Comparison of ACE-FTS and AIRS Temperature Profiles

(Select cases for 2004 over the United States)

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1 Introduction

The purpose of this paper is to describe the comparison of temperature soundings from three different sources. Temperature data from balloon soundings, the ACE-FTS instrument aboard SCISAT-1 and the AIRS instrument aboard AQUA was analyzed for six observations over locations in the U.S. during 2004. An effort was made to find data from all sources that was both collocated and simultaneous for a given observation in order to minimize differences due to spatial and temporal displacements. Descriptions of the instruments and data collection methods are given, as are analyses of the collocated profiles. Conclusions regarding the efficacy of the instruments as well as the respective error in each are provided at the end of the paper.

2 The Sounding Instruments

2.1 ACE-FTS

The Atmospheric Chemistry Experiment - Fourier Transform Spectrometer (ACE-FTS) is a remote sensing instrument on board SCISAT-1, a satellite in circular orbit at an altitude of 650km. The instrument uses a Michelson interferometer to gather spectral intensities of atmospheric constituents in the wavelength band: 2.2\(\mu\m - 13.3\mu\m\). The instrument acts as a limb-sounder, viewing layers of the upper atmosphere (above 12 km) corresponding to tangent heights over a given location on the ground.

During one viewing session, the instrument performs a calibration routine, reading first the deep space view, in order to capture the built-in instrument noise. Then, it views the sun through the exosphere (160km - 225km) so that no atmospheric components absorb intensity from the spectra. Lastly, the instrument views the setting (or rising) sun every 2 seconds through progressively lower levels of the atmosphere, subtracting the deep space
and pure sun spectra out of the signal, so that only absorption spectra remain (see figure 1). (2)

Pressure and temperature values (as well as the volume mixing ratios of various atmospheric constituents) are determined by various means for different levels of the atmosphere. A constant $CO_2$ profile is assumed up to 75 km below 60 degrees latitude (see figure 2), though the VMR of $CO_2$ is assumed to be about 5.5 ppm greater in the troposphere than in the stratosphere. Also, the profile is assumed to increase over time according to:

$$CO_2 VMR (ppm) = 326.909 + 1.50155(t - t_0), \quad (t_0 = \text{January 1, 1977})$$

Although a number of calibration procedures are performed in order to properly interpret the data at each level, the relative intensities of $CO_2$ spectra indicate the temperature values, while the absolute intensities (due to broadening of the line shape) give the pressure. An a priori profile is assumed in order to constrain the retrieval process, which, according to Stephens, suffers from non-uniqueness and instability due to the requisite inverse problem involved in divining pressure and temperature from absorption spectra. Next, various checks are performed on the retrieved $T, P$ values and the calculated tangent height (assuming hydrostatic equilibrium), to ensure that all of the values conspire to effect a physical (realistic) description of the atmosphere. (13)

![Occultation diagram for ACE-FTS limb-sounder (Boone and Bernath, 2002).](image)
Figure 2: The constant profile of $CO_2$ volume mixing ratio (Boone and Bernath, 2002).

The retrieval process is based on the successful separation of the incoming infrared light spectrum into its component peaks via the Fourier-transformed interferogram collected by the interferometer. The spectra is then converted into temperature as a function of height by the assumption that each layer of $CO_2$ in the atmosphere radiates as a blackbody, and that the blackbody curve is attenuated by the local value of the weighting function. Furthermore, it is assumed that the weighting function varies according to the absorption properties of the relevant absorber, which are in turn determined by the local optical depth and the pressure.

In the case of ACE-FTS, the weighting functions are very narrow, as indicated in figure 3. This is due to the small field of view of the satellite, which can only image 3-4 km horizontal layers at a time.

ACE-FTS data is available from the European Space Agency, though the means of acquiring it are a mystery. ACE data used in this study were freely available at the project website, though only from the first year of operation, 2004.
Figure 3: Averaging kernels and error profiles of the ACE-FTS retrieval algorithm (Clerbaux, et al, 2005).

2.2 AIRS

The second instrument is the Atmospheric InfraRed Sounder, or AIRS. It is mounted on the AQUA satellite, in orbit at an altitude of 705 km. Instead of an interferometer, the AIRS has an Echelle spectrometer, which employs a refraction grating to split incident the light into component spectra. Furthermore, unlike the ACE instrument, the AIRS is a nadir sounder, which observes intensities in 2378 spectral samples in 3 bands: 3.74µm – 4.61µm, 6.2µm – 8.22µm, 8.8µm – 15.4µm.

For a nadir sounder, the weighting function can take a form similar to:

\[ W(z) = \frac{2\tau^*}{H} e^{-\tau^*} e^{-\frac{2z}{H}} \]

where \( \tau^* \) is the optical depth at the surface, or the argument to the exponential function that defines the transmission through the absorber at the surface. For a Lorentz line shape (concerning the line wings) under the influence of pressure broadening effects,

\[ \tau^* = \frac{S\pi L_0 \rho_0}{\pi (\nu - \nu_0)^2 2g} \]

In the above weighting function, we can see that as the height increases, one term in the argument of the exponent decreases due to the decreased VMR of the absorber. However,
with increasing height, the second argument increases due to the increase in transmission near the top of the atmosphere. In this way, the weighting function has a bell-curve shape, which finds a maximum at

$$z_{\text{max}} = \frac{H}{2} \ln \tau^*$$

Since $\tau^*$ is a function of frequency, or wavelength, various peaks in the weighting functions can be selected by choosing $\lambda$, so that the intensity at that wavelength is largely due to contributions from the region of peak $W$, i.e. near $z_{\text{max}}$. (13)

The weighting functions for the AIRS instrument, and for nadir sounders in general, are much broader, covering thicker layers of the atmosphere, as is illustrated in figure 4. AIRS data coverage is ubiquitous due to the wide swath of coverage and AQUA’s rapid rate of circumnavigation. It is freely available from the Mirador earth science data search tool at NASA’s Goddard Earth Sciences Data and Information Services Center.

