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Atmospheric Measurement Techniques Discussions
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Technical Note: Detecting outliers in satellite-based atmospheric measurements

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Abstract

The ACE-FTS (Atmospheric Chemistry Experiment – Fourier Transform Spectrometer) instrument on board the Canadian satellite SCISAT has being observing the Earth's limb in solar occultation since its launch in 2003. Since February 2004, high resolution (0.02 cm^{-1}) observations in the spectral region of 750–4400 cm^{-1} have been used to derive volume mixing ratio profiles of over 30 atmospheric trace species and over 20 atmospheric isotopologues. Although the full ACE-FTS level 2 data set is available to users in the general atmospheric community, until now no quality flags have been assigned to the data in order to guide the users. This study describes the two-stage procedure for detecting outliers within the data set for each retrieved species, which is a fixed procedure across all species. Since the distributions of ACE-FTS data across regions (altitude/latitude/season/local time) tend to be asymmetric, the screening process does not make use of the median absolute deviation. Quality flags have been assigned to the data based on fitting error, the outliers described in this study, and known instrumental/processing errors. The quality flags defined and discussed in this study are now available for all level 2 version 2.5 and 3.5 data and will be made available as a standard product for future versions.

1 Introduction

One of the most common techniques for screening out anomalous data from a data set is to calculate the set's mean (μ) and standard deviation (σ). Data that are outside the limits of $\mu \pm k\sigma$, where k is some constant, are deemed to be outliers. Another common, and similar, method is to use the median and MAD (Median Absolute Deviation) (Toohey et al., 2010; and references therein), in place of the mean and standard deviation respectively, where,

$$\text{MAD} = \text{median}_i\left(\left|x_i - \text{median}_j\left(x_j\right)\right|\right) \quad (1)$$

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This method is much less sensitive to extreme outliers, as the presence of outliers typically has an insignificant effect on the median value. However, this technique assumes that the data being analyzed are symmetrically distributed about the median. In the case of data that is asymmetrically distributed and consists of multiple extreme outliers, it is likely that neither the σ nor the MAD will be an appropriate estimate of the variation, or scale, of the measurements. In such cases, they should be avoided in the detection of outliers (Rousseeuw and Croux, 1993).

In satellite remote sensing of the atmospheric limb, measurements inherently suffer from sampling biases. Therefore, isolating geographical/seasonal/local time regions where global satellite-based data are normally distributed can be difficult and/or tedious. This is due to the fact that the atmosphere doesn't necessarily behave in a predictable, periodic manner. Measurements grouped into a given altitude and latitude and month and local time bin can be driven away from normal behaviour by any number of factors – e.g., the polar vortex, a solar proton event, a sudden stratospheric warming, etc.

The ACE-FTS (Atmospheric Chemistry Experiment – Fourier Transform Spectrometer (Bernath et al., 2005) instrument, on board the Canadian satellite SCISAT, is a solar occultation, high-resolution (0.02 cm^{-1}) Fourier transform spectrometer operating between 750 and 4400 cm^{-1}. ACE-FTS observations are used to derive volume mixing ratio (VMR) profiles of over 30 atmospheric trace gases, as well as profiles of over 20 subsidiary isotopologues of atmospheric species (Boone et al., 2005). SCISAT was launched in 2003 and ACE-FTS has been providing consistent measurements since February 2004. Atmospheric profiles range in altitude from ~5–110 km, depending on the species, with a vertical resolution of ~3–4 km and sampling of 2–6 km.

This study outlines the repercussions of screening data based on the standard deviation or the MAD given non-normally distributed data and discusses a two-step process for detecting outliers that is currently carried out on the ACE-FTS level 2 data set. All data presented in this study are ACE-FTS level 2 version 3.5 (v3.5) (Boone et al., 2013) spanning February 2004 to February 2013, however the same processes are used for detecting outliers in version 2.5 (v2.5) data. The main differences in v3.5 from v2.5 are,

– amended sets of microwindows for all molecules, and an increase in the number of allowed interferers in the retrievals;

– improvement in temperature/pressure retrievals, leading to a reduction in unphysical oscillations in retrieved temperature profiles;

– inclusion of $COCl_2$, COClF, H_2CO, CH_3OH, and HCFC-141b and removal of HOCl and ClO VMR retrievals.

The outlier detection and subsequent data flagging procedures discussed in this study have only been performed on the ACE-FTS level 2 data products that have been interpolated onto a 1 km altitude grid (between 0.5 and 149.5 km) (Boone et al., 2005). The philosophical approach for flagging data as potential outliers was one of caution, in that it is better to keep some "bad" data than to reject "good", or "true", data. As well, it was desired that the approach be consistent for all subsets of data being analyzed, i.e. tolerance levels, regional limits, etc. should be the same for all species, for all seasons, at all altitudes.

2 Detection method and results

All distributions of data discussed in this section represent the February 2004–February 2013 data, and all VMRs are given in parts per volume (ppv).

