esa

Ozone_cci+

User Workshop Full Report

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Ozone_cci+

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1 Introduction

Background

The European Space Agency Climate Change Initiative (ESA-CCI) aims to realise the full potential of the long-term global Earth Observation archives that ESA, together with its member states, has established over the past 30 years. This workshop focuses on the generation and exploitation of CCI's harmonised multi-decadal Climate Data Records (CDRs) of atmospheric ozone observations suitable to assess long-term changes in total ozone and its vertical distribution, and their interaction with climate change.

Objectives

The aim of this workshop was to bring together scientists involved in the generation of ozone CDRs, data users of ozone CDRs, and the broader ozone community, in order to

- present the state of the art in ozone CDR production,
- discuss results from major CDR users (e.g. stratospheric and tropospheric ozone assessments, research of the upper troposphere and lower stratosphere (UTLS) region, evaluation of climate modelling results, data assimilation and reanalysis),
- collect and update user requirements for CDRs from current and future Earth Observation (EO) missions, and
- discuss remaining challenges for the generation of ozone CDRs.

The Ozone_cci User Workshop was held on Tuesday 16 and Wednesday 17 March 2021 through 2 half-day virtual sessions via Webex. The organising team was composed of Martin Dameris (DLR), Michel Van Roozendael (BIRA-IASB), Michiel van Weele (KNMI), Melanie Coldewey-Egbers (DLR), Viktoria Sofieva (FMI), Jean-Christopher Lambert (BIRA-IASB), Daan Hubert (BIRA-IASB), Nathalie Kalb (BIRA-IASB), and Christian Retscher (ESA).

The workshop was attended by just over 100 international participants on both days.

The presentations and their abstracts are available on the workshop website and on the Ozone_cci website.

The recordings of the sessions are available here:

Ozone CCI User Workshop 2021 - Climate Data Records and Quality Assessment 1:
https://www.youtube.com/watch?v=y3afwyspGME&list=PLBWo25itnDz-0EpdqMqCxMimgAlw5-wtX&index=5&t=1264s

0:00	Introduction
19:20	Katerina Garane
42:38	Melanie Coldewey-Egbers
58:50	Richard Siddans
1:18:03	Arno Keppens

Ozone CCI User Workshop 2021 - Climate Data Records and Quality Assessment 2:

https://www.youtube.com/watch?v=TzcTkZuEWm4&list=PLBWo25itnDz-0EpdqMqCxMimgAlw5-wtX&index=4&t=3526s
0:00 Viktoria Sofieva
18:57 Daan Hubert
42:43 Jean-Christopher Lambert
58:44 Discussion

Ozone CCI User Workshop 2021 - Scientific use of Ozone_cci data 1:
https://www.youtube.com/watch?v=JLoHly-ZrWY&list=PLBWo25itnDz-0EpdqMqCxMimgAlw5-wtX&index=3&t=5507s
0:00 Introduction
2:38 Birgit Hassler
20:45 Wolfgang Steinbrecht
46:36 Jessica Neu
1:08:42 Peter Hoor
1:31:40 Stacey Frith

Ozone CCI User Workshop 2021 - Scientific use of Ozone_cci data 2:
https://www.youtube.com/watch?v=-cJaCQtGDaI&list=PLBWo25itnDz-0EpdqMqCxMimgAlw5-wtX&index=2
0:00 Hella Garny
25:18 Antje Inness
47:22 Discussion
1:24:30 Closing remarks

2 Workshop Summary

The first day of the workshop program was focused on ***Ozone_cci Climate Data Records (CDRs) and Quality Assessment***. The workshop started with presentations by the CCI team of the ozone climate data records in the CCI portfolio. Further, it was explained how the ozone CDRs are created within Ozone_cci, and data main characteristics and data availability were discussed, together with an overall assessment of data quality.

The workshop was opened by **Martin Dameris**, representing the Climate Research Group (CRG). A welcome note was given by **Christian Retscher**, representative from ESA on the ESA Climate Change Initiative (CCI) programme. Among others he mentioned that more than 10 years of research on ozone Climate Data Records (CDRs) have been successfully carried out. Many ozone CDRs are now available, which were presented and discussed in this workshop.

