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

General guideline: in main text part, only short descriptions. Details can be referencing to literature or hyperlinking to sites where the document can be accessed. New documents or material can be included here as an annex.

Availability

Please give the location where the homogenized time series can be obtained (ftp, data archive, website, doi, e-mail address contact person, etc.). Data format (hdf, NASA-Ames, etc.) but its description in separate document (hyperlink) or annex (possibly refer to code or libraries for reading in the data).

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

Please provide a short description (few lines) of the steps taken to make your dataset (more) homogeneous/harmonized within the network. Give details in an Annex document or the references of the publications (documents) in which the homogenization procedure of the data is described.

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? Overall 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 investigate 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

- *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

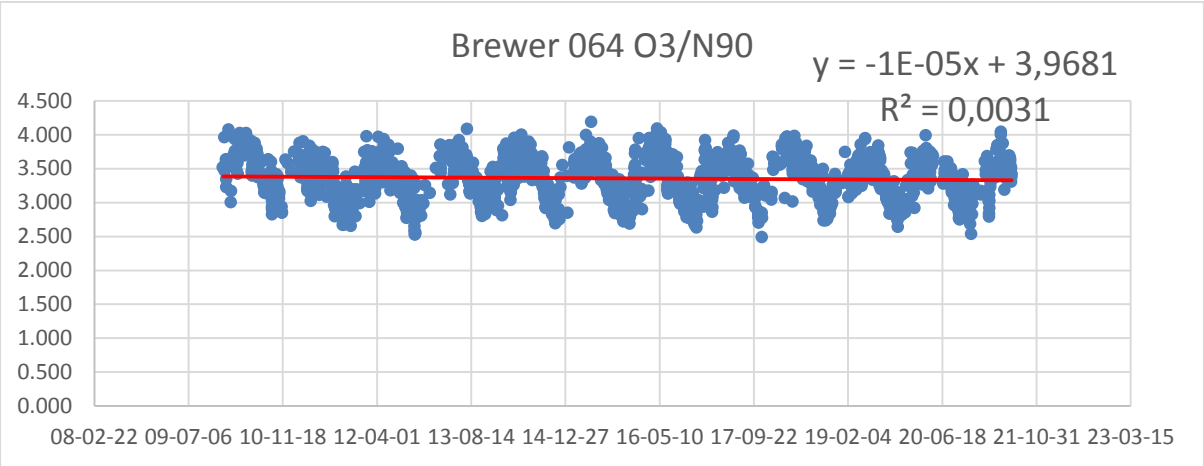
- *Short description or referencing or hyperlinking to a document*
  See Annex 2
- *Factsheet of the performance of the instrument in field operation (only overall specifications, e.g. overall uncertainty xx%) (Table on one page)*
  The uncertainty ranges for the ozone content Umkehr Layers are of about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

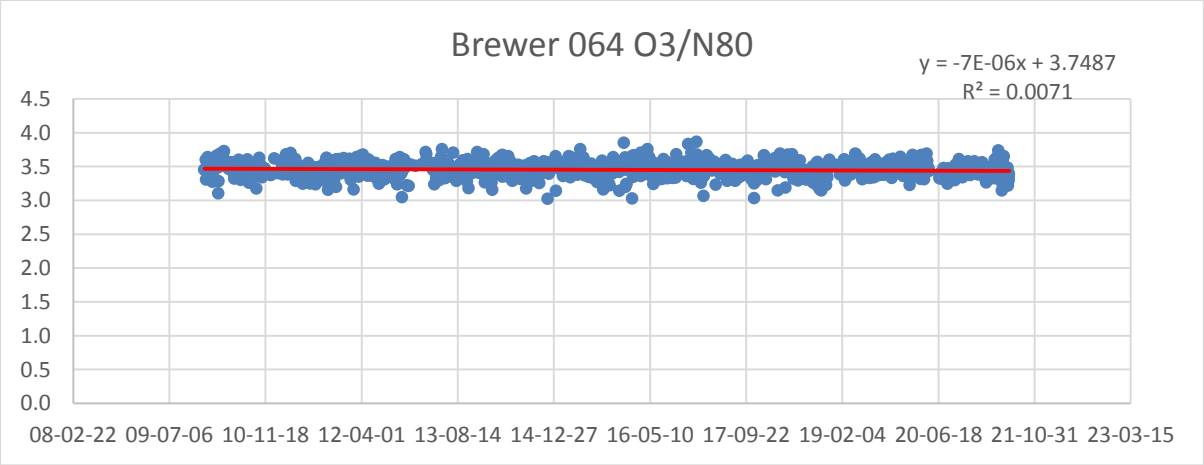
List of homogenized sites (name, geographical location, period of observations)