Global satellite-based measurements of trace gases in the atmosphere typically are not normally distributed. Different regions are governed by different, varying processes, and therefore analysis of the data is typically carried out by breaking down the data into different altitude, latitudinal, etc. bins. Figure 1 shows the ACE-FTS H_2O data at 17.5 and 35.5 km and the corresponding measurement distributions. For both subsets of H_2O data, inlier limits were determined for $\mu \pm 3\sigma$ and median $\pm 3\,\mathrm{MAD} \times 1.428$ (1.428 is the scale factor for a consistent estimate of the variation assuming a normal distribution, Rousseeuw and Croux, 1993). These limits are plotted in Fig. 1a and Fig. 1c and highlight two key points: first, using the standard deviation when there are extreme outliers can allow for the acceptance of data that should clearly be rejected. Second, using the MAD on asymmetrically distributed data can lead to the rejection of "good" data. For instance, as shown in Fig. 1a, the lower cut-off using the MAD of 2.76 ppm clearly excludes the low H_2O concentrations that are observed in Antarctic (austral) spring. As can be seen in Fig. 1b and Fig. 1d, the H_2O data at both altitude levels are not normally distributed.

The data can be separated further into bins based on latitudinal regions and local times. For example, Fig. 2 shows H_2O and O_3 sunset data at 30.5 and 35.5 km, separated into different latitude regions (0–30° S, 30–60° S, and 60–90° S), with dashed lines representing best fits to normal distributions. These regions are representative of bins often used to partition atmospheric data. Figure 2 exemplifies that using a given bin definition that leads to symmetrically distributed data at one altitude level doesn't necessarily lead to symmetrically distributed data at all altitude levels, nor across all species. For instance, in Fig. 2a the 35.5 km O_3 distributions in all three latitude regions are fairly symmetric. However the 35.5 km H_2O distribution (Fig. 2c) in the mid-latitudes is highly skewed, and in Figs. 2b and d we see bimodal, asymmetric distributions for both O_3 and H_2O in the 30–60° S and 60–90° S regions at 30.5 km. For high-latitude data in many species' data sets, distributions can be bimodal due to observing inside and outside of the vortex, and therefore it is not possible to find sub-regions (based on season, latitude, or local time) that will always exhibit symmetric distributions.

Therefore, the ACE-FTS data screening process takes an approach that does not require the distribution of any subset of data to be symmetric. The screening processes starts by analysing the data's probability density functions. The probability density function of data subset x, pdf(x), multiplied by the number of data points, N, gives you the expected number of data points at a given value of x,

$$E(x) = N \times \mathrm{pdf}(x) \tag{2}$$

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The function $E(x)$ is the expectation distribution. Anywhere that the expectation distribution is less than 1 is most likely a statistical outlier, as no data points are expected to be measured at those values of x, given the pdf. Therefore, the criterion for excluding data can be any value of x where $E(x)$ is less than 1. This is similar to Peirce's criterion (Peirce, 1852; Ross, 2003) and Chauvenet's criterion (Chauvenet, 1871), which both assume a normally distributed probability density function. The tolerance level can be varied to suit the desired acceptance level of possible outliers. For ACE-FTS data, a tolerance level of 10^{-4} is used, which corresponds to a 99.99 % confidence of an excluded data point being an outlier – i.e., any value x where $E(x) < 10^{-4}$ is rejected.

This method, however, requires determining an analytical solution for the data's expectation distributions. For each of the 50+ ACE-FTS retrieved species, at each altitude level, the data is separated into sunset and sunrise occultations as well as into four different latitude regions: 60–90° S, 0–60° S, 0–60° N, and 60–90° N. Due to the SCISAT orbital geometry, the majority of ACE-FTS measurements are at high latitudes, and therefore each latitudinal bin has roughly the same number of profiles. The distribution of each subset is then fit to a Gaussian mixed distribution, using three Gaussian distributions. This assumes that the data is at most tri-modally distributed. The fit is performed using the Matlab statistical toolbox, which uses an Estimation Maximization algorithm (McLachlan and Peel, 2000). Figure 3 shows the O_3 distribution at 30.5 km in the 60-90° S and 60–90° N regions, along with the fitted expectation distributions and the three Gaussian distributions derived in the fit. It should be noted that prior to fitting a data subset to a Gaussian mixed distribution, profiles affected by previously determined issues either with the instrument or with the data processing have been excluded, and extreme outliers are screened out by assuming that any data points with absolute values greater than 10 000 times the median of the subset's absolute values are outliers.