Michel Van Roozendael presented an introduction to the ESA project Ozone_cci, which was started over 10 years ago as part of the ESA programme on Climate Change with the ambition for high quality climate data records on Essential Climate Variables. Currently 21 ECVs are addressed in the programme, in close collaboration with the Copernicus Climate Change Service (C3S) led by ECMWF. The Ozone_cci project provides the pre-operational development for the operational climate services. All Climate Data Records are open access.

Melanie Coldewey-Egbers presented the GOME-type Total Ozone Climate Data Record (GTO-ECV) based on GOME/ERS-2, SCIAMACHY/Envisat, GOME-2 (MetOp A/B) and TROPOMI/Sentinel-5P including monthly means on 1x1 degrees spatial resolution covering 25 years. A few scientific highlights on the use of the GOME-type Total Ozone CDR based on the most recent CDR using the GODFITv4 algorithm were presented. See Figure 1 below.

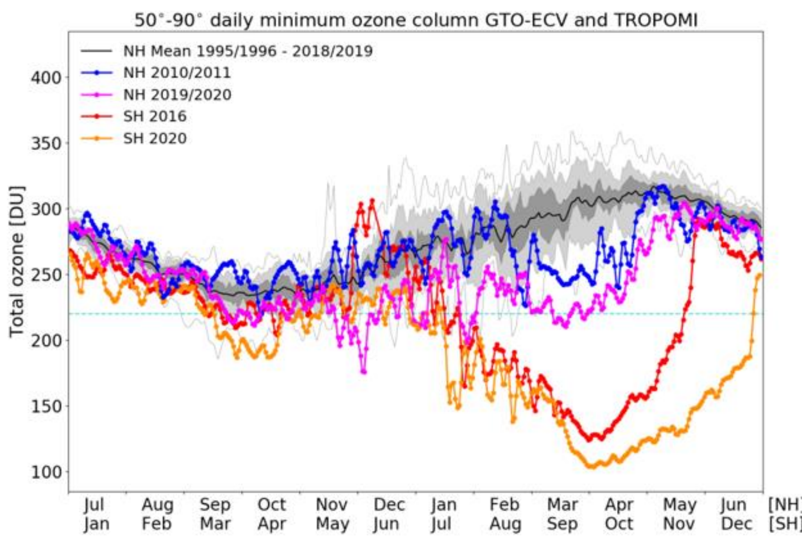

Figure 1: Annual cycle of the daily minimum total column ozone values in the north polar region (50°-90°N) and in the south polar region (50°-90°S) derived from the European satellite data record GOME-type Total Ozone Essential Climate Variable (GTO-ECV) from July 1995 to June 2019 and from TROPOMI/Sentinel-5 Precursor data from July 2019 to December 2020. The thick black line shows the GTO-ECV mean annual cycle in the north polar region and the thin black lines indicate the corresponding maximum and minimum values for the complete time period starting in 1995. The grey shadings denote the 10th and 90th percentile (light grey) and the 30th and 70th percentile (dark grey), respectively. The blue and magenta lines show the minimum values in the north polar region in the years 2010/2011 and 2019/2020. The red and orange curves show the minimum values in the south polar region in the years 2016 and 2020, respectively. The Southern Hemisphere data are shifted by 6 months. Update from Dameris et al. (2021b)

A detailed quality assessment of the Level-2 and Level-3 total ozone column data records (GODFITv4) using the ground-based networks with excellent correlation were presented by **Katerina Garane**. The CDRs shown cover the period from July 1995 (GOME) to the end of 2020 for the subsequent ESA satellite instruments for total ozone column observations. The Level-3 climate data record (GTO-ECV) in the C3S, currently covering 25 years, is in close agreement to the Level-2 CDRs, with no significant drifts over time. It is concluded that both Level-2 and Level-3 Total Ozone products fulfil the requirements in terms of bias uncertainty and long-term stability.

As shown in an overview of the Ozone_cci ozone profile CDRs from nadir sensors, given by Richard Siddans, Nadir UV sensors and Nadir IR sensors both provide tropospheric ozone as well as stratospheric ozone products. Quite a few papers emerge from these data sets and some recent studies related to biomass burning events were highlighted. The longest IASI-based CDRs currently cover close to 15 years since the launch of the first IASI instrument on the MetOp-A platform.

