TOAR-II HEGIFTOM:

Description of the homogenized free-tropospheric ozone times series

IAGOS

Version	Author	Affiliation	Contact	Date
v0	Romain Blot	CNRS, LAERO, UT3	blot.romain@aero.obs-mip.fr	21/12/2021
v1	Romain Blot	CNRS, LAERO, UT3	blot.romain@aero.obs-mip.fr	06/07/2022

Data management plan

The IAGOS Data Management Plan (DMP) document is publicly available here: https://iagos.aeris-data.fr/documents/. The purpose of this document is to describe the data management life-cycle, and the plans for the data collected, processed, generated and published. The goal of the DMP is to describe the present situation and the operational IAGOS Data Centre. Furthermore, the DMP also describes the technical solutions agreed, that are currently under implementation, and outline the strategy and development needed towards making IAGOS data FAIR.TheDMP is a living document that will be updated regularly. The goal is to make the DMP accessible for all stakeholders (repository operators, funders, researchers, publishers, infrastructure providers etc.).

Data availability

The IAGOS ozone time series are in open access using the IAGOS data portal available at http://www.iagos.org/. A registration is mandatory in order to grant access to the data-set (https://iagos.aeris-data.fr/registration/#). This is not a way of restricting access. This is asked to keep track of users and usage, to facilitate access to the database through the web interface, to develop more user-friendly products and to consolidate the research infrastructure in the long term. The person responsible of the website and the IAGOS data center at CNRS in Toulouse (France) is Damien Boulanger (damien.boulanger@obs-mip.fr). The download instructions are provided here: https://iagos.aeris-data.fr/download-instructions/ and the data availability is shown here: https://iagos.aeris-data.fr/data-availability/?level=all&param=all&mission=all.

The data can be downloaded using a web Graphical User Interface (Gui): https://iagos.aeris-data.fr/download/#/. They are provided in NASA ames or NETCDF format. Note that it is possible to download only the profiles data over airports or the data of the entire flights for a selected time series through the IAGOS portal web Gui. The NASA Ames files follow the 1001 format. See the website for more information: https://badc.nerc.ac.uk/help/formats/NASA-Ames. The observations are delimited by the space delimiter.

Data policy

The IAGOS DATA POLICY is described here: https://iagos.aeris-data.fr/data-policy/. To summarize, IAGOS data is licensed under the Creative Commons Attribution 4.0 International licence (CC BY 4.0). Use of the data requires proper reference and citation of the IAGOS data, using the exact citation (including the provided DOI) as provided at the moment of upload from IAGOS, if applicable. By downloading the IAGOS data product you agree to the licensing conditions that apply to the data. Under this license derived products and redistribution are allowed, but you are required to always inform your users of the original source of the data used, refer them to the license text and the original source at IAGOS for possible updates or uploads.

We ask you to inform the data providers, traceable through the metadata connected to the provided DOI, when the data is used for publication(s), and to offer them the possibility to comment and/or offer them co-authorship or acknowledgement in the publication when this is justified by the added value of the data for your results.

In accordance with the IAGOS data policy, users of IAGOS data products are required to:

1. include the following acknowledgements in publications: "MOZAIC/CARIBIC/IAGOS data were created with support from the European Commission, national agencies in Germany (BMBF), France (MESR), and the UK (NERC), and the IAGOS member institutions (http://www.iagos.org/partners). The participating airlines (Lufthansa, Air France, Austrian, China Airlines, Iberia, Cathay Pacific, Air Namibia, Sabena) supported IAGOS by carrying the measurement equipment free of charge since 1994. The data are available at http://www.iagos.fr thanks to additional support from AERIS."
2. offer co-authorship to the IAGOS Principal Investigators if the IAGOS data play a significant role in the publication
3. identify themselves and provide contact information (valid email address)
4. provide a short description of the intended research

Points 3. do not apply to aircraft position data and metadata information that are released by the IAGOS data center for data discovery.

Data field description

- The minimum set of data fields available in the files along with the ozone data are the measurement UTC time, the aircraft longitude, the aircraft latitude, the aircraft barometric altitude, the aircraft radiometric altitude, the air pressure, the aircraft air speed, the aircraft ground speed, the total air temperature, the stagnation temperature, the wind direction, the wind speed, the zonal wind speed and the meridional wind speed. The units are described in the file headers or in the NETCDF file attributes. Additional aircraft data fields can be available in some files. The complete list is found here: https://iagos.aeris-data.fr/parameters/.

- Note that IAGOS program (including IAGOS-CARIBIC) are also known for performing additional atmospheric properties and component measurements such as (currently) relative humidity, water vapor, CO, NO, NOx, NOy, CO2, CH4, aerosol concentrations and cloud particles size distributions. See here for details: https://iagos.aeris-data.fr/parameters/

- The metadata contained in the file headers and in the attributes for the NETCDF format are fully described here: https://iagos.aeris-data.fr/data-format-2/. They provide information about the aircraft carrier (airline, serial number, aircraft type, etc...), the scientific instrument mounted on the aircraft (serial number), the contact information, the default value types for missing data, the measured parameters (short description, units, etc…), the data file downloaded (name, type, revision number, level of processing, etc…), the departure/arrival airports (name, date, location, etc…), etc…

Description of homogenization procedure

The measurement homogenization procedure is part of the IAGOS instrument maintenance and calibration process which are described here:

[1] *Philippe Nédélec, Romain Blot, Damien Boulanger, Gilles Athier, Jean-Marc Cousin, Benoit Gautron, Andreas Petzold, Andreas Volz-Thomas & Valérie Thouret (2015) Instrumentation on commercial aircraft for monitoring the atmospheric composition on a global scale: the IAGOS system, technical overview of ozone and carbon monoxide measurements, Tellus B: Chemical and Physical Meteorology, 67:1, 27791, https://doi.org/10.3402/tellusb.v67.27791.*

[2] *Blot, R., Nedelec, P., Boulanger, D., Wolff, P., Sauvage, B., Cousin, J.-M., Athier, G., Zahn, A., Obersteiner, F., Scharffe, D., Petetin, H., Bennouna, Y., Clark, H., and Thouret, V.: Internal consistency of the IAGOS ozone and carbon monoxide measurements for the last 25 years, Atmos. Meas. Tech., 14, 3935–3951, https://doi.org/10.5194/amt-14-3935-2021, 2021.*

To summarize, for IAGOS-MOZAIC and IAGOS-CORE, all the ozone instruments are compared to the same laboratory reference UV-photometer (ThermoFisher Model 49) before being mounted on the different aircraft that compose the IAGOS fleet. The laboratory ozone reference instrument is hold at the CNRS/LAERO in Toulouse which is the central calibration site for all the IAGOS-CORE/MOZAIC ozone instruments. The calibration and the linearity of the IAGOS reference ozone instrument is periodically checked using a ThermoFisher UV photometric ozone calibrator primary standard which is traceable to a National Institute of Standards and Technology (NIST) reference ozone instrument standard. This procedure remains the same since 1994. For IAGOS-CARIBIC, the UV photometer is controlled by comparison with a KIT custom-made laboratory O3 instrument (using a Hg lamp as light source) and a long-path UV reference photometer (UMEG GmbH) cross checked by the World

Meteorological Organization standard reference photometer no. 15 at the Swiss Federal Laboratories for Materials Science and Technology (EMPA) in Switzerland.

Data management

Flagging

- Both automatic and visual data housekeeping are performed for every fight time series (see [1]).
  - A data flagging scheme is applied and is described here: https://iagos.aeris-data.fr/data-quality/. The flags are also described in the file metadata and a flag value is attributed for each measurement point. However, for ozone, only good data are provided to the users.

Uncertainties

- Since we expect that the homogenization procedure shortly described above removes the possible systematic biases in the long-term time series (see also [2]), the resulting uncertainty should represent only the contribution from random errors.
- Initially, the Package 1 ozone measurement uncertainty results from the contribution of the uncertainty of the Package 1 UV photometer (±1ppbv), the uncertainty of the IAGOS Laboratory reference UV photometer (±1ppbv) and the uncertainty of the ozone calibrator primary standard (±1%). However, flight experience and maintenance experience show that the overall maximum uncertainty is about ±2ppbv ±2% (1σ; integration time is 4 seconds).
- For IAGOS-CARIBIC, the ozone measurement uncertainty is also ±2ppbv ±2%.
- The uncertainty is calculated and provided for each data point as metadata in the NASA AMES files and NETCDF files.

Traceability

Details about the instrument maintenance and calibration traceability are described in [1] and [2] and also in the Standard Operating Procedures (SOPs) documents available here: https://www.iagos.org/iagos-core-instruments/package1/. For each instrument, all maintenance actions are reported in a logbook and each instrument deployment (a flight period) is associated with a QA/QC document that reports:

i. all the flight operation events that could have an impact on the data
ii. the maintenance tasks before deployment
iii. the traceability references of the calibration primary standards
iv. the data corrections applied after calibration

v. the maintenance tasks after the deployment
vi. the internal consistency of the instrument measurements by inter-comparison with other IAGOS aircraft in operation using co-located profiles at airport location (See [2])

Internal consistency

As the homogenized IAGOS time series are traceable to the reference ozone photometer, they are internally consistent within the network. The internal consistency of the 1994 to 2020 IAGOS ozone time series have been furthermore demonstrated in the publication by Blot et al, 2021 [2].

External consistency

During the data validation/harmonization process, we regularly compare the IAGOS O3 profiles with the ozonesondes (WOUDC database) if available at nearby location. In the past, several papers were published showing comparisons between IAGOS, ozone sondes and surface stations in the troposphere. A non-exhaustive list is given below. Note that most of the studies that have used ozone sondes data could be revised using the updated homogenized ozone sondes dataset that is made available by roeland vanmalderen (roeland.vanmalderen@meteo.be) here: ftp://ftp-me.oma.be, accessible with account name “ozonesondes” and password “OzonFeb2021:”.

[3] *Logan, J. A., et al. (2012), Changes in ozone over Europe: Analysis of ozone measurements from sondes, regularaircraft (MOZAIC) and alpine surface sites,J. Geophys. Res.,117, D09301, doi: https://doi.org/10.1029/2011JD016952.*

[4] *Zbinden, R. M., Thouret, V., Ricaud, P., Carminati, F., Cammas, J.-P., and Nédélec, P.: Climatology of pure tropospheric profiles and column contents of ozone and carbon monoxide using MOZAIC in the mid-northern latitudes (24° N to 50° N) from 1994 to 2009, Atmos. Chem. Phys., 13, 12363–12388, https://doi.org/10.5194/acp-13-12363-2013, 2013.*

[5] *Staufer, J., Staehelin, J., Stübi, R., Peter, T., Tummon, F., and Thouret, V.: Trajectory matching of ozonesondes and MOZAIC measurements in the UTLS – Part 1: Method description and application at Payerne, Switzerland, Atmos. Meas. Tech., 6, 3393–3406, https://doi.org/10.5194/amt-6-3393-2013, 2013.*

[6] *Staufer, J., Staehelin, J., Stübi, R., Peter, T., Tummon, F., and Thouret, V.: Trajectory matching of ozonesondes and MOZAIC measurements in the UTLS – Part 2: Application to the global ozonesonde network, Atmos. Meas. Tech., 7, 241–266, https://doi.org/10.5194/amt-7-241-2014, 2014.*

[7] *Hiroshi Tanimoto, Regina M. Zbinden, Valerie Thouret & Philippe Nédélec (2015) Consistency of tropospheric ozone observations made by different platforms and techniques in the global databases, Tellus B: Chemical and Physical Meteorology, 67:1, 27073, DOI: https://doi.org/10.3402/tellusb.v67.270710.3402/*

[8] *H. Petetin, M. Jeoffrion, B. Sauvage, G. Athier, R. Blot, D. Boulanger, H. Clark, J.-M. Cousin, F. Gheusi, P. Nedelec, M. Steinbacher, V. Thouret; Representativeness of the IAGOS airborne measurements in the lower troposphere. Elementa: Science of the Anthropocene 1 January 2018; 6 23. doi: https://doi.org/10.1525/elementa.280*

References (if not given in the text already)

[9] Andreas Petzold, Valerie Thouret, Christoph Gerbig, Andreas Zahn, Carl A.M. Brenninkmeijer, Martin Gallagher, Markus Hermann, Marc Pontaud, Helmut Ziereis, Damien Boulanger, Julia Marshall, Philippe Nédélec, Herman G. J. Smit, Udo Friess, Jean-Marie Flaud, Andreas Wahner, Jean-Pierre Cammas, Andreas Volz-Thomas & IAGOS TEAM (2015) Global scale atmosphere monitoring by in-service aircraft – current achievements and future prospects of the European Research Infrastructure IAGOS, Tellus B: Chemical and Physical Meteorology, 67:1, 28452, DOI: https://doi.org/10.3402/tellusb.v67.28452