Figure 4 shows three examples of ACE-FTS sunset data distributions – NO_2 at 60–90° S and 30.5 km, CH_4 at 0–60° N and 17.5 km, and N_2O at 60–90° N and 20.5 km – and the corresponding fitted expectation distributions. These were chosen in order to illustrate typical results for commonly used ACE-FTS data. The average root-mean-square error (RMSE) between the expectation distributions and actual distributions is 6 % and has a 1σ deviation of 2 %. In the case of rare extreme events present in the data, which tend to be under-sampled in ACE-FTS data, the effect on the distribution can be to skew a tail end of the distribution, driving the shape of the tail away from Gaussian. An additional ad hoc method has been implemented to ensure that no "true" data is excluded in the screening process when rare extreme events occur that are not properly accounted for in the fit. For each subset, the standard deviation is calculated for the inlying data, where $E(x) > 10^{-4}$. This standard deviation we will call σ_{in}. Original upper and lower limiting values, x_{l}, are calculated, where $E(x_{\text{l}}) = 10^{-4}$, and both the upper and lower limiting values are extended by σ_{in}. Hence, $x_{\text{lim}}^{\text{up}} = x_{\text{l}}^{\text{up}} + \sigma_{\text{in}}$ and $x_{\text{lim}}^{\text{low}} = x_{\text{l}}^{\text{low}} - \sigma_{\text{in}}$. Figure 5 shows the inliers and outliers as determined by the expectation distributions for the subsets shown in Fig. 4. As can be seen, not all subsets contain extreme outliers, e.g. NO_2 at 30.5 km (Fig. 5a). When there are obvious outliers, this method does exclude the most extreme outliers, although perhaps not all outliers. For instance, several (potentially) anomalously low values, near 0.75 ppm, in the CH_4 data (Fig. 5b) remain as inliers. This is in part due to the lax tolerance level of 10^{-4}, which is more likely to leave in outliers than if a larger value (but still less than 1) was chosen.

It should be noted that screening using the expectation distribution is a hard-limiting filter, which doesn't necessarily reject data that are non-physically anomalous for a given season. To screen the data of this type of moderate outlier, the 15-day running mean (μ_{15}) and 15-day running standard deviation (σ_{15}) are calculated for each subset, excluding outliers as determined from the expectation distributions. Any data point with a value outside the bounds of $\mu_{15} \pm 5.5\sigma_{15}$ are considered to be outliers. The value of 5.5 was empirically found to maximize the number of discovered outliers without rejecting obviously "true" data. If outliers are detected, they are removed from the data, and a new running mean and standard deviation are calculated for the inlying data in order to determine if there are any more outliers. This process is iterated until all data points are determined to be inliers. The mean and standard deviation are used

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instead of the median and MAD, as it is assumed that the subsets have already been screened for extreme outliers. Figure 6 shows the inliers and outliers as determined by the 15-day running values for the subsets shown in Fig. 4. Clearly this step catches moderate outliers that were not detected using the expectation distributions, although still not all anomalous data have been screened out. The potentially anomalous values near 0.75 ppm in the CH_4 data (Fig. 6b) still remain as inliers. Stricter tolerance criteria in either the expectation distribution or running standard deviation screening process would allow for these data to be screened out; however, they were found to lead to screening out "true" data in other subsets of data, which would be discordant with our philosophical approach.

In order to explore the response to periodic extreme events and to trends, Fig. 7 shows the final inliers and outliers in all ACE-FTS HCN data at 9.5 km, which exhibits periodic increases that could correspond to biomass burning events (e.g. Crutzen and Andreae, 1990; Pommrich et al., 2010), as well as all SF_6 data at 19.5 km, which exhibits a clear positive trend throughout the time series (Rinsland et al., 2005; Brown et al., 2011). Even in these instances of extreme events and a significant trend in the data, the outlier detection method outlined here is robust enough to keep the data as inliers. The top panel in Fig. 7 shows all data points and demonstrates the extreme outliers (red dots) that can occur within the ACE-FTS data set. The middle panel shows the same data as the top panel, however without the more extreme outliers in order to better view the data; and the bottom panel shows the data with all outliers removed.

Stratospheric sudden warmings cause there to be strong descent in the northern high-latitude upper atmosphere. This leads to large concentrations of NO and CO in the upper stratosphere-lower mesosphere, near 50 km (e.g. Manney et al., 2008; Randall et al., 2009). Figure 8 shows the time series of the final inliers and outliers in all ACE-FTS NO and CO data at 55.5 and 50.5 km, respectively. Again, the detection method is robust enough to keep the majority of data during these extreme events as inliers. In a couple extreme cases, NO data in early 2004 at 55.5 km (Fig. 8a–c), seven data points were flagged as extreme outliers that could potentially be "true" data; and similarly in early 2011 CO data at 50.5 km (Fig. 8d–f), eight data points may have been erroneously flagged. Out of all subsets of all 50+ species/isotopologues, these were the most extreme instances of apparent rejection of true data. The down side of not screening out rare extreme events, however, is that this method is less likely to catch sporadic systematic instrument or processing errors. Therefore, continual monitoring of both the rejected and non-rejected data statistics is necessary to determine if any such errors have occurred.

