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ACE-FTS Version 3.0 Data Set: Validation and Data Processing Update

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ACE-FTS version 3.0 data set: validation and data processing update

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I. INTRODUCTION

On 12 August 2003, the Canadian-led Atmospheric Chemistry Experiment (ACE) was launched into a 74° inclination orbit at 650 km with the mission objective to measure atmospheric composition using infrared and UV-visible spectroscopy (Bernath et al., 2005). The ACE mission consists of two main instruments, ACE-FTS and MAESTRO (McElroy et al., 2007), which are being used to investigate the chemistry and dynamics of the Earth's atmosphere. Here, we focus on the high resolution (0.02 cm^{-1}) infrared Fourier Transform Spectrometer, ACE-FTS, that measures in the 750-4400 cm^{-1} (2.2 to 13.3 μm) spectral region. This instrument has been making regular solar occultation observations for more than nine years. The current ACE-FTS data version (version 3.0) provides profiles of temperature and volume mixing ratios (VMRs) of more than 30 atmospheric trace gas species, as well as 20 subsidiary isotopologues of the most abundant trace atmospheric constituents over a latitude range of ~85°N to ~85°S. This letter describes the current data version and recent validation comparisons and provides a description of our planned updates for the ACE-FTS data set.

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II. VALIDATION RESULTS

An extensive validation exercise was undertaken for the ACE-FTS baseline species (VMR profiles of O_3, H_2O, CH_4, N_2O, NO_2, NO, HNO_3, HCl, HF, CO, CCl_3F, CCl_2F_2, N_2O_5, and $ClONO_2$) and temperature for the version 2.2 (+updates for O_3, N_2O_5 and HDO) data set. The retrievals for this version have been described in detail in Boone et al. (2005). The validation results were reported in a special issue of *Atmos. Chem. Phys.* (http://www.atmos-chem-phys.net/special_issue114.html). By building on these comparison results, a newer version of the ACE-FTS data set (version 3.0) was produced that incorporated a new set of microwindows and updated spectroscopic parameters. It addressed the unphysical oscillations that were found in the mesospheric temperature profiles and an artefact (or "glitch") that occurred in the temperature profiles near 23 km. In addition, the altitude ranges for nearly all species have been extended. These increases range from a few km to as much as 35 km for N_2O. These improvements have been briefly summarized in Table 1 and are documented in Boone et al. (2013).

For the version 3.0 data set, work has been undertaken to characterize the results by performing both comparisons between versions and comparisons with measurements by other satellite instruments. Herein, we focus on describing the direct version comparisons for the

ACE-FTS baseline species. These comparisons have been carried out in order to identify the changes to the ACE-FTS retrievals between the new version 3.0 and the previous well-validated (version 2.2 +updates) data set. These results allow users to understand the data quality of the version 3.0 data set in relation to the earlier validation studies for the version 2.2+updates data set.

Table 1: *Summary of the processing differences between ACE-FTS v2.2 and v3.0.*

Retrieval parameter	Version 3.0 (v3.0) versus Version 2.2+Updates (v2.2)
Altitude range	Ranges increased for most species by a few km up to ~35 km for N_2O. Upper altitude limits that varied with latitude were employed for some molecules in v3.0.
Microwindows	Updated to new set for all species, typically using more microwindows in v3.0 to improve the information content on the target constituent.
VMR retrieval	Isotopologues can be treated as separate molecules, i.e., each isotopologue serving as an interferer in a retrieval has an independent VMR profile. In v2.2, different isotopologues of the same molecule were assumed to have the same VMR profile.
Spectral line list	Updated line list using HITRAN 2004 with several updates
Routinely processed species	Number of species routinely processed increased to include COClF, $COCl_2$, O_2, H_2CO, CH_3OH and HCFC-141b, as well as a number of additional subsidiary isotopologues: $^{18}O^{12}C^{16}O$, $^{17}O^{12}C^{16}O$, $^{18}O^{13}C^{16}O$, $^{18}O^{16}O^{16}O$, $^{16}O^{18}O^{16}O$, $^{16}O^{17}O^{16}O$, $N2^{18}O$, $OC^{34}S$, and $O^{13}CS$
Empirical function in ILS calculation	A new empirical function was used to characterize the ACE-FTS's self apodization, one which yielded improved residuals compared to v2.2.
Temperature interpolation in P/T retrieval	Altitude interpolation approach for temperature was changed to match what was used for VMR retrieval. This fixed the unphysical oscillations observed in v2.2 temperature profiles.
Issue at ~23 km	No empirical function is used in the retrieval of pressure below 23 km in v3.0; pressure at each analysed measurement is used as a fitting parameter
Altitude lower limit in P/T retrieval	Changed from 12 km (v2.2) to 15 km (v3.0)
High altitude retrieval in P/T retrieval	The retrieved CO_2 VMR profile at high altitudes was forced to match fixed CO_2 VMR at the interface (near 60 km)
Tangent height separation in P/T retrieval	The tangent height separation is calculated in a way that improves the stability of the retrieval compared to v2.2

