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Ozone_cci+

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1 Introduction

Background

The European Space Agency's Climate Change Initiative (CCI) aims to realize the full potential of the long-term Earth Observation archives collected by ESA and Third Party satellite missions. Since 2010, the Ozone CCI team (https://climate.esa.int/en/projects/ozone) has been developing, maturing, generating and sustaining multiple complementary multi-decadal satellite ozone Climate Data Records (CDRs) tailored for climate monitoring, climate research and climate modelling applications. The CCI portfolio consists of total and tropospheric ozone column data products as well as vertically resolved ozone products by nadir and limb-viewing sensors.

This workshop aimed at

- bringing together scientists involved in the generation of ozone Climate Data Records, as well as (potential) users of such multi-decadal ozone time series, and the broader ozone and climate communities;
- presenting the state of the art in ozone Climate Data Record production;
- discussing results from major Climate Data Record users, e.g., stratospheric ozone assessments for WMO/UNEP, tropospheric ozone assessments for TOAR II, studies focusing on UT/LS, evaluation of climate modelling, data assimilation and reanalysis;
- collecting and updating user requirements for ozone Climate Data Records;
- discussing remaining challenges for the generation of ozone Climate Data Records.

The second Ozone_cci+ User Workshop was held on Tuesday 28 and Wednesday 29 May 2024 through two half-day virtual sessions via Teams. The meeting was organised between 14 UTC and 18 UTC to stimulate international participation. The organising team was composed of Martin Dameris (DLR), Daan Hubert and Nathalie Kalb (BIRA-IASB), Michiel van Weele (KNMI), and Michael Eisinger (ESA). The workshop was divided in two sessions: a tropospheric ozone session on the first day and a stratospheric and total ozone session on the second day. The workshop was attended by 60 international participants for the tropospheric session and by 66 participants for the stratospheric session. A total of 50 participants attended both days with an average attendance time of three and a half hours.

The agenda and the abstracts and video per presentation are available on the workshop website: https://events.spacepole.be/event/185/

The website content including the agenda is copied in the Appendix of this report.



2 Workshop Summary

The first day of the workshop program was focused on *Tropospheric Ozone*.

The workshop was opened by **Martin Dameris** (**DLR**) and the workshop objectives were shortly summarized.

The day started with a Keynote presentation by **Roeland van Malderen** (**KMI/IRM**) on the **Harmonization of tropospheric ozone data for TOAR II.** An overview was given on the key results of the first phase of the Tropospheric Ozone Assessment Report (TOAR-I) and the focus working groups in TOAR-II were shortly introduced. Extra attention was given to the focus working group (FWG) on satellite data and the FWG HEGIFTOM (Harmonization and Evaluation of Ground-based Instruments for Free Tropospheric Ozone Measurements). The harmonization in TOAR-II is coordinated with WMO and WOUDC.

The second presentation was given by **Daan Hubert** (**BIRA-IASB**), science leader of the Ozone_cci+ project. He presented a recent **Overview of tropospheric ozone Climate Data Records by ESA CCI**. Different measurement techniques are employed in the project, which result in CDRs that encode different information about tropospheric ozone:

- Convective Cloud Differential technique, applied to GOME-type sensors (1995-present, 20°S-20°N, 1 column between surface and 270 hPa).
- Limb-Nadir Matching technique, applied to the merged CCI total ozone and limb profile data sets (2004-present, global, 1 column between surface and thermal tropopause, or 3 km below).
- Profile retrieval technique, applied to nadir observations: 1995-present (GOME-type) or 2008-present (IASI), global, two columns in troposphere.

The Intercomparison and validation studies are currently ongoing. Public release of new/improved tropospheric ozone Climate Data Records is expected by late 2024. In 2025 ESA's Climate programme continues with, a.o., further algorithm development for the tropospheric ozone CDRs.

The workshop was continued with presentations by the user community.

The first speaker in this session was **Dave Plummer (ECCC)** on **Bringing chemistry climate models and observations together: Our experience with CCMI.** He showed that models do have biases in their climatological mean state while the sources of these biases can be difficult to understand. Modelers do have a significant interest in analyzing trends. At the same time, trends in observations can be daunting to work with given the internal variability in models and the real world, observational uncertainties and the sampling patterns for observations.

