, and the BUMBA campaign held in April, 2015 in Belgium.

We present preliminary results of an intercomparison study of the tropospheric NO_2 vertical column densities (VCDs) retrieved from the APEX, AirMAP and SWING instruments. Two large NO_2 plumes were detected by all three imaging systems, crossing the city from west to east. Retrieved NO_2 VCDs range between 1.5×10^{15} and 2.4×10^{16} molec cm^{-2}. For the sake of harmonizing the different data sets, efforts are done to agree on a common set of parameter settings and a priori input in the NO_2 retrieval approach. Despite these efforts, some discrepancies can still be observed due to a combination of (1) instrumental differences, e.g. SNR, spatial and spectral resolution; (2) algorithmic differences, e.g. DOAS fitting, RTM; (3) observation differences, e.g. overpass time and viewing geometry. The intercomparison methodology and preliminary results are discussed.

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Effect of Megacities on the Transport and Transformation of Pollutants on the Regional to Global Scales

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Since the industrial revolution, the world's population has increased from 1 billion to over 7.4 billion with an ever increasing standard of living. During this period the relative amount of the population dwelling in the cities has grown while that in rural areas has decreased and urbanization has occurred on an unprecedented scale. The first megacities, defined most frequently as conurbations having over 8-10 million people evolved at the beginning of the 19th century. The increase in population, its longevity and standard of living has been facilitated by the exploitation of fossil fuel for energy and land use change. As a consequence, the emission of primary pollutants, ozone depleting substances, long lived greenhouse gases to the atmosphere, and the generation of short lived climate pollutants in the atmosphere has increased dramatically.

The number and size of growing megacities, large conurbations or agglomerations, called for simplicity in this text major population centres (MPCs), is increasing worldwide. The impact of emissions from MPCs on air pollution and climate change was first recognized as a novel and increasing source of pollution in the past two decades. The investigation of the impact of MPCs on the atmosphere has lately received attention in the scientific community.

The synergetic use of aircraft campaigns, satellites and ground measurements and modelling provides unique scientific insight. Aircraft campaigns deliver unique high spatial resolution snapshots of key atmospheric parameters and trace constituents. Ground based measurements provide typically local information about sources and sinks of pollutants. Satellite data products provide low spatial resolution data of total tropospheric columns but they uniquely provide knowledge at the regional, hemispheric and global scales. The combined set of information synergistically constrains optimally our knowledge and tests our understanding of the outflow from MPC emissions. EMeRGe aims to investigate experimentally the transport and transformation of air plumes coming from MPCs. By comparison with model simulations our understanding of the resultant patterns of pollution resulting from European and Asian MPCs will be tested.

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Active And Passive Remote Sensing Of CH4 (And CO2) Using Airborne Aensors to Support Validation Of Satellite Based Greenhouse Gas Data Products

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In April/May 2017 the Carbon Dioxide and Methane Mission (COMET) campaign will be performed over Europe to deliver new data on large scale CH4 and CO2 distributions to assess sources and sinks of both greenhouse gases as well as to support the validation of the methane column of S5P using aircraft measurements. The German research aircraft HALO will be used as main platform, in combination with lower flying aircrafts. For CoMet the aircrafts will be equipped with a unique payload consisting of a suite of the most sophisticated instruments currently available to measure atmospheric carbon dioxide and methane. Remote sensing instruments, both active and passive, will be complemented by in-situ sensors to obtain maximum synergy. Therefore, this approach can to a significant extent make use of resources already planned to answer the long-term validation needs for Sentinel-5P and GOSAT.

Concerning active remote sensing, the Integrated Path Differential Absorption (IPDA) lidar technique using hard target reflection from the Earth's surface in the near IR (1.64 µm) has been identified in the last few years to measure the column averaged dry air mixing ratio of CH4 (and CO2) and high accuracy and low bias. As a passive remote sensing instrument, the MAMAP airborne spectrometer system capable of direct and quantitative remote column-averaged measurements of atmospheric CH4 (and CO2) complements the payload. This instrument measures reflected and scattered solar radiation in the short wave infrared (SWIR) and near-infrared (NIR) parts of the electro-magnetic spectrum. In order to validate the remote sensing instruments and provide the best possible greenhouse gas profile information, the most sophisticated in-situ instruments to measure CH4 (and CO2) currently available based on cavity-ringdown spectrometry (CRDS) will complement the core payload. Also part of this in-situ package is a flask sampler which will collect air samples for subsequent laboratory analysis and thus provide supplemental information on isotopic composition and other tracers correlated with the emission of GHGs. The above listed instruments are complemented by mini-DOAS which is capable of providing another independent method to measure the greenhouse gases and the aircraft's basis measurements system. The latter will provide precise and quality-assured data of temperature, pressure, and humidity as well as aircraft position and attitude which are required to retrieve the dry-air columnar information.

The CoMet mission will take place in the European air space. Due to HALO's long range capability, gradients can be precisely captured up to sub-continental scales. It is planned to fly over TCCON sites to validate the TCCON CH4 column against the columns retrieved from aircraft. The flight strategy also foresees flights along forecasted CH4 gradients and over methane hotspots like hard coal mining areas.

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Validation Networks / Fiducial Reference Measurements

The Pandonia network for ground validation of satellite-derived trace gas products

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The ESA sponsored Pandonia project was initiated in 2014 with the goal to create a network of ground-based remote sensing instruments, which can provide long, uninterrupted, well-maintained, homogeneously calibrated time-series of trace gas measurements for the validation of satellite-derived data. This presentation describes the capabilities of the main network instrument, the newly developed Pandora-2S spectrometer system, and gives an overview of the current status of the network. We present data and precision estimations for the operational and research data products. Operational products are total columns of O3, NO2, SO2 and HCHO based on direct sun observations and surface concentrations of NO2 and HCHO based on MAXDOAS type measurements. Research products are total columns of water vapor and effective temperatures of O3 and water vapor based on direct sun observations, total columns of O3, NO2, HCHO, and NO3 based on direct moon observations, surface concentrations of O3, SO2, and water vapor based on MAXDOAS type measurements. The Pandonia data are centrally processed in near real time and displayed on the Pandonia web-site.

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Harmonization of HCHO products from NDACC solar absorption FTIR measurements in view of global satellite and model validation

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It has been shown earlier that NDACC (Network for the Detection of Atmospheric Composition Change) solar absorption Fourier-transform infrared (FTIR) measurements can provide high quality formaldehyde (HCHO) products (Jones et al., 2009; Vigouroux et al., 2009; Viatte et al., 2014; Franco et al., 2015). These data can be considered reference measurements for validation of nadir satellite data since they represent comparable quantities, i.e. the integrated total columns. For example, FTIR HCHO total column time-series were compared to collocated GOME data over Wollongong (Jones et al., 2009) and to SCIAMACHY data over Reunion Island (Vigouroux et al., 2009). The diurnal cycle of HCHO at Reunion Island was also used for comparisons with OMI and GOME-2 data in De Smedt et al. (2015).

The provision of consistent HCHO products from all NDACC FTIR stations would allow the sampling of high, mid- and low latitudes, as well as background, sub-urban and urban polluted conditions, which is crucial for satellite validation. This requires a harmonization of the HCHO products across the network, which has not been done up to now: the above four authors used different retrieval settings for their stations, which may lead to possible biases between the derived HCHO columns. To be prepared for the upcoming S5-P validation programme, we set up a harmonization exercise including, up to now, 23 NDACC FTIR stations. This harmonization covers the retrieval settings as well as the uncertainties calculation, the objective being to provide homogenized and well-characterized FTIR HCHO products across the network.

In this presentation, the harmonized retrieval settings will be shortly introduced and the resulting HCHO FTIR products will be discussed including the characterization of their averaging kernels and uncertainty budgets. We will show the HCHO total columns obtained in the network for two selected years (2013-2014) with an emphasis on the seasonal cycle at each station and their potential for future validation work. In addition, we will present the comparisons of the FTIR HCHO total columns to the model IMAGES simulations at the various network stations.

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German contribution to S5P validation via 12 TCCON and NDACC FTIR stations

Sussmann R.[1], Blumenstock T.[2], Feist D.[3], Hase F.[2], Notholt J.[4], Palm M.[4], Rettinger M.[1], Schneider M.[2], Kumar Sha M.[5], Vigouroux C.[5], Warneke T.[4]

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The TCCON and NDACC networks consist of some 30 ground-based observation sites globally. The European FTIR community is running 16 FTIR sites in total, and the 4 German FTIR groups are responsible for 12 out of these, covering latitudes from the high Arctic to the tropics. In this way, the German TCCON and NDACC FTIR community forms an essential part of these networks, and therefore plays a central role in S5P validation.

This paper will highlight the planned German contributions to two ESA-AO projects, i.e. ID 28603 – Validation of S5P Methane and Carbon Monoxide with TCCON Data (TCCON4S5P, lead: Mahesh Kumar Sha, BIRA-IASB) and ID 28607 – 5P NItrogen Dioxide and FORmaldehyde Validation using NDACC and complementary FTIR and UV-Vis DOAS ground-based remote sensing data (NIDFORVal, lead: Corinne Vigouroux, BIRA-IASB).

Proposed tasks of the German contribution comprise, e.g., ground-based solar FTIR measurements and retrievals of CO, CH_4, and H_2CO column data, data stream automatization to achieve a 3-monthly data upload to the CALVAL database, provision of harmonized NDACC CO profiles which allow for improved NDACC and TCCON column validation, validation studies utilizing an a-posteriori correction of satellite and ground XCH_4 retrievals to a realistic common prior in order to reduce intercomparison errors, and provision of TCCON-constrained global XCH4 model fields that are globally consistent with TCCON and the prior. The latter provide an excellent reference for satellite XCH_4 validation – even far away from TCCON sites.

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Relevance of the Total Carbon Column Observing Network (TCCON) for satellite calibration and validation

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The Total Carbon Column Observing Network (TCCON) is a network of ground-based Fourier Transform Spectrometers that record solar absorption spectra at more than 20 globally distributed sites. From these measurements atmospheric columns of CO2, CH4, N2O, CO, H2O, HDO and O2 are retrieved. TCCON retrievals have been calibrated to the in situ calibration scales by a comparison to vertical resolved in situ measurements by AirCore or aircraft. These comparisons also show a very good comparability among the sites arising from the highly standardised measurements and retrieval within TCCON. TCCON represents a vital component in the global observing system for atmospheric trace gases and is an indispensable validation resource for greenhousegas satellite measurements. TCCON can detect a potential temporal drift and/or spatial bias in the satellite retrievals and in addition TCCON is able to link the satellite retrievals to the in situ calibration scales.

Clouds, Water Vapour and Aerosols

Retrieval of aerosol and surface properties from Envisat/MERIS and Sentinel-3/OLCI observations using GRASP algorithm

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We present the results of the study(*) aiming on deriving enhanced aerosol and surface properties from Envisat/MERIS and Sentinel-3/OLCI observations using recently developed GRASP algorithm (Generalized Retrieval of Aerosol and Surface Properties) algorithm described by Dubovik et al. (2014). GRASP derives extended set of atmospheric parameters using multi-pixel concept - a simultaneous fitting of a large group of pixels under additional a priori constraints limiting the time variability of surface properties and spatial variability of aerosol properties. Over land GRASP simultaneously retrieves properties of both aerosol and underlying surface even over bright surfaces. GRAPS doesn't use traditional look-up-tables and performs retrieval as search in continuous space of solution. All radiative transfer calculations are performed as part of the retrieval.

The study includes comprehensive sensitivity tests, as well as analysis of results obtained from real Envisat/MERIS and Sentinel-3/OLCI. The sensitivity tests analyze the accuracy of the retrieval of various aerosol and surface reflectance parameters at different spatial resolutions. The results of aerosol and surface properties retrieval obtained from Envisat/MERIS and Sentinel-3/OLCI at 10 km spatial resolutions discussed and compared with corresponding observations by AERONET sun-photometers, as well as, PARASOL and MODIS satellite sensors. Both the results of numerical tests, as well as results obtained from Envisat/MERIS and Sentinel-3/OLCI data illustrate demonstrate reliable retrieval of AOD (Aerosol Optical Depth) and surface BRDF.

(*) The study has been supported by ESA within framework of CAWA project.

