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## **ACE – FTS**

Atmospheric Chemistry Experiment

*File format description for ACE-FTS level 2 data  
version 2.2 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 27, 2005	Update in Introduction on data processing and ozone update
1	B	Aug. 17, 2006	Added caveats for data use and minor corrections
1	C	Aug. 24, 2006	Updated data use recommendation table
1	D	April 20, 2012	Additional netCDF format description

## 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 retrievals description paper (C. D. Boone *et al.*, “Retrievals for the Atmospheric Chemistry Experiment Fourier Transform Spectrometer”, *Appl. Opt.*, 44(33) 7218-7231 (2005) which is 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 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. A preliminary estimate of the accuracy of these retrievals is provided from the initial validation comparisons done with versions 1.0 and 2.0. In these comparisons, the ACE-FTS temperatures agree to within approximately  $\pm 2$  K with those from other satellite instruments and radiosondes, between approximately 15 and 60 km.

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, 2.1 and 2.2, both the “retrieval” (also called “measurement”) grid and the “1 km” (or “scientific”) grid profiles are available.

This version includes the retrieval of subsidiary isotopologues from the ACE-FTS spectra. There are profiles available for isotopologues of water and methane,  $\text{H}_2^{18}\text{O}$ ,  $\text{H}_2^{17}\text{O}$ ,  $^{13}\text{CH}_4$ , and  $^{12}\text{CH}_3\text{D}$ . Results are also given for HDO but there appears to be a problem with these retrievals. 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 ([www.hitran.com](http://www.hitran.com)). The subsidiary isotopologue profiles are stored separately from the main isotopologue results and are available on both the “retrieval” grid and the “1 km” grid. 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<sub>2</sub><sup>18</sup>O, 171 for H<sub>2</sub><sup>17</sup>O and 162 for HD<sup>16</sup>O.

For each occultation event, 4 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 4 files are given in Table 1.

**Table 1: Table naming convention**

<b>Name</b>	<b>Isotopologues</b>	<b>Data file type</b>
sxXXXX.asc	Most abundant	1 km altitude grid
sxXXXXtangrid.asc	Most abundant	Retrieval altitude grid
sxXXXXiso.asc	Subsidiary	1 km altitude grid
sxXXXXisotangrid.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

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. 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. In previous versions, there was often a discontinuity between the retrieval results and the MSIS data. Version 2.2 resolves this 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.

Version 2.2 Ozone Update:

*Those wanting to use ACE-FTS O<sub>3</sub> should use the data in separate version 2.2 update files instead of the results in the version 2.2 files.* The update version uses microwindows only in the 10 micron region and should represent a significant improvement compared to the version 2.2 results. This change was prompted by preliminary validation comparisons, which found that the ACE-FTS ozone profiles tended to show less ozone than other satellite instruments. *Also, HDO (H<sub>2</sub>O (162)) in the version 2.2 file is incorrect, and one should only use the HDO results from the update files.*

Known issues and recommendations for data use:

*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. Occultations measured prior to January 10, 2004 were for calibration and these occultations should not be used at all. Measurements taken during the Science Commissioning period, during January and most of February 2004, generally should not be used. Since February 21, 2004, there have been a few instances where there were issues with the data and the occultations from these periods should be avoided or used with caution. For example, detector temperatures which are higher than nominal degrade the SNR performance of the ACE-FTS and this can negatively impact the retrievals.

The table below lists occultations with known issues. 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 ([https://database.uwaterloo.ca/validation/data\\_issues\\_report\\_form.php](https://database.uwaterloo.ca/validation/data_issues_report_form.php)).

**Table 2: Data issues and recommendations for use.**

<b>Date Range</b>	<b>Occultation Number(s)</b>	<b>Issue Identified and Recommendation for data use</b>
Before January 10, 2004	ss1439, sr1439, ss1454	These are calibration measurements. <i>They should not be used at all.</i>
January 10 - February 2, 2004	sr2206 to ss2549	Issues with spacecraft clock. The spacecraft clock was being adjusted during this period so the timing is not reliable. <i>These occultations should not be used.</i>
February 2 - 21, 2004	ss2551 to ss2830	Command sequence macros were being adjusted. <i>ACE-FTS results should be treated with caution and ACE-MAESTRO results should not be used.</i>
February 29 – March 2, 2004	ss2968 to ss2978	Issue caused loss of attitude control and science command timeline. The ACE-FTS detector temperature was higher than nominal operating value while recovering from this event. <i>These occultations should be avoided.</i>
May 17 - 29, 2004	ss4108 to sr4281	Closed-loop offsets (for pointing at sun centroid) were set incorrectly. These measurements could have problems because of the offset issue. <i>These occultations should be used with caution.</i>
September 16 – 18, 2004	ss5909 to sr5923	Issue caused attitude control and science command timeline was disabled. The ACE-FTS detector temperature was higher than nominal operating value while recovering from this event. <i>These occultations should be avoided.</i>
March 9-12, 2006	ss13868 to ss13885	Issue caused loss of attitude control and science command timeline. The ACE-FTS detector temperature was higher than nominal operating value while recovering from this event. <i>These occultations should be avoided.</i>
August 14-17, 2006	sr16205 to ss16207	Issue caused loss of attitude control and science command timeline. The ACE-FTS detector temperature was higher than nominal operating value while recovering from this event. <i>These occultations should be avoided.</i>

Prepared by Kaley Walker, August 17, 2006 ([kwalker@atmosph.physics.utoronto.ca](mailto:kwalker@atmosph.physics.utoronto.ca)).