The comparison approach taken for this work follows the method described by Dupuy et al. (2009). Rather than finding pairs of "coincident" measurements by different instruments, the pairs used here are all ACE-FTS occultations for which profiles are available for both data versions. For each trace gas species (or subset of these data), the mean profiles and 1-σ standard deviation of the mean are calculated for each data version. The absolute and relative differences are calculated from individual pairs of profiles and then the means of these differences are calculated (see Eqs. 3 and 4, respectively, in Dupuy et al., 2009). To calculate the relative differences, the mean of the version 2.2+updates and version 3.0 VMR is used as the denominator. As was done for most of the version 2.2+updates validation studies, the standard deviation of the bias-corrected differences (which will be referred to as the "de-biased standard deviation") is calculated for these comparisons (e.g. Eq. 5 in Dupuy et al., 2009). This gives a measure of the combined precision of the two ACE-FTS data versions (von Clarmann 2006). For the results shown here, no data screening has been applied in order to examine all of the profiles produced for the two ACE-FTS data versions.

The ACE-FTS measurements made between 21 February 2004 (beginning of routine operations) and 30 September 2010 have been used in this work. This analysis has been performed for the full latitude range as well as for selected latitude bands (typically using 30° bins) for all fourteen of the ACE-FTS baseline species. An example of the direct version comparisons for O_3 is shown in Figure 1 for the latitude band between 30° S and 60° S. The results shown here are consistent with those seen in all of the different latitude bands. Figure 2 shows two additional examples of these direct version comparisons for CH_4 and H_2O.

In addition to subdividing the data into various latitude bands, the data have also been compared separately for different time periods. Figure 3 shows an example for O_3 where the relative differences for each year are calculated separately to examine the year-to-year

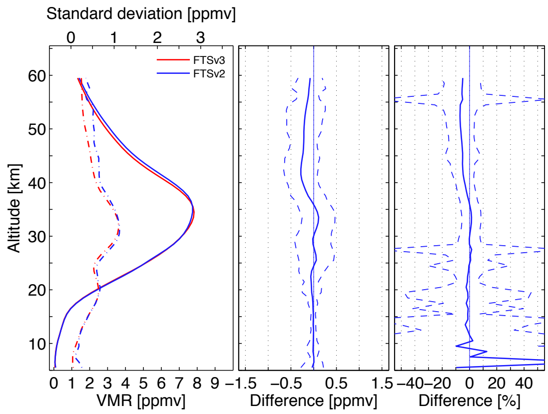

Figure 1: *An example of the ACE-FTS direct version comparisons for O_3 for the 30-60° S latitude range. This compares the version 2.2 O_3 update (blue) product with the version 3.0 (red) product. The mean VMR profiles (solid lines) and the 1-σ standard deviations (dot-dashed lines) are shown in the left panel, the absolute differences are shown in the centre panel and the relative differences are shown in the right panel. The dashed lines in the centre and right panels indicate the de-biased standard deviation of the mean differences.*

changes. It can be seen that these differences are quite consistent for most years, with all years seeing quite large variability below ~20 km. However, above ~20 km, 2008 has larger variability than the other years as shown in the de-biased standard deviation of the mean difference. This is primarily due to increased numbers of outlier profiles, which we are currently in the process of characterizing to understand their origin and to provide guidance to users to allow these to be filtered out as needed. A list of occulations with known issues is provided by the ACE Science Operations Centre (https://databace.scisat.ca/validation/data_issues.php). In addition to consulting this list, users are encouraged to submit reports the ACE team outlining any issues they find.