Table 1 shows what percentage of ACE-FTS level 2 v3.5 profiles contain at least one detected outlier (by either method). For any given species, if all profiles that contained at least one outlier are rejected, less than 6 % of the total number of profiles will be omitted.

3 Conclusions

A two-step process has been developed in order to screen all ACE-FTS level 2 data for outliers. The first step fits an expectation distribution, the superposition of three Gaussian distributions, to actual distributions. Data that have corresponding expectation values that are less than the subset tolerance level are determined to be extreme outliers. The second step iteratively takes the 15-day running mean and standard deviation and screens for moderate seasonal outliers. At each iteration, data that are further than 5.5 times the standard deviation from the mean are determined to be moderate outliers.

Using these methods to screen the ACE-FTS data for outliers, a flagging system has been implemented to give ACE-FTS level 2 data users a guide for how best to use the data. Each VMR data point in each profile is flagged with an integer from 0–9. Table 2 gives the definition for each flag value. Any data with a 0 flag is recommended for use. It is recommended that data points with a corresponding flag greater than 2 be removed before any analysis is performed. This screening method alone may be adequate when only looking at one altitude level, however, profiles that contain an outlier at a given altitude level may also be compromised at lower altitude levels.

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Therefore it is recommended that any profile that contains a flag between 4 and 7 (inclusive) be removed before analysis. However, screening the data using these flags should be done with caution when investigating middle to upper atmospheric NO, CO, and CO isotopologues.

At certain altitude levels for a given species, the data can be either noisy, with a significant number of negative values, or have a strong negative bias. In either case, since the ACE-FTS retrieval allows for negative concentrations, it is possible for valid data to have values close to zero, both positive and negative. When values are systematically near zero, the percent error becomes extremely large. Therefore, in these situations, screening the data based on the percent error may introduce a bias in the data. As such, before analysis, removing data that has a corresponding flag value of 1 is only recommended at altitude levels where the overwhelming majority of data points are greater than zero.

Since the outlier detection methodology was approached with a philosophy that it is better to leave in outliers than to remove inliers, there are outliers that have gone unflagged – especially in data sets that are inherently noisy and at low altitudes (below ~ 10 km). Level 2 data users should use the defined quality flags as a starting point for screening the data and be aware that some outliers may still exist that could be screened out prior to analysis. It is recommended that data users also avoid using the MAD in any attempts to further screen the ACE-FTS level 2 data.

The flag values for all v2.5, v3.0, and v3.5 data are available upon request from the lead author and will soon be made available for download on the ACE-FTS website. It is currently expected that similar flags will be a standard product within the level 2 data of all future products.

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References

Bernath, P. F., McElroy, C. T., Abrams, M. C., Boone, C. D., Butler, M., Camy-Peyret, C., Carleer, M., Clerbaux, C., Coheur, P.-F., Colin, R., DeCola, P., DeMazière, M., Drummond, J. R., Dufour, D., Evans, W. F. J., Fast, H., Fussen, D., Gilbert, K., Jennings, D. E., Llewellyn, E. J., Lowe, R. P., Mahieu, E., McConnell, J. C., McHugh, M., McLeod, S. D., Michaud, R., Midwinter, C., Nassar, R., Nichitiu, F., Nowlan, C., Rinsland, C. P., Rochon, Y. J., Rowlands, N., Semeniuk, K., Simon, P., Skelton, R., Sloan, J. J., Soucy, M.-A., Strong, K., Tremblay, P., Turnbull, D., Walker, K. A., Walkty, I., Wardle, D. A., Wehrle, V., Zander, R., and Zou, J.: Atmospheric Chemistry Experiment (ACE): Mission overview, Geophys. Res. Lett., 32, L15S01, doi:10.1029/2005GL022386, 2005.

Boone, C. D., Nassar, R., Walker, K. A., Rochon, Y., McLeod, S. D., Rinsland, C. P., and Bernath P. F.: Retrievals for the Atmospheric Chemistry Experiment Fourier-Transform Spectrometer, Appl. Optics, 44, 7218–7231, doi:10.1364/AO.44.007218, 2005.

Boone, C. D., Walker, K. A., and Bernath, P. F.: Version 3 Retrievals for the Atmospheric Chemistry Experiment Fourier Transform Spectrometer (ACE-FTS), The Atmospheric Chemistry Experiment ACE at 10: A Solar Occultation Anthology, A. Deepak Publishing, Hampton, Virginia, USA, 103–127, 2013.

Brown, A. T., Chipperfield, M. P., Boone, C. D., Wilson, C., Walker, K. A., and Bernath, P. F.: Trends in atmospheric halogen containing gases since 2004, J. Quant. Spectrosc. Rad. Trans., 112, 2552–2566, doi:10.1016/j.jqsrt.2011.07.005, 2011.

Chauvenet, W.: Manual of spherical and practical astronomy, J. B. Lippincott Company, Philadelphia, USA, 558–563, 1871.