Ozonesondes

Version	Author	Affiliation	Contact	Date
v0	Roeland Van Malderen	RMI	roeland.vanmalderen@meteo.be	13/12/2021
v1	Roeland Van Malderen	RMI	roeland.vanmalderen@meteo.be	26/10/2022
v2	Roeland Van Malderen	RMI	roeland.vanmalderen@meteo.be	26/01/2023
v3	Roeland Van Malderen	RMI	roeland.vanmalderen@meteo.be	05/10/2023

Availability

The homogenized ozonesonde time series for 43 sites are available on the ftp-server "ftp-me.oma.be", accessible with account name "ozonesondes" and password "OzonFeb2021:". In the "ozonesondes" directory, every station has a directory with its name. In case of problems with connecting to the ftp-server, you can contact roeland.vanmalderen@meteo.be. The data is in any of the existing database formats:

- WOUDC (https://woudc.org/home.php, https://guide.woudc.org/en/#334-category-ozonesonde, https://woudc.org/archive/Documentation/Examples-extCSV/Ozonesonde.csv, with Python library code available on https://github.com/woudc/woudc-extcsv),
- NASA-AMES (from NDACC http://www.ndacc.org, see https://ndacc.larc.nasa.gov/data/formats) and,
- SHADOZ (https://tropo.gsfc.nasa.gov/shadoz/)

Data field description

- The minimum data fields that are/should be available are time (s), pressure (hPa), geopotential height (m), temperature (°C), relative humidity (%), pump temperature (°C), ozone partial pressure (mPa), relative uncertainty in ozone partial pressure, wind speed (m/s), and wind direction (degrees), and ozone current (µA). Additional fields possibly available nowadays are GPS height (m), latitude, longitude, pump motor current (mA), and pump motor voltage (V).
- Metadata are available in the headers of the data files and describe the site location, identify the hardware used (manufacturer, model and number of radiosonde, interface, ozonesonde), describe most aspects of the ozonesonde pre-flight preparation and its behaviour during preparation (e.g. background current, pump flow rate, ozonesonde response time), and give details about the processing used (e.g. pump efficiency correction table used). Data quality indicators (e.g. total ozone normalization factor compared to co-located Brewer/Dobson/SAOZ spectrophotometer) might also be present in the metadata header.

Description of homogenization procedure

The aim of the homogenization is twofold: (i) to correct for biases related to instrumental (such as sonde type or sensing solution strength) or processing changes to reduce the uncertainty (from 10–

20% down to 5–10 %), and (ii) provide an uncertainty estimate for every single ozone partial pressure measurement in the profile. The homogenization procedure and guidelines can be found in Annexes C and D of GAW Report No. 268, 2021: Smit, H.G.J., and Thompson, A.M., and the ASOPOS 2.0 Panel, "Ozonesonde Measurement Principles and Best Operational Practices. ASOPOS 2.0 (Assessment of Standard Operating Procedures for Ozonesondes)", WMO Global Atmosphere Watch Report Series, No. 268, World Meteorological Organization, Geneva, https://library.wmo.int/index.php?lvl=notice_display&id=21986#.YbI0xCYo_Ra. The first edition of the guidelines (Dated January 2012) can be found at https://www.wccos-josie.org/en/o3s-dqa, and a Python code that can be used for the homogenization is available at https://github.com/denizpoyraz/o3s-dqa-homogenization/.

Data management

Flagging

- Data cleaning like outlier removal is not systematically applied by every ozonesonde PI; some guidelines exist, but have not been generally implemented across the ozonesonde network.
- A data flagging scheme is proposed on pages 67-68 of GAW Report No. 268, but has not been systematically implemented in the archived data files.
- The total ozone normalization factor w.r.t. a co-located total ozone measuring instrument, if present, is included in the data file header as data quality indicator.

Uncertainties

- Every ozone partial pressure measurement P_{O3} in the ozone profile has an associated relative uncertainty $\Delta P_{O3}/P_{O3}$, following the homogenization guidelines as referred to here above (to be more specific: formula E-3-1 on page 39 in the GAW Report No. 268).
- As the homogenization should have removed all known systematic biases in the ozonesonde time series, the resulting uncertainty should represent only the contribution from random errors.

Traceability

Implementing the homogenization scheme ensures that the processed ozonesonde time series are traceable to the reference ozone photometer OPM (a fast dual-beam UV photometer, Proffitt and McLaughlin, 1983) in the simulation chamber of the World Calibration Centre for Ozonesondes (WCCOS) at FZ-Jülich, with a 1-s response, precision = 0.025 mPa, and uncertainty = 2% – 3%. Since 1996, activities to improve the quality of balloon-borne ozone soundings have been conducted at WCCOS through Jülich OzoneSonde Intercomparison Experiment (JOSIE) campaigns (https://www.wccos-josie.org/en/josie) [Smit et al., 2007; Thompson et al., 2019] and in the WMO/BESOS (Balloon Experiment on Standards for Ozonesondes) campaign [Deshler et al., 2008], in which traceability to the OPM instrument could be established, under the condition of applying the Standard Operating Procedures (SOPs) at the station.

Internal consistency

As the homogenized ozonesonde time series are traceable to the reference ozone photometer OPM, they should be internally consistent within the network. Several publications (see next section) have shown that the homogenization increased the consistency among different networks of ozonesondes with respect to the non-homogenized datasets.

External consistency

In publications describing the homogenization at ozonesonde sites, e.g. the Southern Hemispheric Additional Ozonesondes (SHADOZ) network [1,2,3,4], the Canadian network [5], the US network [4], and some individual sites [6, 7, 8], a comparison with other techniques (mainly measuring total ozone amounts) is made to assess the improvement of the homogenization.

1. Witte, J. C., et al., First reprocessing of Southern Hemisphere ADditional OZonesondes (SHADOZ) profile records (1998-2015) 1: Methodology and evaluation, J. Geophys. Res., 122, doi: 10.1002/2016JD026403 (2017).
2. Thompson, A. M., et al., First reprocessing of Southern Hemisphere ADditional OZonesondes (SHADOZ) Ozone Profiles (1998-2016). 2. Comparisons with satellites and ground-based instruments, J. Geophys. Res., 122, doi: 10.1002/2017JD027406 (2017).
3. Witte, J. C., et al., First reprocessing of Southern Hemisphere Additional Ozonesondes (SHADOZ) Profile Records. 3. Uncertainty in ozone profile and total column, J. Geophys. Res., 123(6), 3243-3268, doi: 10.1002/2017JD027791 (2018).
4. Sterling, C. W., et al., Homogenizing and estimating the uncertainty in NOAA's long-term vertical ozone profile records measured with the electrochemical concentration cell ozonesonde, Atmos. Meas. Tech., 11, 3661–3687, doi: 10.5194/amt-11-3661-2018 (2018).
5. Tarasick, D. W., et al., A re-evaluated Canadian ozonesonde record: measurements of the vertical distribution of ozone over Canada from 1966 to 2013, Atmos. Meas. Tech., 9, 195–214, doi: 10.5194/amt-9-195-2016 (2016).
6. Van Malderen, R., et al., On instrumental errors and related correction strategies of ozonesondes: possible effect on calculated ozone trends for the nearby sites Uccle and De Bilt, Atmos. Meas. Tech., 9, 3793–3816, doi: 10.5194/amt-9-3793-2016 (2016).
7. Witte, J. C., et al., The NASA Wallops Flight Facility digital ozonesonde record: Reprocessing, uncertainties, and dual launches. J. Geophys. Res., 124, 3565–3582, doi:10.1029/2018JD030098 (2019).
8. Ancellet, G., et al., Homogenization of the Observatoire de Haute Provence electrochemical concentration cell (ECC) ozonesonde data record: comparison with lidar and satellite observations, Atmos. Meas. Tech., 15, 3105–3120, doi:10.5194/amt-15-3105-2022 (2022).

Data quality indicators

In the GAW Report No. 268, on page 71, the following table 5.1 with some data quality indicators based on the available (meta)data of the ozonesonde is presented.

Table 5‒1: Criteria to evaluate the reliability of vertical ozonesonde profiles made using the two major ozonesonde types used in GAW-ozonesonde networks. The here marked indicators are independent of the sensing solution types used but are related to the ozonesonde types deployed (For details see text in Section 5.2).

Indicator	ECC SPC	ECC ENSCI-Z	Identifier in WOUDC
Total ozone normalization factor	0.9‒1.1	0.9‒1.1	TotalOzoneNormalizationFactor
Time to pump 100 ml [s]	25‒35	25‒35	FlowRateTime
Pump flowrate [ml/min]	170‒240	170‒240	PumpFlowRate
Response time (1/e) [s]	18‒28	18‒28	ResponseTimeFast
Pump temperature [K]	278‒310	283‒310	SampleTemperature
Background current before exposure to ozone [μA]	< 0.03	< 0.03	I_{B0}
Background current after exposure to ozone [μA]	< 0.07	< 0.07	I_{B1}
Pump motor current [mA]	50‒120	50‒120	PumpMotorCurrent
Pump motor voltage [V]	12‒18	12‒18	PumpMotorVoltage

The overall performance of the ozonesonde (see section 3.2 in GAW Report No. 268) can be summarized as

	Precision	Uncertainty
Troposphere	3%-5%	5% (in Tropics: 5-10%)
Stratosphere (< 28 km)	3%-5%	5%-10%

List of homogenized sites (name, geographical location, period of observations)

Site	Lat	Lon	Time range	#	Instrument	Homogenized?	Instrument PI	Contact
Alert, Canada	82.49	-62.34	1987 – Apr 2020	1587	ECC	Yes	David Tarasick	david.tarasick@canada.ca
Eureka, Canada	79.98	-85.94	1992 – Mar 2021	1873	ECC	Yes	David Tarasick	david.tarasick@canada.ca
Ny-Ålesund, Norway	78.92	11.93	1992 - 2022	2670	ECC	Yes	Peter von der Gathen	peter.von.der.gathen@awi.de
Thule, Greenland	76.53	-68.74	1992 - 2015	0	ECC	No	Nis Jepsen	nje@dmi.dk
Resolute, Canada	74.7	-94.96	1966/1979 – Mar 2021	2190	BM/ECC	Yes	David Tarasick	david.tarasick@canada.ca
Summit, Greenland	72.34	-38.29	2006 - 2018?	0	ECC	No	Bryan Johnson	bryan.johnson@noaa.gov
Scoresbysund, Greenland	70.48	-21.97	1989 - 2022	1611	ECC	Yes	Nis Jepsen	nje@dmi.dk
Sodankylä, Finland	67.37	26.65	1994 - 2022	1446	ECC	Yes	Rigel Kivi	rigel.kivi@fmi.fi
Lerwick, United Kingdom	60.13	-1.18	1992 - 2022	1637	ECC	Yes	Norrie Lyall	norrie.lyall@metoffice.gov.uk