An in-depth analysis of the quality assessment of the Level-2 nadir ozone profile CDRs from Ozone_cci and the Level-3 CDRs made available within C3S were given by **Arno Keppens**. Various validation data sources were considered including ground-based networks of WOUDC, SHADOZ, NDACC (a.o.). Biases and drifts of the nadir sensor derived CDRs relative to ozone sondes were shown as function of altitude.

Viktoria Sofieva presented an overview of the Level-2 and Level-3 ozone profile CDRs based on Limb and Occultation sensors including MIPAS, GOMOS, SCIAMACHY, OMPS-LP and ACE-FTS. Harmonized individual and merged CDRs were presented ultimately covering the period 1984 to 2020, including SAGE II data (a.o.). For individual instruments monthly zonal-mean data sets have been created. Recent results on altitude-dependent and regional ozone trends were presented in order to evaluate (the presence of significant) ozone recovery. See Figure 2 below.

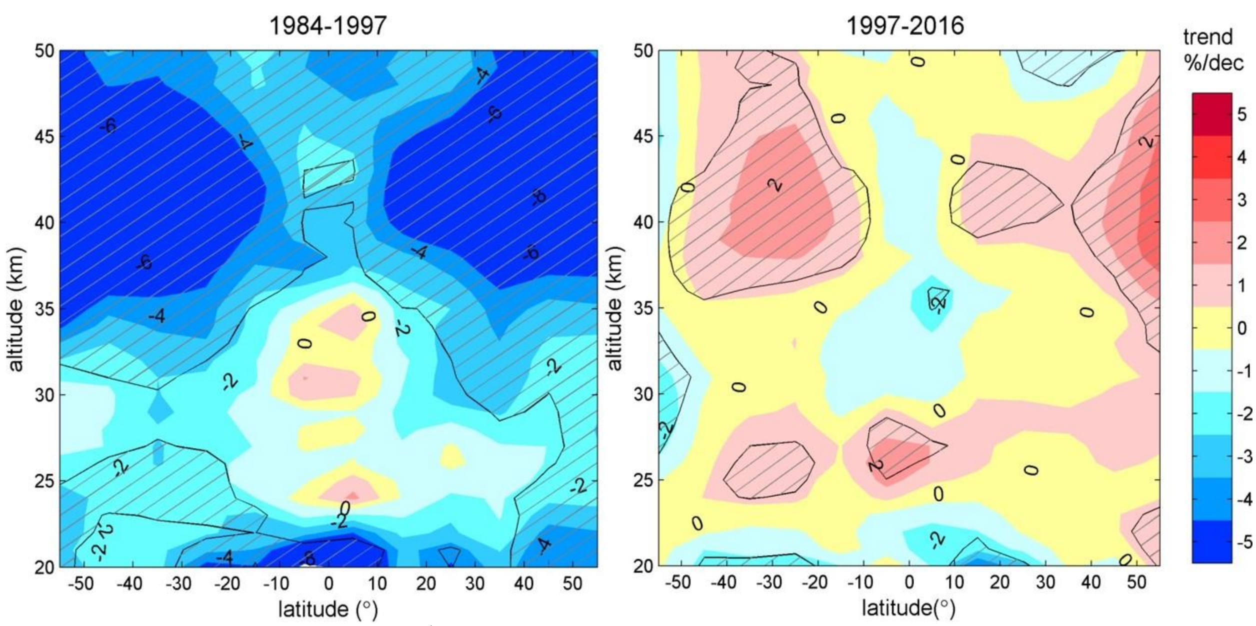

Figure 2: The ozone trend (% decade^{-1}) for different latitudes for 1984–1997 (left) and 1997–2016 (right). Shaded areas show regions where trends are statistically different from zero at the 95% level. Reproduced from (Sofieva et al., 2017).

A detailed quality assessment of the Ozone_cci Limb ozone profile CDRs by independent ground-based networks was discussed by **Daan Hubert,** including observations from ozone sonde, microwave radiometer and lidar ground-based networks. Results on bias, dispersion and drift were reported for a set of instruments and the derived CDRs. For Level-3 CDRs covering the 2001-2019 time period the granularity of the data record is most coarse because limb-based profiles are merged and gridded mostly to zonal monthly mean profiles. Most limb-based CDRs provided through Ozone_cci comply with user requirements. Detailed evaluation of the (merged) gridded limb CDRs is still considered a challenge. Recommendations on how to make best use of the Ozone_cci CDRs were given.