Crutzen, P. J. and Andreae, M. O.: Biomass burning in the tropics: impact on atmospheric chemistry and biogeochemical cycles, Science, 250, 1669–1678, doi:10.1126/science.250.4988.1669, 1990.

Manney, G. L., Daffer, W. H., Strawbridge, K. B., Walker, K. A., Boone, C. D., Bernath, P. F., Kerzenmacher, T., Schwartz, M. J., Strong, K., Sica, R. J., Krüger, K., Pumphrey, H. C., Lambert, A., Santee, M. L., Livesey, N. J., Remsberg, E. E., Mlynczak, M. G., and Russell III, J. R.: The high Arctic in extreme winters: vortex, temperature, and MLS and ACE-FTS trace gas evolution, Atmos. Chem. Phys., 8, 505–522, doi:10.5194/acp-8-505-2008, 2008.

McLachlan, G. and Peel, D.: Finite Mixture Models,John Wiley & Sons, Inc., Hoboken, New Jersey, USA, 2000.

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Peirce, B.: Criterion for the rejection of doubtful observations, Astronomical J., 2, 161–163, 1852.
Pommrich, R., Müller, R., Grooß, J.-U., Günther, G., Konopka, P., Riese, M., Heil, A., Schultz, M., Pumphrey, H.-C., and Walker, K. A., What causes the irregular cycle of the atmospheric tape recorder signal in HCN?, Geophys. Res. Lett., 37, L16805, doi:10.1029/2010GL044056, 2010.
Randall, C. E., Harvey, V. L., Siskind, D. E., France, J., Bernath, P. F., Boone, C. D., and Walker, K. A., NO_x descent in the Arctic middle atmosphere in early 2009, Geophys. Res. Lett., 36, L18811, doi:10.1029/2009GL039706, 2009.
Rinsland, C. P., Boone, C., Nassar, R., Walker, K. A., Bernath, P., Mahieu, E., Zander, R., McConnell, J. C., and Chiou, L.: Trends of HF, HCl, CCl_2F_2, CCl_3F, $CHClF_2$ (HCFC-22), and SF_6 in the lower stratosphere from Atmospheric Chemistry Experiment (ACE) and Atmospheric Trace Molecule Spectroscopy (ATMOS) measurements near 30° N latitude, Geophys. Res. Lett., 32, L16S03, doi:10.1029/2005GL022415, 2005.
Ross, S. M.: Peirce's criterion for the elimination of suspect experimental data, J. Eng. Tech., 20, 38–41, 2003.
Rousseeuw, P. J. and Croux C.: Alternatives to the Median Absolute Deviation, J. Amer. Stat. Assoc., 88, 1273–1283, 1993.
Toohey, M., Strong, K., Bernath, P. F., Boone, C. D., Walker, K. A., Jonsson, A. I., and Shepherd T. G., Validating the reported random errors of ACE-FTS measurements, J. Geophys. Res., 115, D20304, doi:10.1029/2010JD014185, 2010.

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Table 1. Percent rejection of ACE-FTS level 2 v3.5 profiles that contain one or more detected outlier (either by running mean or expectation distribution).

Species	% reject	Species	% reject	Species	% reject
C_2H_2	1.71	HCFC141b	2.03	$C^{17}O$	1.95
C_2H_6	1.81	HCFC142b	1.81	$C^{18}O$	2.54
CCl_2F_2	2.09	HCl	2.19	$O^{13}CO$	4.46
CCl_3F	1.66	HCN	2.50	$O^{13}C^{18}O$	1.30
CCl_4	1.81	HCOOH	2.09	$OC^{17}O$	1.33
CF_4	2.35	HF	1.53	$OC^{18}O$	4.90
CFC113	1.50	HNO_3	2.65	$H^{17}OH$	2.95
CH_3Cl	2.39	HNO_4	2.49	$H^{18}OH$	3.08
CH_3OH	2.83	N_2	2.62	HDO	2.76
CH_4	2.95	N_2O	4.29	^{15}NNO	2.39
CHF_2Cl	2.35	N_2O_5	2.16	$N^{15}NO$	2.37
$ClONO_2$	1.68	NO	4.91	$NN^{17}O$	1.88
CO	4.10	NO_2	2.34	$NN^{18}O$	2.91
CO_2	5.70	O_2	2.23	$O^{17}OO$	3.03
$COCl_2$	2.37	O_3	2.40	$O^{18}OO$	1.97
COClF	1.35	OCS	1.42	$OO^{18}O$	1.85
COF_2	1.26	SF_6	2.31	$O^{13}CS$	2.17
H_2CO	3.43	$^{13}CH_4$	3.00	$OC^{34}S$	1.92
H_2O	3.97	CH_3D	2.01		
H_2O_2	3.16	^{13}CO	3.08		

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Table 2. 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 outlier detected from running mean, percent error within limits
5	Extreme outlier detected from expectation distribution, percent error within limits
6	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)