A summary of the results obtained for the direct version comparisons of the ACE-FTS baseline species is shown in Table 2. For each species, the reference describing the version 2.2+updates validation study and the altitude range for the version 3.0 retrievals are listed.

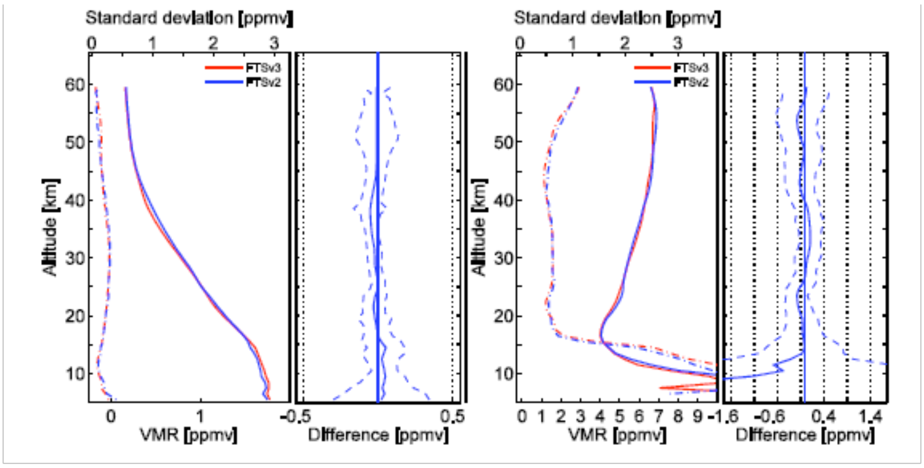

Figure 2: *Two further examples of version 2.2 versus version 3.0 comparisons (mean profiles and absolute differences) for CH_4 (left panels) and H_2O (right panels). The legend for each pair of panels is the same as given for the corresponding panel in Fig. 1. Measurements from all latitudes are included in these comparisons.*

In addition, brief summaries of the version 2.2+updates validation results are given in Jones et al. (2012). The differences described for the version 3.0 data set, compared to version 2.2+updates, are consistent with the need to reduce the bias seen in the version 2.2+updates validation studies. A more detailed validation paper is in preparation in which the ACE-FTS v3.0 dataset is compared to the ACE-FTS v2.2+updates dataset as well as several other satellites (SAGE II, SAGE III, POAM III, HALOE, OSIRIS and MLS).

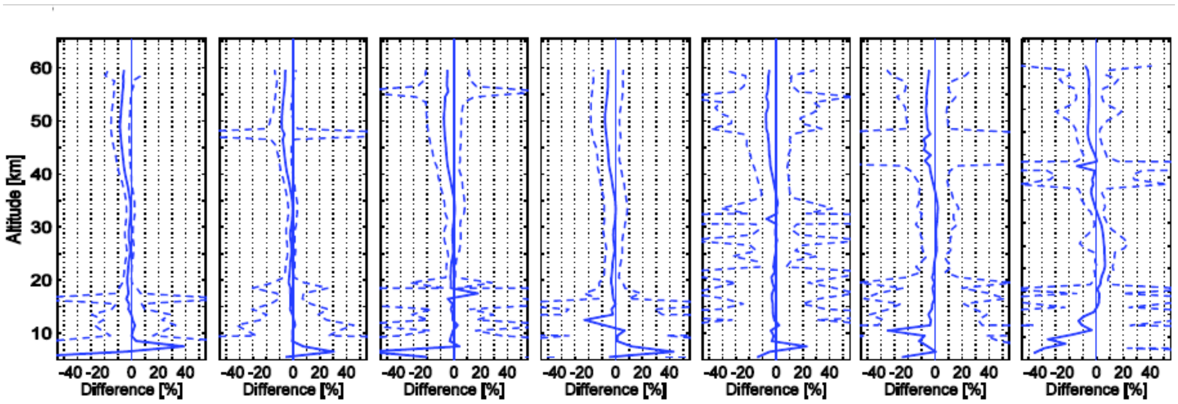

Figure 3: *The mean relative differences for the direct version comparisons for O_3 are shown for each year from 2004 (far left) to 2010 (far right).*