The next presentation was by Kazuyuki Miyazaki (NASA JPL) on Shifting patterns of global emissions and tropospheric ozone linked to human activity and natural processes derived from a decadal chemical reanalysis. He showed the results from JPL's Tropospheric Chemical Reanalysis and preparation for the new reanalysis (TCR-3) in preparation using the decadal Aura



era as well as data from newer satellites, e.g. to study global shifts in the anthropogenic NOx emissions.

This presentation was followed by the talk by **Viktoria Sofieva (FMI)** on **Tropospheric ozone column datasets by combining nadir and limb satellite measurements**. Viktoria Sofieva derived a tropospheric ozone data record by subtracting the stratospheric integrated profile based on limb observations from a total ozone record based on nadir observations. The tropospheric ozone column is defined either up to the tropopause, to 3 km below the tropopause and/or to the ozonopause determined by a criterium (3.5 DU / km) on the ozone vertical gradient in the UTLS. The presented uncertainties in the tropospheric ozone column is typically of the order of ~5 DU. The trends per latitude band are mostly not significant.

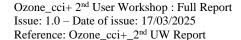
After the break, the first speaker was **Natalya Kramarova** (**NASA GSFC**) on **Decade-long ozone record from Suomi NPP OMPS.** The ozone data records based on MLS v5 and OMPS v2.6 were presented. A lower limit of about 12.5 km for OMPS limb is given, although this limit might be lowered to 8.5 km in the future. The 8.5 - 12.5 km layer typically contains 5 - 30 DU, i.e. large relative variability with sometimes quite significant ozone amounts. There is a broad averaging kernel using limb observations below 12.5 km.

This talk was followed by the presentation by **Andrea Orfanoz-Cheuquelaf (IUP Bremen)** on **Long-term tropospheric ozone column from SCIAMACHY+OMPS.** Andrea Orfanoz-Cheuquelaf presented the limb and nadir data records of both SCIAMACHY (ESA Envisat) for 2002-2012 period and OMPS for 2012 up to present day. To remove the bias from the combined time series the OMI-MLS data set has been used as a transfer function, also making use of the seasonal cycle.

Next, Elyse Pennington (NASA JPL) presented on the Quantification and evaluation of tropospheric TROPESS ozone trends using CrIS, AIRS, and OMI satellite products. Elyse Pennington focused on the use of CrIS, AIRS and OMI (collections 3 and 4) in common retrievals. Differences are related to e.g. sampling and vertical sensitivity of the instruments. Satellite-sonde biases are found on the order of 10% using sonde observations within 300 km/9 hours distance.

In his contribution to the user workshop Klaus-Peter Heue (DLR) presented on Tropical Tropospheric Ozone observed by European Satellites from ERS-2/GOME (1995) to S5P/TROPOMI (2024) and resulting trends. Klaus-Peter Heue presented homogenized tropospheric ozone data records capped at either the 200 hPa or the 270 hPa pressure level. Derived ozone trends are positive for the period 1995-2007 (+1 DU/decade) and negative for the period 2008-2023 (-0.6 DU/decade). For the analysis of the monthly mean data records a minimum of 20 sonde measurements per month is proposed. The SHADOZ ozone sonde network is essential for such evaluations, as well as the HEGIFTOM initiative on data homogenization.

The last presentation of the first day of the workshop was given by **Paul Griffiths (NCAS Cambridge)** on **Tropospheric ozone in CMIP6**. Paul Griffiths explained the model intercomparisons taking place e.g. in the framework of AerChemMIP and the importance of a





better understanding of the cause of model-to-model differences. He observed that over time the number of models participating in the intercomparisons is decreasing which is unfortunate. Although model validations with satellite data are typically considered more complex than using in-situ data sets such as ozonesondes, these data sets provide a complementary perspective. The comparisons are sensitive to a consistent definition of the tropopause in the data sets and models. Models indicate that the stratospheric ozone recovery will lead to an increase in tropospheric ozone after 2040 even in case ozone precursors would turn over before 2040. Also, surface ozone is found sensitive to stratospheric ozone. Climate change will also impact the tropospheric ozone burden and better insight is needed in the ozone production and loss terms and their changes for which satellite-based ozone precursor data sets could play an important role.