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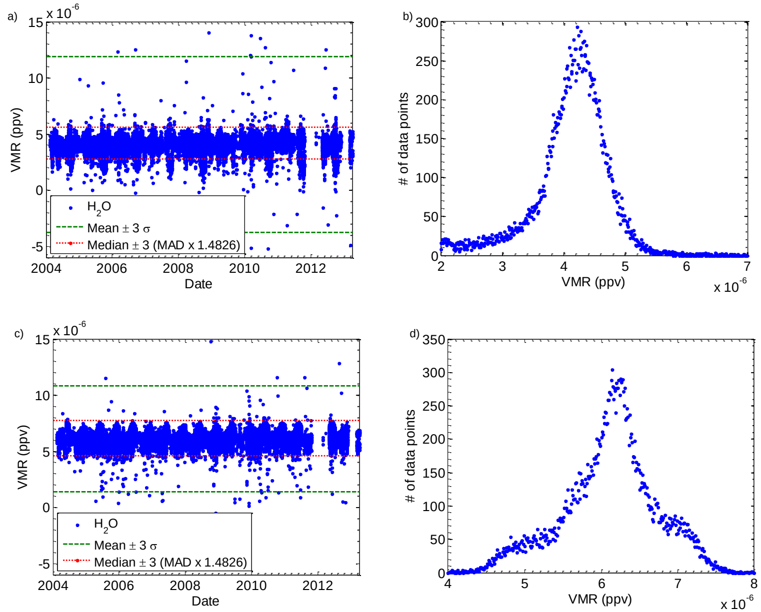

Figure 1. ACE-FTS level 2 v3.5 H_2O data (left) and corresponding distributions (right). Top panel shows data at 17.5 km, and the bottom panel shows data at 35.5 km.

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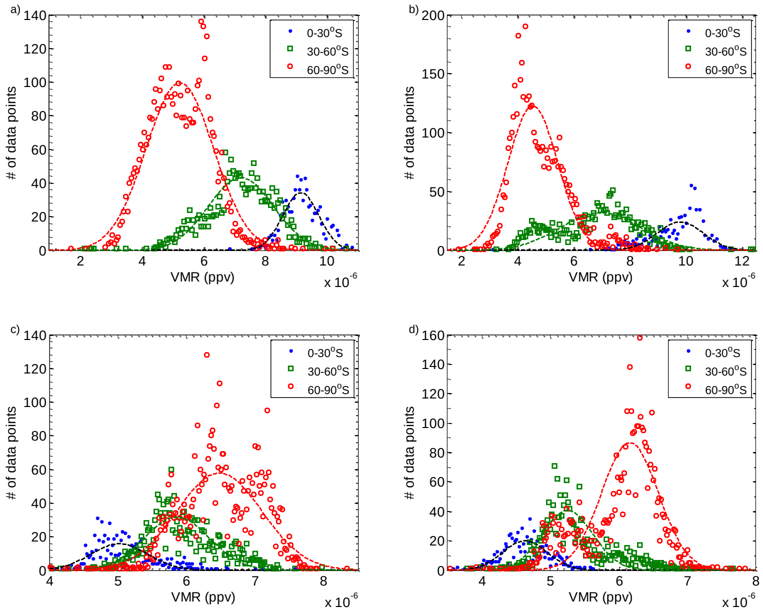

Figure 2. 2004-2013 ACE-FTS VMR distributions for sunset occultations (symbols) in the Southern hemisphere and corresponding best fits to normal distribution (dashed lines). **(a)** O_3 at 35.5 km, **(b)** O_3 at 30.5 km, **(c)** H_2O at 35.5 km, **(d)** H_2O at 30.5 km.

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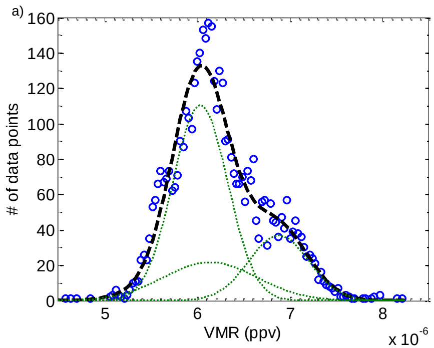

Figure 3. Sunrise ACE-FTS O_3 VMR distributions at 30.5 km (blue circles) and fitted expectation distributions (dashed black lines) for **(a)** 60–90° N, and **(b)** 60–90° S. Dotted green lines are the fitted Gaussian distributions in calculating the expectation distributions.