Dubovik, O., T. Lapyonok, P. Litvinov, M. Herman, D. Fuertes, F. Ducos, A. Lopatin, A. Chaikovsky, B. Torres, Y. Derimian, X. Huang, M. Aspetsberger, and C. Federspiel "GRASP: a versatile algorithm for characterizing the atmosphere", SPIE: Newsroom, DOI:10.1117/2.1201408.005558, Published Online: September 19, 2014. http://spie.org/x109993.xml .

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Evaluation of Aerosol Properties of Satellite Retrievals

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Retrievals of aerosol properties from satellite retrievals through detected changes in solar reflection to space are difficult. Signal changes are small (compared to those by clouds), attributions require accurate knowledge about the background (e.g. surface contributions to the signal) and the interpretation of the aerosol amount also depends on the aerosol composition (aerosol size, shape and absorption). Fortunately, data of sun-/sky-photometer ground networks (e.g. AERONET, Skynet) provide accurate reference data (at more than 400 sites worldwide). And aside from AOD references via direct solar attenuation data, inversion methods applied to detected sky-radiance data offer detailed information on average microphysical aerosol properties and on average aerosol absorption. These reference data are applied to examine the quality of available aerosol products from satellite sensors. The retrieval evaluations focus retrievals developed during ESA's CCI effort for retrievals for ESA sensors and also relate the accuracy and usefulness of these aerosol products to commonly used NASA products.

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Cloud Top Pressure Retrieval from MERIS and OLCI: Global Assessment

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Cloud top pressure (CTP) retrievals from measurements within the O2 A-band of MERIS (*Medium Resolution Imaging Spectrometer* on board ENVISAT) have been analysed with respect to a decadal variability on a global scale. Clouds are subject of climate studies, because they have a large impact on the earth radiation budget and it is very likely that clouds respond on climate change. Due to the high variability of clouds no significant trend in cloud cover and cloud properties has been identified so far. Nevertheless, recent climate studies indicate that the vertical structure of clouds and zonal shifts of clouds might be caused by climate change. Since the MERIS and OLCI measurements within the O2 A-band are sensitive to the vertical cloud profile, we assessed the global MERIS CTP product during its 10 years of operation to detect regional cloud anomalies. We also compared the single MERIS CTP product with the synergistic MERIS and AATSR CTP product, which is less sensitive to the vertical cloud profile.

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Day 3 : 20 October 2016

Stratospheric and Mesospheric Composition

An Overview of Recent ACE-FTS Version 3.5 Validation Studies

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The Atmospheric Chemistry Experiment – Fourier Transform Spectrometer (ACE-FTS) is a solar occultation limb sounding instrument on the Canadian SCISAT satellite. Measurements in the infrared, between 750 and 4400 cm^{-1} with a 0.02 cm^{-1} spectral resolution, are used to derive profiles of pressure, temperature, and concentrations of over 30 atmospheric trace gases and over 20 subsidiary isotopologues. This study focuses on the most recent ACE-FTS version 3.5 validation work that compares ACE-FTS to correlative data sets from other satellite-based limb viewing instruments (GOMOS, HALOE, MAESTRO, MIPAS, MLS, OSIRIS, POAM III, SABER, SAGE III, SCIAMACHY, SMILES, SMR, and SOFIE). This includes comparisons of O_3, H_2O, and CH_4 in the lower troposphere to the upper mesosphere, stratospheric comparisons of five different NO_y species (NO, NO_2, HNO_3, N_2O_5, and $ClONO_2$) using a photochemical model to compensate for diurnal variations between instrument local times, as well as comparisons of temperature, NO, CO, and CO_2 in the stratosphere to the lower thermosphere. Where possible, we use the satellite comparison to identify and quantify any diurnal or hemispheric biases inherent in the ACE-FTS data. In addition, an error characterization procedure is being developed for the ACE-FTS version 3.5 baseline species. The current status of this work will also be presented.

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Ground-based Validation Of Altitude, Temperature, And Four Primary Trace Gas Products Of The Operational MIPAS Level-2 Processors

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Infrared observations at Earth's limb by the MIPAS instrument on Envisat have resulted in a unique data record to study physical and chemistry processes in the atmosphere. Profile retrievals are made of pressure, temperature and 15 trace gas species. The operational processor chain (Level-1b: IPF 7.11 + Level-2: ML2PP 7.03) recently completed the reprocessing of the entire MIPAS mission. This new version includes several significant improvements; we name just two: The non-linearity correction scheme in the Level-1 processor is now based on actual MIPAS observations, and the microwindow selection for Level-2 retrievals was reoptimized to enlarge their information content. Such changes potentially have an important impact on the quality of the Level-2 data products: their bias, precision or long-term stability, and their dependence on geophysical parameters.

Here, we present the first consolidated results of the validation of five primary ML2PP 7.03 Level-2 data products (temperature, O_3, HNO_3, CH_4 and N_2O) and the altitude scale. Our analyses are based on comparisons to co-located ground-based observations by ozonesonde, stratospheric temperature and ozone lidar and FTIR instruments operating within the Network for the Detection of Atmospheric Composition Change (NDACC), WMO's Global Atmospheric Watch (GAW) and the Southern Hemisphere ADditional OZonesonde programme (SHADOZ). These networks provide well-characterized data records of different atmospheric constituents with appropriate accuracy and spatio-temporal sampling and resolution properties to act as a transfer standard for the validation of satellite data products. The considerable correlative statistics allowed an in-depth study of the structure of bias and short-term variability in the spatial (vertical, latitudinal) and temporal domain at various scales. In addition, they permitted us to characterize the quality of the different MIPAS spectral resolution modes and the different vertical sampling modes. For temperature, we show non-negligible changes in the long-term stability of ML2PP 7.03 relative to earlier MIPAS data versions (ML2PP 6.0 and IPF 5.05). We discuss whether this change also affects the stability of other trace gas products (especially ozone). Another important topic is the consistency between MIPAS data from 2002-2004 and from 2005-2012, for all species. We conclude by showing that the ML2PP 7.03 altitude scale is superior to that reported in previous data releases.

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Long-term Validation Of MIPAS ESA Operational Products Using MIPAS-B Measurements

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The re-processing of the full MIPAS mission Level 2 data from 2002 to 2012 was recently performed with the ESA processor ML2PP version 7. The current MIPAS data set not only includes retrieval results of pressure-temperature and the standard species H_2O, O_3, HNO_3, N_2O, CH_4, and NO_2, but also vertical profiles of volume mixing ratios of the more difficult to retrieve molecules $ClONO_2$, N_2O_5, CFC-11, CFC-12 (all already included in the version 6 processing), HCFC-22, CCl_4, CF_4, HCN, and COF_2.

Several flights with MIPAS-B, the balloon-version of MIPAS, have been carried out during the 10 years operational phase of ENVISAT at different latitudes and seasons, including both operational periods where MIPAS measured with full spectral resolution (FR mode) and with optimized spectral resolution (OR mode). All MIPAS operational products are compared to results inferred from dedicated validation limb sequences of MIPAS-B. To enhance the statistics of vertical profile comparisons, a trajectory match method has been applied to search for MIPAS coincidences along 2-day forward/backward trajectories running from the MIPAS-B measurement geolocations.

This paper will give an overview of the comprehensive validation activities and results on the basis of the ESA operational version 7 data comprising the MIPAS FR and OR observation periods. This includes an assessment of the data agreement of both sensors taking into account combined errors of the instruments.

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The Polar Stratosphere in a Changing Climate (POLSTRACC): A HALO mission to explore the Arctic lowermost stratosphere in the extraordinary winter 2015/16

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The aircraft campaign POLSTRACC studied the bottom of the polar vortex and the high-latitude UTLS (upper troposphere / lower stratosphere) along with their impact on lower latitudes throughout the entire winter/spring cycle during the extraordinarily cold Arctic winter 2015/16. The overarching mission goal has been to provide new scientific knowledge on the Arctic lowermost stratosphere and upper troposphere under the present load of halogens and state of climate variables several years after the last intensive Arctic campaigns.

POLSTRACC employed the German High Altitude and LOng range research aircraft (HALO) offering a payload capacity of more than 3t, a range of almost 10.000 km and a maximum altitude of about 15 km. The payload comprised an innovative combination of remote sensing techniques providing 2- and 3-D distributions of a large number of substances above and underneath the flight level and precise in-situ instruments measuring T, O_3, H_2O, tracers of different lifetimes and chemically active species at the aircraft level with high time-resolution. Drop sondes added information about the vertical structure of the tropopause region. The POLSTRACC consortium includes national (KIT, Forschungszentrum Jülich, DLR, PTB and the Universities of Frankfurt, Heidelberg, Mainz and Wuppertal) and international partners (e.g. NASA).

The field campaign was divided into three phases for addressing (i) the early polar winter vortex and its wide-scale vicinity in December 2015, (ii) the evolution of the mid-winter polar vortex from January to early March 2016, and (iii) the late winter dissipating vortex and its impact on the lower latitude UTLS in March 2016. The airborne field observations were complemented by ground-based activities (e.g. lidars, radars and radio soundings) and satellite observations (e.g. CALIPSO, MLS and ACE-FTS). Mission and flight planning was supported by a variety of model tools and satellite observations.

First results for the winter 2015/16 from the POLSTRACC observations show extended polar stratospheric clouds reaching sometimes even down to HALO flight levels at 13-14 km during almost all HALO sorties in January and February. Particulate NO_y and redistribution of gas-phase NO_y was observed down to HALO flight levels. Significant chlorine activation in the lowermost stratosphere was deduced from observations of HCl and $ClONO_2$, along with halogen source gas observations which indicated the presence of high levels of inorganic chlorine of more than 1 ppb in the lowermost stratosphere. Aged vortex air masses characterized by high amounts of inorganic chlorine and indications of ozone loss down to potential temperature levels of 380-400K were probed before the major warming starting around mid-March.

The presentation is intended to give a brief overview of the mission along with first results and to put this into perspective with past, present and future satellite missions

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Analysis of Seasonal Differences in the Recent Satellite Ozone Records in the Upper Atmosphere

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The upper stratospheric and mesospheric ozone is expected to increase as a result of declining level of human-produced chlorine and bromine and rising greenhouse gas concentrations in the lower atmosphere. However, a detection of the ozone recovery requires the analysis of combined record from multiple instruments and is complicated by measurement uncertainties and inter-instrumental biases. One source of uncertainties, that we will tackle in the study, manifests from the seasonally varying biases which have been observed between different satellite observations in the upper stratosphere and mesosphere. Often these seasonal biases are ignored. In this study we examine recent satellite ozone observations - since 2005 up to date - from a number of satellite sensors (Aura MLS, SBUV, OMPS LP and MIPAS). We will focus our analysis on contrasting ozone seasonal cycles derived from individual instruments in the upper stratosphere and mesosphere. The satellite sensors use different techniques to retrieve ozone vertical profiles. SBUV and OMPS LP operates in UV spectral range and measures solar scattered radiances. While MLS and MIPAS derived ozone profiles by measuring emissions in microwave and infrared spectrum. The sensors vertical resolutions also vary from ~6 km for SBUV around 3 hPa to ~2 km for OMPS LP. In addition these named sensors perform measurements at different local solar times. All these factors can contribute to the observed seasonal differences. To sort out different sources of uncertainties in the seasonal biases we will analyze the relationship between temperature and ozone variability at various time scales from daily to seasonal. For these purposes we will consider temperature measurements from MIPAS and MLS and model simulations from the Global Chemistry-Transport model. Model simulations will help to establish a benchmark for ozone-temperature relationship at different time scales and conditions (seasons, local time) and help to isolate different sources of uncertainties. Finally, we will estimate how sensitive ozone trend estimates to the seasonal biases by testing different approaches to handle seasonal differences in the SBUV Merged Ozone Dataset.