Churchill, Canada	58.74	-94.07	1973/1979 – Mar 2021	1790	BM/ECC	Yes	David Tarasick	david.tarasick@canada.ca
Edmonton, Canada	53.54	-114.1	1970/1979 – Mar 2021	2175	BM/ECC	Yes	David Tarasick	david.tarasick@canada.ca
Goose Bay, Canada	53.31	-60.36	1969/1980 – Mar 2021	2358	BM/ECC	Yes	David Tarasick	david.tarasick@canada.ca
Legionowo, Poland	52.4	20.97	1979/1993 - 2022	1749	OS/ECC	Yes	Bogumil Kois	Bogumil.Kois@imgw.pl
Lindenberg, Germany	52.21	14.12	1974/1992 - present	0	OS/ECC	No	Peter Oelsner	Peter.Oelsner@dwd.de
De Bilt, Netherlands	52.1	5.18	1992 - 2020	1489	ECC	Yes	Ankie Piters	Ankie.piters@knmi.nl
Valentia, Ireland	51.94	-10.25	1994 - 2022	790	ECC	Yes	Michael Gill	michael.gill@met.ie
Uccle, Belgium	50.8	4.35	1969/1997 - 2022	3748	BM/ECC	Yes	Roeland Van Malderen	roeland.vanmalderen@meteo.be
Port Hardy	50.69	-127.38	2018 – Mar 2021	110	ECC	Yes	David Tarasick	david.tarasick@canada.ca
Bratt's Lake, Canada	50.2	-104.7	2003 - 2011	0	ECC	No	David Tarasick	david.tarasick@canada.ca
Praha, Czech Republic	50.01	14.45	1994 - present	0	ECC	No, in progress	Pavla Skrivankova	pavla.skrivankova@chmi.cz
Kelowna, Canada	49.93	-119.4	2003 – Jun 2017	700	ECC	Yes	David Tarasick	david.tarasick@canada.ca
Hohenpeissenberg, Germany	47.8	11.01	1967 – Sep 2023	6452	BM	Yes	Wolfgang Steinbrecht	Wolfgang.Steinbrecht@dwd.de
Payerne, Switzerland	46.49	6.57	1968/2002 - 2022	3114	BM/ECC	Yes	Eliane Maillard-Barras	Eliane.MaillardBarras@meteoswiss.ch
Egbert, Canada	44.23	-79.78	2003 - 2011	0	ECC	No	David Tarasick	david.tarasick@canada.ca
Haute Provence, France	43.94	5.71	1991 – Sep 2023	1497	ECC	Yes	Gerard Ancellet	gerard.ancellet@latmos.ipsl.fr
Yarmouth, Canada	43.87	-66.11	2003 – Mar 2021	795	ECC	Yes	David Tarasick	david.tarasick@canada.ca
Sapporo, Japan	43.06	141.33	1990/2010 - ???	0	KC/ECC	No	Masamichi Nakamura	mnakamura@met.kishou.go.jp
L'Aquila, Italy	42.3	13.31	1994 – May 2023	340	ECC	Yes	Vincenzo Rizi	vincenzo.rizi@aquila.infn.it
Trinidad Head, California, USA	40.8	-124.16	1997 – Aug 2023	1354	ECC	Yes	Bryan Johnson	bryan.johnson@noaa.gov
Madrid, Spain	40.47	-3.58	1994 - 2022	1180	ECC	Yes	Ana Diaz Rodriguez	adiazr@aemet.es
Boulder, Colorado, USA	40	-105.25	1967 – Sep 2023	2043	ECC	Yes	Bryan Johnson	bryan.johnson@noaa.gov
Wallops Island, Virginia, USA	37.93	-75.48	1995 – Nov 2020	1477	ECC	Yes	Ryan Stauffer	ryan.m.stauffer@nasa.gov
Tateno (Tsukuba), Japan	36.06	140.13	1990/2010 - present	0	KC/ECC	No	Masamichi Nakamura	mnakamura@met.kishou.go.jp
Huntsville, Alabama, USA	34.72	-86.64	1999 - present	0	ECC	No	Bryan Johnson	bryan.johnson@noaa.gov
Izana, Tenerife, Spain	28.3	-16.5	1995 - 2022	1412	ECC	Yes	Carlos J. Torres García	ctorresg@aemet.es
Naha, Japan	26.21	127.69	1990/2009 - ???	0	KC/ECC	No	Masamichi Nakamura	mnakamura@met.kishou.go.jp
Hong Kong, China	22.31	114.17	2000 - present	0	?	No	?	
Hanoi, Vietnam	21.01	105.8	2004 – Nov 2021	350	ECC	Yes	Ryan Stauffer	ryan.m.stauffer@nasa.gov
Hilo, Hawaii, USA	19.43	-155.04	1982 – Sep 2023	1885	ECC	Yes	Bryan Johnson	bryan.johnson@noaa.gov
Costa Rica	9.94	-84.04	2005 – Mar 2023	687	ECC	Yes	Holger Vömel	voemel@ucar.edu
Paramaribo, Suriname	5.8	-55.21	1999 - 2022	880	ECC	Yes	Ankie Piters	ankie.piters@knmi.nl
Kuala Lumpur, Malaysia	2.73	101.27	1998 - 2022	501	ECC	Yes	Ryan Stauffer	ryan.m.stauffer@nasa.gov
San Cristobal, Ecuador	-0.92	-89.62	1998-2022	468	ECC	Yes	Bryan Johnson	bryan.johnson@noaa.gov
Nairobi, Kenya	-1.27	36.8	1998 – May 2022	968	ECC	Yes	Eliane Maillard Barras	Eliane.MaillardBarras@meteoswiss.ch
Natal, Brazil	-5.42	-35.38	1998 - 2022	724	ECC	Yes	Ryan Stauffer	ryan.m.stauffer@nasa.gov
Watukosek, Java, Indonesia	-7.5	112.6	1998 - 2022	370	ECC	Yes	Masatomo Fujiwara	fuji@ees.hokudai.ac.jp
Ascension Island, United Kingdom	-7.58	-14.24	1998 – Sep 2022	379	ECC	Yes	Ryan Stauffer	francis.j.schmidlin@nasa.gov
Pago Pago, American Samoa	-14.23	-170.56	1986 – Sep 2023	1149	ECC	Yes	Bryan Johnson	bryan.johnson@noaa.gov
Suva, Fiji	-18.13	178.4	1997 – Jun 2023	517	ECC	Yes	Bryan Johnson	bryan.johnson@noaa.gov

Réunion Island, France	-21.06	55.48	1998 - 2022	805	ECC	Yes	Jérome Brioude	jerome.brioude@univ-reunion.fr
Irene, South Africa	-25.9	28.22	1998 – Mar 2023	415	ECC	Yes	Gerrie Coetzee	gerrie.coetzee@weathersa.co.za
Broadmeadows, Australia	-37.69	144.95	1965/1989 - present	0	BM/ECC	No	Matt Tully	matt.tully@bom.gov.au
Lauder, New Zealand	-45	169.68	1986 – Jun 2021	1973	ECC	Yes	Richard Querel	Richard.Querel@niwa.co.nz
Macquarie Island, Australia	-54.5	158.95	1994 - present	0	ECC	No	Matt Tully	matt.tully@bom.gov.au
Marambio, Antarctica	-64.24	-56.62	1988 - present	0	ECC	No	Rigel Kivi	rigel.kivi@fmi.fi
Dumont d'Urville, Antarctica	-66.7	140	1991 - present	0	ECC	No	Julien Jumelet	jumelet@latmos.ipsl.fr
Davis, Antarctica	-68.58	77.97	2003 - present	0		No	Matt Tully	matt.tully@bom.gov.au
Syowa, Antarctica	-69	39.58	1966 - present	0		No	Masamichi Nakamura	mnakamura@met.kishou.go.jp
Neumayer, Antarctica	-70.62	-8.37	1992 - present	0	ECC	No, TBD	Peter von der Gathen	peter.von.der.gathen@awi.de
McMurdo, Antarctica	-77.85	166.67	1986- Oct 2010	822	ECC	Yes	Terry Deshler	Richard.Querel@niwa.co.nz
Belgrano, Antarctica	-77.87	-34.63	2016 - present	0	ECC	No	Margarita Yela	yelam@inta.es
South Pole, Antarctica	-90	169.68	1967 – Sep 2023	2360	ECC	Yes	Bryan Johnson	bryan.johnson@noaa.gov

References (if not given in the text already)

Deshler, T., J. Mercer, H.G.J. Smit, R. Stübi, G. Levrat, B.J. Johnson, S.J. Oltmans, R. Kivi, J. Davies, A.M. Thompson, J. Witte, F.J. Schmidlin, G. Brothers, T. Sasaki, 2008: Atmospheric comparison of electrochemical cell ozonesondes from different manufacturers, and with different cathode solution strengths: The Balloon Experiment on Standards for Ozonesondes, *Journal of Geophysical Research*, 113, D04307, https://doi.org/10.1029/2007JD008975

Proffitt, M.H., and R.J. McLaughlin, Fast response dual-beam UV-absorption photometer suitable for use on stratospheric balloons, *Rev. Sci. Instrum.*, 54, 1719-1728, 1983.

Smit, H.G.J., W. Straeter, B. Johnson, S. Oltmans, J. Davies, D.W. Tarasick, B. Hoegger, R. Stübi, F. Schmidlin, T. Northam, A. Thompson, J. Witte, I. Boyd, F. Posny (2007), Assessment of the performance of ECC ozonesondes under quasi-flight conditions in the environmental simulation chamber: Insights from the Jülich Ozone Sonde Intercomparison Experiment (JOSIE), *J. Geophys. Res., 112, D19306, doi:10.1029/2006JD007308*

Thompson, A. M., H. G. J. Smit, J. C. Witte, R. M. Stauffer, B. J. Johnson, G. A. Morris, P. von der Gathen, R. van Malderen, J. Davies, A. Piters, M. Allaart, F. Posny, R. Kivi, P. Cullis, Nguyen T. H. Ahn, E. Corrales, T. Machinini, F. Raimundo daSilva, G. Paiman, K Thiong'o, A. Zainal, G. B. Brothers, K. R. Wolff, T. Nakano, R. Stübi, G. Romanens, G. J. R. Coetzee, J. A. Diaz, S. Mitro, M. 'bt Mohamad, S-Y. Ogino (2019), Ozonesonde Quality Assurance: The JOSIE-SHADOZ (2017) Experience, *Bull. Am. Meteor. Society*, *100(1)*, https://pubmed.ncbi.nlm.nih.gov/33005057/

Brewer Umkehr

Availability

The homogenized data (daily), total column ozone, N-values and Umkehr profiles can be obtained per request: Belsk – Janusz Krzyścin, januszj@igf.edu.pl, Thessaloniki (also Madrid, Warsaw and Hradec Kralove) – Kostas Fragkos, kfragkos@gmail.com, Arosa/Davos – Eliane Maillard -Barras, Eliane.MaillardBarras@meteoswiss.ch

The data format for the Umkehr is Excel or csv (Belsk, Warsaw, Madrid, Hradec Karlove, Thesalonikis), .txt (Arosa/Davos).

Data field description

- *Please describe shortly all the data fields (and their units) that are available, also auxiliary data fields.*

The short output format for all stations includes:

Daily Umkehr ozone profiles (DU) are profiled in 16 layers (pressure based), 16 pressure levels (mbar) for Umkehr layers, a priori (DU) in 16 layers, AK (16 layers), date (dd/mm/yyyy), time of the day (AM or PM), total ozone observed (DU), total ozone integrated from profile (DU), SZA range 70°-90°.

The long format is available per request, in addition to information in the short format it also include N values, a priori profiles, residuals, AK in 16x16 format.

Additional data from Belsk are available for the period January 2010 - October 2021:

- Total column ozone (DU) – homogenized time series of the intra-day total column ozone measurements. The homogenization procedure accounts for instrument's sensitivity changes recorded during intercomparisons with Brewer #017 on yearly basis.
- Profiles and N-values obtained from Brewer Spectrophotometer Umkehr Analysis Program based on UMK04 algorithm, by Martin Stanek software package, the latest version available on this website http://www.o3soft.eu/o3bumkehr.html

- *Describe the metadata that is available*
  a. The metadata for the Belsk total column ozone data are included in the header (txt format).
  b. Daily N-values and Umkehr ozone profiles are in standard format used by the UMK04 retrieval, similar to the WOUDC Level 2 format.
- *Are there derived products (e.g. tropospheric columns) available for HEGIFTOM? Where?*
  a. Umkehr layer 1 is representative of the tropospheric layer (surface to 250 mbar). This information is included in the 10-layer standard output, it can be also obtained by combining layers 0 and 1 from the 16 layer profile output.

Description of homogenization procedure

Belsk

Umkehr ozone profile records are homogenized using simulated ozone record over the station (i.e. M2GMI model) as a reference to remove step changes in observations (N-values) when caused by changes in the stray light contribution or from other instrumental artifacts, or in association with data re-processing before and after instrument calibrations. The reference paper is in the reviews. https://amt.copernicus.org/preprints/amt-2021-203/#discussion

The standard approach is used i.e., homogenization is done using time series of the ratio between $N(SZA_i)$ values (calculated at selected SZA_i) and total column ozone. No significant trend in the above mentioned ratio has been found for the period 2010-2021.

Arosa

B040 Umkehr ozone profile record has been compared to simultaneous and collocated Dobson and Brewer ozone records. No significant anomaly related to any technical issues has been detected. No significant steps changes have been detected. The reference paper is in preparation (Maillard Barras et al., 2022).

Thessaloniki (also Madrid, Warsaw and Hradec Kralove)

The consistency of the Brewer data has been assured by comparisons against the OMI, IASI and GOME satellite records. The paper is in preparation (2022).

Data management

Flagging (Data cleaning (outlier removal)?