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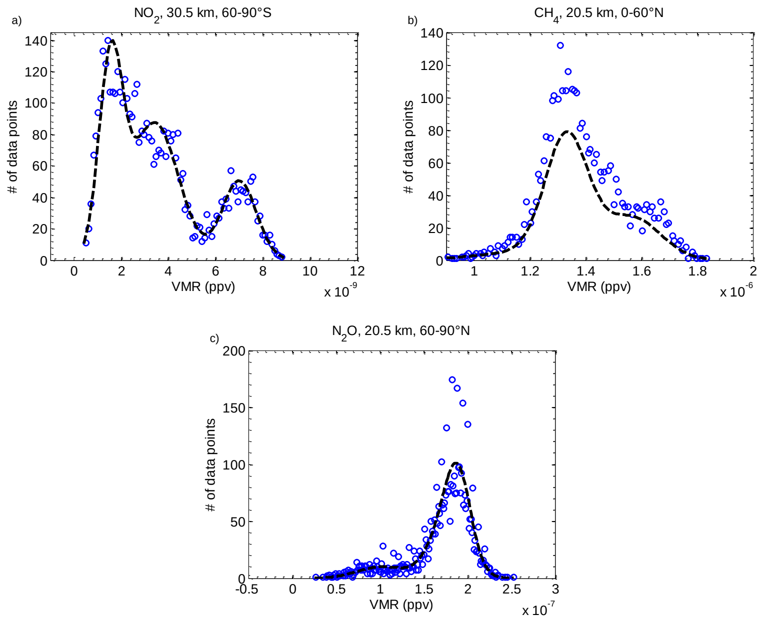

Figure 4. Sunrise ACE-FTS VMR distributions (blue circles) and fitted expectation distributions (black dashed lines) for **(a)** NO_2 at 30.5 km in the latitude region 60–90° S; **(b)** CH_4 at 20.5 km, 0–60° N; and **(c)** N_2O at 20.5 km, 60–90° N.

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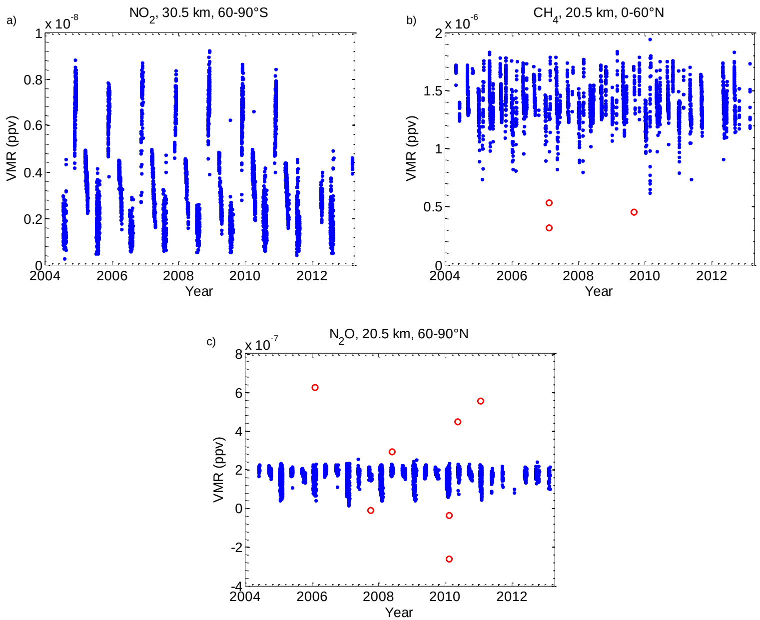

Figure 5. Sunrise ACE-FTS data for the same data subsets as Fig. 4. Red circles are data that have been determined to be outlying data as per the expectation distributions, and blue dots are the inlying data.

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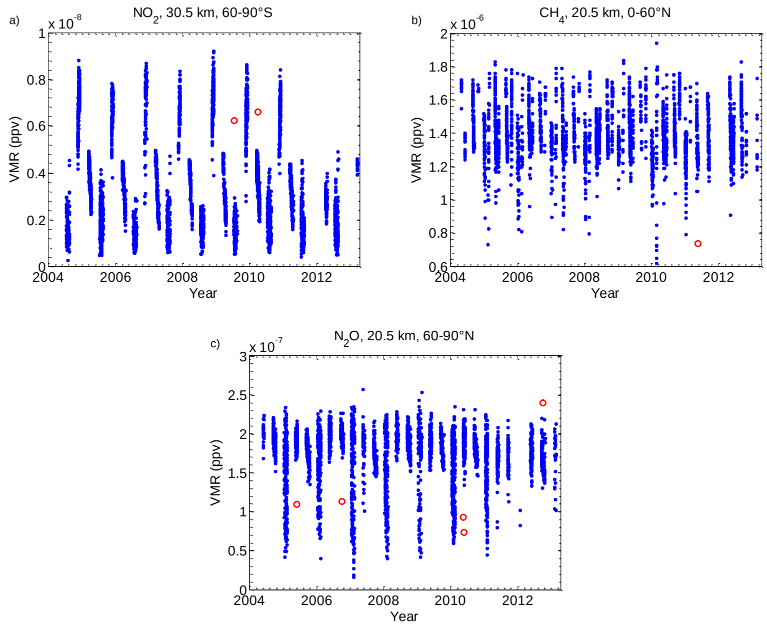

Figure 6. Sunrise ACE-FTS data for the same data subsets as Fig. 4. Red circles are data that have been determined to be outlying data as per the 15-day running mean and standard deviation, and blue dots are data that have been determined to be inliers.