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Particle size distribution of the stratospheric aerosol from SCIAMACHY: sensitivity studies and first results

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Stratospheric aerosols play important role not only in the radiative budget of the Earth by changing the radiative transfer through the atmosphere, but also they affect crucially the stratospheric chemical processes which lead to the ozone layer depletion. It is well known, that tropical upwelling of SO_2, COS and sulfate particles from the troposhere determine the background stratospheric aerosol composition, which is occasionally perturbed by vast SO_2 emissions, caused by strong volcanic eruptions. The most common characteristics of the stratospheric aerosols are the particle size distribution parameters (mode radius and distribution width) and particles number density. The information on these parameters is important among other for various modeling activities related to stratospheric processes including stratospheric models validation. One of the most important sources of the global information on spatial and vertical distribution of the stratospheric aerosol characteristics are the measurements of the transmitted or scattered solar light in visible and near infrared spectral region performed by satellite instruments in occultation and limb viewing geometries. We used limb measurements from space borne spectrometer SCIAMACHY, operated on board the ENVISAT satellite from August 2002 to April 2012, to derive stratospheric aerosol characteristics. We present a retrieval method, sensitivity studies and first results on the aerosol particle size distribution parameter retrieval from SCIAMACHY limb measurements. The presented data set is unique as there is no other similar instrument measuring scattered solar light which is capable to provide both parameters of the aerosol particle size distribution. We have analyzed the time series of the mode radius and distribution width in the unperturbed background period of time as well as in the period after the volcanic eruptions. These analysis showed an increase of mode radius and a widening of whole particle size distribution function after the volcanic eruption. Also, we observed a temporal shift in the increased values of the stratospheric aerosol characteristics with the height, or the so-called tape recorder. The initial validation of the SCIAMACHY limb aerosol retrieval is done using data from the occultation space borne instrument SAGE II.

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Results from the second SPARC water vapour assessment (WAVAS II) on satellite data quality

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Water vapour is one of the most important trace constituents of the Earth's atmosphere and plays a fundamental role in the climate system. The second SPARC water vapour assessment on satellite quality focused on the observations that have become available since the start of the new millennium. Overall more than 40 data sets from 15 individual instruments have been considered. They were compared in comprehensive way ranging from profile-to-profile comparisons to comparisons of climatologies and time series. Besides that secondary parameters as tropopause ascent rates or amplitudes of various variability patterns were compared. Here a selection of results will be presented and the quality of the current set of data will be discussed.

Tropospheric Composition / Air Quality

Potential For Observing Ozone Pollution By A Three-band Synergism UV+VIS+TIR Of Satellite Measurements From IASI And GOME-2

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Tropospheric ozone is currently one of the air pollutants posing greatest threats to human health and ecosystems (e.g. EEA, 2011). Exposure to ground-level ozone may irritate the respiratory system, aggravate asthma and other lung diseases and even lead to premature mortality. Monitoring tropospheric ozone at regional and global scales is a crucial societal issue, and only spaceborne remote sensing offer the potential to do it.

At the LISA laboratory, a first multispectral method has been developed in order to observe lowermost tropospheric ozone by synergism of thermal infrared (TIR) observations by IASI and ultraviolet (UV) measurements from GOME-2 (Global Ozone Monitoring Experiment-2). This new approach has been used with real observations and it allowed observing ozone pollution down to 2 km of altitude (Cuesta et al., 2013). A further step to enhance sensitivity to near-surface ozone may be probably achieved by using as well the Chappuis band in the visible (VIS) spectrum (Chance et al., 1997, and Sellitto et al., 2012). However, difficulties to exploit this visible band are related to the relatively small absorption by ozone in this band and the uncertainties associated to the spurious spectral signatures of water vapour, nitrogen dioxide, aerosols, surface albedo, etc.

The objective of this work is to evaluate the potential of a new ozone retrieval based on the synergism of the 3 spectral bands: UV+VIS+TIR. In order to do so, two sensitivity studies are performed: i) an estimation of sensitivity and retrieval errors (including systematic and cross-state errors) based on the optimal estimation theory (Rodgers, 2000) and ii) the implementation of a so-called OSSE (Observing System Simulation Experiment) by applying the 3-band multispectral retrieval on simulated satellite observations of IASI and GOME-2, for realistic atmospheric scenes of ozone outbreaks over Europe (provided by the MOCAGE chemistry-transport model). The performance of the multispectral approaches using three bands (UV + VIS + TIR) is compared to that of two bands (UV + VIS and TIR + VIS) and with single-band approaches. The implementation of this new UV+VIS+TIR synergism allows to define two key aspects of the method: i) spectral micro-windows selected by maximising the ozone information content, thus minimising the spurious effects of uncertain variables (water vapour, NO2, etc) and ii) the set variables (in addition to the ozone profile) that should be simultaneously adjusted in order to retrieve ozone with acceptable errors.

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Validation of OMI and TROPOMI SO2 VCD measurements using emission inventories

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Sulfur dioxide (SO_2) plays an important role in Earth's atmospheric chemistry and climate. It is also one of the major pollutants that can be measured from space. However, validation of satellite SO_2 measurements is a challenge: in most countries, SO_2 levels measurable by satellites can only be seen in close proximity to emission sources and the measurement noise is high. Moreover, comparisons of coincident satellite and ground-based vertical column density (VCD) measurements are not very informative for a localized source and their interpretation requires a proper accounting of satellite viewing geometry, SO_2 vertical distribution, wind direction, satellite pixel size, and measurement uncertainties even for cloud-free conditions. Our comparison of Pandora sunphotometer SO_2VCDs and Aura OMI VCDs over Fort McKay, Alberta, Canada, over a two-year period demonstrated a low correlation (R= 0.2), although the site was located 20 km from two relatively large sources with emitting about 50 kt yr^{-1} total. This is not surprising given the large pixel size, high uncertainties of OMI measurements relative to the range of SO_2 variations, and heterogeneity of the SO_2 spatial distribution at this location.

As another approach, available emission data from emissions inventories can be used for satellite SO_2 VCD validation. Such inventories in U.S. and Canada are based on accurate direct stack measurements. These emissions can be directly compared with emission estimates from satellite data. Alternatively, SO_2 VCD calculated from reported emissions can be compared to satellite SO_2 measurements using a new method, described here, linking these two quantities. The method is based on fitting satellite SO_2 vertical column density (VCD) to a set of functions of OMI pixel coordinates and wind speeds where each function represents a plume from a single source. The method is also used to calculate seasonal and annual mean VCD distributions from the emissions inventories that are compared with OMI measurements over the eastern US and southern Canada. The approach can be further used for Sentinel 5P TROPOMI SO_2 VCD validation.

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Comparison of OMI NO2 Observations And Their Seasonal And Weekly Cycles With Ground-Based Measurements In Helsinki: Results From ESA Living Planet Fellowship ILMA

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Finnish Meteorological Institute, Finland

We present the comparison of satellite-based OMI (Ozone Monitoring Instrument) NO2 products with ground-based observations in Helsinki. OMI NO2 total columns, available from standard product (SP) and DOMINO algorithm, are compared with the measurements performed by the Pandora spectrometer in Helsinki in 2012. The relative difference between Pandora #21 and OMI SP retrievals is 4 % and −6 % for clear sky and all sky conditions, respectively. DOMINO NO2 retrievals showed slightly lower total columns with median differences about −5 % and −14 % for clear sky and all sky conditions, respectively. Large differences often correspond to cloudy autumn-winter days with solar zenith angles above 65°. Nevertheless, the differences remain within the retrieval uncertainties. Furthermore, the weekly and seasonal cycles from OMI, Pandora and NO2 surface concentrations are compared. Both satellite- and ground-based data show a similar weekly cycle, with lower NO2 levels during the weekend compared to the weekdays as result of reduced emissions from traffic and industrial activities. Also the seasonal cycle shows a similar behaviour, even though the results are affected by the fact that most of the data are available during spring-summer because of cloud cover in other seasons.

This is one of few works in which OMI NO2 retrievals are evaluated in a urban site at high latitudes (60° N). Despite the city of Helsinki having relatively small pollution sources, OMI retrievals have proved to be able to describe air quality features and variability similar to surface observations. These results add confidence in using satellite-based atmospheric observations for air quality monitoring also at high latitudes. Future missions such as TROPOMI on Sentinel 5 Precursor will provide improved information on the atmospheric composition, increasing the possible exploitation and applications of such data at high latitudes. This work is supported by ILMA-project (under ESA Living Planet fellowship programme), which aims at evaluating satelite-based air quality observations and increasing their scientific exploitation at high latitudes.

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Validation and Verification of S5P NO2 Using Ground-based, Airborne and Satellite Data

Richter A.[1], Wittrock F.[1], Peters E.[1], Schönhardt A.[1], Meier AC.[1], Bovensmann H[1], Burrows JP.[1], Vrekoussis M.[1], Schreier SF.[2], Gratsea M.[3], Gerasopoulos E.[3]

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The TROPOMI instrument, to be launched on Sentinel-5P in fall 2016 will continue the time series of GOME / SCIAMACHY / OMI / GOME-2 nadir UV/vis observations. It will provide both tropospheric and stratospheric NO_2 columns with much improved spatial resolution compared to current sensors.

Validation of S5P NO_2 measurements is essential to assess and characterise data quality and its change over the instrument lifetime. In addition to the usual requirements for satellite NO_2 validation, the high spatial resolution of the observations adds additional challenges as it requires high resolution a priori data in the S5P tropospheric NO_2 retrieval.

In this project, validation of S5P NO_2 data using different approaches is proposed to address the different aspects of validation:

1) Validation with MAX-DOAS measurements of the BREDOM network. This network includes measurement stations in Ny-Alesund, Bremen, Athens, Vienna (from 2017) and Nairobi (currently not operational). Ground-based observations provide long-term high quality data of tropospheric and stratospheric columns as well as profile information close to the ground. In some stations also the horizontal inhomogeneity is measured. These data provide seasonal and long-term validation at a small number of locations.

2) Validation with measurements from the airborne AirMap DOAS instrument. This instrument can be operated on campaign basis and provides maps of NO_2distributions of cities or other targets with spatial resolution of better than 100 x 100 m^2. This data can be used to validate individual S5P observations and to

investigate sub-pixel variability and its impact on a priori assumptions in the S5P retrieval.

3) Verification of global NO_2 distributions using satellite observations. By comparison with IUP NO_2 retrievals on data from other satellite such as OMI and GOME-2, global comparison can be performed covering all relevant geometries, seasons and latitudes. While this is not a strict validation as many uncertainties are similar between instruments, the results can provide valuable insight into the quality of the S5P NO_2 product

In this presentation, the planned validation measurements and approaches will be described and examples of validation results on data from existing sensors will be shown.

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Validation of CO vertical columns from SCIAMACHY and TROPOMI shortwave infrared measurements

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Netherlands Institute for Space Research (SRON)

The Tropospheric Monitoring Instrument (TROPOMI), to be launched at the end of 2016 onboard of ESA's Sentinel-5 Precursor (S-5P) mission, will pursue the 10-year measurement record of ESA's Scanning Imaging Absorption Spectrometer for Atmospheric Chartography (SCIAMACHY) instrument in the 2.3 µm spectral range but with a superior signal-to-noise performance and a higher spatial resolution of 7x7 km2. The S-5P operational data processing employs the SICOR algorithm, which will infer CO total columns from 2.3 µm Earth radiance measurements for clear sky and cloudy sky conditions. In this study, we will demonstrate the validation strategy for this operational S-5P data product applying on the one hand the SICOR algorithm to the 10-year SCIAMACHY data set and on the other hand using CO ground-based Fourier Transform Spectrometer measurements of the TCCON and NDACC network. Here, validating the CO product from cloudy ocean observations is challenging because of the lack of sensitivity to the atmospheric CO concentration below the cloud. However, comparison with CO measurements at remote TCCON and NDACC sites shows that including retrievals for cloudy land and ocean scenes to the SCIAMACHY CO data set improves the data coverage with consistent and valuable data quality. It allows us to estimate the seasonality of CO from SCIAMACHY measurements even over the ocean and for low albedo scenes over land. To validate our CO product for urban polluted areas, information on the vertical distribution of CO is required. To this end, we use MOZAIC/IAGOS profile measurement close to the airports Teheran, Beijing, and Windhoek as reference measurements and show that applying the column averaging kernel to the data confirms the validity of the data product even in case of high and optically thick clouds.

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Poster Session

Calibration of Measured Radiences

In-Flight calibration of SCIAMACHY Polarization Sensitivities

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In order to correct the radiometric response of SCIAMACHY for polarization effects, the linear polarization has to determined accurately. However, most notably the UV-VIS polarization measured in the limb mode deviates significantly from expectations. This is still the case, even when the reanalyzed on-ground calibration data [1] and a sophisticated model for the degradation of the scanner unit are used. In order to investigate this feature, the polarization response of the Polarization Measurement Devices (PMDs) has been determined for both limb and nadir modes from a statistical analysis of the corresponding in-flight data, using a combination of radiative transfer model (RTM) and extrapolation to known limits. The analysis method, the derived polarization sensitivities and their uncertainties are presented. In the UV-VIS region, the accuracy is high enough to reveal an on-ground to in-flight phase shift introduced by stress birefringence within the optical bench of the instrument. The observed time dependence and its possible interpretations will also be discussed.