The user requirements in relation to data validation and quality assessment were introduced by **Jean-Christopher Lambert**. Validation requirements include aspects on the data products including e.g. altitude registration and important diagnostics such averaging kernel, viewing geometry and many other quantities that affect retrievals. Validation of merged and assimilated data sets has specific issues requiring specific attention w.r.t. propagation of uncertainties to trace back analyses e.g. to the underlying observations used for the merging/assimilation. Lessons learnt w.r.t. validation, and remaining challenges, were discussed, as well as validation requirements for upcoming satellite missions such as Altius and the observations from geostationary platforms.

The **discussion** at the end of Day 1 was moderated by **Jean-Christopher Lambert** and **Viktoria Sofieva**. It was remarked that the long-term GOME-type nadir-based profile data records might become more and more valuable for trend studies, complementing (or challenging) the unique NASA SBUV-type ozone profile data record. However earlier limitations w.r.t. stability of shortest UV bands and the limited vertical resolution in nadir, were also highlighted. This is particularly critical in the UTLS, a region very sensitive to climate that cannot be properly resolved with nadir sensors. Moreover, other species as measured e.g. by MLS are also needed to understand ozone chemistry. Long-term limb observations are certainly not a luxury.

While merged and gridded data sets are a logical choice for many users including chemistry-climate modelers, for other applications such as assimilation individual instrument-specific Level-2 data records qualify best. Continuation from reanalysis to near-real time data provision with only weeks to at most a month delay would prevent sudden changes in the prolongation of existing reanalysis records. The use of a data set in assimilation is further dependent on its uniqueness and long-term consistency (do not change versions too often). Bias and stability are very important in the evaluation of data set performance within the assimilation framework. A concrete recommendation was to create overlap periods for subsequent CDRs of a few years for consistency in reanalysis data sets.

Representativeness in validation was considered important. Concurrently the need to increase the frequency and spatial coverage of FRM data was pointed out, raising questions on how to ensure their sustainability. It was stressed that a more structural cooperation is needed across agencies. Finally, the potential impact on satellite validation of the recently reported post-2013 drop-off in total ozone at some stations of the ozone sonde network was highlighted.

Research applications of the Ozone_cci climate data records

The **second day** of the workshop focused on the use of Ozone_cci data in various studies and frameworks. The presentations were given by invited external researchers on selected scientific topics and international initiatives to which Ozone_cci climate data records provide (or could provide) important contributions.

Birgit Hassler in her presentation emphasized the specific need of consistent long-term data sets for ozone research. She introduced the main research questions of the upcoming 2022 WMO/UNEP Ozone Assessment, as well as the overall timeline of the report preparation. She pointed out where ESA-CCI ozone data was already used in analyses for previous WMO/UNEP Ozone Assessments, the SPARC project Long-term Ozone Trends and Uncertainties in the Stratosphere (LOTUS; https://www.sparc-climate.org/activities/ozone-trends/), and the Tropospheric Ozone Assessment Report, Phase I (TOAR-I, 2014-2019; https://igacproject.org/activities/TOAR/TOAR-I).

