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ACE – FTS

Atmospheric Chemistry Experiment

Data usage guide and file format description for ACE-FTS level 2 data version 3.5 ASCII format

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DOCUMENT CHANGE RECORD

Issue	Rev.	Date	Change Detail
1	-	26 Aug. 2014	First Issue of document – for version 3.5 preliminary data release
1	A	12 Feb. 2015	Update to data flag information
1	B	15 Mar. 2016	Addition of information on research data products

1. Introduction, Data Usage Information and Format Description

The user is **strongly encouraged** to read the README files (produced by Chris Boone for each version of the ACE-FTS retrievals and reproduced in this document) and the ACE-FTS retrieval paper (C. D. Boone *et al.*, "Retrievals for the atmospheric chemistry experiment Fourier-transform spectrometer", *Appl. Opt.*, **44**(33), 7218-7231, (2005) available from the ACE Mission website (http://www.ace.uwaterloo.ca/publications.html)) for more information on the ACE-FTS retrievals. In particular, the ACE-FTS version 3.5 retrievals are described in C. D. Boone et al. "Version 3 Retrievals for the Atmospheric Chemistry Experiment Fourier Transform Spectrometer (ACE-FTS)" in *The Atmospheric Chemistry Experiment ACE at 10: A Solar Occultation Anthology* (Peter F. Bernath, editor, A. Deepak Publishing, Hampton, Virginia, U.S.A., 2013).

Relationship between version 3.5 and version 3.0 ACE-FTS datasets:

The reason for the version 3.5 data version is to correct a processing issue that impacted all ACE-FTS data (versions 3.0 and 2.2+updates) from October 2010 forward. This arose from the pressure and temperature data from the Canadian Weather Service Model from the Canadian Meteorological Center (CMC) that is utilized in the retrieval (see *Use of a priori data* section below). This issue has been resolved and the affected data has been reprocessed. In addition, recommended research products have been included in this new version including high altitude CO, HCFC-22, C_2H_6, and polar N_2O. **Version 3.5 replaces version 3.0 for the entire ACE mission period and this is the recommended version to use for research purposes.**

General comments on the file formatting and data usage:

In all of these files, the start and end times given (either time stamp or date and time) correspond essentially to the start and end of the command sequence. They cannot and should not be used to derive the length of an occultation since they include warm up time and calibration measurements (deep space and exo-atmospheric). The location given for each occultation is obtained from the latitude, longitude and time of the 30 km tangent point (calculated geometrically).

A fill value of -999 is used when at each altitude where a retrieval is not performed. The user should be careful to distinguish fill values (-999) reported in the VMR statistical error columns from flagged values (-888). This is not a typographical error! For VMR retrievals, the profile above the highest analyzed measurement is taken as a constant times the input guess profile. These data are flagged with an error of -888 and should be treated with caution.

It should be noted that there are no errors provided for the temperature or pressure retrievals because of amount of time required to calculate them. The user is directed to the Applied Optics paper by C. D. Boone for details on how the temperature and pressure retrievals are done. The accuracy of these retrievals was assessed for version 2.2 and is reported in the validation paper by R. J. Sica *et al.* ("Validation of the Atmospheric Chemistry Experiment (ACE) version 2.2

temperature using ground based and space-borne measurements", *Atmos. Chem. Phys.*, **8**, 35-62, 2008; available from the ACE website using the link given above).

The ACE-FTS measurements are recorded every 2 s. This corresponds to a measurement spacing of 2-6 km which decreases at lower altitudes due to refraction. The typical altitude spacing changes with the orbital beta angle. For historical reasons, the retrieved results are interpolated onto a 1 km "grid" using a piecewise quadratic method. For ACE-FTS version 1.0, the results were reported only on the interpolated grid (every 1 km from 0.5 to 149.5 km). For versions 2.0 through 3.5, both the "retrieval" grid and the "1 km" grid profiles are available.

This version includes the retrieval of subsidiary isotopologues from the ACE-FTS spectra. The line strengths in the HITRAN 2004 database are scaled according to natural isotopic abundance. For the subsidiary isotopologues, in order to obtain the actual VMR values, the user will need to scale the retrieved profile with the isotopic abundances assumed by HITRAN (http://www.hitran.com). We have adopted the same notation as used by HITRAN to label the subsidiary isotopologues. For example, the minor water vapor isotopologues are labeled, 181 for $H_2{}^{18}O$, 171 for $H_2{}^{17}O$ and 162 for $HD^{16}O$.

For each occultation event, four ASCII formatted data files are produced: the "1 km" and "retrieval" grid results for the most abundant or main isotopologues and the "1 km" and "retrieval" grid results for the subsidiary isotopologues. The file naming conventions for the four files are given in Table 1. The file formats are provided in Table 5 (main isotopologues) and Table 6 (subsidiary isotopologues).