[1] Krijger, J. M., Snel, R., van Harten, G., Rietjens, J. H. H., and Aben, I.: Mirror contamination in space I: mirror modelling, Atmos. Meas. Tech., 7, 3387-3398, doi:10.5194/amt-7-3387-2014, 2014.

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SCIAMACHY: The new Level 0-1 Processor

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SCIAMACHY (SCanning Imaging Absorption spectroMeter for Atmospheric CHartographY) is a scanning nadir and limb spectrometer covering the wavelength range from 212 nm to 2386 nm in 8 channels. It is a joint project of Germany, the Netherlands and Belgium and was launched in February 2002 on the ENVISAT platform. After the platform failure in April 2012, SCIAMACHY is now in the postprocessing phase F. SCIAMACHYs originally specified in-orbit lifetime was double the planned lifetime. SCIAMACHY was designed to measure column densities and vertical profiles of trace gas species in the mesosphere, in the stratosphere and in the troposphere (Bovensmann et al., 1999). It can detect a large amount of atmospheric gases (e.g. O3 , H2CO, CHOCHO, SO2 , BrO, OClO, NO2 , H2O, CO, CH4 , among others) and can provide information about aerosols and clouds.

The operational processing of SCIAMACHY is split into Level 0-1 processing (essentially providing calibrated radiances) and Level 1-2 processing providing geophysical products.

The operational Level 0-1 processor has been completely re-coded and embedded in a newly developed framework that speeds up processing considerably. In the frame of the SCIAMACHY Quality Working Group activities, ESA is continuing the improvement of the archived data sets. Currently Version 9 of the Level 0-1 processor is being implemented. It will include

- An updated degradation correction
- Several improvements in the SWIR spectral range like a better dark correction, an improved dead & bad pixel characterisation and an improved spectral calibration
- Improvements to the polarisation correction algorithm
- Improvements to the geolocation by a better pointing characterisation

Additionally a new format for the Level 1b and Level 1c will be implemented. The version 9 products will be available in netCDF version 4 that is aligned with the formats of the GOME -1 and Sentinel missions. We will present the first results of the new Level 0-1 processing in this paper.

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SCIAMACHY Lunar Observations for Intercalibration

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The moon: Stable and always present, with highly predictable variations due to lunar phase, liberation and polarisation. This makes the moon a very good satellite (inter)calibration source.
With this goal in mind we will provide absolute radiometric calibrated hyperspectral lunar observations by SCIAMACHY (on board ENVISAT), including the new degradation correction derived from contaminated mirror analysis, that will allow accounting for the differences in spectral response between instruments to be inter-calibrated. Comparision with (lower resolution) lunar spectra and Apollo lunar soil spectra will provide independent verification of the employed SCIAMACHY calibrations.

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Impact of the Discontinuities of Radiometric Gain Calibration on the MIPAS Retrieved Species in Band-A and Band-B

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This work is meant to analyze a list of periods along the ENVISAT-MIPAS mission (2002-2012) affected by discontinuities of HNO_3, CH_4 and N_2O retrievals contained in the ESA Level 2 v7.03 dataset. As shown in the study, the discontinuities are related to radiometric gain variations in band-A and band-B.

During MIPAS operational phase, a number of blackbody and cold space measurements were acquired daily, and used during on-ground processing to calibrate the instrument responsivity and to correct for the instrument self-emission. Although the radiometric gain calibrations were performed c.a. once per day, the gain calibration function has been typically considered stable and updated once per week in the processing from Level 0 to Level 1b. Sometimes big variations of the gain function between two consecutive calibration measurements have been detected, and causing jumps > c.a. 3% of the radiance and therefore discontinuities of the amount of retrieved species.

The gain measurements in band A and band B have been extracted from the Level 1b v7.11 dataset; a coverage analysis (of Level 0 and gain files) along the mission has been performed in order to obtain information on both gain validity time periods and time windows where gains are not acquired.

Each two consecutive gain functions of band A and band B are compared and the percentage variation calculated. Big gain variations (>2%) are detected typically in correspondence of instrument interruptions, but also for periods where no operations' interruptions took place: this analysis provides a list of periods where retrievals can potentially be affected. The radiances corresponding to these periods are also extracted from Level 1b v7.11 products and the discontinuities analyzed. Finally the profiles relative to species retrieved in band A (HNO_3) and band B (CH_4 and N_2O) are extracted from the ESA Level 2 v7.03 dataset and statistically analyzed by the analysis of variance method (ANOVA) in order to understand the impact of the gain variation. Furthermore, the mean daily column density is estimated and bias analyzed in order to investigate potential drifts/trends on the mean values.

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Evaluation of OMI Surface UV Irradiances against NILU-UV Measurements: in preparation for TROPOMI/S5P.

Zempila M.M.[1,2], Koukouli M.E.[2], Bais A.[2], Arola A.[3], Fountoulakis I.[2], Kouremeti N.[4], Kazadzis S.[4], Balis D.[2]
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In this study we evaluate the surface UV irradiances derived from the Ozone Monitoring Instrument (OMI) onboard the AURA satellite with a Norwegian Institute for Air Research UV multi-filter actinometer (NILU-UV) situated in the Laboratory of Atmospheric Physics (LAP) in the Aristotle University of Thessaloniki (40.69°N, 22.96°E). The NILU-UV performs measurements in 5 UV spectral regions with full width at half maximum (FWHM) of ~10 nm and a time resolution of 1 minute. Although the NILU-UV channels' highest sensitivity is obtained at 302, 312, 320, 338 and 376 nm, the measured irradiances are wavelength shifted with the use of a Brewer UV double monochromator spectroradiometer, in order to confront with the UV irradiances measured by the OMI. Then, the NILU-UV QA/QC data were compared with the OMI/Aura overpass and local noon irradiances at 305, 310, 324 and 380 nm for a 10 year period (2005-2014) over Thessaloniki.

For the comparisons a set of restrictions was applied and tested. The cloudiness conditions were investigated along with the averaging time period applied to the ground-based data (10 minute and 1 hour mean values were examined). The influence of a strict and a less strict radius (10 and 25km) was also studied while effects of restrictions on OMI flagging were analyzed (according to the OMUVB Levels Format554 Specification Document). Overall, our findings, using the NILU-UV actinometer in Thessaloniki, Greece, are well in-line with other validation studies of the OMI/Aura UVB irradiances product. Similar methods and techniques can provide useful information and pointers for the further improvement of the nominal satellite retrieval algorithm.

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Evaluation of Satellite Photobiological Effective Dose Products with a ground-based NILU-UV Radiometer: in preparation for TROPOMI/S5P.

Zempila M.M[1,2], Taylor M.[2], Koukouli M.E[2], Fountoulakis I.[2], Bais A.[2], Arola A.[3], van Geffen J.[4], van Weele M.[4], van der A R.[4], Meleti C.[2], Balis D.[2], Kouremeti N.[5], Kazadzis S.[5]

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This study aims to assess and investigate the accuracy of ground-based and satellite-based models of three photobiological effective dose products: the erythemal UV, Vitamin-D and DNA damage. A suite of UV measuring instruments are operating at the Laboratory of Atmospheric Physics of the Aristotle University of Thessaloniki (LAP/AUTh) in Greece (40.63oE, 22.96oN). In particular, ground data provided by a Brewer UV double monochromator spectroradiometer (used as a reference for calibration), a NILU-UV multi-filter radiometer, and a YES UVB-1 pyranometer are used to produce the surface time series of photobiological effective dose products.

Novel methodologies are applied to the multi-filter data as well to the broadband derived measurements in order to obtain the three doses. In particular, a neural network is trained to simulate the Brewer-based photobiological effective dose products based on the NILU-UV solar measurements. The model is subjected to sensitivity analysis, is validated, and used to generate long coincident time series originated from the NILU-UV 5 irradiance measurements (nominal wavelengths: 305, 312, 320, 340 and 380 nm). For the UVB-1 derived measurements an empirical relationship was developed with appropriate correction factors applied in order to obtained the desired doses. Both retrieved datasets provide a time analysis of 1-minute estimations.

Then, satellite data are used to provide a comparison for the surface-based estimates. Specific, OMI/Aura surface UV irradiance data from 2004 to 2014 is used which includes the erythemally-weighted dose and erythemal dose rate at the overpass time and also at local solar noon. The same daily integrated sub-products provided by the SCIAMACHY/Envisat and GOME2/Metop-A joint UV product, are used for this purpose. Erythemal, Vitamin D and DNA damage daily doses are provide by the joint UV product also, and are compared with the daily doses derived from the NILU-UN and UVB-1 instruments. Time series analysis and correlation statistics of the comparisons provide a basis for a thorough assessment of model limitations as well as atmospheric, algorithm-related and/or technical factors responsible for sources of discrepancy among the retrievals.

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Evaluation of Satellite Total Ozone Observations with a ground-based NILU-UV Radiometer: in preparation for TROPOMI/S5P.

Zempila M.M.[1,2], Taylor M.[2], Koukouli M.E.[2], Lerot C.[3], Bais A.[2], Fragkos K.[2], Fountoulakis I.[2], Balis D.[2], van Roozendael M.[3], Kouremeti N.[4], Kazadzis S.[4]

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A novel approach to retrieve total ozone at high temporal frequency from surface irradiance measurements performed with a NILU-UV multi-filter radiometer is presented. A neural network model utilizes time series of 1-minute NILU-UV irradiances at central wavelengths of 302, 312, 320, 340 and 376 nm along with collocated solar zenith angles calculated at Thessaloniki, Greece (40.63E, 22.96N) and the day of the year and its sinusoidal components as temporal variables. The target value (outputs) of the model during its training are a decade of coincident Brewer total ozone measurements (TOCs). The agreement between the NN estimates and Brewer derived TOC for the training data is denoted by the high correlation statistics (R2 = 0.94, RMSE = 8.21 D.U. and bias = -0.15 D.U.).

After the training session, the model is fed with unseen real (noisy) inputs to estimate TOCs for the decade 2005-2014. Satellite total ozone from the GOME/ERS-2, SCIAMACHY/Envisat, OMI/Aura, and GOME2/MetopA GODFIT_v3 Ozone-CCI ESA algorithm are used to provide a comparison at each overpass time for TOC estimates produced by the neural network model from NILU-UV irradiances. The NILU TOC estimates agree with the satellite TOC retrievals with coefficients of determination found to be in the range $0.88 \leq R^2 \leq 0.90$ for all sky and $0.95 \leq R^2 \leq 0.96$ for clear sky conditions. For the cloud free circumstances, the mean fractional differences (satellite-ground/ground TOCs %) were found equal to -0.67% ± 2.15%, -1.44% ± 2.25%, -2.09% ± 2.06% and -0.85% ± 2.19% for GOME, SCIAMACHY, OMI and GOME2 respectively. Furthermore, the high Pearson correlation coefficients ($0.94 < R < 0.98$) is evidence of the linearity between the satellite algorithm retrievals of TOC and ground-based estimates, while biases of less than 5 D.U. prove that systematic errors are low. This methodology provides a new approach to the ongoing assessment of the quality and consistency of ground and space-based measurements of total ozone columns and can be used as a benchmark for the new satellite instrument generation.

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Methods and Instruments for Validation

Ground-based Assessment Of The SCIAMACHY Operational L2 SGP V6.01 Full Mission Dataset And Its Evolution With Respect To Preceding Processor Versions

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ESA's Envisat satellite has provided an important contribution to the global atmospheric composition monitoring from 2002 to 2012. The SCIAMACHY (SCanning Imaging Absorption spectroMeter for Atmospheric CHartographY) instrument is one of the three on-board passive remote sensing spectrometers that enabled measuring the abundance of a variety of trace gases and parameters, including reactive and greenhouse gases. Although Envisat currently resides in its post-flight Phase F, the development of the algorithms used for the retrieval of these atmospheric abundances is still ongoing. This continuous evolution of data products requires appropriate independent data quality assessment and validation. In particular, the uncertainties and geophysical consistency of the SCIAMACHY data must be assessed for the wider range of atmospheric states and over the relevant spatial domain, vertical range, and mission lifetime. Every upgrade of the data products and associated data processors must be verified through delta-validation studies of the expected improvement. The outcome of validation studies of successive data products furthermore provides highly valuable feedback to the respective data retrieval teams.