Yes, only good data are provided in the output (i.e. less than 4 iterations, RMSE less than 1, no negative ozone, no missing observations between 70 and 90 degrees SZA)

- *Flagging applied? Description of data flags*
  No flagging
  Arosa: Clear sky day measurement only i.e. flagged using simultaneity with flagged collocated D051 data record.
- *Data quality indicators?*
  No

Uncertainties

- Which? Distinction random vs. systematic?
  Total uncertainty, no distinction.
- How determined?
  Rodgers (2000) equations for measurement and smoothing errors, similar to calculations discussed in Bhartia et al, 2013 paper.
  Bhartia, P. K., McPeters, R. D., Flynn, L. E., Taylor, S., Kramarova, N. A., Frith, S., Fisher, B., and DeLand, M.: Solar Backscatter UV (SBUV) total ozone and profile algorithm, Atmos. Meas. Tech., 6, 2533–2548, https://doi.org/10.5194/amt-6-2533-2013, 2013.

Belsk: Total uncertainty for each layer was estimated from the statistics of the differences between the am and pm Umkehr taken during one day (see Table1 in Annex 2)

Traceability

Are the data of an instrument traceable to a reference instrument? Traceable to SI units?

Belsk:

Brewer 064 measurements during yearly intercomparisons have been focused on total ozone and UV traceability to the reference instrument (Brewer # 017), as well as on control of absolute sensitivity of the instrument through the calibration by the NIST traceable UV lamps. No intercomparison of Umkehr measurements have been done so far.

Arosa/Davos:

Since 1988, biennial calibrations are carried out (Stubi et al., 2017) towards the traveling reference instrument B017 (SCI-TEC/IOS) and, since 2008, towards the traveling reference instrument B185 (RBCC-E).

Other stations:

Biennial calibrations towards the traveling standard instrument (?)

Internal consistency

- *Are the time series of different instruments within the network internally consistent?*

Processed with O3Brewer v2.7 algorithm which is adapted from the Dobson umk04 (Petropavlovskikh et al, 2005) algorithm (M. Stanek, http://www.o3soft.eu/o3bumkehr.html)

- *References of intercomparison campaigns of different instruments within the network? Over-all conclusions of such studies?*

GAW Report, 180. Towards a Better Knowledge of Umkehr Measurements: a Detailed Study of Data from Thirteen Dobson Intercomparisons. Conclusion: individual instruments have different out-of-band light rejection (aka stray light), which can result in relative biases (up to 6 % or larger) between Umkehr retrieved profiles measured simultaneously by several instruments.

Belsk

Comparison between Dobson Umkehrs with those by the collocated Brewer at Belsk was possible for the period 2011-2016 (Annex 3). There was a good correspondence between the profiles by both spectrophotometers as biases (Brewer minus Dobson) are in the range -2.7% (Layer 2) and 2.2% (Layer 7). For Layer 1, bias is -1.7%. and the 10^{th}-90^{th} percentile range is of [-7.1%; 4.7%], i.e. close to the uncertainty range of the Dobson Umkehr in layer 1.

Arosa/Davos

In good agreement with the travelling references (TCO deviations <=1%, (Stubi et al., 2017a)). Total ozone ADD: time series of relative difference with collocated Brewer

Other stations

- *World Meteorological Organization (WMO) - WMO, 2008 (WMO/TD-No. 1456) How much inconsistency is left over after homogenization: details in Annex or referencing.*

To be investigated during HEGIFTOM activity. Potential biases are expected from the interference of large amounts of stratospheric (i.e. volcanic, scattering) and tropospheric aerosols (i.e. urban, absorbing).

External consistency

9. *References of intercomparison studies between your technique and other techniques measuring free-tropospheric ozone? Overall conclusions of such studies?*
   Petropavlovskikh et al (2021) shows that homogenized Dobson Umkehr profiles have less than +/- 5 % biases from other techniques (i.e. COH, MLS, SAGE III and ozonesonde) in the stratosphere. The biases increase in the lower stratosphere and troposphere depending on station: -5 % at Lauder, near zero at Boulder and MLO, 5% at OHP. The biases in Thessaloniki Brewer Umkehr data appear to be of a similar magnitude (Fragkos – PhD).
   Up to now, there were no intercomparisons of the Belsk's tropospheric ozone by the Brewer spectrophotometer at Belsk with other techniques.

   Arosa/Davos profiles were regularly compared with the Aura MLS satellite overpass record (since 2005) and with collocated Dobson (since 1994).

Data quality indicators

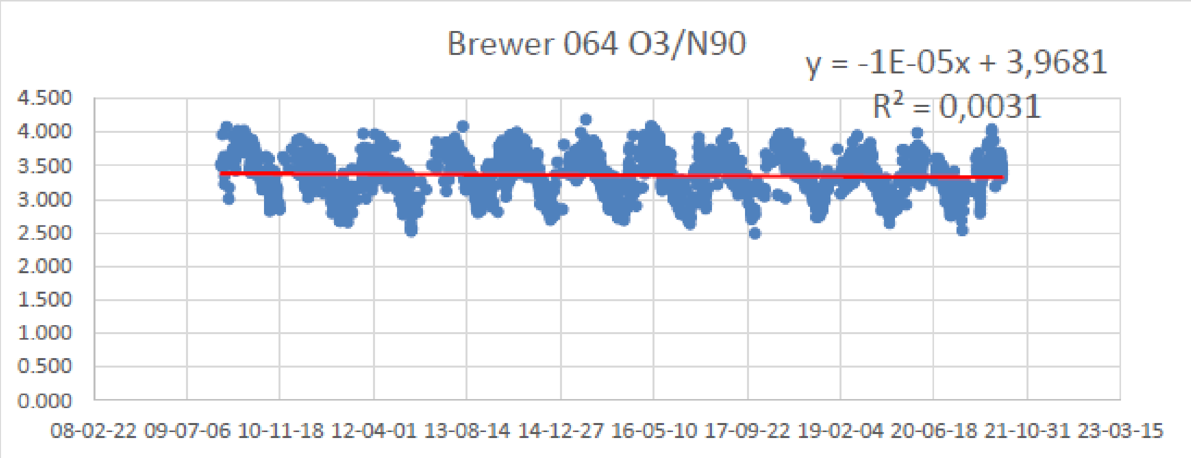
10. *Short description or referencing or hyperlinking to a document*
    See Annex 2
11. *Factsheet of the performance of the instrument in field operation (only overall specifications, e.g. overall uncertainty xx%) (Table on one page)*
    The uncertainty ranges for the ozone content Umkehr Layers are of about ± 5% for layer 2-10, and only slightly above this range for Layer 1 (-7.5%- 5.8%). (see Annex 2 and 3)

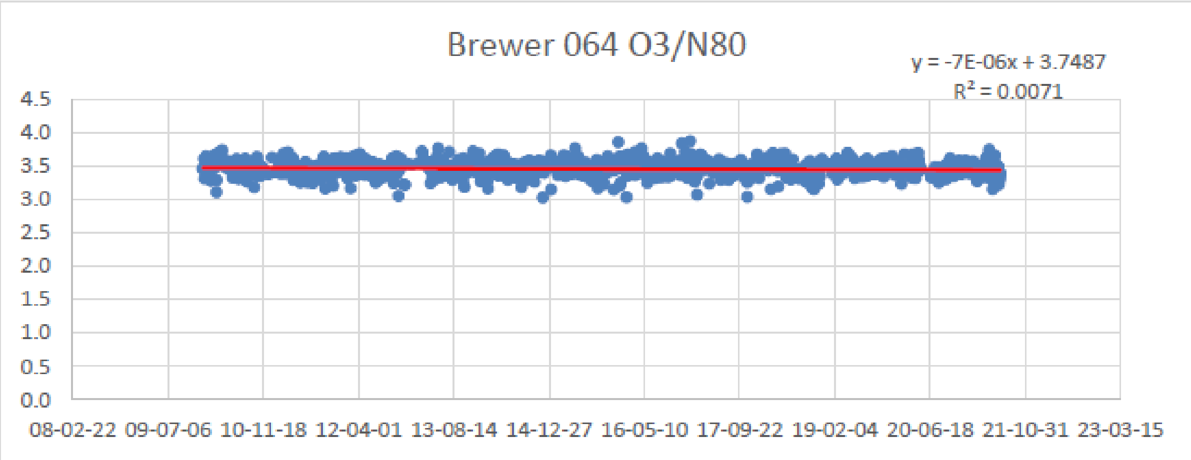
List of homogenized sites (name, geographical location, period of observations)

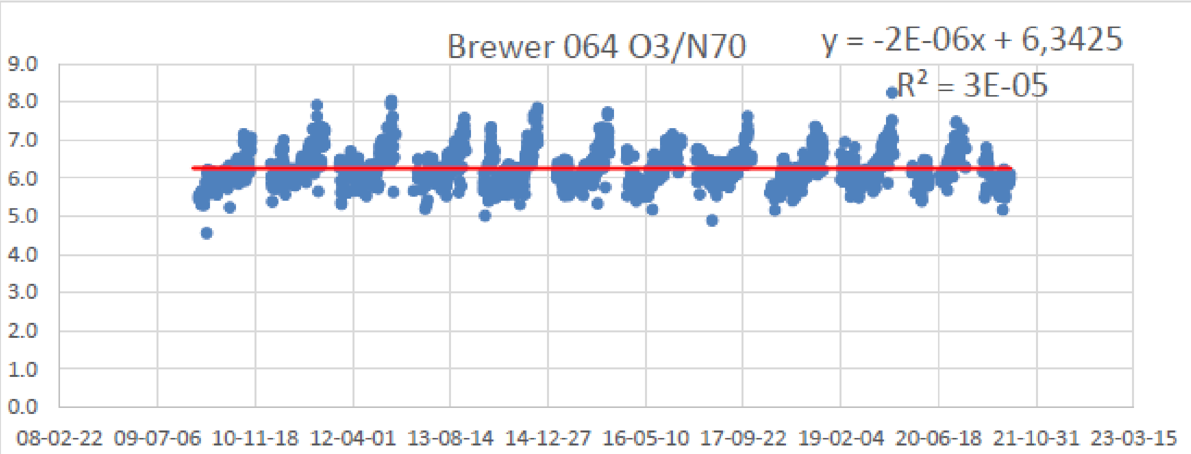
Station	Instrument Type/ Number	Observational period	Latitude	Longitude
Thessaloniki	Brewer MKII (#005)		40.63 N	22.96 E
Hradec Kralove	Brewer MKIII (#184)		50.18 N	15.84 E
Madrid	Brewer MKIII (#186)		40.45 N	3.72 W
Warsaw	Brewer MKIII (#207)		52.25 N	20.94 E
Belsk	Brewer MKII (#064)	01/2010 -10/2021	51.84 N	20.79 E
Arosa/Davos	Brewer MKII (#040)	01/1998 – 12/2021	46.77° N/ 46.81 N	9.67° E/ 9.84E

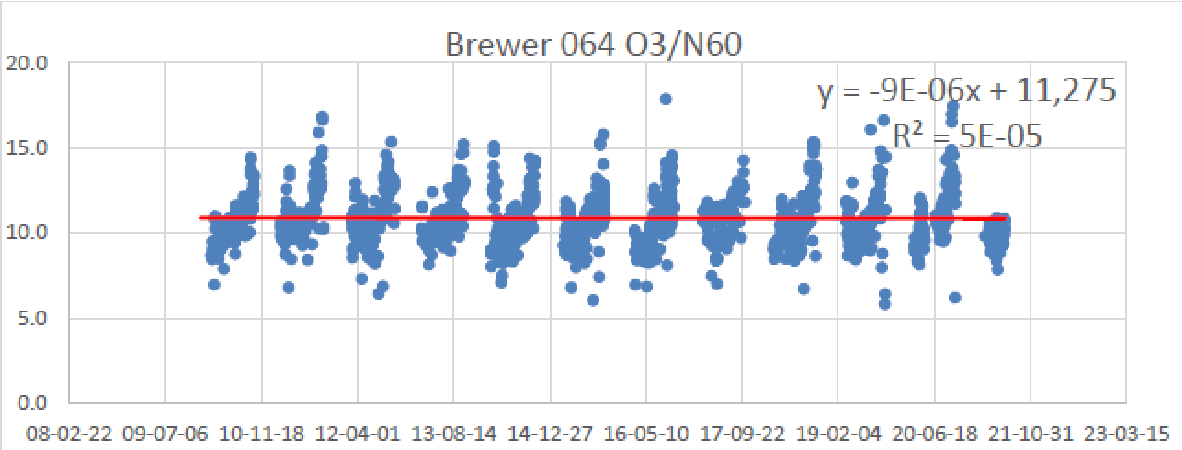
Annex 1

Below the ratios of N values for different SZA's and total ozone are shown for the whole dataset (2010-2021)









Annex 2

Total uncertainty in the Umkehr profiles over Belsk is estimated empirically by examining set of differences between am and pm profiles taken during one day. Table 1 shows the difference between am and pm values (for all Umkehr layers and total column ozone) in percent of the daily mean value, i.e. (pm+am)/2. The following statistical characteristics (N=639) are used, mean value, standard deviation, median, 10th and 90th percentile. It is assumed that the range between 10th and 90th percentile provides the uncertainty. This value probably overestimates the "true" uncertainty as it is possible that the profile could change during the day. However, the Umkehr profiles are taken during perfect clear-sky days with a stable weather conditions and we do not expects also abrupt changes in the stratosphere. It is possible to eliminate days with large intraday changes in the ground-based profiles examining differences in the satellite ozone profile for three consecutive days (*t*-1, *t*, *t+1*) and select only days (*t)* for calculations of the ratio differences when the change between the triad values are below a threshold. This is left for future consideration.