The discussion on user needs for tropospheric ozone at the end of Day 1 was moderated by Michiel van Weele (KNMI). Seed questions were used to open the discussion. The seed questions presented included:

- Would you prefer one unified ('best') multi-instrument tropospheric ozone data set, or would you consider multiple single instrument-based data sets as more useful?
- For multiple single instrument-based data sets: what (additional) information would you need to intercompare/analyze these data sets?
- What experiences in using tropospheric ozone data sets do you have? What challenges do you foresee? And:
- What do you think would be needed to increase the quality and usefulness of tropospheric ozone data products as provided by ESA ozone_cci? Finally:
- How could we further increase the use and visibility of the ESA's ozone data sets and which actions should the team prioritize?

An important element of the discussion on the first day was to receive further feedback on the different tropospheric ozone products developed through the ESA Ozone_cii+ project.

The second day of the workshop program was focused on *Stratospheric Ozone and Total Ozone*.

The workshop was re-opened by **Martin Dameris** (**DLR**). The stratospheric session started with two Keynote presentations.

The first Keynote was presented by **Susan Solomon (MIT)** under the title **On today's challenges** in understanding the ozone layer. In this talk, Susan Solomon provided a personal perspective on current challenges in the field of stratospheric ozone science and observing. She summarized her view of current challenges, inspired by both expected and unexpected events, including the evaluation of the emergence of ozone recovery (or not), wildfire smoke, and the eruption of the Hunga Tonga volcano. Important events included the prolonged ozone holes in recent years and the key role of chemical ozone depletion during the month of September, wildfires that are reaching (or not) the stratosphere and the uncertainty in the ozone trends, even in the upper stratosphere and more evident in the lower stratosphere. Systematic model evaluations are needed, e.g. to address the differences between modeled and observed ozone in the lowermost stratosphere.



The second Keynote was presented by **Paul Newman** (**NASA GSFC**) on **The 2026 WMO/UNEP Ozone Assessment.** Paul Newman has been co-chairing the WMO UNEP ozone assessments for 17 years. In 2022, one of the key findings was on the decline in the ODS emissions, while policy action in 2019/2020 on lingering CFC-11 emissions was successful. Recovery of the ozone layer in the 21st century will be dependent on increasing greenhouse gases, most notably N₂O, CH₄ and CO₂. Scientifically, uncertainties in lower stratospheric ozone and concerns of the impact of a reduction in tropical total ozone will need further attention. In the 2026 ozone assessment similar aspects will be important as in the 2022 assessment, including strengthened controls, new substances, and the more general question: are the implemented policies working?

In the next presentation **Daan Hubert** (**BIRA-IASB**), science leader of the Ozone_cci+ project, gave an **Overview of stratospheric and total ozone Climate Data Records by ESA CCI.** Daan Hubert explained the relation between the operational production of ozone data records by C3S and the research and development in the Ozone_cci project of ESA. The GTO-ECV product is currently based on 7 ESA sensors and 1 NASA sensor (OMI). The multi-sensor reanalysis by KNMI (MSR-2) has been extended backwards to the 1960s using ground-based observations. For the nadir-based ozone profiles a data release is expected in early 2025 based on 5 sensors. Through HARMOZ a common format is provided for all limb sensors measuring stratospheric ozone.

These introductions were followed by a couple of presentations by the user community.

First, May Chim (NCAS Cambridge) presented a talk with the title: Future volcanic eruptions delay healing of the Antarctic ozone layer. May Chim explained that in CMIP6 constant volcanic forcings are applied instead of zero forcing as before. A question to pose is: do future eruptions in stochastic scenarios lead to an earlier or a delay in Antarctic ozone recovery? A few years (3 to 6 years) delay could be possible. As a side note, she also reminded of the volcanic forcings other than SO₂.

In the next presentation, Samuel Benito-Barca (U. Madrid) presented on the Role of natural variability and ozone transport in understanding recent trends in lower stratosphere ozone. Samuel Benito-Barca presented results from the CCMI-2022 models and observed trends over 1998-2018 including negative trends at tropical latitudes due to increased upwelling, while at midlatitudes the situation is still unclear, mainly because the CCMs are not able to reproduce the observed patterns. However, models in CCMI-2022 are doing better on natural variability.