This work reports on the quality assessment of the continuous evolution of operational SCIAMACHY L2 data products that include the nadir-observed vertical column of O_3, NO_2, BrO, CO and CH_4, and the limb profile measurement of O_3 and BrO. Validation analyses are based on comparisons to co-located ground-based observations by ozonesonde, lidar, DOAS spectrometers, and FTIR instruments operating within the Network for the Detection of Atmospheric Composition Change (NDACC), WMO's Global Atmospheric Watch (GAW) and the Southern Hemisphere ADditional OZonesonde programme (SHADOZ). These networks provide well-characterized data records of different atmospheric constituents with appropriate accuracy and spatio-temporal sampling and resolution properties. The studies conclude with (wherever possible) altitude and latitude-resolved estimates of bias, spread, long-term stability, and their dependence on geophysical parameters.

The focus of this validation exercise is on the latest SGP V6.01 processor full mission data and its improvement with respect to previous operational products. It is to be verified whether the quality of the V6 data is similar to that of the previous SGP V5.02 processor for all studied products, as suggested by a delta-validation study on a diagnostic dataset selection of 5000 orbits. This would be in line with the expectations from the code changes made in the new Level-1 and Level-2 processors. The delta-validation however also pointed at the appearance, at middle latitudes in the northern hemisphere, of a negative drift of about 1.5 % over the mission lifetime in the updated ozone column data relative to correlative observations, most likely related to the changes in the IPF 8.01 Level-1 processor. This result must be reconsidered for the complete SGP V6.01 reprocessing. For other products and quality indicators no degradation is expected relative to SGP 5.02, but not a substantial improvement either, since there have been no major changes in the Level 2 algorithms.

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NO2 Cross Satellite Validation: The New SCIAMACHY L2V6 Products And The Road To S5P

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Nitrogen dioxide (NO_2) plays an important role in the troposphere. As part of NOx (= NO2 + NO) it is one of the key players in the formation of photochemical smog during pollution episodes and contributes to acid rain. Locally, it may also add to radiative forcing. In the stratosphere, nitrogen dioxide acts both as an ozone destroying substance (through the catalytic NOx cycle) and as a buffer against halogen catalysed ozone loss (through formation of chlorine and bromine nitrates).

Several satellites today are capable of measuring NO2. Aura Ozone Monitoring Instrument (OMI) launched in 2004 and Metop-A Global Ozone Monitoring Experiment (GOME-2) instrument launched in 2006 are still operating, while the ENVISAT SCIAMACHY instrument measured from 2002 to 2012.

The SCIAMACHY Level 2 (L2) Version 6 (V6) dataset was reprocessed for the full SCIAMACHY mission 2002-2012 at the Data Processing and Analysis Consortium (DPAC). Due to changes in the Level 1B data, slight changes in the NO2 columns of L2V6 are expected. A different NO2 data product using GOME-2 and SCIAMACHY measurements (IUP Bremen) will be taken for intercomparisons. This is based on DOAS technique using SCIATRAN for the AMF calculations.

One aspect that needs to be further investigated is the time dependency of the NO2 column during the day. While the comparison of the algorithms with one satellite dataset is independent of time issues, cross comparisons of NO2 data from two satellites needs a time dependent conversion factor. This depends not only on the equator crossing time of the satellite, but also on the latitude and azimuth angle of the measurement.

The start of the Sentinel 5P instrument at the end of 2016 will add another high resolution NO2 dataset with a equator crossing time similar to the OMI instrument (1:10 PM) in the afternoon (1:30 PM)). SCIAMACHY and GOME-2 have crossing times in the morning at 10:30 AM and 9:30 AM, respectively.

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Aurora Project: Simulation And Validation Of Synergistic Products From Sentinel-4 And Sentinel-5(p)

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AURORA (Advanced Ultraviolet Radiation and Ozone Retrieval for Applications) is a three-year project supported by the European Union in the frame of its H2020 Call (EO-2-2015) for “Stimulating wider research use of Copernicus Sentinel Data”. The overarching objective of AURORA is to simulate the provision of synergistic data products, having unprecedented accuracy, for the vertical profile of atmospheric ozone and to assess their quality with respect to the one expected for the operational products of the geostationary mission Sentinel-4 and of the Low Earth Orbit missions Sentinel-5p and Sentinel-5. The project data cover the lower layers of the atmosphere over Europe, North Africa and the Middle East, where ozone acts as a pollutant and as a greenhouse gas.

This work provides a brief overview of the project, highlighting its first priority scientific and technological objectives, along with the envisaged impact strongly oriented towards pre-market activities and applications. The main scientific purpose of AURORA is to investigate the potential of synergistic exploitation of complementary measurements of ozone acquired in different spectral regions – from the UV to the visible to the thermal infrared - through the assimilation of fused GEO and LEO ozone profile products resulting from application of the innovative method of complete data fusion. A technological infrastructure, based on virtual machines, cloud data sharing, a geo-database, and web-services for data access, will be developed to implement the full AURORA data processing chain. This infrastructure represents a best practice that plays a key role in ensuring the wider use of Copernicus Sentinel data for academia and industry. Such broad combination will stimulate the development of innovative downstream applications with high commercial potential, mainly exploiting derived tropospheric ozone and UV radiation data.

A pivotal role in the AURORA project will be played by QA/validation activities, which are elucidated secondly: Before being used in operational applications, the fitness-for-purpose of the AURORA ozone profile, tropospheric ozone, and UV radiation data products must be warily verified and documented by means of in-depth QA/validation studies. To that purpose, an extensive ozone product validation system has been developed on the heritage of various validation activities. The end-to-end approach of this system combines data content studies, information content studies, information-content based co-location procedures, and data harmonization, to conclude with the more traditional data comparisons with respect to reference measurements acquired by ground-based networks of ozonesonde and lidar stations (NDACC, SHADOZ, WMO GAW). The validation of surface UV on the other hand has been well established during almost two decades of satellite-based UV product quality assessment. The validation requires the use of ground-based spectral measurements, which are of better quality than the more widely used broadband instruments. There are several databases available for this activity, e.g. EUVDB hosted by FMI and NSF’s UV Network. These spectral data form the backbone for the UV radiation validation, while the broadband data from FMI’s COST UV Index Database are also considered.

The status and future evolution of AURORA can be followed on the official web site of the project at http://www.aurora-copernicus.eu/.

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Remote Sensing in the O2 A-band

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Atmospheric remote sensing using oxygen absorption is a technique already existing for 55 years. Because oxygen is a well-mixed gas, its measurement provides altitude information. Since the idea of using the strongest oxygen absorption band - the O2 A-band around 760 nm - for cloud altitude determination was proposed by Yamamoto and Wark (JGR, vol. 66, 1961), many theoretical studies, laboratory investigations, ground-based and aircraft measurements of the O2 A-band have been performed. In addition other oxygen absorption bands, like the O2 B-band at 680 nm and the O2-O2 collision complex bands at UV-visible wavelengths, can be used to provide vertical information of clouds.
Satellite observations of the O2 A-band have been performed since 1995, when GOME on ESA's ERS-2 satellite was launched. Since then, the number of satellite spectrometers measuring the O2 A-band has been steadily increasing. Multi-directional observations of the O2 A-band provided by POLDER have proven another way of exploiting the information of the O2 A-band. For current and upcoming satellite instruments which measure the greenhouse gases CH4 and CO2, the O2 A-band is chosen for light path correction. Especially GOSAT and OCO-2 provide more detailed O2 A-band spectra. At the same time, high spectral resolution measurements from the ground have been used to study photon path statistics in clouds.
The potential of the O2 A-band is high, since oxygen absorption provides a unique method for passive remote sensing of cloud height and cloud profile information. Latest developments are aerosol profile retrieval and fluorescence retrieval. All these O2 A-band applications need a good basis in spectroscopy and radiative transfer, and need appropriate retrieval techniques.
In the workshop "Remote sensing in the O2 A-band", held from 6-8 July 2016 at KNMI, De Bilt (NL), around 55 experts on O2 A-band observations, radiative transfer, and retrieval algorithm development from different applications came together to inform each other about state-of-art methods and observations, and to prepare for the coming years with many more O2 A-band data, especially from satellite. New and approved satellite instruments measuring the O2 A-band (and/or B-band) include: OLCI on Sentinel-3, TROPOMI on Sentinel-5P, UVN/Sentinel-4 on MTG, UVNS/Sentinel-5 on Metop-SG, TANSO-FTS2 on GOSAT-2, TANSAT, TEMPO, 3MI on Metop-SG, and MetImage on Metop-SG.

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The GreenHouse gas Observations of the Stratosphere and Troposphere (GHOST) airborne shortwave infrared spectrometer as a validation tool for satellite observations of greenhouse gases

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GHOST is a novel, compact shortwave infrared grating spectrometer, designed for remote sensing of tropospheric columns of greenhouse gases (GHGs) from an airborne platform. This is achieved by observing solar radiation at high spectral resolution which has been reflected by the surface. One of the main science requirements determining the design of the GHOST system was the capability to validate GHG column observations obtained using polar orbiting satellites such as the JAXA GOSAT mission, NASA's OCO-2 and the forthcoming Copernicus Sentinel 5-Precursor. GHOST observes carbon dioxide in spectral bands centred around 1.61 µm and 2.06 µm, the same spectral regions used by OCO-2 and GOSAT, whilst simultaneously measuring methane absorption at 1.65 µm (also observed by GOSAT) and 2.30 µm (to be observed by Sentinel 5-P once launched in late 2016). The overlapping spectral ranges and comparable spectral resolutions mean that GHOST has unique potential for providing validation opportunities for these platforms, particularly over the ocean where ground-based validation measurements are not available.

Here we present some of the latest retrievals of carbon dioxide and methane from GHOST radiance spectra using the 1.6 µm band, which incorporate new laboratory calibration data (measured at the UK Astronomy Technology Centre in June 2016) into the post-processing chain. In March 2015 GHOST took part in two science flights on board the NASA Global Hawk unmanned aerial vehicle based at the Armstrong Flight Research Centre in Edwards, California, which comprised long approximately north-south transects over the eastern Pacific Ocean. In addition to providing observations of spatial trends in GHG column concentrations over a regional scale, the second of these flights (on 10th March) allows inter-comparisons of GHOST retrievals with observations from OCO-2 and GOSAT, which both passed directly over the Global Hawk during clear sky conditions. We also, for the first time, look at the potential for using GHOST's 2.3 µm band for methane observations as a future validation opportunity for Sentinel 5-P.

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Combined Lidar and Ceilometer Networks for Cloud and Aerosol Monitoring

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Initially, Lidar networks formed the basis of the Global Atmosphere Watch Lidar Observation Network (GALION) that is currently complemented and enhanced by operational ceilometer networks of National Meteorological Services and aviation control entities. However, triggered by the eruptions of the Icelandic volcanoes Eyjafjallajökull and Grimsvötn in 2010 and 2011 European national meteorological services (e.g. Deutscher Wetterdienst, UK Meteorological Office, KNMI, RMI, few others) partially replaced existing instruments and upgraded their ceilometer networks to online capabilities. Based on the lidar principle, not only cloud base height and boundary layer heights but also aerosol layers can be detected by these instruments and their four-dimensional structure and dispersion can be tracked. Elastic backscatter profiles are retrieved by calibrating the devices absolutely, i.e. applying Rayleigh or liquid water cloud calibration. A Lidar and ceilometer inventory has recently been established and serves as a tool for monitoring qualitatively and quantitatively the transport of aerosol particles across Europe and other parts of the world, provided that profiling instruments are on-line. Currently (October 2016) instruments of Deutscher Wetterdienst (DWD), the KNMI, the UK Met. Office and several instruments operated by Meteo-France in France, RMI in Belgium, Met.No in Norway and Italy are on-line and provide quick looks of e.g., the range corrected signal and the attenuated backscatter coefficient. These quick looks are accessible through the ceilomap web page (www.dwd.de/ceilomap) hosted by DWD It is possible to further customize the page by overlying trajectories, satellite information (cloud coverage, cloud-top height) and model charts from the COPERNICUS Atmospheric Monitoring Service (CAMS).

Two European initiatives are currently working on data harmonization/data format and data transfer issues (E-PROFILE, a EUMETNET project led by MeteoSwiss, http://www.eumetnet.eu/e-profile) while harmonization of aerosol retrievals from ceilometers and assimilation of profiles into models are foci of TO-PROF, a European COST action (ES 1303, http://www.toprof.imaa.cnr.it/). Supported by EARLINET a first operationally running ceilometer network across national borders is anticipated as the main result of E-PROFILE and TO-PROF in 2017/2018. It will be based on a central processing and monitoring facility hosted by the UK Met. Office.