**Table 2: File format for “1 km” and “retrieval” grid data files – Version 2.2 for main isotopologues**

Filename for “1 km” grid data: sxXXXX.asc or sxXXXXXX.asc			
Filename for “retrieval” grid data: sxXXXXtangrid.asc or sxXXXXXXtangrid.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.sxXXXXXX	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
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 <i>a priori</i> value (0)	0 (not fit), 1 (fit)	Integer
P (atm)	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, HO2NO2, H2O2, HOCl, N2			

Note: These files contain retrievals for 28 species. HCOOH, H2CO, CCl4, CFC13, and HCFC142b are not included in Version 2.2. Columns were included but no data is available

**Table 3: File format for “1 km” and “retrieval” grid data files – Version 2.2 for subsidiary isotopologues**

Filename for “1 km” grid data: sxXXXXiso.asc or sxXXXXXXiso.asc			
Filename for “retrieval” grid data: sxXXXXisotangrid.asc or sxXXXXXXisotangrid.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.sxXXXXXX	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
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 <i>a priori</i> value (0)	0 (not fit), 1 (fit)	Integer
P (atm)	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 (181), H2O (171), H2O (162), CH4 (311), CH4 (212)			

Note: These files contain retrievals for 5 isotopologues. Columns are included for more isotopologues but no data is available. These columns remain as place holders.



**Table 4: File format for “1 km” and “retrieval” grid data files – Version 2.2 Ozone Update**

<b>Filename for “1 km” grid data: sxXXXXv2.2_Ozone_Update.asc or sxXXXXXv2.2_Ozone_Update.asc</b>			
<b>Filename for “retrieval” grid data: sxXXXXv2.2_Ozone_Update_tangrid.asc or sxXXXXXv2.2_Ozone_Update_tangrid.asc</b>			
<b>Field name</b>	<b>Description</b>	<b>Acceptable values / units</b>	<b>Type</b>
<b>Header section</b>			
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 ( $\pm 90$ , 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
O3	Retrieved volume mixing ratio for ozone	ppv (parts per volume) NOT ppm or ppb	Float
O3_err	Statistical error for ozone 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

## 2. Readme Files

### 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<sup>-1</sup> range and a set in 1830-2130 cm<sup>-1</sup> 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<sup>-1</sup> region. The software was upgraded to allow subsidiary isotopes as interferers. Ozone isotopologues 2 and 3 were included as interferers 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, H<sub>2</sub>O<sub>2</sub>, and HO<sub>2</sub>NO<sub>2</sub>. 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 C<sub>2</sub>H<sub>6</sub>, 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 C<sub>2</sub>H<sub>6</sub> 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.

C<sub>2</sub>H<sub>2</sub> was retrieved only for a small number of occultations. The software occasionally crashed during C<sub>2</sub>H<sub>2</sub> retrievals, and so it was taken out of the retrieval list.

Low altitude O<sub>3</sub> (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 HNO<sub>3</sub> 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 CO<sub>2</sub> 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. 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. (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.

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.

Chris Boone

### 3. netCDF formatting update

In coordination with the public release of the version 2.2 data, a preliminary netCDF format has been prepared in close analogy to the existing ASCII data. Each occultation is written to a single file with the following properties:

- netCDF-4/HDF5 binary format
- UDUNITS library-compatible units
- A *Global Attributes* section containing the entire ASCII header field section, as well as additional self-descriptive parameters
- ‘Data-L2\_1km\_grid’ group for the 1-km altitude grid data
- ‘Data-L2\_retreival\_grid’ group for the retrieval grid data

Users who are familiar with the netCDF or HDF formats should have very little difficulty opening and extracting ACE data from this product. For example, Figure 1 shows the data that’s immediately available to the *HDFView* utility, and the interface to several high-level programming languages ( *MATLAB*, *IDL* ) is very similar.

For ACE-FTS vertical profiles, the primary coordinate axis is altitude, which is available in the ‘z’ coordinate variable. Each retrieved species then has two entries in the above groups’ data sections, containing VMR and error values.