Table 1: File naming convention

Name	Isotopologues	Data file type
sxXXXXv3.5.asc	Most abundant	1 km altitude grid
sxXXXXv3.5tangrid.asc	Most abundant	Retrieval altitude grid
sxXXXXv3.5iso.asc	Subsidiary	1 km altitude grid
sxXXXXv3.5isotangrid.asc	Subsidiary	Retrieval altitude grid

where: sx is the type of occultation sunrise (sr) or sunset (ss)
and XXXX (or XXXXX) is the orbit number

Preliminary version 3.5 release dataset:

There are some data gaps and processing issues that are still being dealt with for the ACE-FTS version 3.5 processing. Note that for this "preliminary" version 3.5 dataset, the following are still being processed.

Data gaps: Not all ACE-FTS occultations have yet to undergo level 1 → 2 processing. There is a data gap in 2011 and another in 2012, as well as a minor data gap in 2009. These are currently being back-filled and all successfully processed occultations will be made available in the coming months.

Processing errors: There were batches of data where errors occurred in the level 0 → 1 processing. These are included in the current release, however a list of affected occultations is given on the website, and have been flagged as a 7 in the v3.5 flag files. These occultations should not be used. These will be reprocessed and will be released in the future.

Spectral calibration errors: There were occultations where one or more spectra used in calculating the average reference solar spectrum contained significant errors, leading to increased variability in multiple species. Many of these occultations (mostly in Jan 2006 and Oct-Nov 2008 and 2009) have been identified and are included in the current release. A list of occultations known to be affected by this issue is given on the website, and have been flagged as a 7 in the v3.5 flag files. These occultations should not be used. These will be reprocessed in the coming months.

Retrieval failures: The retrieval failure rate for most species is on the order of 1%. However, in v3.5 there are 10 species with a significantly higher failure rate, with the majority of failures occurring in 2004-2005. Table 2 shows the affected species and associated failure rates. We aim to provide research versions of the N_2O_5, $ClONO_2$, and CCl_3F for this period of time. These will be made available in the next months.

Table 2: Retrieval failure rates for 10 different ACE-FTS species.

Species	Total (%)	Before 2006 (%)	2006 and on (%)
N_2O_5	23.68	79.34	6.27
$ClONO_2$	23.72	79.33	6.33
CF_4	23.86	79.31	6.52
CCl_3F	25.06	79.47	8.05
SF_6	23.79	79.33	6.42
CCl_4	24.53	79.44	7.35
CFC-113	27.78	80.15	11.41
HCFC-141b	25.94	79.48	9.20
HCFC-142b	27.34	79.93	10.90
CH_3D	47.87	8.79	60.43

Research Version Data Products:

For some species, data products are not produced routinely. However, "research versions" of these data products are made available to the Science Team, upon request. These products can be reprocessed versions of species with improved spectroscopic parameters or adjusted microwindows (e.g. CH_4) or data products that have not yet been incorporated into the routine processing stream (e.g. SO_2). The Science Operations Centre can provide detailed information on the processing used for these research version products.

In version 3.5, there are five research products available, namely peroxyacetyl nitrate (PAN), acetonitrile (CH_3CN), acetone (CH_3COCH_3), methane (CH_4), and sulfur dioxide (SO_2). These are available in ascii format (without data quality flags included) and in netCDF format (with data quality flags included). For the SO_2 product, the data quality flags should be used with caution around the 2008 and 2009 volcanic eruptions.

Use of a priori data:

For the temperature and pressure profiles, the reported values come from different sources depending on the altitude range. Below 15 km, these are fixed to meteorological data from the CMC (Canadian Meteorological Center). Between 15 km and ~120 km, pressure and temperature are retrieved. Above ~120 km, they are fixed to data from MSIS model calculations. These regions are identified by the T_fit parameter. If this is true, then the temperature and pressure have been retrieved from the measurements. In version 1.0, the T_fit parameter had values of T or F whereas in later versions these have been changed to 1 or 0.

It should be noted that the only places that we use *a priori* profiles are the areas described above: p/T is fixed to *a priori* below 15 km and above ~120 km, and the VMR above the highest analyzed measurement for the given molecule is taken as a constant times the *a priori* (in this case, only the shape of the *a priori* profile is important). The operational retrieval employs a weighted non-linear least squares fit with appropriately bounded constraints to invert the spectral measurements and produce atmospheric profiles of pressure, temperature and constituent species. Beyond the exceptions described above, *a priori* profiles are used only as a first guess.