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Tools and Methods for Validation

HARP - a toolkit for inter-comparing atmospheric data

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HARP is a freely available and open source toolkit for ingesting, processing and inter-comparing earth observation data.

The main goal of HARP is to assist in the inter-comparison of data sets. By appropriately chaining calls to HARP command line tools one can preprocess data files such that two datasets that need to be compared end up having the same temporal/spatial grid, same data format/structure, and same physical unit. At the end of the tool chain you will have a set of data files that can be directly compared in e.g. Python, IDL or MATLAB.

In order for the HARP command line tools to handle each others output, the toolset uses its own data format conventions for intermediate files.

This HARP data format is a set of conventions for files stored in netCDF-3, HDF4, or netCDF-4/HDF5 format. The HARP conventions can generally be combined with other conventions that do not contradict it. The aim is that a file can be compliant with e.g. both netCDF-CF and the HARP data format conventions at the same time. HARP already includes converters for a wide range of satellite products such as Sentinel-5P, OMI, GOME-2, IASI, CCI, etc.

Once data products are converted to HARP compliant files, further processing can be done in the same way for each dataset. The standard also allows users to develop their own custom components and integrate these with the tool chain.

HARP is one of the components of the ESA Atmospheric Toolbox, and is used as a core toolset for the automated validation servers within projects such as CAMS, S5P-MPC, and QA4ECV. It is available on GitHub at https://github.com/stcorp/harp

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The Technology and Atmospheric Mission Platform (TAMP) for Atmospheric Sciences Cal / Val activities

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The scientific and industrial communities are being confronted with a strong increase of Earth Observation (EO) satellite missions and related data. This is in particular the case for the Atmospheric Sciences communities, with the upcoming Copernicus Sentinel-5 Precursor, Sentinel-4, -5 and -3, and ESA's Earth Explorers scientific satellites ADM-Aeolus and EarthCARE.

The challenge is not only to manage the large volume of data generated by each mission / sensor, but to create synergies among the different datasets to exploit the full potential of the available information, integrating EO data with ground based observations and numerical models is essential for Cal/Val activities as well as for the creation of combined products.

As a preparation activity supporting scientific data exploitation for Earth Explorer and Sentinel atmospheric missions, ESA is funding the technology study and prototype implementation of the "Technology and Atmospheric Mission Platform" (TAMP). The TAMP test-bed environment offers data access, visualization, processing and analysis services for the "data triangle" consisting of (1) EO satellite products, (2) model data provided by chemical weather forecast, and (3) reference / validation data sets.

Data analysis tools allow e.g. comparing the same variable as measured by different data sources (various satellite sensors and ground measurements) or comparing measured data (e.g. lidar data) with numerical simulations. Specific functions (e.g. bias, RMS, spatial and temporal averages) have been implemented to simplify the data comparison; moreover the user is allowed to upload his/her own data assessment tool in a dedicated virtual environment for (massive) data processing and assessment.

The implementation pursues the "virtual workspace" concept: all resources (data, processing, visualization, collaboration tools) are provided as "remote services", accessible through a standard web browser, to avoid the download of big data volumes and for allowing utilization of provided infrastructure for computation (processors close to data), analysis and sharing of results.

It is proposed to provide TAMP demonstration desk, where the TAMP platform is introduced by means of three use cases:

- SO2 volcanic emissions monitoring via different satellite platforms, models and ground measurements,
- global stratospheric Ozone (model, satellite data, lidar data)
- tropospheric aerosol from satellite, model and ground measurements (stations, lidar)

The workshop's participant are allowed to interact with the platform, playing I real time with the data to test the visualization and analysis capabilities.

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Fiducial Reference Measurements

Terms and Definitions for Uncertainty in Atmospheric Composition Measurements

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High-quality satellite observational datasets provide an essential input to the Copernicus Climate Change Service (C3S) and the Copernicus Atmosphere Monitoring Service (CAMS) of the European Earth Observation programme Copernicus. These services must provide users with reliable and up-to-date information related to environmental and safety issues.

The satellite data products have to developed with a view to fulfilling user requirements expressed by international bodies (e.g., Global Climate Observing System, WMO rolling requirements), by dedicated projects (e.g., ESA's CCI Climate Modelling User Group), and from user surveys as carried out within the FP7 QA4ECV project. These target requirements are a guideline for data validators and potential data users to verify the fitness-for-purpose of the data product.

Understanding of, and common agreement on, the actual meaning of these requirements are a prerequisite for obtaining quality-assured satellite data products. Lists of applicable terms and definitions have been set up within QA4ECV and other EU FP7/H2020 projects like FIDUCEO, GAIA-CLIM and CLIPC. Unfortunately, as will be shown here, the definitions used in the different lists are not always mutually consistent, and the terms (like error, uncertainty, accuracy, …) are not always applied rigorously in documents and product (meta)data.

Regarding the communication of metrological aspects, we advocate the use of the International Vocabulary of Metrology (VIM) and the Guide to the Expression of Uncertainty in Measurement (GUM). Set-up by the authoritative Joint Committee for Guides in Metrology, these works provide a comprehensive vocabulary on metrology. Here, we will present examples of both consistent and inconsistent terminology usage with respect to these reference works, for three of the future TROPOMI atmospheric L2 data products which are also the atmospheric output of QA4ECV: formaldehyde, nitrogen dioxide and carbon monoxide.

Not only the use of terminology of uncertainty must be consistent, but also the calculation of uncertainties. Satellite L2 data are no direct measurements, but rather result from several non-trivial transformation steps of L1 data, and themselves serve as input to derive other products. Each transformation step introduces some uncertainty that propagates itself to the final result. This uncertainty and the way it impacts the end product must be evaluated. In the case of comparisons of satellite with reference correlative data, uncertainties of the satellite and reference data must assume the same meaning. Therefore, clear communication on and -to the extent possible- harmonization of uncertainties are essential, e.g., touching their nature, their format within the data product, their contributions (random noise, parameter errors, model errors,…), as well as the error correlations and the level of approximation of the uncertainty calculation. As will be shown here with QA4ECV illustrations, efforts are made to reach a clear communication and consistent use of uncertainty between (i) satellite and correlative data and (ii) among the different atmospheric data products.

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HCHO and NO2 MAXDOAS retrieval harmonization as part of the QA4ECV project

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Over the last years, ground-based MAXDOAS measurements have played an increasing role for the ground truthing of space-nadir observations of air quality relevant trace gases such as NO_2 and HCHO. Current MAXDOAS network data however lack harmonization in terms of data acquisition, data processing and data reporting. This issue is addressed as part of the ongoing EC FP7 QA4ECV project (*Quality Assurance for Essential Climate Variables*; see http://www.qa4ecv.eu/) which aims at developing standardized quality control procedures for Climate Data Records generation. In particular, tools and best-practices for MAXDOAS measurements are developed and tested on a selected number of sites to be used as Fiducial Reference Measurement (FRM) as part of the project.

We present a status of the QA4ECV MAXDOAS harmonization activities addressing spectral fitting and air mass factor calculations. Results from a large scale intercomparison exercise involving 15 groups are presented for both NO_2 and HCHO. We also introduce an approach allowing for harmonized conversion of slant columns into vertical columns through application of generic look-up tables of air mass factors parameterized as a function of solar and viewing angles, wavelength, boundary layer height, aerosol optical depth (AOD) and surface albedo. The advantages and drawbacks of the LUT approach are investigated and the application of the resulting data set for comparison with OMI and GOME-2 satellite measurements is discussed.

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Validation of OMI and GOME-2A and GOME-2B tropospheric NO2, SO2 and HCHO products using MAX-DOAS observations from 2011 to 2014 in Wuxi, China

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Tropospheric vertical column densities (VCDs) of NO_2, SO_2 and HCHO derived from Ozone Monitoring Instrument (OMI) on AURA and Global Ozone Monitoring Experiment 2 aboard METOP-A (GOME-2A) and METOP-B (GOME-2B) are widely used to characterize the global distributions, trends, dominating sources of the trace gases and for the comparison with chemical transport models (CTM). We use tropospheric VCDs and vertical profiles of NO_2, SO_2 and HCHO derived from MAX-DOAS measurements from 2011 to 2014 in Wuxi, China, to validate the corresponding products derived from OMI, GOME-2A/B by different scientific teams (daily and bimonthly averaged data). Prior the comparison we investigate the effects of the spatial and temporal coincidence criteria for MAX-DOAS and satellite data on the comparison results. We find that the distance of satellite data from the location of the MAX-DOAS station is the dominating effect, and we make suggestions for the spatial and temporal averaging. We also investigate the effect of clouds on both MAX-DOAS and satellite observations. Our results indicate the discrepancies between satellite and MAX-DOAS results increase with increasing effective cloud fractions and is dominated by the cloud effect on the satellite products. Our comparison results indicate a systematic underestimation of all SO_2 and HCHO products and an overestimation of the GOME-2A/B NO_2 products (the DOMINO NO_2 product is only slightly underestimated). To better understand the reasons for the differences, we recalculated the AMFs for satellite observations based on the shape factors (SFs) derived from MAX-DOAS. The recalculated satellite VCDs agree better with the MAX-DOAS VCDs than those from the original products, especially for large VCDs. Finally we investigate the effect of aerosols on the satellite retrievals. We find that an increasing underestimation of the OMI NO_2, SO_2 and HCHO products with increasing AOD. One reason for this finding is that aerosols systematically affect the satellite cloud retrievals and can lead to apparent eCFs of up to 10% and apparent cloud top pressures (CTP) of down to 830 hPa for the typical urban region in Wuxi. We show that in such cases it might be better to apply AMFs for clear sky conditions than AMFs based on the satellite cloud retrievals.

We find that the satellites systematically overestimate the magnitude of the diurnal variations of NO_2 and HCHO. No significant weekly cycle for all trace gases is found by either the satellites or the MAX-DOAS measurements.

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Fiducial Reference Measurements for Ground-Based Infrared Greenhouse Gas Observations (FRM4GHG) at the Sodankylä TCCON site

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Ground-based infrared remote sensing greenhouse gas (GHG) observations are extensively used for the validation of GHG measurements from satellites like SCIAMACHY, GOSAT and OCO-2. TCCON (Total Carbon Column Observing Network) is a network of about 23 stations distributed globally and measuring the total column abundances of GHGs using a Fourier-transform infrared (FTIR) solar absorption spectrometer of the type Bruker IFS 125HR. TCCON was set up with the aim to provide precise and accurate measurements of GHGs to be used primarily for satellite validation. However, the TCCON network has shown some deficiencies in terms of the gaps in the coverage, especially in remote locations, locations with high/low albedo. The TCCON spectrometer is very expensive, not so easy to move, and requires special operational conditions, trained personnel for operation and maintenance, therefore, it is very costly if further expansion of the network is desired. Presently, several new portable spectrometers have been developed that

have the potential to eliminate those deficiencies of the TCCON network: they are low cost, portable, easy to operate and maintain and require low operational cost. However their performances have not yet been fully characterized. In order to characterize the performance of these low cost portable spectrometers performing TCCON-type measurements simultaneously under different atmospheric conditions in comparison with a TCCON instrument, a campaign has been planned for approximately one year in 2017. In this campaign, the teams will install these candidate instruments together at the TCCON site in Sodankylä. In addition, regular AirCore launches will also be performed from that site and will provide in-situ reference profiles of the target gases, which will be useful to verify the instruments calibration. The focus of this campaign will be on CO and CH4 in support of the S5P validation. The campaign will provide a significant dataset of GHG measurements which can be used for validation purposes during the S5P commissioning phase. Furthermore, it will also provide a comparative characterization of the participating instruments with respect to the standard TCCON instrument in terms of the precision, accuracy, stability, portability and ease of deployment, cost factor, etc. The outcome of the campaign will then be a guideline for the further development of new observation sites to complement the TCCON network and provide better support for the validation of the existing and future satellite missions. This talk will focus on the objectives of the campaign and give an overview of the current status of the campaign.

