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## **ACE – FTS**

Atmospheric Chemistry Experiment

*File format description for ACE-FTS level 2 data  
versions 1.0, 2.0 and 2.1 ASCII format*

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## DOCUMENT CHANGE RECORD

Issue	Rev.	Date	Change Detail
1	-	Sept 15, 2005	First Issue of document
1	A	Oct 25, 2005	Update in Introduction on data processing

## 1. Introduction 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 paper accepted by Applied Optics (“Retrievals for the Atmospheric Chemistry Experiment Fourier Transform Spectrometer” by C. D. Boone *et al.* available from <http://www.ace.uwaterloo.ca/data> for more information on the ACE-FTS retrievals.

### General comments on the file formatting and data:

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 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 first guess profile. These data are flagged with an error of -888 and should be treated with caution.

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 version 2.0 and 2.1, both the “retrieval” grid and the “1 km” grid profiles were made available.

### Use of *a priori* data:

For the temperature and pressure profiles, the reported values come from different sources depending on the altitude range. Below 12 km, these are fixed to meteorological data from the CMC (Canadian Meteorological Center). Between 12 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. There can often be a discontinuity between the retrieval results and the MSIS data. The next version will try to fix this problem by scaling the MSIS results above ~120 km during the retrieval process.

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 12 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.

**Table 1: File format – Version 1.0**

Field name	Description	Acceptable values / units	Type
<b>Header section</b>			
Name	Occultation identifier using mission name (ace), orbit number (XXXX) and type of occultation (sx)	ace.sxXXXX	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 ( $\pm 90$ , N = +, S = -)	Float
longitude	Longitude of 30 km geometric tangent point for occultation	Degrees ( $\pm 180$ , E = +, W = -)	Float
beta_angle	Beta angle of occultation (at 30 km tangent point)	Degrees	Float
<b>Data section</b>			
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 (T) or is set to the <i>a priori</i> value (F)	F (not fit), T (fit)	String
P	Pressure	atm (1 atm = 1.01325 bar)	Float
dens	Atmospheric density	cm <sup>-3</sup>	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 <i>a priori</i> value)	Ppv	Float
Species and statistical errors are entered in order of retrieval H2O, O3, N2O, CO, CH4, NO, NO2, HNO3, HF, HCl, N2O5, ClONO2, HCN, CF4, CCl2F2, CCl3F, COF2, CHF2Cl, HDO, SF6			

Note:

These files contain retrievals for 18 species. HCN and CF4 were not included in Version 1.0. Columns were included as place holders for future retrieval results.

**Table 2: File format – Version 2.0**

Field name	Description	Acceptable values / units	Type
<b>Header section</b>			
name	Occultation identifier using mission name (ace), orbit number (XXXX) and type of occultation (sx)	ace.sxXXXX	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	YYYY-MM-DD hh:mm:ss.ms+00	String
end_time	End date and time of occultation measurement sequence	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 ( $\pm 90$ , N = +, S = -)	Float
longitude	Longitude of 30 km geometric tangent point for occultation	Degrees ( $\pm 180$ , E = +, W = -)	Float
beta_angle	Beta angle of occultation (at 30 km tangent point)	Degrees	Float
<b>Data section</b>			
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 <i>a priori</i> value (0)	0 (not fit), 1 (fit)	Integer
P	Pressure	atm (1 atm = 1.01325 bar)	Float
dens	Atmospheric density	cm <sup>-3</sup>	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 <i>a priori</i> 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, C2H6, C2H2, CHF2Cl, SF6, N2			

Note:

These files contain retrievals for 24 species. HCOOH, HO2NO2, ClO, H2O2, HOCl, H2CO, CCl4, CFC-13 and HCFC-142b were not included in Version 2.0. Columns were included as place holders for future retrieval results.

**Table 3: File format – Version 2.1**

Field name	Description	Acceptable values / units	Type
<b>Header section</b>			
name	Occultation identifier using mission name (ace), orbit number (XXXX) and type of occultation (sx)	ace.sxXXXX	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	YYYY-MM-DD hh:mm:ss.ms+00	String
end_time	End date and time of occultation measurement sequence	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 ( $\pm 90$ , N = +, S = -)	Float
longitude	Longitude of 30 km geometric tangent point for occultation	Degrees ( $\pm 180$ , E = +, W = -)	Float
beta_angle	Beta angle of occultation (at 30 km tangent point)	Degrees	Float
<b>Data section</b>			
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 <i>a priori</i> value (0)	0 (not fit), 1 (fit)	Integer
P	Pressure	atm (1 atm = 1.01325 bar)	Float
dens	Atmospheric density	cm <sup>-3</sup>	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 <i>a priori</i> 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, C2H6, C2H2, CHF2Cl, SF6, ClO, N2			

Note:

These files contain retrievals for 25 species. HCOOH, HO2NO2, H2O2, HOCl, H2CO, CCl4, CFC-13 and HCFC-142b were not included in Version 2.0. Columns were included as place holders for future retrieval results.

## 2. File naming conventions

All files are named using the occultation “name”. This name identifies the occultation using the orbit number (XXXX or XXXXX) and type of occultation (sx = sr or ss).

For version 1.0, data was made available in both ASCII (space delimited) and CSV (comma separated) formats. Only ASCII (space delimited) format was used for versions 2.0 and higher.

<b>Version Number</b>	<b>Data file type</b>	<b>Name</b>	<b>Format</b>
1.0	“1 km” altitude grid	sxXXXX.asc	ASCII
1.0	“1 km” altitude grid	sxXXXX.csv	CSV
2.0	“1 km” altitude grid	sxXXXX.asc	ASCII
2.0	“Retrieval” altitude grid	sxXXXXtangrid.asc	ASCII
2.1	“1 km” altitude grid	sxXXXX.asc	ASCII
2.1	“Retrieval” altitude grid	sxXXXXtangrid.asc	ASCII

### 3. Readme Files

#### 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. ClONO<sub>2</sub> 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. Note that the same issue exists for version 2.0.

CIO 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 CIO present during the Arctic spring occultations in this data set.

C<sub>2</sub>H<sub>2</sub> 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 (HO<sub>2</sub>NO<sub>2</sub>, H<sub>2</sub>O<sub>2</sub>, HOCl, H<sub>2</sub>CO, 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.

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

O<sub>3</sub>: 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 O<sub>3</sub> concentration peak.

N<sub>2</sub>O: More microwindows at lower altitudes, particularly for the troposphere.

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

NO<sub>2</sub>: The upper altitude limit was increased, mostly to capture the enhanced high altitude NO<sub>x</sub> observed during February, 2004.

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

COF<sub>2</sub>: Microwindows were adjusted to avoid residual solar features. More lines were included in the retrieval.

SF<sub>6</sub>: 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, CF<sub>4</sub>, CH<sub>3</sub>Cl, C<sub>2</sub>H<sub>2</sub>, C<sub>2</sub>H<sub>6</sub>, and N<sub>2</sub>

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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 column 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., N<sub>2</sub>O<sub>5</sub> and SF<sub>6</sub>), 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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