Use of CO_2 profiles provided in data files:

Care should be taken in use of the CO_2 profiles provided in these data files. Above ~60 km, CO_2 VMR is retrieved from the ACE-FTS spectra and can be used for scientific studies. For altitudes below ~60 km, CO_2 VMR is held fixed during the pressure/temperature retrieval process, and the retrieved CO_2 in that altitude region will therefore simply reproduce the input assumptions for the molecule's VMR profile. **CO_2 VMRs below 60 km are not to be used for scientific studies.**

Validation results for ACE-FTS:

The ACE mission website contains links to all of the papers produced using ACE data and current validation results: http://ace.uwaterloo.ca/publications.html.

Specific issues with certain species based on preliminary validation assessment:

Nitrous oxide (N_2O): Some N_2O measurements inside the Antarctic vortex, when derived temperatures are below 196 K, are anomalously large. These occultations have been flagged as a 7 in the v3.5 flag files.

Nitric oxide (NO): Between ~35 and 50 km, NO VMRs (volume mixing ratios) spike to significant negative values during times of increased NO. It is recommended that negative values not be removed, as to not skew the mean. There is a known low bias for NO below about 20 km, with the VMR often going negative, likely a consequence of the fact that we do not account for diurnal effects in our retrievals.

Carbon monoxide (CO): Between ~20 and 50 km, CO VMRs spike to significant negative values. It is recommended that negative values not be removed, as to not skew the mean.

Chlorine nitrate ($ClONO_2$): There is an increase in noise at 33.5 km (interpolated grid files). This is likely due to interfering species HNO_3 at this altitude level. This issue is under investigation.

CFC-113: At altitudes above 12 km in the Antarctic winter, VMRs increase to unrealistic values. This is most likely due to an unaccounted for interfering species.

Availability of Geolocation Information for ACE profiles:

With this release of ACE-FTS data, geolocation information (GLC files) is being provided for the 1 km and tangrid profiles. These are calculated using a refraction model and Satellite Toolkit (STK). If the model calculation failed, it is recommended to use the 30 km tangent point (calculated geometrically) information in the file headers. The GLCs can be used with the ACE-Imager and ACE-MAESTRO profiles (interpolating in altitude as necessary). The file format for the GLC files is provided in Table 7.

Recommendations for data use and availability of data flags:

The ACE Science Operations phase started on February 21, 2004. ACE measurements taken in late 2003 and early 2004 were done as part of the Satellite Commissioning phase. Since February 21, 2004, there have been instances where there were issues with the data and the occultations from these periods should be avoided or used with caution.

The occultations with known issues are listed on the ACE Data Issues webpage (https://databace.uwaterloo.ca/validation/data_issues.php). This list is updated as new issues are reported so please check it frequently. You can download a csv version of this using the button at the bottom of the page.

If you find any problems or issues with the ACE data please let the ACE Science Operations Centre know by submitting a Data Issue Report via:
(https://databace.uwaterloo.ca/validation/data_issues_report_form.php).

In addition to the Data Issues List, a system of data quality flags have been developed for the ACE-FTS version 3.5 dataset. These are provided for each level for each 1 km grid profile in self-descriptive netCDF files (one for each species/isotopologue including both flags and data). The fields in each of the files are as follows in Table 3.

A description of the flagging method and flags has been published in P. E. Sheese *et al.* ("Detecting physically unrealistic outliers in ACE-FTS atmospheric measurements", *Atmos. Meas. Tech.*, **8**, 741-750, 2015). The current version of these flags is v1.1 (dated 7 Jan. 2015). This version uses a calculation method that is slightly modified from that of the first release (described in P. E. Sheese *et al.* "Technical Note: Detecting outliers in satellite-based atmospheric measurements", *Atmos. Meas. Tech. Discuss.*, **7**, 8398-8414, 2014 that was released in early September 2014).

Table 3: netCDF fields included in data quality flagging files.

Parameter	Definition
Altitude	Tangent altitude for retrieved species, temperature and pressure (in km)
ss (0) or sr (1)	Type of occultation flag (ss = 0; sr = 1)
Orbit	Orbit number for occultation
Year	Year of occultation 30 km geometric tangent point (YYYY in UTC)
Month	Month of occultation 30 km geometric tangent point (MM in UTC)
Day	Day of occultation 30 km geometric tangent point (DD in UTC)
Hour	Time of occultation 30 km geometric tangent point (hh.xxxx in UTC)
Latitude	Latitude of 30 km geometric tangent point (in degrees; ±90, N = +, S = -)
Longitude	Longitude of 30 km geometric tangent point (in degrees; ±180, E = +, W = -)
beta angle	Beta angle of occultation at 30 km tangent point (in degrees)
Species	Retrieved volume mixing ratio for species (in ppv; parts per volume)
species_error	Statistical error for species retrieval from fitting (in ppv; if this value is -888, vmr is not retrieved. It is the value obtained by scaling the *a priori* value)
quality flag	Flag value as per Table 4
Temperature	Temperature (in K)
temperature_fit	Values indicating if temperature was retrieved from data (1) or is set to the *a priori* value (0)
Pressure	Pressure (in atm; 1 atm = 1.01325 bar)
flag_version	Version of flag product for ACE-FTS v3.5

It is recommended that any profile known to be affected by instrument or processing errors (flag values of 7) or any profile containing a data point determined to be an unnatural outlier (flag value in the range of 4-6) be excluded from the analysis. Data users are directed to the Sheese *et al.*, 2015 paper for further recommendations and caveats for usage.

