Product Specification Document for ACE-FTS MesosphEO L2 data sets

Prepared by Patrick Sheese, 7 Nov 2017
psheese@atmosp.physics.utoronto.ca
(Based on document: ACE-SOC 0030-1A Data usage guide and file format description for ACE-FTS level 2 data version 3.5/3.6 ASCII format, dated 16 Janaury 2017)

Contents

1. File formatting

The files are in netCDF format and contain all profiles (on the 1 km altitude grid) with associated data quality flags. The file format for these files is provided in Table 1 and the definition of the data quality flags is given in Table 2.

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.

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.

The occultation labels are generated using the satellite orbit number calculated by a program called Systems Tool Kit (STK). For example, ss12345 would be the sunset observed on the satellite's 12345th orbit. On occasion, STK glitches when counting the number of orbits, and two occultations end up getting the same name. Because we are constrained to use unique identifiers in occultation names, a number of measured occultations wound up not being processed because an existing occultation with the name it 'wanted' already existed.

To recover these missed occultations (and avoid renaming thousands of occultations in the version 3.6 processing), an 'a' was appended to the occultation label wherever an occultation of the same name already existed, in order to generate a unique identifier. Occultations with the

same orbit number in the label (e.g., ss12345 and ss12345a) are completely different occultations, collected at different times and locations that just happened to be assigned the same orbit number through a glitch in STK calculations. The measurement time and location reported in the file header is the important information for making use of these data.

2. General data usage information

Data gaps: There is a data gap for version 3.5 in 2011 and in 2012, as well as a minor data gap in 2009.

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 in the next version.

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 data issues page (https://databace.scisat.ca/validation/data_issues.php), and these occultations have been flagged as a 7 in the flag files. These occultations should not be used.

Upper altitude data: Pressure and temperature profiles calculated from the US Naval Research Laboratory's MSIS model, used in the ACE-FTS pressure/temperature retrieval, require F10.7 (a measure of solar flux at wavelength 10.7 cm) and Ap index (a measure of geomagnetic activity) as inputs. In version 3.6 processing, measured Ap index values were used only up to January 2013, and measured F10.7 was used up to January 2015. Average values for the quantities were used whenever current values were not available (i.e., after January 2013 for the Ap index and after January 2015 for F10.7). Errors in one or both of these parameters will impact retrieval results at very high altitudes, above about 90 km. Expect systematic errors the order of 1 percent when using average values for the Ap index and a few percent when using average values for both F10.7 and Ap index. As such, it is not recommended to use ACE data for trend studies at very high altitudes for time frames extending beyond January 2013.

3. Species dependent information

Temperature: 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. There are no errors provided for the temperature retrievals because of amount of time required to calculate them.

Carbon dioxide (CO_2): 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.

Nitrous oxide (N_2O): Some N_2O measurements inside the Antarctic vortex, when derived temperatures are below 196 K, are anomalously large. These result from a failure to converge because the first guess for the VMR of an interferer (H_2O isotopologue 3) is too far from the true value, a consequence of water levels being extremely low in these occultations. These occultation profiles have been flagged as a 7 in the quality 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.

4. Using the 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.scisat.ca/validation/data_issues.php). In addition to the Data Issues List, a system of data quality flags have been developed for the ACE-FTS version 3.5/3.6 dataset. These are provided for each level for each 1 km grid profile. 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 v2.1. This version uses a calculation method that is slightly modified from that of the first release.

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 4-5) be excluded from the analysis. Data users are directed to the Sheese *et*

al., 2015 paper for further recommendations and caveats for usage. [Note: The flags involving percent errors (e.g. 1 and 6) have been removed in this version as they were not a robust flag for all species.]

Table 1: netCDF fields included in data quality flagging files.

Parameter	Definition
altitude	Tangent altitude for retrieved species, temperature and pressure (in km)
sunset_sunrise	Type of occultation flag (ss = 0 or 2; sr = 1 or 3)
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 v3.5/3.6

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

Flag value	Definition
0	No known issues with data
2	Not enough data points in the region to do statistical analysis
4	Moderate unnatural outlier detected from running MeAD
5	Extreme unnatural outlier detected from EDF
7	Instrument or processing error
8	Error fill value of –888 (data is scaled a priori)
9	Data fill value of –999 (no data)