Therefore, to access altitude, VMR and error values for an ozone profile on the 1 km grid, one just needs to access the variables:

```
ACE-FTS-v2.2/Data-L2_1km_grid/z(0:149:1)
ACE-FTS-v2.2/Data-L2_1km_grid/O3(0:149:1)
ACE-FTS-v2.2/Data-L2_1km_grid/O3_err(0:149:1)
```

within the file.

The CDL ( Common Data Language ) representation of a VMR product is given for reference:

```
float O3(z) ;
    O3:long_name = "ozone" ;
    O3:isotopologue_name = "(16)O (16)O (16)O" ;
    O3:units = "1" ;
    O3:missing_value = -888.f ;
    O3:_FillValue = -999.f ;
float O3_err(z) ;
    O3_err:long_name = "ozone" ;
    O3_err:isotopologue_name = "(16)O (16)O (16)O" ;
    O3_err:units = "1" ;
    O3_err:missing_value = -888.f ;
    O3_err:_FillValue = -999.f ;
```

This data format is considered to be preliminary, and will be extended and enhanced when possible.



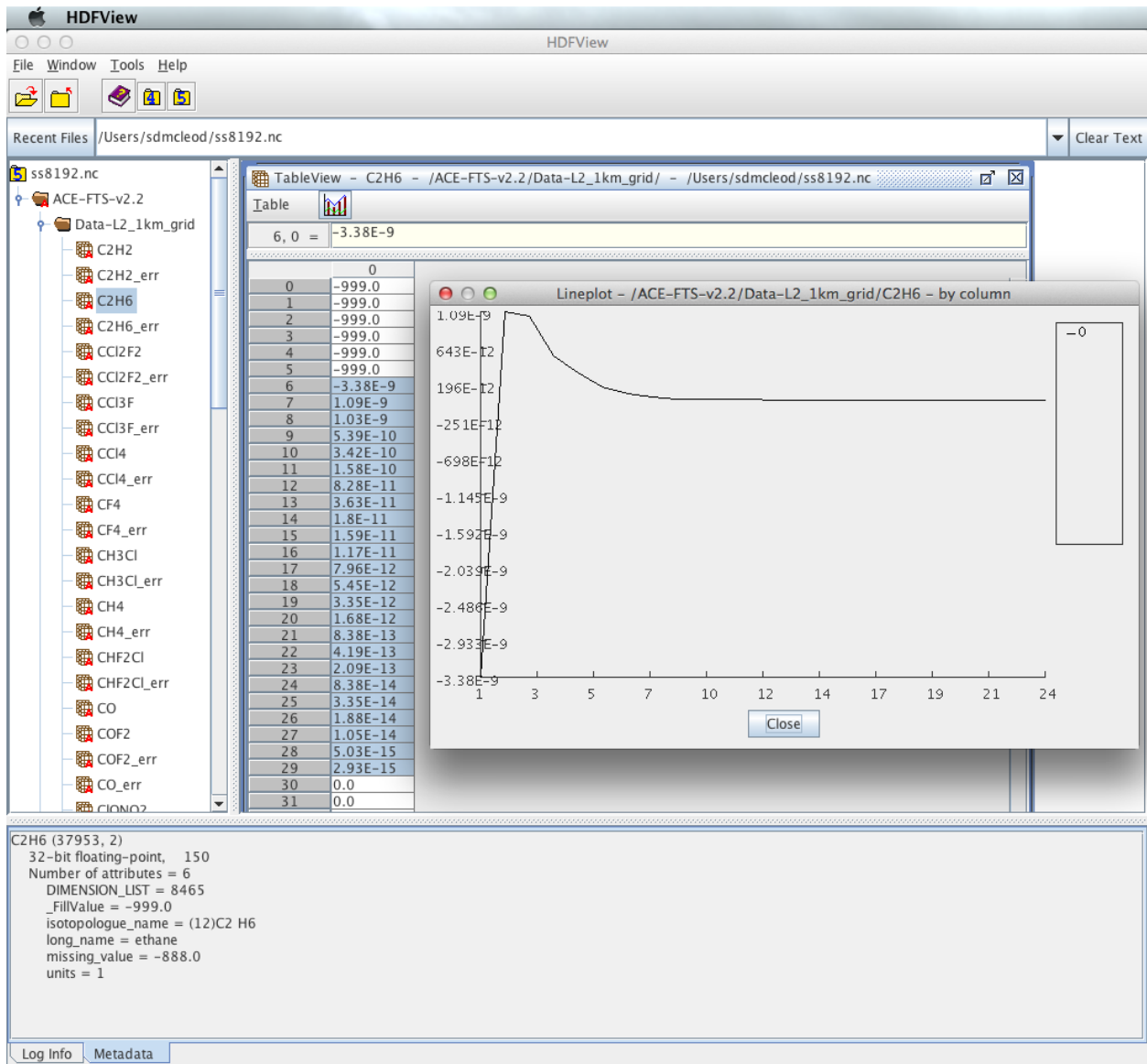


Figure 1. Example netCDF data file loaded into HDFView utility