Table 4: Definition of flag values associated with ACE-FTS level 2 data.

Flag value	Definition
0	No known issues with data
1	Percent error is not within 0.01–100 %, and no other category of flag applies
2	Not enough data points in the region to do statistical analysis, and percent error is within 0.01–100 %
3	Not enough data points in the region to do statistical analysis, and percent error is not within 0.01–100 %
4	Moderate unnatural outlier detected from running MeAD, percent error within limits
5	Extreme unnatural outlier detected from EDF, percent error within limits
6	Unnatural outlier detected and percent error is outside of limits
7	Instrument or processing error
8	Error fill value of −888 (data is scaled a priori)
9	Data fill value of −999 (no data)

Table 5: File format for “1 km” and “retrieval” grid data files – Version 3.5 for main isotopologues

Filename for “1 km” grid data: sxXXXXv3.5.asc or sxXXXXXv3.5.asc			
Filename for “retrieval” grid data: sxXXXXv3.5tangrid.asc or sxXXXXXv3.5tangrid.asc			
Field name	**Description**	**Acceptable values / units**	**Type**
Header section			
Name	Occultation identifier using mission name (ace), orbit number (XXXX or XXXXX) and type of occultation (sx)	ace.sxXXXX or ace.sxXXXXX	String
start_timetag	Time stamp for start of measurement sequence for the occultation	Mission elapsed seconds	Float
end_timetag	Time stamp for end of measurement sequence for the occultation	Mission elapsed seconds	Float
start_time	Start date and time of occultation measurement sequence (UTC)	YYYY-MM-DD hh:mm:ss.ms+00	String
end_time	End date and time of occultation measurement sequence (UTC)	YYYY-MM-DD hh:mm:ss.ms+00	String
Date	Date and time of occultation 30 km geometric tangent point (UTC)	YYYY-MM-DD hh:mm:ss.ms+00	String
Latitude	Latitude of 30 km geometric tangent point for occultation	Degrees (±90, N = +, S = -)	Float
Longitude	Longitude of 30 km geometric tangent point for occultation	Degrees (±180, E = +, W = -)	Float
beta_angle	Beta angle of occultation (at 30 km tangent point)	Degrees	Float
Data section			
Z	Tangent altitude grid for retrieved parameters and species	Km	Float
T	Temperature	K	Float
T_fit	Values indicating if temperature was retrieved from data (1) or is set to the *a priori* value (0)	0 (not fit), 1 (fit)	Integer
P (atm)	Pressure	atm (1 atm = 1.01325 bar)	Float
Dens	Atmospheric density	cm^{-3}	Float
Species	Retrieved volume mixing ratio for species	ppv (parts per volume) NOT ppm or ppb	Float
species_err	Statistical error for species retrieval from fitting (if this value is -888, the vmr is not retrieved. It is the value obtained by scaling the *a priori* value)	ppv	Float
Species and statistical errors are entered in order of retrieval H2O, O3, N2O, CO, CH4, NO, NO2, HNO3, HF, HCl, OCS, N2O5, ClONO2, HCN, CH3Cl, CF4, CCl2F2, CCl3F, COF2, COCl2, COClF, C2H6, C2H2, CHF2Cl, HCOOH, SF6, HO2NO2, H2O2, H2CO, CH3OH, CCl4, N2, O2, CFC113, HCFC141b, HCFC142b, HFC134a, CO2			

Note: The HFC-134a column is included but no data is available

Table 6: File format for "1 km" and "retrieval" grid data files – Version 3.5 for subsidiary isotopologues