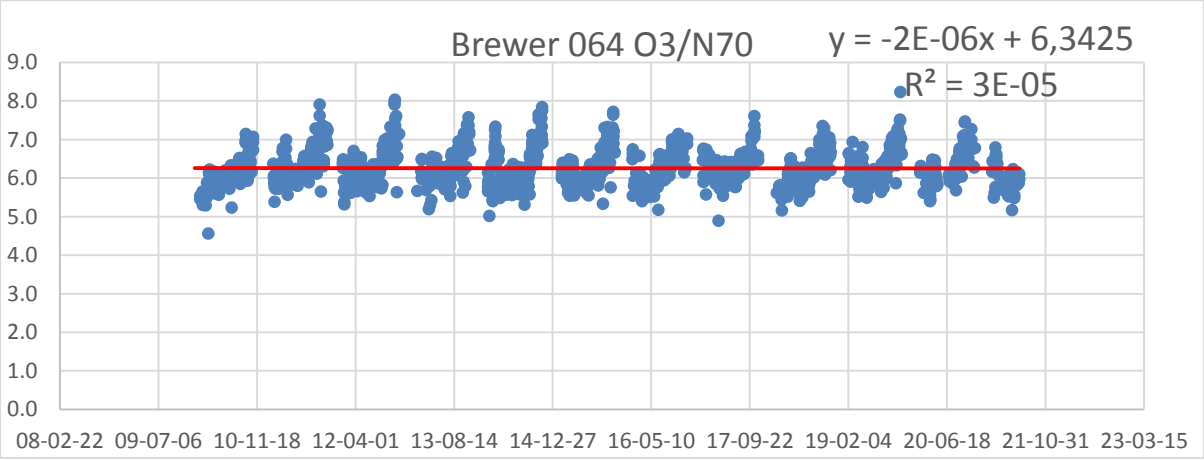
Station	Instrument Type/ Number	Observational period	Latitude	Longitude
Thessaloniki	Brewer MKII (#005)		40.63 N	22.96 E
Hradec Kralove	Brewer MKIII (#184)		50.18 N	15.84 E
Madrid	Brewer MKIII (#186)		40.45 N	3.72 W
Warsaw	Brewer MKIII (#207)		52.25 N	20.94 E
Belsk	Brewer MKII (#064)	01/2010 -10/2021	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

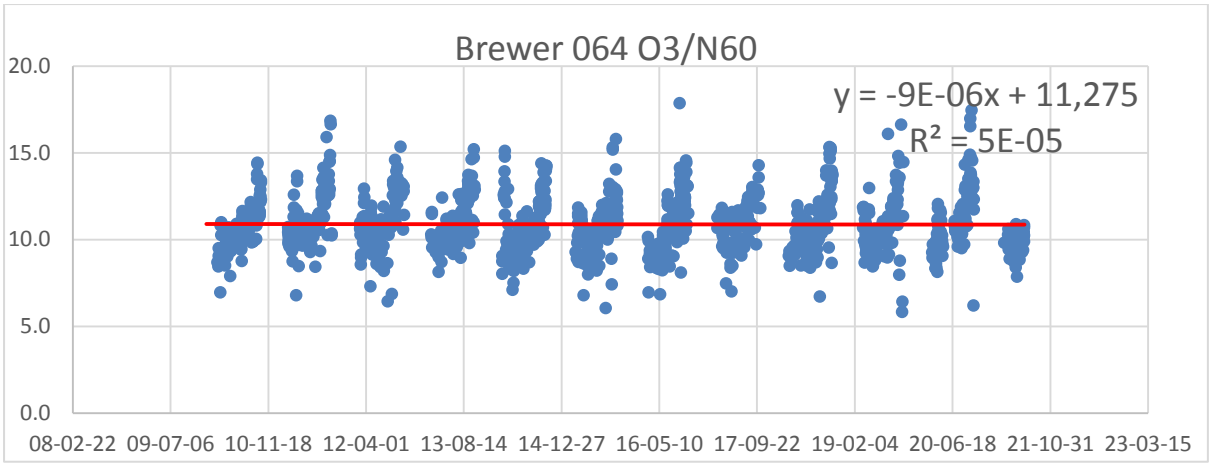
Annex 1

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, 10^{th} and 90^{th} percentile. It is assumed that the range between 10^{th} and 90^{th} 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**	**10^{th}**	**90^{th}**
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