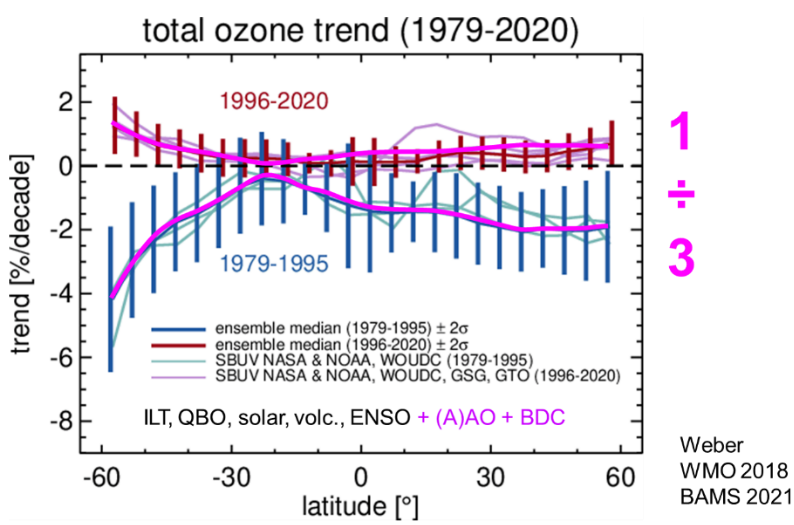

Figure 3: Total ozone trends as a function of latitude, and for the two periods 1979 to 1995 (blue colours, negative trends), and 1996 to 2020 (reddish colours, positive trends). Trends were estimated by multiple linear regression, using proxies for independent linear trends, QBO, solar cycle, volcanic aerosol, El-Nino/Southern Oscillation, Arctic and Antarctic Oscillation (AO and AAO), and strength of the Brewer-Dobson Circulation (BDC). The thin lines show observed trends from individual merged satellite data sets. The thick lines with error bars show the latitude dependent trends of the median of the different merged satellite datasets. From the long-time increase and decline of effective equivalent stratospheric chlorine loading (EESC), a fast increase until 1995, and a three times slower decline since 1996, one might expect a 3 to 1 ratio also for the ozone trends. The magenta lines in the figure show that simulated and observed ozone trends indeed follow this expectation, provided dynamical proxies are included in the multiple linear regression (AO, AAO, BDC). Update from Weber et al. (2018) and WMO (2018).

In his talk **Wolfgang Steinbrecht** focused on trends in total column and stratospheric ozone. While ground- and space-based observations show that the large ozone decline from the 1970s to the 1990s has been stopped, thanks to the international ban of ozone depleting substances by the Montreal Protocol and its amendments, so far only the regions of largest ozone depletion, the upper stratosphere and the Antarctic ozone hole, show clearly improving trends. The slope of the expected recovery is about three times slower than the fast decline from the 1970s to the 1990s (Figure 3).

In her presentation of an assessment of tropospheric ozone by TOAR-II, **Jessica Neu** Introduced the intercomparison of time series from multiple satellite instruments undertaken as part of the Tropospheric Ozone Assessment Report – Phase I (TOAR-I), which shows substantial differences in the net change in ozone over the past decade. Given the importance of tropospheric ozone as a greenhouse gas and a hazardous pollutant that impacts human health and ecosystems, it is critical to quantify and understand long-term changes in its abundance. In TOAR-II the possible sources of differences in these datasets are discussed and methodologies will be developed for quantifying expected differences in the ability of each product to better capture long-term variations in tropospheric ozone.

Based on OCTAV-UTLS, **Peter Hoor** mentioned that the ozone distribution in the UTLS is affected by the Brewer-Dobson Circulation (BDC) as well as transport across the tropopause and the jets. Complications arise particularly from the short-term variability of the tropopause and jet locations, which introduce variability in the ozone distribution. Examples of the remapping of the observations in jet- or tropopause-based coordinates with the JETPAC tool using MERRA-2 reanalysis data demonstrate a reduction in the ozone variability.

Stacey Frith showed a comparison of GTO-ECV and MERRA-2 including further plans. The adjusted MERRA-2 product combines the high spatial and temporal resolution of the MERRA-2 assimilation with the long-term consistency of the SBUV merged satellite record. The consistency between both products spatially and in time was discussed.

The results of an interesting comparison of observational ozone data to chemistry-climate models was discussed by **Hella Garny**. Chemistry-climate models have been developed and used extensively over the last decades to project the future development of the stratospheric ozone layer. At time periods shorther than about 2 decades, internal variability strongly influences ozone trends and therewith complicates conclusions on (dis-)agreement between modelled and observed time series. In the lower stratosphere observational data indicate a decline in ozone mixing ratios in a broad latitudinal region extending well into the mid-latitudes, while models predict an ozone decline only in the tropics, but an increase in mid-latitudes. It is concluded that the observed mid-latitude lower stratospheric ozone trend is an extreme value given the model distribution. Possible reasons explaining this discrepancy are reviewed, including a possible misrepresentation of chemistry in models.

Finally, **Antje Inness** explained the CAMS current and planned ozone data assimilation activities, including plans for a CAMS-II reanalysis. In addition to meteorological reanalyses, reanalyses of the atmospheric composition have been emerging in the last decade. The EU funded Copernicus Atmosphere Monitoring Service (CAMS), implemented by ECMWF, has recently produced the so-called CAMS reanalysis (CAMSRA), which can be used to assess ozone anomalies, e.g. related to the ozone hole. The importance of good quality, long term datasets as input for future reanalysis activities was stressed, including the CAMS-II reanalysis production, which is scheduled to start in 2023 and the ERA6 reanalysis scheduled to start in 2024.