It is supposed that the am and pm profiles should be quite similar as the Dobson total column ozone (last row in Table 1) changes only slightly during a day (i.e., mean=0.2% with the uncertainty range between -0.7% and 1.1%. The uncertainty ranges for all layers are about ± 5%, and only slightly above this range for Layer 1 (-7.5%- 5.8%).

Table 1. Statistical characteristics of the relative differences, Δ, between am and pm Dobson Umkehr and total column ozone measured during one day at Belsk for the period 1963-2020, Δ=(am – pm)/(am+pm)/2 *100% .

Layer	Mean	SD	Median	10th	90th
Difference between Ozone Content in the Umkehr Layer					
1	-0.8	5.9	-0.6	-7.5	5.8
2	-0.6	3.8	-0.6	-5.5	3.9
3	-0.1	2.9	-0.1	-3.5	3.3
4	0.6	3.4	0.5	-3.5	4.7
5	0.8	2.1	0.9	-1.6	3.3
6	0.8	2.0	0.8	-1.6	3.3

7	0.7	2.3	0.7	-1.9	3.3
8	0.4	3.6	0.4	-3.9	4.7
9	0.1	3.3	0.2	-3.7	4.0
10	0.0	1.7	0.0	-2.0	2.0
Difference between Total Column Ozone					
	0.2	0.8	0.3	-0.7	1.1

Annex 3.

The column ozone monitoring with the Brewer spectrophotometer serial no. 64 (BS64) mark II (single monochromator) was launched at Belsk in 1991 but the Umkehr observations in 2010. The full series of the Brewer Umkehrs (2010 -2021) is under construction. At the moment, a comparison with the concurrent Dobson data is available for the period 2011-2016 (N=328, including am and pm Dobson-Brewer pairs). Statistics of the relative differences between Brewer and Dobson Umkehrs and total column ozone is shown in Table 2. There is a good agreement between the instruments. Standard deviations and the uncertainty ranges (10th-90th percentile of the differences) are similar to those for the relative differences between am and pm Dobson profiles for one day (Table 1). This allows to determine a universal uncertainty range pertaining the Umkehr retrieval for any ground-based spectrophotometer measuring N-values regardless of its type.

Table 2. Statistical characteristics of the relative differences, Δ, between Brewer and Dobson ozone content in Umkehr Layers and the column amount of ozone measured simultaneously by both instruments at Belsk for the period 2011-2016, Δ= (Brewer-Dobson/(Brewer+Dobson)/2 *100%

Layer	**Mean**	**SD**	**Median**	**10^{th}**	**90^{th}**
Difference between Ozone Content in the Umkehr Layer					
1	-1.7	5.2	-2.1	-7.1	4.7
2	-2.7	3.9	-2.9	-6.9	2.4
3	-0.1	3.1	-0.2	-3.7	3.7
4	0.3	2.8	0.2	-3.0	3.4
5	0.0	2.0	0.1	-2.4	2.4
6	0.8	2.0	0.9	-1.8	3.1
7	2.2	2.7	2.0	-1.1	5.8
8	2.0	3.4	1.8	-1.7	6.3
9	1.4	3.6	1.4	-2.6	5.4
10	0.7	2.0	0.7	-1.6	3.1
Difference between Total Column Ozone					
11	0.0	1.0	0.0	-1.3	1.0

Dobson Umkehr

Availability

There are several version of Umkehr processing software: the WinDobson is used at NOAA, Martin Stanek software is used at Belsk, and MeteoSwiss is using their own software for Arosa/Davos Umkehr data processing. All have the standard (aka WOUDC) and supplementary output formats.

The homogenized Umkehr ozone profile data for **NOAA stations at Boulder, US; MLO, US; OHP, France; and Lauder, New Zealand** (Petropavlovskikh et al., 2022, https://amt.copernicus.org/preprints/amt-2021-203/) are available from https://gml.noaa.gov/aftp/data/ozwv/Dobson/AC4/Umkehr/Optimized/ as monthly mean time series in the .csv and netcdf formats, and as daily profiles in AMES (WOUDC) format. The netcdf files for daily ozone profiles can be obtained from irina.petro@noaa.gov or peter.effertz@noaa.gov.

The homogenized data including total column ozone, N-values and Umkehr profiles for **Belsk, Poland** can be obtained from jkrzys@igf.edu.pl or bonia@igf.edu.pl. The data format for the Umkehrs is according to input/output used by the UMK04 retrieval. Two output options are possible: short (measured and retrieved total column ozone, the profile, indices describing the quality of the profile) and long (as short output plus N-values, a priori profiles, residuals, AK in 8x8 format). The data format is ".txt".

2 different homogenized Umkehr data records for **D051 Arosa/Davos, Switzerland** are available

1) from eliane.maillard@meteoswiss.ch as monthly mean time series and as daily profile in the .txt format.

2) from the LOTUS website (ftp://Phase-2_2022-2019/Umkehr/optimized/ARO_*) as monthly mean time series in the .csv format.

Data field description

- *Please describe shortly all the data fields (and their units) that are available, also auxiliary data fields.*

WOUDC format (i.e. *.txt file for NOAA record)

Daily Umkehr profiles in the WOUDC standard output have the following format:

DD MM YY M/A LAM TO_OB TO_RT LO3(10:1)*100 NUMIT SZA_b SZA_num RMSD(DIF) RMSD(CONV) RMSD(err) STN_num

Example:

30 12 18 1 3 289 2906 147 371 960 1848 3418 6491 7580 4496 2096 1649 3 3 10 0 3 16 67
where
DD is day
MM is month
YY is year
M/A is morning or afternoon (1/2)

TO_OB is observed total ozone (TO)
TO_RT is retrieved TO
LO3(10:1) is 100*ozone amount (DU*100) in Umkehr layers 10, 9,...1 (layer 1 is a double layer 0+1)
NUMIT is number of iterations
SZA_b is the SZA number for the first available measurement (1 is 60, 2 is 65, 3 is 70 etc)
SZA_nub is the number of measurements (12 is the maximum number)
RMSD(DIF) is the root-mean square deviation (RMSD) of the difference of the solution profile from the previous iteration
RMSD(CON) is the RMSD of the convergence of the forcing factor
RMSD(err) is the RMSD of the residual fit (difference between OB and RT N-values)
STN_num station number.

NOAA datasets

Supplementary Daily Umkehr ozone profile files (netcdf format, per request) have output for all quality assured (less than 5 iterations, RMSD(err) less than 100, not negative ozone) profiles. The files contain a collection of profiles for a single year. The following parameters are included: the date (Julian day of the year), time of the day (1 for AM or 2 for PM), total ozone observed (DU), total ozone integrated from profile (DU), pressure for 10 and 16 Umkehr layers (pressure is at the bottom of the layers, mbar), Umkehr profile in 10 and 16 layers (DU), type of observation (i.e. 3 is for Dobson C-pair wavelengths), measurement code (30 means AD zenith measurement with clear sky).

Monthly mean files (.csv) contain the following information: Date (DD/MM/YYYY), Year, Month, Layer 1 through 10 mean ozone (DU), Layer 1 through 10 standard deviation (DU), Count (number of profiles). #N/A indicates missing data.

Belsk dataset

The following data from measurements taken at Belsk, Poland, by the Dobson spectrophotometer serial no.84, are available for the period March 1963-December 2020:

- Total column ozone (DU) – homogenized time series of the intra-day total column ozone measurements. The homogenization procedure accounting for the instrument aging, dependence on ozone absorption on temperature, stray light is described in the paper: Krzyścin, J. W., Rajewska-Więch, B., and Jarosławski, J.: Total column ozone measurements by the Dobson spectrophotometer at Belsk (Poland) for the period 1963–2019: homogenization and adjustment to the Brewer spectrophotometer, Earth Syst. Sci. Data, 13, 4425–4436, https://doi.org/10.5194/essd-13-4425-2021, 2021

- N-values - homogenized time series based on the Umkehr observations for C pair during clear-sky conditions. The data are coded using standard for the UMK04 input

- Daily Umkehr ozone profiles (DU) – output of the UMK04 retrieval using the homogenized series of total column ozone and N values. The data are coded using standard for the UMK04 output: date (year, month, day), time of the day (1 or 2 for AM or PM), total ozone observed (DU), total ozone integrated from profile (DU), type of observation (i.e. 3 is for Dobson C-pair wavelengths), ozone content in 10 layers (DU), number of N values used the retrieval (max 10 for all possible N values between 70°-90°SZA, and 7 for the so-called short-Umkehr), indices for the profile quality. In addition to standard UMK04 output, the flag is added (see flagging section)

Extended output of the UMK04 retrieval contains also a priori profiles, residuals, AK values in 8x8 format.

Arosa/Davos

Daily Umkehr ozone profiles (DU) are made in 16 pressure-based layers. For each layer record the pressure (mbar), a priori (DU), and AK. Date (Julian day of the year), time of the day (1 for AM or 2 for PM), total ozone observed (DU), total ozone integrated from profile (DU), pressure for 10 Umkehr layers (pressure is at the bottom of the layers, mbar), Umkehr profile in 10 layers (DU), for 2) type of observation (i.e. 3 is for Dobson C-pair wavelengths), measurement code (for (1)clear sky or cloudy sky).

- *Describe the metadata that is available*

NOAA data

Monthly mean files have the header. Some station and instrument information is included in the netcdf file description of the fields.

Further information about datasets and instruments used in homogenized records can be found in Petropavlovskikh et al., 2022, https://amt.copernicus.org/preprints/amt-2021-203/

Belsk data

Daily N-values and Umkehr ozone profiles are in standard format used by the UMK04 retrieval. Concerning the total column ozone data, the metadata are included as the data header (txt format).

Arosa/Davos

For 1) Some information is included in the file header.

For 2) Some information is included in the netcdf file description of the fields

- *Are there derived products (e.g. tropospheric columns) available for HEGIFTOM? Where?*

Both NOAA and Belsk files

Umkehr layer 1 is representative of the tropospheric layer (surface to 250 mbar).

Description of homogenization procedure

NOAA data

Umkehr ozone profile records are homogenized using simulated ozone record over the station (i.e. M2GMI model) as a reference to remove step changes in observations (N-values) when caused by changes in the stray light contribution or from other instrumental artifacts, or in association with data re-processing before and after instrument calibrations. The reference paper is in the reviews. Petropavlovskikh et al., 2022, https://amt.copernicus.org/preprints/amt-2021-203/

Belsk data

The standard approach is used i.e., homogenization is done using time series of the ratio between N(SZAi)- values (calculated at selected SZAi) and total column ozone. Two steps procedure is proposed. In the first step, the ratio is corrected for a slight decline in the ratio values since the early 2000s. After the first step, the corrected ratio values are examined for a step change in the data. To eliminate step changes in 1990, 1996, 2003 year, constant values are added to the time series. (Annex 1)

Arosa/Davos

1) D051 Umkehr ozone profile record is homogenized using simultaneous and collocated Dobson and Brewer ozone records. Steps changes are corrected on the raw data level (N values) under the express condition that the anomaly is confirmed by a technical issue in the metadata. The reference paper is in preparation (Maillard Barras et al., 2022).