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Fiducial Reference Measurements for Ground-Based DOAS Air-Quality Observations

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We present the recently awarded ESA FRM$_4$DOAS (Fiducial Reference Measurements for Ground-Based DOAS Air-Quality Observations) project. The main objective of this project is to improve and harmonize data products from UV-Visible ground based MAXDOAS spectrometers to arrive at Fiducial Reference Measurements (FRMs) for satellite observations of air-quality variables. By providing centrally-processed quality-controlled MAXDOAS measurements from a demonstration network of 11 sites, the FRM4DOAS project will directly contribute to the validation of the Sentinel-5 Precursor mission scheduled for launch in mid-2016 and prepare the establishment of an essential ground-truth reference measurement capacity in support of the future Copernicus Sentinels 4 and 5 that will provide operational air quality observations for the next 15 years. Activities will include a round-robin NO_2, O_3 and HCHO profiling retrieval algorithm selection and its implementation into a processing chain which will have the capability to ingest data from a large number of MAXDOAS sites. The system will be fully documented and tested on 11 stationary sites belonging to the project partners as well as using data from the large scale CINDI-2 MAXDOAS intercalibration campaign which will take place in September 2016 in Cabauw, The Netherlands.

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TCCON Measurements From Ascension Island - Challenges Of Running A Remote Site

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The Total Carbon Column Observation Network (TCCON) has become the reference network for all total-column observations of greenhouse gases (GHGs) like CO_2 , CH_4, CO, N_2O and others. Within TCCON, the Max Planck Institute for Biogeochemistry (MPI-BGC) has been operating a Fourier-Transform Spectrometer (FTS) on Ascension Island (8°S, 14° W) since May 2012. This is currently the only TCCON station covering the South Atlantic Ocean. So far, the measurements cover more than two complete seasonal cycles.

Due to its location the southern trade wind zone, the station is downwind from Africa most of the time. A detailed trajectory analysis shows that different parts of the total air column typically have different origins. Air in the Planetary Boundary Layer (PBL) typically comes from the deep southern Atlantic Ocean and had only little GHG exchange with land surfaces. However, air in the free troposphere above the PBL usually comes from tropical and southern Africa and sometimes also from South America.

Ascension Island is certainly a key site to understand the Southern Hermisphere Carbon Cycle. It is also a key site for the calibration and validation of GHG satellite observations over the ocean. However, running a TCCON site at such a remote place is also very challenging: the harsh environment destroys standard equipment in weeks, technical support can only be provided 1-2 times per year, utility costs are high, the measured data cannot be transmitted online, and qualified personnel is hard to find and keep. For long term operation, remote sites like Ascension Island need more support - also from their data users.

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Stratospheric and Mesospheric Composition

Stratospheric and mesospheric measurements of O3 above Ny Alesund/Spitsbergen

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Ny Alesund is a research village on Spitsbergen in the Arctic at 79°N. Among other instruments, an millimeterwave radiometer, OZORAM, to measure stratomesospheric Ozone, is operated continuously in cooperation of the University Bremen and the AWI Bremerhaven. The OZORAM is an NDACC - affiliated instrument since 1994 and has been adapted to measure the Ozone emission line at 142 GHz with a high resolution of 60 kHz. This allows to retrieve profile information from 30 km up to 70 km altitude.

The independence of the measurements of light and the ability to measure at overcast conditions enable Ozone measurements with an time resolution of 1 hour all year around. This allows for detailed studies of the variation of Ozone on the solar zenith angle during polar day, but also the dynamical change connected with the descent of polar air due to the establishment of the polar vortex.

In this poster, a comparison with MLS and SABER time series will be shown, as well as some highlights which could be studied using the OZORAM time series. This includes a detailed study of the sun zenith angle dependency of Ozone during polar day which shows that the variation is underestimated by models.

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SCIAMACHY nadir ozone profile retrievals and their validation

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We have carried out stratospheric nadir ozone retrievals of SCIAMACHY version-8 level-1 data in the ultra-violet range [265-330nm] using the *Opera* optimal estimation algorithm developed in KNMI. We will show time-series for the ozone retrievals for the collocated gelocations with (WOUDC) ozone sondes from years 2002 to 2012. We also include comparisons to these ozone sondes to evaluate the accuracy of the retrieved ozone datasets. We have also investigated spectral slit functions (soft calibration) for the instrument using Dobber's solar reference (Dobber et al. 2008, textit{Solar Phys}, 249). We find that applying a spectral shift and squeeze to the UV wavelengths of solar spectra significantly improves the residuals which are the differences between convolved modeled and measurement spectra.

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Validation of the new Limb Ozone product SCIAMACHY ESA V6

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The validation of new limb ozone product from SCIAMACHY mesurement onboard the Envisat satellite is presented and the improvements toward the last version (V 5.2) are shown. In addition the comparison is performed toward different limb ozone measuring instruments which cover the period of SCIAMACHY lifetime, i.e. 2002-2012.

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Validation of MIPAS IMK/IAA Version 7 ozone profiles

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We present the results of validation exercise on Version V7R_O3_240 of ozone vertical profiles retrieved with IMK/IAA MIPAS scientific level 2 processor from the new version 7 of spectral Level 1 files provided by ESA. The time period covered corresponds to Reduced Resolution period of MIPAS instrument, i.e. January 2005-April 2012. The comparison with satellite instruments includes ACE-FTS, GOMOS, MLS, OMPS, OSIRIS and SAGE II. Also, the comparison with ozonesondes data from 15 stations from networks SHADOZ, WOUDC and NDACC will be presented. For each reference dataset, bias determination and precision validation are performed.

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Performance of the horizontal gradient model implemented in the MIPAS ESA v8 processor

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Recent studies have shown that neglecting the horizontal variability of the atmosphere in the forward model for the simulation of limb emission radiances causes a systematic error in MIPAS retrieved profiles. While not visible in the individual profiles, this systematic effect is noticeable as a difference between zonal averages obtained from the ascending and descending parts of the satellite orbit. To improve the quality of MIPAS products, it is desirable to take into account the horizontal variability of the atmosphere in the forward model. There are several methods to account for the atmospheric horizontal variability, one of them is to introduce an altitude dependent horizontal gradient for the quantities used to describe the atmospheric state.

The introduction of the horizontal gradient model into the Optimized Retrieval Model (ORM), the scientific prototype of the processor used by ESA to obtain MIPAS level 2 products, required a new design of the code itself. Several optimizations exploiting the spherical symmetry of the atmosphere could no longer be used. Therefore, both the ray tracing and the radiative transfer integration algorithms had to be adapted.

In this work we show the effect of the implemented horizontal gradient model in the retrieval results. Depending on the accuracy of the input horizontal gradient gradient, the model permits to achieve a smaller chi-square of the fit, and to reduce the systematic differences in the zonal averages computed from the ascending and descending parts of the MIPAS orbits. The new model is more demanding from the computational point of view. We characterize the increase of computing load with respect to the old 1d model.

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Validation of ozone vertical distributions retrieved from SCIAMACHY limb measurements: IUP Bremen scientific processor V3.5

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Measurements of the scattered solar light performed by the Scanning Imaging Absorption Spectrometer for Atmospheric CHartographY (SCIAMACHY) instrument, which was operated on board the European Environmental Satellite (ENVISAT) from August 2002 to April 2012, provide a global information on vertical distributions of important stratospheric constituents such as O_3, NO_2, H_2O, BrO as well as stratospheric aerosols. This presentation focuses on the investigation of the quality of the newly developed ozone profile retrieval algorithm (V3.5) using measurements from the space borne Aura MLS instrument of NASA and ozone sondes. V3.5 of the ozone profile retrieval algorithm is intended to fix the issues previously identified in both V2.9 IUP Bremen retrieval and operational processor of DLR/ESA. The new retrieval version exploits the spectral information from three ozone absorption bands (Hartley, Huggins and Chappuis) and makes an independent estimation of the surface albedo in the UV and visible spectral ranges. First investigations show a substantial improvement in the retrieval quality, in particular the artificial drift and overestimation of the QBO signal in tropical ozone around 35 km are eliminated in the newest retrieval version.

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Validation of SCIAMACHY limb NO2 profiles: accounting for differences in the local solar time

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Nitrogen dioxide (NO2) has significant impacts on the chemistry of the stratosphere being major ozone-depleting substance, thus requires accurate global monitoring and high-quality datasets.

The aim of this study is to validate the SCIAMACHY (**Sc**anning Imaging **A**bsorption spectro**M**eter for **A**tmospheric **Ch**artograph**Y**) limb NO2 product (version 3.1) and to assess systematic uncertainties. For 10 years of SCIAMACHY NO2 observations, we analyze data from the three-dimensional Bremen Chemistry Transport Model (B3DCTM) and the photochemical box model PRATMO to provide validation and photochemical conversions of measured NO2 profiles.

Both models have also been applied to consider measurements from SCIAMACHY solar occultation observations. We also compare SCIAMACHY limb NO2 profiles to collocated observations from the limb-sounders MIPAS (Michelson Interferometer for Passive Atmospheric Sounding), OSIRIS (Optical Spectrograph and Infrared Imager System), and solar occultation measurements SAGE-II (Stratospheric Aerosol and Gas Experiment II).

The two models B3DCTM and PRATMO are currently used to develop a better approach for receiving qualitatively improved conversion factors for the photochemical conversion of data from different instruments. Thus, we expect that the quality of comparisons between limb and occultation measurements of NO2 will be refined.

B3DCTM is driven by ECMWF (European Centre for Medium-Range Weather Forecasts) meteorological reanalysis ERA-Interim in spatial resolution of 2.5° lat. × 3.75° lon., using 29 isentropic levels in the vertical, ranging from 335K to 2726K (about 11-55 km). Horizontal transport has been calculated from meteorological wind fields, and the vertical transport from EI diabatic heating rates using the Prather advection scheme.

PRATMO is driven by climatological ozone and temperatures and enables NO2 scaling in the altitude range from 0 to 70 km.

Here, we show first results of our current photochemical conversion approach and assess potential deficits in order to further develop the work flow and incorporated systems and approaches.

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Assessment of MIPAS ESA V7 Products And First Verification Of MIPAS ESA V8 Products

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The Michelson Interferometer for Passive Atmospheric Sounding (MIPAS) on ESA's ENVISAT satellite performed almost continuous measurements of the global atmospheric composition for approximately 10 years, from July 2002 to April 2012. The operational ESA data retrieval processor, based on the algorithm ORM (Optimized Retrieval Model), originally designed for the Near Real Time analysis and developed by an European Consortium led by IFAC, is currently used for the reanalysis of the full MIPAS mission. The maintenance and the upgrade of the ESA processor are made in the frame of the Quality Working Group, where a fruitful collaboration among Level 1, Level 2 and validation teams can be exploited. This collaboration is essential to pursue improvements in the accuracy of the products and their characterization.

This paper is meant to describe the most recent upgrades in the ESA processor performed to improve the quality of ESA products. In particular, the full mission was recently reprocessed with the L1 V7 and L2 V7 processors, and further improvements are in preparation, that will be collected in version 8 of the ESA processors. With respect to V6, V7 and V8 products take advantage of significant improvements in both L1 and L2 processors, as well as in the auxiliary data. Improvements in the L1 processor consist in the correction of the instrumental drift, improved spike detection algorithm and new Instrument Line Shape, as well as in the use of measured daily gain calibration instead of weekly gain. Improvements in the L2 processor include a different approach for retrieving atmospheric continuum, the use of an a posteriori regularization with altitude dependent constraint, a better approach for handling interfering species, a reduced bias in CFC-11, the handling of horizontal inhomogeneities and the use of ECMWF altitude/pressure relation for determining more accurate tangent altitudes. Improvements in the auxiliary data consist in the use of microwindows with larger information content, more accurate non-LTE errors, new spectroscopic database and diurnally varying climatological dataset. Furthermore, with each new version additional trace-gases are provided, leading to 20 retrieved species by the L2 V8 processor.

Improvements in the V7 products will be revised in the light of the results of the validation with correlative measurements, and, by comparing the first new L2 V8 products with the L2 V7 ones, a preliminary assessment of the performance of the new V8 processors will be presented.

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Validation of SCIAMACHY Limb Water Vapour V4.2

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SCIAMACHY, an instrument on borad Envisat observed the earth atmosphere with differnt observation geometries for nearly and decade between 2002 and 2012. The limb geometry was used to retrieve water vapour profiles in the UTLS, between about 11 and 23km height. The UTLS (upper troposphere and lower stratosphere) is a region of special interest for the radiative transfer and a variety of dynamical and chemical processes in the atmosphere.

At the same time it is challanging to measure water vapour in this altitude, therefore only few long and consistent time series exist.

The new SCIAMACHY limb water vapour version V4.2 is currently processed. Compared to V3.01 the aerosol correction retrieval and the regularization were improved. Additionally, updates of the Level 1c data (L1V8),

the spectral data base and other minor setup changes were applied. Due to the time-consuming retrieval process, calculations are using a Message Passing Interface (MPI) on the massively parallel supercomputing system.