After the break, Melanie Coldewey-Egbers (DLR) kicked off by presenting for the Ozone_cci project The coherent set of total ozone and ozone profile climate data records based on a series of GOME-type nadir UVN satellite sensors. Melanie Coldewey-Egbers presented the total ozone data record (GTO-ECV) that fulfils the GCOS stability requirement of less than 1% per decade. The long-term ozone profile record (GOP-ECV) record uses the GTO-ECV as extra constraint on the integrated profile to produce profiles for 14 layers on 5x5 lat-lon grid.



After this presentation Lawrence Flynn (NOAA) presented on the Performance of NOAA S-NPP OMPS Nadir Instruments for Long-term Ozone Records. Lawrence Flynn presented the V8TOz algorithm used for OMPS nadir instruments and discussed the importance of an analysis of instrument drift for nadir UV ozone profile observations. The S-NPP V8TOz ozone record is compared to ground-based Dobson stations.

Representing the Ozone_cci+ project, **Viktoria Sofieva** (**FMI**) presented on the **Merged long-term datasets of ozone profiles developed in the ESA Climate Change Initiative.** The merged SAGE-CCI-OMPS+ data record is an important achievement of Ozone_cci and encompasses multiple limb instruments starting from observations by SAGE II in 1984 and includes currently operating instruments such as OMPS-LP on SNPP and SAGE III on ISS. The record is used to study long-term trends in the stratospheric ozone profile as well as in the stratospheric ozone column for which a monthly-mean data set has been made available. While recently positive trends in the stratospheric ozone profiles are found e.g. at 25 km in the Southern Hemisphere, negative ozone trends pertain below 25 km at tropical latitudes.

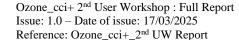
The next presentation was by Yue Jia (NOAA) on SWOOSH ozone updates, their implications for variability and trends, and preparing for the loss of the Aura Microwave Limb Sounder. Yue Jia presented the SWOOSH (Stratospheric Water and OzOne Satellite Homogenized) updated (V2.7 beta release) merged data record for 1984 to present day based on Aura MLS v5.0. The data set consists of monthly mean profiles on a grid of 5 degrees latitude and 20 degrees longitude with 3.3 km steps in the vertical dimension ranging from 10 to 60 km altitude. Long-term stability of the combined data set is achieved. OMPS-LP is considered the primary ozone data source for SWOOSH after MLS.

The discussion on user needs for stratospheric and total ozone at the end of Day 2 moderated by Michiel van Weele (KNMI) and followed the same structure as on Day 1. Seed questions were also very similar as for the discussion on tropospheric ozone (see the questions presented above). An important element of the discussion on the second day was to receive further feedback on the different stratospheric and total ozone products developed through the ESA Ozone_cci+ project.

3 Workshop Outcome and Recommendations

The outcome of this second workshop, synthesized in a set of recommendations, will be taken on board when preparing the next phase of the Ozone_cci+ programme of ESA.

A general recommendation of the workshop participants to the team is to come up with a clear strategy on how to promote the new Ozone_cci data records as soon as these become available (end 2024/early 2025) and also to provide a concise guide to users on how to access and reference these data sets.





Specific recommendations on **tropospheric ozone** include:

- For all tropospheric ozone products provide the days/orbits (sampling) contributing to the monthly mean data sets of Ozone_cci;
- On the longer term, investigate together with modellers if/how ozone production and ozone loss changes and variability might be inferred from the ozone data records, potentially including data sets from the Precursors CCI team in the analysis.

Specific recommendations on **total ozone** include:

 For the Level-3 long-term total ozone data records, including the backward extended MSR data set, it is considered important that these records are being continued and that Level-2 total ozone data is made readily available for assimilation by modellers. The Ozone_cci total ozone data records are considered a welcome and important contribution in support of the upcoming WMO/UNEP ozone assessment.

Specific recommendations on **stratospheric ozone** include:

- Long-term stratospheric ozone profile data products, including the merged limb products of Ozone_cci are a crucial input to the upcoming WMO/UNEP ozone assessment and need to be extended in time;
- The stratospheric ozone column is considered by some users as an important CDR as well, i.e. next to the total ozone products and tropospheric ozone products provided by the team. Users suggest to investigate how this product could be added to the portfolio of Ozone_cci on top of the existing products, e.g. as the integrated vertical profile and/or the difference between total and tropospheric ozone. For some products this could be equivalent.
- On the longer term, investigate the role of transport processes together with modellers for how ozone changes and variability at different altitudes next to the trends related to the stratospheric chlorine loading (EESC)



Appendix

This appendix contains a copy of the information contained on the website of the user workshop: https://events.spacepole.be/event/185/

On the website of the user workshop the abstracts and videos per presentation are provided in addition.