2) D051 Umkehr ozone profile record is homogenized using simulated ozone record over the station (i.e. M2GMI model) as a reference to remove step changes in observations (N-values) when caused by changes in the stray light contribution or from other instrumental artifacts, or in association with data re-processing before and after instrument calibrations. The reference paper is in the reviews. https://amt.copernicus.org/preprints/amt-2021-203/#discussion

Data management

Flagging

- *Data cleaning (outlier removal)?*

NOAA data

Yes, only good quality data are provided in the output (i.e. less than 4 iterations, RMSD less than 100, no negative ozone, no missing observations between 70 and 90 degrees SZA)

Belsk data

YES, no data with missing observations at 90 degree SZA

Arosa/Davos

Yes, only good data are provided in the output (i.e. less than 4(3 for (1)) iterations, RMSD less than 100, no negative ozone, for 2) no missing observations between 70 and 90 degrees SZA

- *Flagging applied? Description of data flags*

NOAA data

No flagging

Belsk data

YES

1 - good standard Umkehr, all possible N values (10) between 70°-90 SZA, less than 4 iterations, and RMSE <1,

2 -good short Umkehr, all possible N values (7) between 80°-90 SZA, less than 4 iterations, and RMSE <1,

3 - bad Umkehr, number of N values different than 10 or 7 for SZA in the range 70-90 SZA and 80-90 SZA, respectively, or more than 3 iterations, or RMSE >1

Arosa/Davos

For 1) Clear sky day measurements considered: flagging using a nearby UV/VIS lux meter.

- *Data quality indicators?*

Both NOAA and Belsk data

No

Arosa/Davos

For 1)

3=clear sky

5=corrected for cloud effect

Uncertainties

- Which? Distinction random vs. systematic?

Total uncertainty, generic

- How determined?

NOAA data and Arosa/Davos

Rodgers (2000) equations for measurement and smoothing errors, similar to calculations discussed in Bhartia et al, 2013 paper.

Bhartia, P. K., McPeters, R. D., Flynn, L. E., Taylor, S., Kramarova, N. A., Frith, S., Fisher, B., and DeLand, M.: Solar Backscatter UV (SBUV) total ozone and profile algorithm, Atmos. Meas. Tech., 6, 2533–2548, https://doi.org/10.5194/amt-6-2533-2013, 2013.

Total uncertainties based on synthesized Umkehr data as discussed in Petropavlovskikh et al. (2005, see Figure 2 for monthly mean record and three cases with different normalization SZAs) and in Petropavlovskikh et al. (2022, Figure 1 c)

Belsk data

Total uncertainty for each layer was estimated from the statistics of the differences between the morning (am) and afternoon (pm) Umkehr profiles taken during one day (see Table1 in Annex 2)

Traceability

Are the data of an instrument traceable to a reference instrument? Traceable to SI units?

NOAA data

Yes, Dobson 083 instrument is WMO GAW world standard instrument. During intercomparisons, Umkehr observations are compared between the station and standard instrument and results are included in the report. The optical wedge calibration is done with standard lamps (NIST traceable).

All Dobson instruments are compared against either Dobson 083 (MLO, Boulder, Fairbanks) or regional standard (D064 in Hohenpeissenberg, Germany for OHP and Perth, and Dobson standard in Melbourne, Australia for Lauder).

The **Belsk' Dobson** (serial no.84) has been calibrated against standard instrument since 1974 during regular (almost every four year) international inter-comparison campaigns including also calculations of new R-N tables after optical wedge calibrations. The calibrations supported long-term stability of total column ozone measurements (Krzyścin et al., 2021). There were no such inter-comparisons with the Belsk's Dobson concerning measurements of N-values for different SZAs.

Dobson 051 instrument at Arosa is regularly intercompared within the Dobson network wrt two regional secondary standard Dobson instruments (D064 from the Hohenpeissenberg Observatory (MOHp, Germany) and D074 from the Solar and Ozone Observatory in Hradec Kralove (SOO-HK, Czech Republic) (Stubi et al., 2021, https://doi.org/10.5194/amt-14-4203-2021). The optical wedge calibration is done with standard lamps (NIST traceable).

Internal consistency

- *Are the time series of different instruments within the network internally consistent?*

NOAA data

Yes, they are processed with the same UMK08 algorithm that is based on the source code (Fortran 77, WOUDC) but also incorporates the stray light correction look up tables (Petropavlovskikh et al, 2011). The Umkehr retrieval algorithm is incorporated in the WinDobson software. The optimization corrections to the N-values are applied outside of the WinDobson software. Corrections for NOAA record homogenization are published in Petropavlovskikh et al. (AMTD, under the review).

Belsk data

The source program (in FORTRAN 77) was copied from WOUDC resources.

Arosa/Davos

Processed with umk04 (Petropavlovskikh et al, 2005). For 1) No stray light correction.

- *References of intercomparison campaigns of different instruments within the network? Overall conclusions of such studies?*

NOAA data

GAW Report, 180. Towards a Better Knowledge of Umkehr Measurements: a Detailed Study of Data from Thirteen Dobson Intercomparisons. Conclusion: individual instruments have different out-of-band light rejection (aka stray light), which can result in relative biases (up to 6 % or larger) between Umkehr retrieved profiles measured simultaneously by several instruments.

Belsk data

Comparison between Dobson Umkehrs with those by the collocated Brewer at Belsk was possible for the period 2011-2016 (Annex 3). There was a good correspondence between the profiles by both spectrophotometers as biases (Brewer minus Dobson) are in the range -2.7% (Layer 2) and 2.2% (Layer 7). For Layer 1, bias is -1.7%. and the 10th-90th percentile range is of [-7.1%; 4.7%], i.e. close to the uncertainty range of the Dobson Umkehr in layer 1 (Annex2).

Arosa/Davos

The biases increase in the lower stratosphere and troposphere depending on station: 5% for D051/LKO.

- *World Meteorological Organization (WMO) - WMO, 2008 (WMO/TD-No. 1456) How much inconsistency is left over after homogenization: details in Annex or referencing.*

Under investigation.

External consistency

- *References of intercomparison studies between your technique and other techniques measuring free-tropospheric ozone? Overall conclusions of such studies?*

NOAA data

Petropavlovskikh et al (2021) shows that homogenized Umkehr profiles have less than +/- 5 % biases from other techniques (i.e. COH, MLS, SAGE III and ozonesonde) in the stratosphere. The biases increase in the lower stratosphere and troposphere depending on station: -5 % at Lauder, near zero at Boulder and MLO, 5% at OHP.

Belsk data

Up to now, there were no intercomparisons of the Belsk's tropospheric ozone by the Dobson spectrophotometer with other techniques.

Data quality indicators

- *Short description or referencing or hyperlinking to a document*

See Annex 2

- *Factsheet of the performance of the instrument in field operation (only overall specifications, e.g. overall uncertainty xx%) (Table on one page)*

The uncertainty ranges for the ozone content in Umkehr Layers are of about ± 5% for layers 2-10, and only slightly above this range for Layer 1 [-7.5%; 5.8%). (see Annex 2).

List of homogenized sites (name, geographical location, period of observations)

Table 1. NOAA Dobson Umkehr data information: Name of the station, WMO code, dates of the record (month and year), geolocation of the ground-based stations.

Location	Site Code	Data Record (MM/YEAR)	Latitude	Longitude	Elevation (m)
Fairbanks, Alaska	FBK	03/1984 - 10/2020	64.86 N	147.85 W	133
Haute Provence, France	OHP	09/1983 - 12/2020	43.93 N	5.71 E	685
Boulder, Colorado	BDR	02/1978 - 12/2020	40.02 N	105.25 W	1634
Mauna Loa, Hawaii	MLO	05/1982 - 12/2020	19.53 N	155.58 W	3400
Perth, Australia	PTH	03/1969 - 07/2016	31.92 S	115.96 E	2
Lauder, New Zealand	LDR	02/1987 - 12/2020	45.04 S	169.68 E	370

Belsk, Poland, BEL, 03/1963 – 12/2020 , 51.84 N, 20.79 E, 173

Arosa/Davos, LKO/PMOD , 1/1956- 12/2021 , 46.77N 9.67E/46.81N 9.84E, 1860m/1550m

Belsk data

Annex 1 – Homogenization of the Umkehr series

Umkehr retrieval (UMK04) requires total column ozone (TCO) and series of N-values measured at selected solar zenith angles (SZA) ≥70° before and/or in the afternoon. Here, TCO were taken from the re-evaluated TCO intra-day values for the period 1963-2020. The long-term stability of TCO measurements was supported by frequent (almost every 4 years) intercomparisons of the Belsk's Dobson (serial no. 84) with the reference spectrophotometer. The corrections to the original TCO data accounted for less accurate Dobson observations under low solar elevation (mi>3), presence of clouds, and the temperature dependence of ozone absorption (Krzyścin et al., 2021). TCO measured at the moment closest to SZA=70° in the morning and afternoon were used by the Umkehr retrieval. For some days (late autumn-early winter), the noon SZA values at Belsk were above 70°. In such cases, the daily mean TCO values were used both for calculations of am and pm Umkehrs. Previously, corresponding TCO values for the Umkehr observations were calculated manually from the intra-day TCO series based on the Bass-Paur ozone absorption coefficients calculated at the fixed effective temperature of -46.3°C.

The Umkehr homogenization procedure follows standard approach (used in many previous papers) to examine time series of the ratio between N(SZA_i) values (calculated at selected SZA_i for C pair) and the corresponding TCO. The long-term smoothed series of the ratio (for SZA≥70°) should be a trendless line without step changes. Therefore, two steps homogenization procedure is proposed. In the first step, corrections to N values were added to remove a decline found in the smoothed pattern of the ratio that was found in the period 2004-2020 (Figure 1). The differences between the smoothed ratio values and the constant value (smoothed N value in 1963) were subtracted from the raw ratios. After this correction, the resulting smoothed time series of the ratios was close to a trendless line (Figure 2).

Next step of the homogenization of the Umkehr data is adding corrections for step changes in the ratio time series. These were found in 1990, 1996, and 2003. The mean value of the decline from the smoothed pattern was calculated for the period 1990-1995 and 1996-2002. For these periods, the mean values were subtracted from the time series of the ratio obtained after the first step of homogenization. The next smoothed curve of the corrected ratios was calculated for each SZA. Finally, this smoothed curve was close to a constant line and the ratio values were scattered around this line (Figure 3). In the homogenized data , there were no periods of several years in which the ratios were mostly above or below the line as it was observed after the first step of the homogenization (Figure 2).

Figure 1. Ratios between raw N-values (for SZA=70,77, and 90) and total column ozone measured at Belsk for the period 1963-2020 (points). Curve show the corresponding smoothed values by the LOWESS smoother. Vertical dashed lines mark periods with step changes.

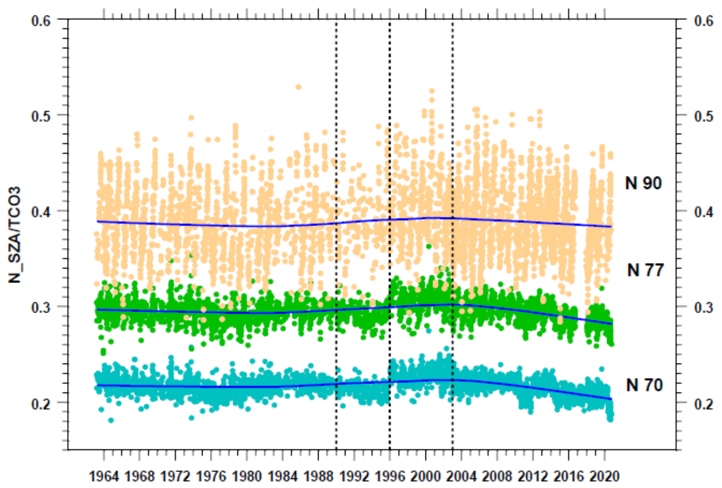


Figure 2. The same as Fig.1 but after elimination of a decline in the ratios for the period 2004-2020 (first step of the homogenization).