To validate the new data version, we present comparisons to in situ measurements, water vapour profiles from other satellites, and from the occultation measurements of SCIAMACHY.

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Improved Algorithm Baseline For The Generation Of Total Ozone Climate Data Records: Application To GOME And OMI.

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The direct-fitting total ozone retrieval algorithm GODFIT developed at BIRA-IASB has been applied in the past years on nadir observations from the instruments GOME, SCIAMACHY, GOME-2A/B and OMI to generate climate data records characterized by a high level of accuracy, temporal stability and inter-sensor consistency. As part of the on-going activities within the ESA Ozone_cci project, new developments in the algorithm baseline have been carried out. A new total column-classified ozone profile climatology recently released by Labow et al. (2015) is now used in the GODFIT forward model. Covariance matrices associated to this climatology have been built and are used to estimate smoothing errors on a pixel-basis. Also, a better treatment of the instrumental slit functions and their time variation and an optimized correction for the I0-effect have been implemented in the algorithm. This improved baseline has been used to reprocess the full GOME/ERS-2 and OMI/Aura missions and we present here the new version of the corresponding GODFIT total ozone data sets. The quality of the products is evaluated by comparisons with other total ozone products, such as OMI-TOMS, SBUV v8.6 and also with the previous version of the CCI data sets. They have also been validated using ground-based Brewer and Dobson measurements, and preliminary main findings are highlighted here. This improved algorithmic baseline will also be used in the coming months to generate a new version of multi-sensor L2 and L3 total ozone data records.

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Tropospheric Composition / Air Quality

Validation Of The ESA-CCI Harmonized Tropospheric Ozone Column Data Product, Using Balloon Sounding Data

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Within the ESA Ozone-CCI project, a Convective Cloud Differential (CCD) algorithm has been used to derive a harmonized dataset of 20 years (July 1995 –December 2015) of Tropical Tropospheric Ozone Column (TTOC) data for the Tropical latitude belt (20° S – 20° N). This homogenized dataset can be used in climate research studies, e.g. validating chemical transport models, helping us to understand the processes which are responsible for the variability of tropospheric ozone in the Tropical belt. The accuracy of this CCD method has been assessed by comparing the tropospheric ozone columns with ozonesonde measurements obtained from the SHADOZ network. Validation results of this Tropical Tropospheric Ozone Column (TTOC) product will be presented. The tropospheric ozone retrieval is based on the consistent ESA-CCI total ozone dataset retrieved from the successive GOME, SCIAMACHY, GOME-2A, GOME-2B and OMI sensors, applying the GODFITv3 algorithm. The TTOC product is available as monthly averages with a horizontal resolution of 1.25° latitude x 2.5° longitude. The TTOC time series will be extended in the future with the upcoming Sentinel 5 Precursor data. For S5P both the GODFIT and the TTOC will be an operational offline product. The validation results reveal that the merged TTOC product is after comparison with ozonesonde data for most of the stations within 10 % relative difference error. The correlation varies between 0.43 and 0.84 with a rmse between 3.3 and 5.1 DU. When comparing the total uncertainty among the different sensors with the harmonized dataset, it is shown that the harmonized dataset leads towards a better agreement between the different instruments.

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Validation of ATSR Total Column Water Vapour (AIRWAVE v1 and v2) using sondes, GPS and independent satellite datasets

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The ATSR water vapour dataset consists in Total Columns of atmospheric Water Vapour (TCWV) retrieved for cloud-free sea surface scenes using the two Thermal InfraRed (TIR) channels of the Along Track Scanning Radiometer (ATSR) instrument series. The retrieval scheme, named Advanced InfraRed WAter Vapor Estimator (AIRWAVE, version 1 and 2), uses the instrument physical characteristics in combination with advanced radiative transfer models and a sea surface spectral emissivity database. The native spatial resolution of the retrieved TCWV is 1x1 km^2 with a water vapour column accuracy of about 15%; AIRWAVE products at lower spatial resolution (e.g. 0.25x0.25deg) are also available.

The global validation of the AIRWAVE TCWV dataset, spanning from 1991 to 2012, is carried out using the WMO soundings located on islands or close to coasts. The validation exercise comprises the SUOMINET GPS dataset, freely available at http://www.suominet.ucar.edu/data.html#netcdf. Preliminary results show that the AIRWAVE version 1 dataset is bias-free and highly sensitive to the water vapour content in the atmospheric boundary layer, a part from the polar regions where version 1 is affected by dry biases for latitudes > 60 degrees. This problem has been solved in version 2 adopting a dynamic and self-consistent selection of the retrieval parameters.

Inter-comparison with the Remote Sensing Systems Special Sensor Microwave Imager Level 2 products (RSS SSM/I, http://www.remss.com/missions/ssmi) has also been carried out, showing excellent agreement at global scale.

Validation and inter-comparison methods and results for both AIRWAVE version 1 and 2 will be critically analysed and discussed.

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An ECV algorithm for the retrieval of tropospheric HCHO from OMI, GOME(-2), and SCIAMACHY within the Quality Assurance For Essential Climate Variables (QA4ECV) project.

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One of the main goals of the QA4ECV project is to define community best-practices for the generation of multi-decadal ECV data records from satellite instruments. QA4ECV will develop retrieval algorithms for the Land ECVs surface albedo, leaf area index (LAI), and fraction of active photosynthetic radiation (fAPAR), as well as for the Atmosphere ECV ozone and aerosol precursors nitrogen dioxide (NO_2), formaldehyde (HCHO), and carbon monoxide (CO).

Here we present the first results of the QA4ECV HCHO product for the OMI, GOME-2, SCIAMACHY and GOME sensors. We use a fitting window covering the 328.5-346 nm spectral interval for the morning sensors (GOME, SCIAMACHY and GOME-2) and an extension to 328.5-359 nm for OMI and GOME-2, allowed by improved quality of the recorded spectra. The use of a mean background radiance as DOAS reference spectrum allows for a stabilization of the retrievals. The selection of reference spectra is line-of-sight dependent. A background correction based on the reference sector method has been implemented in the QA4ECV HCHO algorithm, as it further reduces retrieval uncertainties. As for NO_2, HCHO profiles from the TM5 model are used as a priori in the AMF calculation. These are provided on a 1°x1° latitude-longitude grid.

Every step of the retrieval algorithm is documented via traceability diagrams available on the QA4CV website, providing very detailed information on the algorithm settings and auxiliary data sources, in order to be used for quality assurance and validation within the QA4ECV project.

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Recent Developments in the Aerosol Layer Height Algorithm for the Sentinel-4 mission

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The Sentinel-4 mission is a part of the European Commission's Copernicus programme, the goal of which is to provide geo-information to manage environmental assets, and to observe, understand and mitigate the effects of the changing climate. The Sentinel-4/UVN instrument design is motivated by the need to monitor trace gas concentrations and aerosols in the atmosphere from a geostationary orbit. The on-board instrument is a high resolution UV-VIS-NIR (UVN) spectrometer system that provides hourly radiance measurements over Europe and northern Africa with a spatial sampling of 8 km. The main application area of Sentinel-4/UVN is air quality. One of the data products that is being developed for Sentinel-4/UVN is the Aerosol Layer Height (ALH). The goal is to determine the height of aerosol plumes with a resolution of better than 0.5 - 1 km. The ALH product thus targets aerosol layers in the free troposphere, such as desert dust, volcanic ash and biomass during plumes. KNMI is assigned with the development of the Aerosol Layer Height (ALH) algorithm. Its heritage is the ALH algorithm developed by Sanders and De Haan (ATBD, 2016) for the TROPOMI instrument on board the Sentinel-5 Precursor mission that is to be launched in Oct/Nov 2016. The retrieval algorithm designed so far for the aerosol height product is based on the absorption characteristics of the oxygen-A band (759-770 nm). The algorithm has heritage to the ALH algorithm developed for TROPOMI on the Sentinel 5 precursor satellite. New aspects for Sentinel-44/UVN include the higher spectral resolution (0.116 nm compared to 0.4 nm for TROPOMI) and hourly observation from the geostationary orbit. The algorithm uses optimal estimation to obtain a spectral fit of the reflectance across absorption band, while assuming a single uniform layer with fixed width to represent the aerosol vertical distribution. The state vector includes amongst other elements the height of this layer and its aerosol optical thickness. We will present the development work around the ALH retrieval algorithm in the framework of the Sentinel-4/UVN instrument. The main challenges are highlighted and retrieval simulation results are provided. Also, an outlook towards application of the S4 bread board algorithm to Sentinel-5 Precursor data later this year will be discussed.

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New Developments in the SCIAMACHY L2 Ground Processor

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SCIAMACHY (SCanning Imaging Absorption spectroMeter for Atmospheric ChartographY) aboard ESA's environmental satellite ENVISAT observed the Earth's atmosphere in limb, nadir, and solar/lunar occultation geometries covering the UV-Visible to NIR spectral range. It is a joint project of Germany, the Netherlands and Belgium and was launched in February 2002. SCIAMACHY doubled its originally planed in-orbit lifetime of five years before the communication to ENVISAT was severed in April 2012, and the mission entered its post-operational phase.

In order to preserve the best quality of the outstanding data recorded obtained by SCIAMACHY, data processors are still being updated. This presentation will highlight three new developments that are currently being incorporated into the forthcoming Version 7 of ESA's operational Level 2 processor:

1. Tropospheric BrO, a new retrieval based on the scientific algorithm of (Theys et al., 2011). This algorithm had been originally developed for the GOME-2 sensor and later adapted for SCIAMACHY. The main principle of the new algorithm is to utilize BrO total columns (already the operational product) and split them into stratospheric VCDSTRAT and tropospheric VCDTROP fractions. BrO VCDSTRAT is determined from a climatological approach, driven by SCIAMACHY O3 and NO2 observations. VCDTROP is then determined simply as a difference: VCDTROP = VCDTOTAL – VCDSTRAT.

2. Improved cloud flagging using limb measurements. Limb cloud flags are already part of the SCIAMACHY L2 product. They are currently calculated based on the scientific algorithm SCODA developed by (Eichmann et al., 2015). Clouds are categorized into four types: water, ice, polar stratospheric and noctilucent clouds. Recently the scientific version of SCODA has been reviewed and further improved. These latest modifications are currently being implemented into the operational processor.

3. A new, future-proof file format for the level 2 product based on NetCDF. Although the final concept for the new format is still under discussion within the SCIAMACHY Quality Working Group, main features of the new format have already been clarified. The data format should be aligned and harmonized with other missions (esp. Sentinels and GOME-1/2). Splitting of the L2 products into profile and column products is also considered. Additionally, reading routines for the new formats have to be developed and provided.

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Water Vapour Retrievals from MERIS and OLCI: Validation and Representativeness

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Total Column Water Vapour (TCWV) retrievals from measurements of the polar orbiting, sun-synchronous satellite spectrometers MERIS (*Medium Resolution Imaging Spectrometer* on board ENVISAT), MODIS (*Moderate Imaging Spectro-radiometer* on board Aqua and Terra) and OLCI (*Ocean and Land Colour Instrument* on board Sentinel-3) enable observations of high spatial resolution and accuracy over land surfaces on a global scale. Only those observations provide information on regional variations of water vapour as well as the detection of local and global anomalies. But, depending on the swath width of the sensor, the temporal sampling is low and the observations of TCWV are limited to cloud free land scenes.

The representativeness of the satellite retrieved TCWV has been investigated by the use of 10 years of a 2-hourly TCWV data-set, estimated from measurements of the global GNSS (Global Navigation Satellite System). It turns out, that the TCWV observed, i.e., at 10:30 local time is generally lower than the daily mean TCWV by -0.65mm on average for cloud-free cases. Averaging over all GNSS stations, the monthly mean TCWV, constrained to cases that are cloud-free at 10:30 LT (Local Time), is by 25 % lower than the monthly mean TCWV of all cases. For the majority of GNSS stations, the amplitude of the averaged diurnal cycle ranges between 0-5 % of the 15 daily mean with a minimum between 6 and 10 LT and maximum between 16 and 20 LT. However, the features of the diurnal cycle of TCWV vary significantly between individual locations.

The TCWV retrieval scheme has been extended for OLCI applications, whereby the algorithm includes the additional, strongly absorbing water vapour channel at 940nm. This results of TCWV retrievals from OLCI measurements will be discussed.

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