Filename for "1 km" grid data: sxXXXXv3.5iso.asc or sxXXXXXv3.5iso.asc			
Filename for "retrieval" grid data: sxXXXXv3.5isotangrid.asc or sxXXXXXv3.5isotangrid.asc			
Field name	**Description**	**Acceptable values / units**	**Type**
Header section			
Name	Occultation identifier using mission name (ace), orbit number (XXXX or XXXXX) and type of occultation (sx)	ace.sxXXXX or ace.sxXXXXX	String
start_timetag	Time stamp for start of measurement sequence for the occultation	Mission elapsed seconds	Float
end_timetag	Time stamp for end of measurement sequence for the occultation	Mission elapsed seconds	Float
start_time	Start date and time of occultation measurement sequence (UTC)	YYYY-MM-DD hh:mm:ss.ms+00	String
end_time	End date and time of occultation measurement sequence (UTC)	YYYY-MM-DD hh:mm:ss.ms+00	String
Date	Date and time of occultation 30 km geometric tangent point (UTC)	YYYY-MM-DD hh:mm:ss.ms+00	String
Latitude	Latitude of 30 km geometric tangent point for occultation	Degrees (±90, N = +, S = -)	Float
Longitude	Longitude of 30 km geometric tangent point for occultation	Degrees (±180, E = +, W = -)	Float
beta_angle	Beta angle of occultation (at 30 km tangent point)	Degrees	Float
Data section			
Z	Tangent altitude grid for retrieved parameters and species	km	Float
T	Temperature	K	Float
T_fit	Values indicating if temperature was retrieved from data (1) or is set to the *a priori* value (0)	0 (not fit), 1 (fit)	Integer
P (atm)	Pressure	atm (1 atm = 1.01325 bar)	Float
Dens	Atmospheric density	cm^{-3}	Float
Species	Retrieved volume mixing ratio for species	ppv (parts per volume) NOT ppm or ppb	Float
species_err	Statistical error for species retrieval from fitting (if this value is -888, the vmr is not retrieved. It is the value obtained by scaling the *a priori* value)	ppv	Float
Species and statistical errors are entered in order of retrieval H2O (181), H2O (171), H2O (162), H2O (182), CO2 (636), CO2 (628), CO2 (627), CO2 (638), CO2 (637), O3 (668), O3 (686), O3 (667), O3 (676), N2O (456), N2O (546), N2O (448), N2O (447), CO (36), CO (28), CO (27), CO (38), CH4 (311), CH4 (212), OCS (624), OCS (632), OCS (623)			

Table 7: File format for “1 km” and “retrieval” grid geolocation (GLC) files.

Filename for “1 km” grid GLC files: ace.sxXXXX.txt			
Filename for “retrieval” grid GLC files: ace.sxXXXXtangrid.txt			
Field name	**Description**	**Acceptable values / units**	**Type**
Header section			
!OCCULTATION_NAME	Occultation identifier using mission name (ace), orbit number (XXXX or XXXXX) and type of occultation (sx)	ace.sxXXXX or ace.sxXXXXX	String
!SCALAR_DATE	Date and time of occultation 30 km geometric tangent point (UTC)	YYYY-MM-DD hh:mm:ss.ms+00	String
!SCALAR_LATITUDE	Latitude of 30 km geometric tangent point for occultation	Degrees (±90, N = +, S = -)	Float
!SCALAR_LONGITUDE	Longitude of 30 km geometric tangent point for occultation	Degrees (±180, E = +, W = -)	Float
!BETA_ANGLE	Beta angle of occultation (at 30 km tangent point)	Degrees	Float
!COLUMNS	Definition of columns included in file altitude (z), pressure (p), temperature (T), latitude (Lat), longitude (Lon), sun heading (SunHeading)	z p T Lat Lon SunHeading	String
!FORMAT_STRING	Fortran format string for columns	%12.5 for each of the six fields	String
Data section (each line)			
Z	Tangent altitude for retrieved parameters and species	Km	Float
P	Pressure at tangent altitude	atm (1 atm = 1.01325 bar)	Float
T	Temperature at tangent altitude	K	Float
Lat	Latitude of tangent altitude	Degrees (±90, N = +, S = -)	Float
Lon	Longitude of tangent altitude	Degrees (±180, E = +, W = -)	Float
SunHeading	Angle from the ACE-sun pointing vector to the meridional direction (vector tangent to a longitude circle)	Degrees NOTE: The SunHeading parameter calculation is not fully implemented in the v3.5 GLCs and should not be used for analyses.	Float
• In files for “1 km” grid data, z provided from 0.5 to 149.5 km • In files for “retrieval” grid data, altitudes below the lowest retrieved ACE-FTS altitude (0.5 km to lowest retrieved altitude) are provided from the “1 km” grid files and noted “(SCI)” at the end of the line in the Data section.			
When refraction model calculation failed, only the first four lines are provided in the file.			

2. Readme Files

ACE-FTS version 3.5

August 26, 2014

From October 2010 onward, bad low-altitude pressure and temperature inputs had an adverse affect on version 3.0 ACE-FTS results. Version 3.0 data from that time period should not be used.

ACE-FTS version 3.5 fixes this problem by using better pressure and temperature inputs, which were generated from the analysis run of the Canadian Meteorological Center's "global model."

Research products from ACE-FTS version 3.0 were also incorporated into the version 3.5 results:

1) In version 3.0, the shape of the CO volume mixing ratio (VMR) profile above the highest analyzed measurement was wrong, increasing too rapidly with increasing altitude, causing problems near the upper altitude limit of the CO retrievals. In version 3.5, a constant VMR as a function of altitude is assumed above the highest analyzed measurement.