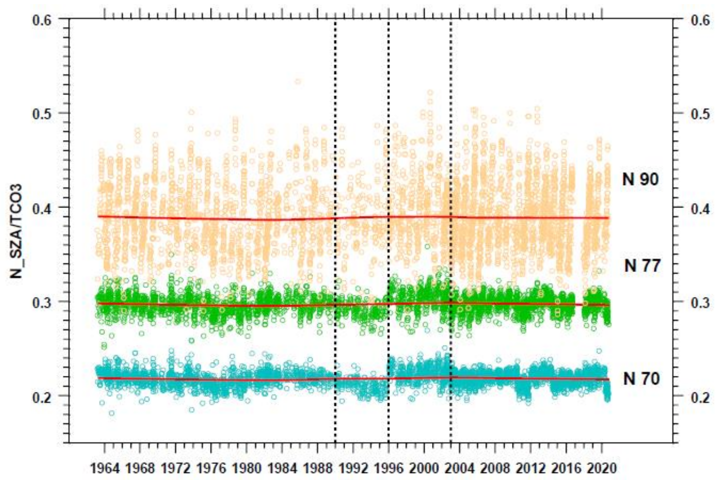
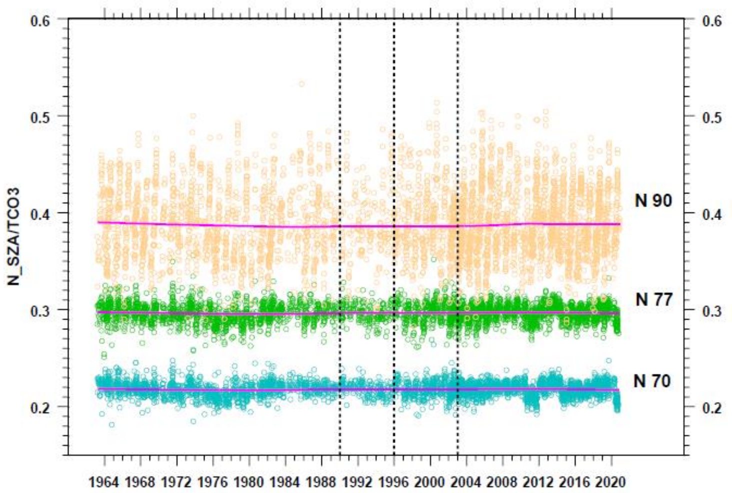


Figure 3. The same as Fig. 1 but the ratios were corrected for step changes in the ratios found after the first step of the homogenization (second step of the homogenization).



Annex 2 - Uncertainty of the Umkehr profile

Total uncertainty in the Umkehr profiles over Belsk is estimated empirically by examining set of differences between am and pm profiles taken during one day. Table 1 shows the difference between am and pm values (for all Umkehr layers and total column ozone) in percent of the daily mean value, i.e. (pm+am)/2. The following statistical characteristics (N=639 for the period 1963-2020) are used, mean value, standard deviation, median, 10th and 90th percentile. It is assumed that the range between 10th and 90th percentile provides the uncertainty. This value probably overestimates the "true" uncertainty as it is possible that the profile could change during the day. However, the Umkehr profiles are taken during perfect clear-sky days with a stable weather conditions and we do not expect also abrupt changes in the stratosphere. It is possible to eliminate days with large intra-day changes in the ground-based profiles examining differences in the satellite ozone profile for three consecutive days (*t*-1, *t*, *t+1*) and select only days (*t)* for calculations of the ratio differences when the change between the triad values are below a threshold. This is left for future consideration.

It is supposed that the am and pm profiles should be quite similar as the Dobson total column ozone (last row in Table 1) changes only slightly during a day (i.e., mean=0.2% with the uncertainty range between -0.7% and 1.1%. The uncertainty ranges for all layers are about ± 5%, and only slightly above this range for Layer 1 [-7.5%; 5.8%].

Table 1. Statistical characteristics of the relative differences, Δ, between am and pm Dobson Umkehr and total column ozone measured during one day at Belsk for the period 1963-2020, Δ=(am – pm)/(am+pm)/2 *100% .

Layer	**Mean**	**SD**	**Median**	**10th per**	**90th per**
Difference between Ozone Content in the Umkehr Layer					
1	-0.8	5.9	-0.6	-7.5	5.8
2	-0.6	3.8	-0.6	-5.5	3.9
3	-0.1	2.9	-0.1	-3.5	3.3
4	0.6	3.4	0.5	-3.5	4.7
5	0.8	2.1	0.9	-1.6	3.3
6	0.8	2.0	0.8	-1.6	3.3
7	0.7	2.3	0.7	-1.9	3.3
8	0.4	3.6	0.4	-3.9	4.7
9	0.1	3.3	0.2	-3.7	4.0

10	0.0	1.7	0.0	-2.0	2.0
Difference between Total Column Ozone					
	0.2	0.8	0.3	-0.7	1.1

Annex 3 – Comparison between the Dobson and Brewer Umkehr profiles.

The column ozone monitoring with the Brewer spectrophotometer serial no. 64 (BS64) mark II (single monochromator) was launched at Belsk in 1991 but the Umkehr observations began in 2010. The full series of the Brewer Umkehrs (2010 -2021) is under construction. At the moment, a comparison with the concurrent Dobson data is available for the period 2011-2016 (N=328 inluding am and pm Dobson-Brewer pairs). Statistics of the relative differences between Brewer and Dobson Umkehrs and total column ozone is shown in Table 2. There is a good agreement between the instruments. Standard deviations and the uncertainy ranges (10th-90th percentile of the Brewer-Dobson differences) are similar to those for the relative differences between am and pm Dobson profiles for one day (Table 1). This allows to determine a universal uncertainty range pertaining the Umkehr retrieval for any ground-based spectrophotometer measuring N-values regardless of its type.

Table 2. Statistical characteristics of the relative differences, Δ, between Brewer and Dobson ozone content in Umkehr Layers and the column amount of ozone measured simultaneously by both instruments at Belsk for the period 2011-2016, Δ= (Brewer-Dobson)/(Brewer+Dobson)/2 *100%

Layer	**Mean**	**SD**	**Median**	**10th per**	**90th per**
Difference between Ozone Content in the Umkehr Layer					
1	-1.7	5.2	-2.1	-7.1	4.7
2	-2.7	3.9	-2.9	-6.9	2.4
3	-0.1	3.1	-0.2	-3.7	3.7
4	0.3	2.8	0.2	-3.0	3.4
5	0.0	2.0	0.1	-2.4	2.4
6	0.8	2.0	0.9	-1.8	3.1
7	2.2	2.7	2.0	-1.1	5.8
8	2.0	3.4	1.8	-1.7	6.3
9	1.4	3.6	1.4	-2.6	5.4
10	0.7	2.0	0.7	-1.6	3.1
Difference between Total Column Ozone					
11	0.0	1.0	0.0	-1.3	1.0

FTIR

Availability

The FTIR ozone retrieval settings have been harmonized within the NDACC IRWG (Infra-Red Working Group), and published in Vigouroux et al. (2015). Most of the data can be found in NDACC IRWG website (https://www2.acom.ucar.edu/irwg/sites). The data are public but required a registration for downloading.

However, for TOAR-II users' convenience, and because a few sites are not yet affiliated to NDACC, we give in the HEGIFTOM ftp-server all relevant FTIR O3 files. This has also the advantage that a few sites providing doubtful data in the NDACC database are not given in the HEGIFTOM ftp-server. So, all the FTIR data (at 23 stations) provided in the HEGIFTOM ftp-server have been quality controlled.

The files are in GEOMS hdf format. General information on GEOMS format can be found here: https://avdc.gsfc.nasa.gov/PDF/GEOMS/geoms-1.0.pdf

Specific information on GEOMS file for FTIR measurements can be found here: https://git.nilu.no/geoms/templates/blob/master/GEOMS-TE-FTIR-002.csv

Data field description

- All the data fields and their units are given in the document: https://git.nilu.no/geoms/templates/blob/master/GEOMS-TE-FTIR-002.csv

They are, in summary, the time (in Julian day, starting from 1 Jan 2000), latitude, longitude and altitude of the instrument, the O3 a priori and retrieved total columns and associated random and systematic uncertainties (in molec/cm^2 or a scaled unit), the altitude grid, the O3 a priori and retrieved vertical profiles (volume mixing ratio – vmr; in ppmv or a scaled unit) and associated random and systematic uncertainty covariance matrices (in $ppmv^2$ or a scaled unit), the averaging kernel matrix (in vmr/vmr), the altitude boundaries of each layer and the corresponding O3 vertical profiles in molec/cm^2, the pressure and temperature profiles (auxiliary data used for the retrievals; from NCEP), the H_2O profiles from NCEP. Additional information can also be added (measured surface pressure and temperature if available).

- Some metadata are included in the GEOMS files. Their description is given here: https://avdc.gsfc.nasa.gov/PDF/GEOMS/geoms-1.0.pdf

In summary, they are divided in 3 kinds: the global originator attributes (name, affiliation, email,… of the PI of the instrument, of the person that generated the data, and of the person that has created the file), the global dataset attributes (short description of the data, location name, instrument name, list of the data fields, start and end of date of measurements, file version, rules of use, acknowledgements to be used in case the data are included in a publication, data quality information, software used for the retrievals,…), and the global file attributes (file name, generation date, file access - database).

Additional metadata information can be found (one unique file per station) at the NDACC website (https://www.ndaccdemo.org/stations/), with more details on the instrument (type, detectors, possible failures, …), relevant publications, …

- For the users' convenience, some derived products will be put in the HEGIFTOM ftp-server. Depending on the outcomes of the discussion within the TOAR-II WG, it will be 0-8 km columns and/or tropospheric columns (with tropopause height definition to be harmonized within the WGs).

Description of homogenization procedure

Most of the FTIR NDACC instruments are from the same manufacturer (Bruker), and of the same type (120 or 125 HR; for High Resolution). Furthermore, only 2 different retrieval codes are used within the network (PROFFIT and SFIT), and provide retrieved columns and profiles in excellent agreement when the same retrieval parameters are used (Hase et al., 2004). The FTIR retrieval parameters have been harmonized within the IRWG and can be found in Vigouroux et al. (2015). A modification of these parameters can occur during the HEGIFTOM timeframe (e.g. use of an updated spectroscopy), but in that case, all FTIR sites will make the modification to ensure homogenization within the network. At the time of Vigouroux et al. (2015), homogenization of the uncertainties was not complete (the same Rodgers theory was used within the network, but not necessarily with the same input uncertainty parameters). The next update of the FTIR products in the NDACC database will include this homogenization of uncertainties.

Data management

Flagging

- Before archiving in the NDACC database, FTIR data providers perform a quality check of their data (using a threshold filtering on e.g. RMS, Degrees of Freedom for Signal, uncertainties, convergence of the fit, …). A quality control of the FTIR archived files concludes that indeed in most cases, no or very few outliers remain. Two sites were found however to provide doubtful profiles and/or columns and are not put in the HEGIFTOM ftp-server (in agreement with the PIs).
- No flagging is available in the GEOMS files.
- A metadata attribute is given in the GEOMS file (DATA_QUALITY) where the information is provided whether or not the instrumental line shape is regularly controlled. (this is mostly the case since this is mandatory for becoming an official NDACC site)

Uncertainties

- For each individual measurement, separate random and systematic uncertainties are provided in the GEOMS files for the O3 total columns, and for the O3 profiles (error covariance matrices are given because the uncertainties at different heights of the profiles are correlated, i.e. there are off-diagonal elements). Note that the smoothing error is not included in the GEOMS file, but can be calculated by the users using the provided averaging kernel and a variability covariance matrix to be built by the users (Rodgers 2000). The covariance matrices will be used to derived the random and systematic uncertainties on the dedicated partial columns for HEGIFTOM (0-8 km, and/or tropospheric columns). Since the smoothing error is the dominant random error source for the tropospheric O3 columns, it should be added in these dedicated HEGIFTOM products.
- The uncertainties are derived from the Rodgers theory. Details can be found in e.g. García et al. (2012) and Tarasick et al. (2019, Supplemental material).

Traceability

- Some retrieval parameters are available in the GEOMS HDF files archived in NDACC (a priori ozone profiles, p, T)
- A metadata file is also available at each site with information such as the instrument / instrument change; the retrieval code; some publications with informations on retrievals,…
- Some guidelines for FTIR retrievals are given at the IRWG website: https://www.acom.ucar.edu/irwg/IRWG_Uniform_RP_Summary-3.pdf; and for O3 specifically, in Vigouroux et al. (2015).
- A process chain with full traceability is in progress within the project ACTRIS.

Internal consistency

- The homogenization of the instrument type, retrieval codes and parameters (see above) should lead to an internal consistency of the FTIR network.
- However, no inter-comparison campaign has been made, except for the retrieval codes (Hase et al., 2004).
- The consistency in the uncertainty parameters needs to be improved.

