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

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.

References

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