2) In version 3.0, the microwindow for C_2H_6 extended up to 20 km, but there were additional windows employed in the retrieval (intended to provide extra information for a number of interferers in the C_2H_6 window and therefore improve the convergence stability) that extended up to 22 km. The software therefore attempted to retrieve C_2H_6 up to 22 km. With minimal spectral information between 20 and 22 km, the results in that altitude region were often wildly oscillatory. For version 3.5, the upper altitude limits for the extra microwindows were lowered to 20 km, removing the bad results between 20 and 22 km.

3) In version 3.0, HCFC-22 retrievals employed microwindows from two spectral regions: near 815 and 1115 cm^{-1}. The region near 1115 cm^{-1} has a much higher signal-to-noise ratio, and therefore this window dominated the retrieval, yielding an unexpected slope for the HCFC-22 results in the troposphere, likely a result of an unidentified interferer in the 1115 cm^{-1} microwindows. In version 3.5, the HCFC-22 retrievals only make use of the microwindow near 815 cm^{-1} for the tropospheric altitude region.

4) For some occultations in version 3.0 with low levels of tropospheric H_2O, particularly in the polar regions, the first guess for one of the interferers (H_2O isotopologue 3, $^{17}OH^{16}O$) was too far off. As a result, the retrieval would "get stuck," stopping without moving very far from the first guess parameters. The first guess VMR profile for N_2O is quite different from what you would expect in the polar region. However, the N_2O retrieval works fine for most (but not all occultations) when the H_2O retrieval is carried out first for a particular occultation, giving a much better first guess for the weak H_2O isotopologue 3 interferer. For version 3.5, N_2O retrievals were run a second time for all version 3.0 occultations, using the same software with the same N_2O microwindow set. For occultations after September 2010, H_2O retrievals are always implemented prior to N_2O retrievals to ensure a good first guess for the weak interferer.

For occultations prior to October 2010, version 3.5 results will be the same as version 3.0 results except for the above four molecules. For occultations from October 2010 onward, the version 3.0 results have been discarded, and the retrievals have been redone from scratch with improved pressure and temperature inputs. The data from October 2010 onward employ the exact same retrieval software as was used in version 3.0, except for CO, C_2H_6, and HCFC-22. For version 3.5, the microwindow sets for C_2H_6 and HCFC-22 have been adjusted as described above, and the shape of the CO VMR profile for altitudes above ~120 km has been changed as described.

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ACE-FTS version 3.0

March 18, 2010

Please read the readme files for previous version of ACE-FTS processing.

In version 3.0 pressure/temperature retrievals, there should be a significant reduction in the occurrence of unphysical oscillations in the retrieved temperature profiles compared to version 2.2. Also, version 3.0 removed the empirical function employed for pressure at low altitudes in the pressure/temperature retrievals, which should remove a minor glitch near 23 km that was sometimes observed in version 2.2 results.

The microwindow sets for all of the molecules have been upgraded. The maximum number of interferers allowed in the software for version 3.0 is 17 (compared to 5 in version 2.2). When multiple isotopologues of a given molecule serve as interferers in the retrieval, they are now treated separately in version 3.0, with a different VMR profile attributed to each isotopologue. Upper altitude limits for volume mixing ratio profile retrievals have been increased for most molecules, pushing the retrievals as much as possible into the noise limit.

A CO2 volume mixing ratio (VMR) profile is retrieved in version 3.0. The differences between this retrieved profile and the CO2 VMR profile derived during pressure/temperature retrievals (employing the same set of CO2 microwindows) is used to assess limitations of the retrievals. The error reported for the VMR retrievals on the 1 km grid is now a root-mean-square combination of the least-squares (random) fitting error and the percentage difference observed for CO2 in the given layer (i.e., the difference between the retrieved CO2 VMR and the value employed in the pressure/temperature retrievals). Errors for data reported on the tangent grid are still the straight least-squares fitting errors.

Version 3.0 VMR retrievals include the following molecules not available in version 2.2: COCl2, COClF, H2CO, CH3OH, and HCFC-141b. The molecules HOCl and ClO were removed from the list of molecules studied on version 2.2 due to a lack of quality. Columns that were always empty in the version 2.2 outputs (CFC-113, HCFC-142b, etc.) will contain results in version 3.0. The only column in the version 3.0 outputs that will remain empty (for the set of main isotopologues) will be HFC-134a while I work on issues with the retrievals for that molecule. A research product will follow for the molecule in the future.

There are results for many isotopologues in version 3.0, including subsidiary isotopologues of H2O, CO2, O3, N2O, CO, CH4, and OCS.

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ACE version 2.2 O3 update
October 26, 2005

Preliminary validation efforts with ozone suggested that the ACE-FTS retrieval results showed a low bias. The ozone microwindow set consisted of a set in the 1000-1150 cm-1 range and a set in 1830-2130 cm-1 range. Upon closer inspection, it seems that the spectroscopic information in the two regions is not entirely consistent. The latter microwindow set received a higher weighting in the fitting process (because the SNR was higher in that region) and ended up dominating the fit.