External consistency

- Comparisons between FTIR and sondes have been made in Vigouroux et al. (2008) at 6 sites. For the ground-10 km layer, the bias was from +1 up to +9% (FTIR higher), and the standard deviation of 11-20%. An even smaller standard deviation with sondes was found in García et al. (2012) for the ground-13km layer (9%).
- Inter-comparison study will be performed within HEGIFTOM (FTIR vs Umkehr, Lidar,…), to better conclude on the external consistency of FTIR measurements (in particular drifts have never been studied yet).

Data quality indicators

- We give in Table 1, the estimated uncertainties at Izaña for the ground-8km layer. But note that, since the smoothing uncertainty is dominant, and since it is smaller when the partial column's width increase, the random uncertainty for a complete tropospheric column would be 5-6% only. Systematic and random parameter errors would stay similar.

	Errors [%]
Theoretical Random Parameter Error (TPE)	3
Theoretical Smoothing Error (SE)	10
Theoretical Random Error (TRE)	~11
Theoretical Systematic Error (TSE)	4
Experimental Random Error –ECC sondes	9

Experimental Systematic Error –ECC sondes	4

Table 1. Estimated random and systematic errors relative to the FTIR retrieved ozone tropospheric partial column (2.37-8.0 km) [in %] for the IZO Bruker 120/5HR (TOAR-I, Omaira García, private comm.) as well as experimental errors by comparing to coincident ECC sondes obtained in García et al. (2012) for 2.37-13 km columns.

List of homogenized sites (name, geographical location, period of observations)

The list of FTIR stations measuring tropospheric ozone (as well as total ozone and profiles) is given in Table 2. The stations with homogenized data ready to be used within TOAR-II are in green. The data will be provided in the HEGIFTOM ftp-server. When the data are not available in NDACC, it is mentioned in red in the appropriate column.

Site	Latitude (deg)	Longitude (deg)	Altitude (km)	Time range	Did not pass yet completely my quality check and/or in discussion with PI	Instrument	Archived in NDACC ?	Instrument PI	Contact
Eureka, Canada	80,05	-86,42	0,61	2006 - present		Bruker 125HR	Yes	Kim Strong	strong@atmosp.physics.utoronto.ca
Ny-Ålesund, Norway	78,92	11,92	0,02	1995 - present		Bruker 120/5HR	Yes	Justus Notholt	jnotholt@iup.physik.uni-bremen.de
Thule, Greenland	76,53	-68,74	0,22	1999 - present		Bruker 120M	Yes	Jim Hannigan	jamesw@ucar.edu
Kiruna, Sweden	67,84	20,4	0,42	1996 - present		Bruker 120/5HR	Yes	Thomas Blumenstock	thomas.blumenstock@kit.edu
Harestua, Sweden	60,2	10,8	0,6	1995-2008	X	Bruker 120M	No (sent to me in 2010)	Johan Mellqvist	johan.mellqvist@chalmers.se
				2009- present		Bruker 125M	Yes		
StPetersburg, Russia	59,88	29,82	0,02	2009 - present		Bruker 125HR	Yes	Yana Virolainen	yana.virolainen@spbu.ru
Bremen, Germany	53,1	8,85	0,03	2004 - present		Bruker 125HR	Yes	Justus Notholt	jnotholt@iup.physik.uni-bremen.de
Zugspitze, Germany	47,42	10,98	2,96	1995 - present		Bruker 120/5HR	Yes	Ralf Sussmann	Ralf.Sussmann@imk.fzk.de
Jungfraujoch, Switzerland	46,55	7,98	3,58	1984 - 1994	X	Home-made HR	No (in the future)	Emmanuel Mahieu	Emmanuel.Mahieu@ulg.ac.be
				1995 - 1999	X	Bruker 120HR	No (in the near future)		
				2000 - present		Bruker 120HR	Yes		
Toronto, Canada	43,6	-79,36	0,17	2002 - present	X	Bomem DA8	Yes	Kim Strong	strong@atmosp.physics.utoronto.ca
Rikubetsu, Japan	43,46	143,77	0,38	2010 (few) ; 2014-present		Bruker 120/5HR	Yes	Tomoo Nagahama	nagahama@isee.nagoya-u.ac.jp
Boulder, USA	40,04	-105,24	1,61	2010 - present		Bruker 120/5HR	No (not an NDACC site yet)	Jim Hannigan	jamesw@ucar.edu
Tsukuba, Japan	36,05	140,12	0,03	2014 - present		Bruker 125HR	No (not an NDACC site yet)	Isao Murata	murata@pat.gp.tohoku.ac.jp
Hefei, China	31,91	117,17	0,045	2015 - present		Bruker 125HR	No (not an NDACC site yet, but soon)	Cheng Liu	ywsun@aiofm.ac.cn, chliu81@ustc.edu.cn
Izaña, Spain	28,3	-16,48	2,37	1999 - 2005		Bruker 120M	Yes	Omaira García	ogarciar@aemet.es
				2005 - present		Bruker 125HR			
Mauna Loa, Hawaï	19,54	-155,57	3,4	1995-2001	X	Bruker 120/5HR	Yes	Jim Hannigan	jamesw@ucar.edu
				2001-present					
Mexico City, Mexico	19,33	-99,18	2,26	2013 - present	X	Bruker Vertex80 (not NDACC compliant)	No (not a NDACC site)	Michel Grutter	grutter@unam.mx
Altzomoni, Mexico	19,12	-98,68	3,98	2012 - present		Bruker 120/5HR	Yes	Michel Grutter	grutter@unam.mx
Paramaribo, Suriname	5,81	-55,214	0,03	2004-2016 (sparse)		Bruker 120/5M	Yes	Justus Notholt	jnotholt@iup.physik.uni-bremen.de
PortoVelho, Brazil	-8,77	-63,87	0,09	2019 only. Restart 2022		Bruker 120M (125HR in 2022)	No (not an NDACC site)	M. De Mazière	corinne.vigouroux@aeronomie.be
St-Denis, Reunion Island	-20,9	55,48	0,08	2004-2011		Bruker 120M	Yes	M. De Mazière	corinne.vigouroux@aeronomie.be
Maïdo, Reunion Island	-21,08	55,38	2,16	2013 - present		Bruker 125HR	Yes	M. De Mazière	corinne.vigouroux@aeronomie.be
Wollongong, Australia	-34,41	150,88	0,03	1996 - 2007	X	Bomem DA8	No (sent to me in 2013)	Nicholas Jones	njones@uow.edu.au
				2007 - present		Bruker 125HR	Yes		
Lauder, New-Zealand	-45,04	169,68	0,37	2001 - present		Bruker 120HR	Yes	Dan Smale	Dan.Smale@niwa.co.nz
Arrival Heights, Antartica	-77,82	166,65	0,2	1997 - 2016		Bruker 120M	No (strato profiles to be improved)	Dan Smale	Dan.Smale@niwa.co.nz
				2014 - present		Bruker 125HR		Dan Smale	Dan.Smale@niwa.co.nz

Table 2: List of FTIR stations measuring tropospheric ozone.

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TOAR-II HEGIFTOM: Description of homogenized TMF Tropospheric Ozone Lidar (TMTOL) time series

This document refers to the ozone profiles obtained from the JPL tropospheric ozone differential absorption lidar located at the Table Mountain Facility, California (Lat. 34.4N; Long. 117.7W; Elev. 2285 m a.s.l.; PI: T. Leblanc), also referred to as "TMTOL". This long-term dataset (historically archived at NDACC) consists of 2-hour-averaged nighttime ozone profiles measured routinely 3 to 4 times per week, totaling an average of 150 profiles per year between 2000 and present. Typical altitudes covered are 3-22 km (extended down to 100 m above ground for the most recent years).

Availability

As of February 2023, the complete homogenized time series (2000-present) in hdf-5 format can be obtained via ftp from the TOAR-II HEGIFTOM ftp server "ftp-me.oma.be", accessible with account name "ozonesondes" and password "OzonFeb2021:", in the subdirectory "Lidar". The 2018-present segment of this dataset is also available in GEOMS-compliant HDF4 format at the NDACC data handling center (the 2000-2017 segment will be uploaded to NDACC shortly, so that the full dataset will also be available at NDACC).

Data field description (HDF5 format)

- See Table 1 below for the most essential variables.

HDF name	Description	Unit	Dim	Comment
Altitude	Geometric altitude	m (a..s.l.)	1D	Primary independent variable
O3_ND	Ozone number density	mol.m-3	1D	Primary dependent variable
Vertical_resolution	Effective vertical resolution (see ref. 1)	m	1D	NDACC-standardized (see ref. 1)
uO3_ND	Uncertainty components (see ref. 2)	mol.m-3	2D	Total uncertainty is in row 1 Individual contributions are in rows 2-14
u_contributions	Sources of uncertainty components	STRING	1D	The only random component is detection noise (row 2)
u_recommended_treatment	Advise how to use uncertainty components	STRING	1D	Useful for computing Level 3 and 4 datasets

Time_start	Measurement start time	MJD	1D	Same time for all altitudes
Time_end	Measurement end time	MJD	1D	Same time for all altitudes
O3_MR	Ozone Volume mixing ratio	m-3.m-3	1D	Derived from O3_ND, xT_O3MR and xP_O3MR
xT_O3MR	Ancillary temperature	K	1D	Used to derive O3_MR
xP_O3MR	Ancillary pressure	Pa	1D	Used to derive O3_MR
xT_O3MR_source	Source of ancillary temperature	STRING	1D	By default: MERRA-2
xP_O3MR_source	Source of ancillary pressure	STRING	1D	By default: MERRA-2

Table 1: Most essential variables

- Metadata file available at NDACC
- Simultaneous surface ozone measurement reported in HDF5 files since 2018

Description of homogenization procedure

Homogenization is done by using the GLASS Data Processing Algorithm, which follows the NDACC Vertical resolution and Uncertainty Budget Standardization Guidelines provided in refs. 1-3. Dataset was re-analyzed with same version of GLASS (v1). The GLASS data processor can analyze raw lidar signals produced by about 15 different lidar instruments contributing to 3 global networks: NDACC, TOLNet and GRUAN. Besides the TMTOL system, lidars relevant to HEGIFTOM and for which data has already been analyzed by GLASS are: OHP tropospheric ozone lidar, Reunion Island tropospheric ozone lidar, all TOLNet lidars, and Mauna Loa, Table Mountain, Lauder, and Eureka stratospheric ozone lidars. However, the re-analysis of multiple large datasets is time-consuming, and full homogenized datasets currently exist only for the JPL-operated lidars.

Data management

Flagging

- Data cleaning: Visual check and cut-off at bottom and top of profiles, as well as cloud-clearing
- No actual flagging, but cloud-contaminated layers are systematically set to missing values
- Data quality indicators: All given by uncertainty

Uncertainties

- NDACC-standardized: All uncertainty components (random and systematic) are explicitly computed following the BIPM Guide to Uncertainty in Measurements (GUM, see refs 2-3)
- Unaccounted uncertainty sources: Aerosols contamination and receiver misalignment

Traceability

- No lidar instrument is traceable to a reference instrument
- TMTOL instrument initial set up description can be found in ref. 4
- Data processing is traceable to GLASS documentation (refs. 1-2 and ref. 5) and references therein

Internal consistency

- Time series of different instruments are internally consistent if analyzed by GLASS, or if algorithms were validated within a network (true for TOLNet, partly true for NDACC)
- References of intercomparison campaigns of different instruments within the same network? Overall conclusions of such studies: SCOOP Campaign (see ref. 6)
- How much inconsistency is left over after homogenization: Aerosol uncertainty.

External consistency

- References of intercomparison studies between TMTOL and ozonesonde: SCOOP Campaign (ref. 6)
- Overall conclusions: TMTOL instrument within 5% of other lidars and ozonesondes

Data quality indicators

- Dataset used by multiple authors for climatology and trend studies (e.g., refs. 7-9)
- Overall: Total uncertainty ranging from 3% to 10% and higher. Larger uncertainty is found at the very top of the profiles (lower STNR), and occasionally at the very bottom (signal saturation or incomplete telescope/laser overlap).
- Longer integration times reduce random noise and improves quality

Current homogenized sites (expansive datasets):

- JPL-Table Mountain Facility (TMF) TMTOL lidar 1999-present
- JPL-Table Mountain Facility (TMF) StratO3 Lidar TMSOL 2018-present (homogenized)
- Mauna Loa Observatory (MLO) StratO3 Lidar MLSOL 1998-present

Potential/future expansion of homogenized sites:

- Observatoire de Haute-Provence (OHP) Trop.O3 lidar 1990-present
- All five TOLNet lidars : dates TBD
- JPL-Table Mountain Facility (TMF) StratO3 Lidar TMSOL 1988-2017

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