Background and Workshop Objectives

Background

The European Space Agency's Climate Change Initiative (CCI) aims to realise the full potential of the long-term Earth Observation archives collected by ESA and Third Party satellite missions. Since 2010, the Ozone CCI team (https://climate.esa.int/en/projects/ozone) has been developing, maturing, generating and sustaining multiple complementary multi-decadal satellite ozone Climate Data Records (CDRs) tailored for climate monitoring, climate research and climate modelling applications. The CCI portfolio consists of total and tropospheric ozone column data products as well as vertically resolved ozone products by nadir and limb-viewing sensors.

Workshop objectives

This second user workshop will be an online event, aimed at

- bringing together scientists involved in the generation of ozone Climate Data Records, as well as (potential) users of such multi-decadal ozone time series, and the broader ozone and climate communities;
- presenting the state of the art in ozone Climate Data Record production;
- discussing results from major Climate Data Record users, e.g., stratospheric ozone assessments for WMO/UNEP, tropospheric ozone assessments for TOAR II, studies focusing on UT/LS, evaluation of climate modelling, data assimilation and reanalysis;
- collecting and updating user requirements for ozone Climate Data Records;
- discussing remaining challenges for the generation of ozone Climate Data Records.



Scientific Programme

The workshop consisted of two MS Teams sessions with a duration of 3:45, both starting at 14h UTC on 28 and 29 May 2024, respectively.

Tropospheric ozone (Tue 28 May)

- **Keynote Dr. Roeland Van Malderen** (KMI, Belgium): *Harmonization of tropospheric ozone data for TOAR II*
- Overview of tropospheric ozone Climate Data Records by ESA CCI
- Oral presentations by user community
- Discussion of user needs and requirements

Stratospheric (and total) ozone (Wed 29 May)

- **Keynote Prof. Susan Solomon** (MIT, USA): *On today's challenges in understanding the ozone layer*
- **Keynote Dr. Paul Newman** (NASA GSFC, USA): *The 2026 WMO/UNEP Ozone Assessment*
- Overview of stratospheric and total ozone Climate Data Records by ESA CCI
- Oral presentations by user community
- Discussion of user needs and requirements

Organising Committee

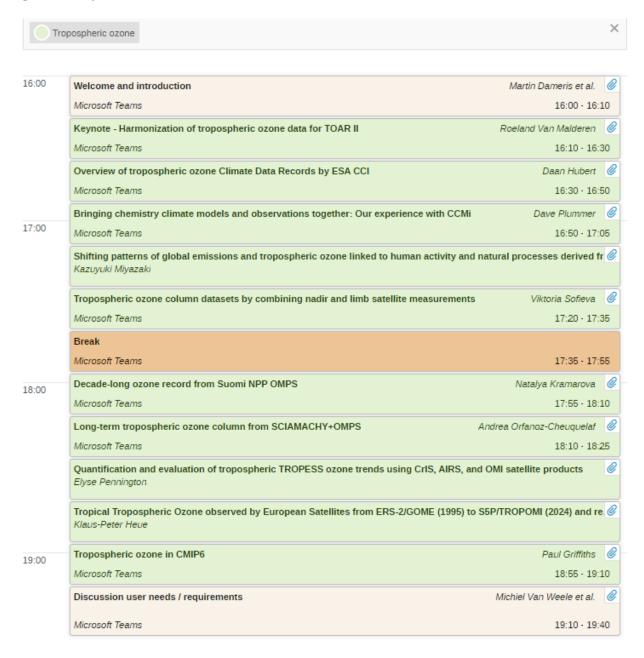
- Dr. Martin Dameris (DLR, Germany)
- Dr. Michiel van Weele (KNMI, The Netherlands)
- Dr. D. Hubert (BIRA-IASB, Belgium)
- Mrs. N. Kalb (BIRA-IASB, Belgium)
- Mr. Michael Eisinger (ESA ECSAT, UK)



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Reference: Ozone_cci+_2nd UW Report

Agenda (Day 1)





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Reference: Ozone_cci+_2nd UW Report

Agenda (Day 2)\