Table 2: *Summary of the version 2.2+updates and version 3.0 direct version comparisons.*

Molecule	Altitude Range (km)	Comparison Result (behavior of version 3.0 relative to version 2.2+updates)	Previous Validation Results (Version 2.2)
O_3	5-95	A reduction of ~5% is seen above the peak, at ~35 km and higher altitudes.	Dupuy et al. (2009) (version 2.2 O_3 update)
CH_4	5-62	A reduction of ~10% is seen near ~35-40 km and slight reduction is seen at ~23 km.	De Mazière et al. (2008)
H_2O	5-89	Small differences of ~±2% are seen over the altitude range between ~20 and ~55 km	Carleer et al. (2008)
NO	12-105	A slight increase of ~2 % is seen between ~25 and ~40 km and reduction of ~2% is seen above ~40 km.	Kerzenmacher et al. (2008)
N_2O	5-60	A reduction of ~10% is seen above ~35 km	Strong et al. (2008)
NO_2	13-45	A reduction of ~10% is seen in the altitude range of ~40-45 km.	Kerzenmacher et al. (2008)
N_2O_5	15-40	Above ~20 km, an increase is seen that is up to ~0.04 ppbv at ~26-30 km. Below ~20 km, a reduction is seen that is up to ~0.035 ppbv at ~15 km.	Wolff et al. (2008) (version 2.2 N_2O_5 update)
HF	10-50	A reduction of ~5% is seen over profile.	Mahieu et al. (2008)
HCl	8-57	A reduction of ~5% is seen over profile	Mahieu et al. (2008)
CCl_3F	2-22	A slight increase is seen around ~15 km.	Mahieu et al. (2008)
CCl_2F_2	6-28	An increase of ~2-5% is seen over the ~6-22 km altitude range.	Mahieu et al. (2008)
$ClONO_2$	12-35	From ~17-22 km, a ~20-30% reduction is seen. A ~7% reduction was also seen above the peak, at ~30-32 km.	Wolff et al. (2008)
CO	5-105	Below ~10 km and between ~35 and ~45 km, a small decrease is seen. Between ~14 and ~18 km, a small increase is seen.	Clerbaux et al. (2008)
HNO_3	5-37	Above ~25 km, an increase of ~5% is seen.	Wolff et al. (2008)

III. ACE-FTS Processing Plans

The next processing version (version 4.0) is now in development (Boone et al., 2013). The primary motivation for this update is to develop a data set that is more appropriate for studying longer-term changes and investigating trends. In ACE-FTS processing versions 3.0 and earlier, the assumed rate of change in CO_2 as a function of time is too low and will therefore be changed to match better with observations. In version 4.0, the shape of the CO_2 VMR profiles at low altitudes will vary with latitude, and a seasonal cycle will be included, features that were not present in previous processing versions.

An issue was identified in the input a priori temperature/pressure profiles for low altitudes that has affected all ACE-FTS retrievals beginning in October 2010 (Boone et al., 2013). Because of this, data from both version 2.2+updates and version 3.0 should not be used after 30 September 2010. New processing versions (2.5 and 3.5) are being produced to provide corrected results for the affected time period (October 2010 onward). These new versions do not include any changes in the retrieval process other than employing more appropriate a priori pressure and temperature information (Boone et al., 2013).

IV. Conclusion

ACE-FTS and the SCISAT satellite continue to perform well in their tenth year in orbit and produce a valuable data set for investigating the composition of the Earth's atmosphere. Through direct profile comparisons, the current ACE-FTS v3.0 data set is generally seen to improve on the v2.2+updates data set. Comparisons with other satellite data sets are in progress and these results are being used to provide feedback for future ACE-FTS data versions.

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