A new set of ozone microwindows was selected, restricting the selection to the 980-1130 cm-1 region. The software was upgraded to allow subsidiary isotopes as interferers. Ozone isotopologues 2 and 3 were included as interfers for the updated ozone retrievals.

Tropospheric ozone results showed higher than expected variability. A method used to accelerate the retrieval process runs into trouble where there are significant baseline effects. The speedup was removed for the ozone update.

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ACE version 2.2
May 24th, 2005

Please read the readme files from versions 1.0, 2.0, and 2.1 ACE-FTS processing.

The high altitude portion (i.e., above ~90 km) should be improved in this version.

The bug for the output on the retrieval grid (i.e., the tangrid files) has been fixed. One can use either the results on the retrieval grid or the results on the 1-km grid.

The following weak molecules have been added to the processing: HOCl, H2O2, and HO2NO2. This is a testing phase for these molecules. As with ClO, averaging results from different occultations may be required.

The retrieval of subsidiary isotopologues begins with this version. Note, however, that there appears to be a problem with HDO retrievals.

A change in the VMR retrieval approach made VMR profiles more susceptible to unphysical oscillations in version 2.0. Care should be taken when comparing to the results for a single ACE occultation. However, comparisons that employ average results from several ACE occultations should not be strongly affected. This problem is not present for any other version of the ACE-FTS processing.

August 24, 2005
Problems reported for version 2.2

In occultations with elevated levels of C2H6, there was on occasion a failure of the cross-correlation approach used to align the calculated and measured spectra. With the given first guess for the C2H6 profile, the measured and calculated spectra did not look similar enough for the cross-correlation approach to work properly. This will be fixed in the next processing version by increasing the microwindow width to include lines from interfering molecules, to better constrain the cross correlation approach.

C2H2 was retrieved only for a small number of occultations. The software occasionally crashed during C2H2 retrievals, and so it was taken out of the retrieval list.

Low altitude O3 (below ~10 km) sometimes shows variability higher than expected. An approach used to speed up the processing reduced the effectiveness of the retrieval for molecules with little information content at low altitudes when there were large baseline effects (i.e., the baseline was not close to 1 and/or had a large slope). There could be problems for other molecules with low information content at low altitudes such as HNO3 or HCl (i.e., molecules with much higher VMRs in the stratosphere than in the troposphere), although this has not been investigated fully.

Some occultations exhibited errors in temperature at high altitudes (above ~90 km). The cause was compensating errors in the retrieved temperature and CO2 VMR. Be prepared to discard some occultations when working above 90 km.

Some polar winter exhibited (likely unphysical) oscillations in the retrieved pressure and temperature in the stratosphere. Note, however, that the errors should compensate and should not translate to large errors in retrieved VMRs.

In the VMR retrievals, if there are two values reported in the lowest layer in the results on the retrieval grid (the tangrid files), it is an output error. There should only be one retrieved quantity in the middle of the layer. If, for example, it reports VMR values at 9.2 and 9.8 km, the value reported at 9.2 km should be ignored, and the value reported for 9.8 km actually corresponds to the middle of the layer (9.5 km).

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ACE version 2.1
May 24th, 2005

Please read the readme files from versions 1.0 and 2.0 ACE-FTS processing.

Version 2.1 processing was only performed on a subset of the measured occultations, mostly concentrating on the Arctic measurements during January-March 2005. There was significant ice contamination on the detectors during this time period. Results for some molecules are expected to be noisier than usual, particularly HCN. ClONO2 below 18 km could also exhibit increased noise.

The results on the retrieval grid (i.e., the "tangrid" files) did not always output properly. Use the results on the 1-km grid. (Only these results were submitted to the AVDC). Note that the same issue exists for version 2.0.

ClO was added to the retrievals. This is a very weak absorber, and so it may be better to average results for several occultations with similar conditions rather than considering the results from a single occultation. There only appears to be significant ClO present during the
Arctic spring occultations in this data set.

C2H2 does not appear to be processing properly.

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ACE version 2.0
January 20, 2005

Please read the ACE_readme.txt file from ACE-FTS version 1.0 processing. The setup of the output files is the same as for version 1.0, although there are more molecules. Recall the papers available for background information:

Bernath, P.F et al., Atmospheric Chemistry Experiment (ACE): mission overview, Geophys. Res. Lett., submitted (2005)

Boone, C.D. et al., Retrievals for the Atmospheric Chemistry Experiment Fourier Transform Spectrometer, Geophys. Res. Lett., submitted (2005)

Pre-prints of the papers can be found on the following Web site:
http://www.ace.uwaterloo.ca/data

In the T_fit column, 1 and 0 are used to replace T and F, respectively, from the version 1.0 output format.

