TOAR-II HEGIFTOM: Description of homogenized IAGOS free-tropospheric ozone time series

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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*

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[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