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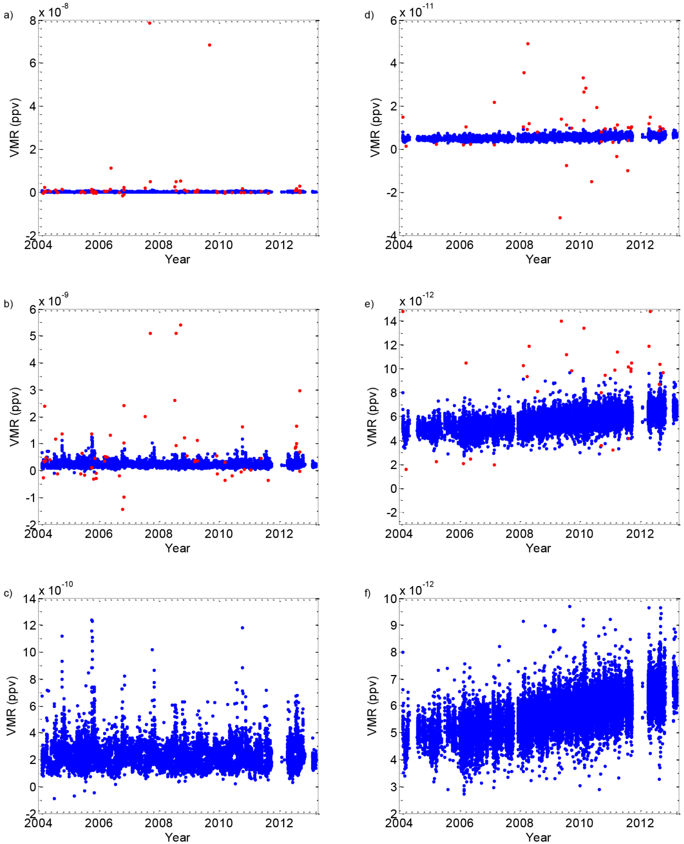

Figure 7. The final inlying (blue dots) and outlying (red dots) data for all ACE-FTS HCN data at 9.5 km (left) and SF_6 data at 19.5 km (right). The top panel shows all data, the middle panel is the same as the top panel only zoomed in for clarity, and the bottom panel is all data excluding the outliers.

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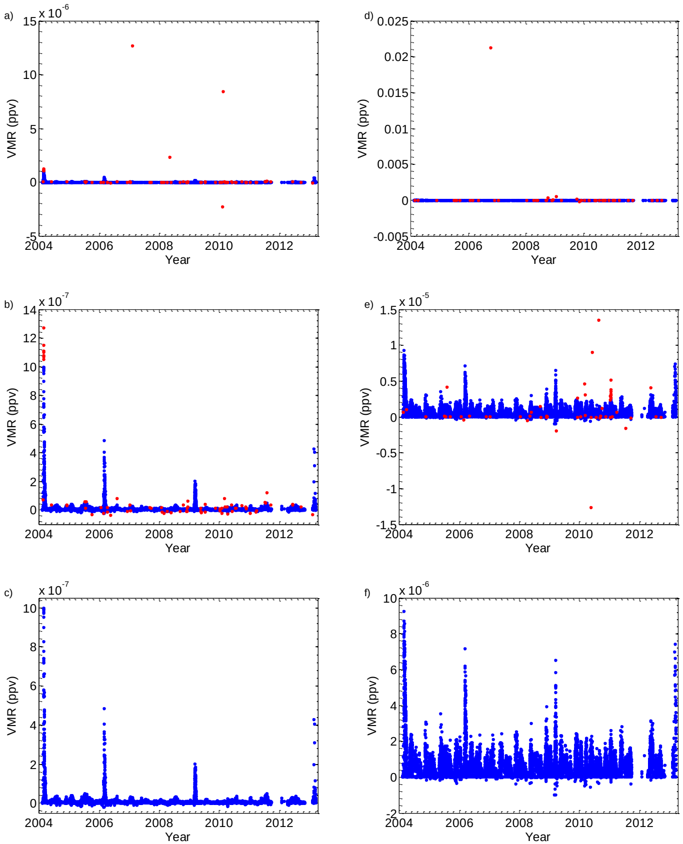

Figure 8. The final inlying (blue dots) and outlying (red dots) data for all ACE-FTS NO data at 55.5 km (left) and CO data at 50.5 km (right). The top panel shows all data, the middle panel is the same as the top panel only zoomed in for clarity, and the bottom panel is all data excluding the outliers.

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