The **discussion** at the end of Day 2 was moderated by **Michiel van Weele** and **Martin Dameris**

The importance of the continuation of research activities within Ozone_cci was stressed, as well as the ongoing cooperation on the creation, intercomparison and analysis of the ozone CDRs deriving from the different space agencies.

The workshop participants consider the user needs on forecast and reanalysis as important as feeding long-term monitoring needs. Further, the participants stress the continued need of independent validation data records. These are needed next to satellite data records being used in the assimilation.

Continuation of limb observation capacity is required to mitigate important drawbacks of nadir-based ozone vertical profiles based trends for the UTLS vertical resolution and instrument stability at the shortest UV bands.

For the potential production of data sets in non-standard coordinates (useful for attribution studies), attention was drawn on a proper error propagation in the production of such climate data records.

Finally, the most important cross-ECV components that were mentioned by the participants for the use of the ozone CDRs were the ozone precursors in the troposphere (e.g. NO_2 and CO) as well as stratospheric water vapor and stratospheric aerosols in the stratosphere.

3 Workshop Outcome

In his concluding remarks, **Christian Retscher** stressed the importance of the ozone ECV project for the European Space Agency. Based on the presentations given during the two days of the workshop, it is clear that the project has gained a high visibility at the international level.

Among the important points that were raised in the discussions, he points out that:

- The community calls for new and improved merged data products
- There is a high potential for cross ECV work, in particular regarding ozone precursors (NOx, CO, HCHO), water vapour and aerosols
- CCI data are used as an independent validation data in a growing number of studies

He appreciates the comments from the users on the quality of the work performed in the Ozone_cci project. Users consider this activity as very useful for their work. The high impact of the project is also reflected in the number of scientific publications. People are specifically happy with the support the Ozone_cci consortium provides on related data sets. Further, they recommend pursuing the ongoing efforts and look forward to new and improved data sets. Nonetheless, users specifically stress the need for further developing merged products of vertically-resolved ozone data. They also express the specific interest on incorporating data from S-NPP and the future JPSS and Copernicus Sentinel-4 and -5 missions as well as the need for more cross ECV work.

Finally **Christian Retscher** acknowledges the important work of Claus Zehner, who managed the Ozone_cci project for ESA from the beginning of the CCI programme in 2010 until 2018.

The outcome of this workshop, synthesized in a set of recommendations, will be taken on board when preparing the next phase of the CCI+ programme and the future follow-up climate programme of ESA.

A shortened version of this report was published in the SPARC newsletter of July 2021 (Dameris et al, 2021).

4 Recommendations

R-1 Continue to deliver high quality data products, easy to access and well documented.

R-2 The quality and representativeness of the data products should be improved in the troposphere and in the UTLS.

R-3 Merged data sets are most useful for many users and motivate their further development. In particular, the production of a merged level-3 product of ozone profiles derived from GOME-type nadir sensors should be of high priority.

R-4 Level-2 data products are very important for assimilation in models (e.g. the CAMS reanalysis). The continuity and the consistency of the times series are critical for such applications. Moreover, interim climate data records should be produced with a maximum latency of one month after acquisition.

R-5 Overpass data series over known FRM sites should be made available to users

R-6 To help in data interpretation and process attribution, it is recommended to generate advanced ozone data sets in alternative coordinates (e.g. sorted according to equivalent latitude, tropopause altitude, PV, etc) with attention to the error propagation in such transformations. Alternatively, the ancillary parameters necessary to transform the data should be included in the product, as supporting information.

R-7 To support validation activities, the requirements on ozone data products should be refined and better categorised. E.g. requirements should distinguish between individual measurements, monthly means, etc.

R-8 There is a need to increase the frequency and coverage (representativeness) of Fiducial Reference Measurement (FRM) datasets.

R-9 A better use should be made of airborne reference data (e.g. IAGOS/CARIBIC) for evaluation of both satellite and model data.

R-10 The cooperation between related atmospheric ECV projects should be reinforced. A practical recommendation is to promote the use of common vertical coordinates across ECVs and use common data formats.

5 References

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