Version 2.0 output files give results on both the standard 1-km grid and on the measurement grid.

For version 2.0, problems encountered when measurement spacings were less than 1 km (the altitude grid spacing) have been addressed.

A slightly improved approach is used for interpolating onto the 1-km grid for forward model calculations. In version 1.0, you could get a (maximum 0.5 km) extrapolation that would serve to slightly enhance unphysical oscillations in the results (when they were present).

For pressure/temperature retrievals below 25 km, an empirical expression with four parameters is used for pressure retrievals (instead of using a parameter for each measurement).

For P/T processing, a bug was fixed whereby during retrievals below the "crossover", P and T were fixed to the results of the retrieval above the crossover (rather than being fixed to the a priori P and T).

The software was converted to use exclusively HITRAN molecule numbering (rather than using ATMOS molecule numbering with the HITRAN 2004 linelist). A mismatch between the assumed molecule numbering and the molecule numbers in the linelist caused some issues in the troposphere (because of "phantom interferences").

The ability to retrieve subsidiary isotopologues was implemented in the software. As of January 20th, 2005, the isotopologues were not being retrieved, awaiting completion of microwindow selection. A second pass with the software will fill in the isotopologue results. Note that HDO, which was included in the regular output files for version 1.0, will now be in a separate file with all of the other subsidiary isotopologues.

Columns in the output files exist for some weak absorbers (HO2NO2, H2O2, HOCl, H2CO, and HCOOH) that are not being retrieved. They will also be retrieved on a second pass of processing, once I am comfortable with the ability to retrieve them reliably.

With a broader sample of atmospheric conditions available for evaluating microwindows, the microwindow selection was revised to avoid instances of saturation. More microwindows were added at low altitudes for several molecules to improve tropospheric results.

H2O: Microwindows changed to (1) avoid saturation experienced for some occultations, (2) avoid the 3200 cm-1 region (which was strongly impacted by detector contamination), (3) improve tropospheric retrievals, and (4) have fewer interferences in the multiple molecule retrievals

O3: The upper altitude limit of the retrieval range was increased to 95 km. Microwindow selection was redone to avoid significant interference from the 668 and 686 isotopologues and to get more microwindows in the troposphere. More windows were also added in the vicinity of the O3 concentration peak.

N2O: More microwindows at lower altitudes, particularly for the troposphere.

CO: Microwindows were adjusted improve results at low altitudes, particularly for the troposphere.

NO2: The upper altitude limit was increased, mostly to capture the enhanced high altitude NOx observed during February, 2004.

HCl: More microwindows were added, particularly at high altitudes.

COF2: Microwindows were adjusted to avoid residual solar features.
More lines were included in the retrieval.

SF6: The upper altitude limit was lowered to improve retrievals.

The following molecules have been added for version 2.0 that were not retrieved in version 1.0:

OCS, HCN, CF4, CH3Cl, C2H2, C2H6, and N2

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ACE version 1.0
September 11, 2004

Some issues to be aware of with the ACE data

In the vmr results, an entry of -999 indicates that no retrieval was performed at that altitude. At high altitudes, above the highest measurement used in the analysis for a given molecule, I include a VERY rough estimate of the molecule's vmr (it is a constant times the a priori value, with the same constant used for all altitudes above the highest analysed measurement). These data are flagged by the uncertainties being set to -888. Do not trust these results too far above the highest analyzed measurement.

Pressure and temperature values were retrieved down to no lower than 12 km (the columun labelled T_Fit indicates whether temperature was retrieved at that altitude: T for True and F for False). Below 12 km, temperature and pressure were fixed to data from the Canadian Meteorological Center.

High altitude results (above about 95 km) should be viewed with skepticism. The temperature profiles above this altitude require further work.

No provision was made for identifying occultations with significant ice contamination on the FTS detectors. Therefore, some occultations (particularly earlier ones) could experience a deterioration of results at low altitudes, some molecules worse than others.

Uncertainties provided for the vmr results are statistical errors from the fitting process (1-sigma), and do not include systematic contributions. A more detailed error budget will be determined later.

The molecule NO sometimes has extremely low absorption through the mesosphere (increasing for both higher and lower altitudes). For such occultations, the retrieved NO profile through the mesosphere will look quite ugly. The results are to be ignored when this happens.

For occultations that cut out above 10-17 km (due to clouds), the bottom-most measurement often gives results that are clearly out (presumably from the clouds affecting the measurement just before the suntracker loses lock). Simply ignore the bottom point if it looks inconsistent.

For molecules with significant interferences (e.g., N2O5 and SF6), the vmr for the highest analyzed measurement is sometimes suspiciously high. I am investigating the cause of this. If you see a sharp increase in the highest retrieved points, don't trust it.

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