### 2.3 Rawinsondes

The last instrument is the rawinsonde, or balloon sounder. These devices are all slightly different, depending on the launching station, though the stations are required to keep certain standards of accuracy. The instruments are in direct contact with the atmosphere,
so they are not remote sensors, but in situ sensors. The balloons tend to reach an altitude of approximately 35 km before they rupture due to the low pressure at that height. However, according to the Federal Meteorological Handbook, which expresses regulations for balloon soundings in the U.S., the temperature accuracy must be between 0.4 and 1.0 degrees Celsius, while the pressure must be accurate to within 1.5 hPa above the 300hPa level. (16) A brochure by Sippican Inc., a manufacturer of balloon sondes, and one of the recommended devices by NOAA, claims even better accuracy values of approximately half those given above. (12)

Balloon sondes are launched in the U.S. at many stations around the country regularly at 00Z and 12Z. Furthermore, the data is freely available from several websites, such as that of the University of Wyoming’s Department of Atmospheric Science, from which rawinsonde data was procured for this experiment.

3 Data Collection

In order to find parallel data across the three data types, it was necessary to begin with the most sparse data set, and select soundings that would match up with observations in the next most sparse set. Those data sets were from the ACE-FTS and the rawinsondes, respectively. Figure 5 illustrates the scarcity of ACE-FTS data for the period 01/01/04 to 01/11/04. The reason for the scarcity is the need for ACE-FTS to observe absorption spectra while facing a sunrise or sunset event. When this doesn’t occur during the passage of SCISAT-1, no observation can occur. Having plotted the ACE observations, the next step was to compare them to the map of rawinsonde observations at the University of Wyoming’s Department of Atmospheric Science website, in order to find matching sites. There were six ACE sites that had reasonable matches with rawinsonde observations. Those sites are: Alabama, Georgia, Louisiana, South Dakota, Texas and Wisconsin.
Lastly, I used NASA’s Mirador search tool to locate AIRS observations that approximately matched the locations and times of the six compound observations. The data is summarized in the table, below, in which the times are all UTC. According to the table, the greatest spatial difference is 2.04 degrees latitude, though the mean change in longitude is 0.5 degree, and the mean change in latitude is 0.95. Also, the greatest temporal difference is 5.32 hours, though the mean is 4.7 hours. The large temporal differences are strictly due to the scarcity of AIRS data near the UTC times 00Z and 12Z, since the ACE and rawinsonde data matched within 1 hour of each other at the largest time difference.

<table>
<thead>
<tr>
<th>Location</th>
<th>ACE (lon/lat)</th>
<th>ACE date</th>
<th>Bal. (lon/lat)</th>
<th>Bal. date</th>
<th>AIRS (lon/lat)</th>
<th>AIRS date</th>
<th>max Δ(lon/lat)</th>
<th>max Δ t</th>
</tr>
</thead>
<tbody>
<tr>
<td>Alabama</td>
<td>(-86.58, 33.45)</td>
<td>7/31/04, 00:42</td>
<td>(-86.76, 33.16)</td>
<td>7/31/04, 00</td>
<td>(-87.01, 33.03)</td>
<td>7/30/04, 19:35</td>
<td>(0.43, 0.42)</td>
<td>5:07h</td>
</tr>
<tr>
<td>Georgia</td>
<td>(-83.94, 31.43)</td>
<td>4/01/04, 23:51</td>
<td>(-84.30, 30.45)</td>
<td>4/02/04, 00</td>
<td>(-83.96, 31.38)</td>
<td>4/01/04, 18:41</td>
<td>(0.36, 0.98)</td>
<td>5:19h</td>
</tr>
<tr>
<td>Louisiana</td>
<td>(-92.60, 29.51)</td>
<td>2/09/04, 23:50</td>
<td>(-93.20, 30.11)</td>
<td>2/10/04, 00</td>
<td>(-92.85, 30.31)</td>
<td>2/09/04, 19:05</td>
<td>(0.60, 0.80)</td>
<td>4:55h</td>
</tr>
<tr>
<td>S. Dakota</td>
<td>(-100.45, 45.78)</td>
<td>6/28/04, 11:00</td>
<td>(-100.75, 46.76)</td>
<td>6/28/04, 12</td>
<td>(-100.59, 45.85)</td>
<td>6/28/04, 8:29</td>
<td>(0.30, 0.98)</td>
<td>3:31h</td>
</tr>
<tr>
<td>Texas</td>
<td>(-102.15, 37.09)</td>
<td>2/11/04, 00:18</td>
<td>(-101.69, 35.22)</td>
<td>2/11/04, 00</td>
<td>(-102.32, 37.26)</td>
<td>2/10/04, 19:53</td>
<td>(0.63, 2.04)</td>
<td>4:25h</td>
</tr>
<tr>
<td>Wisconsin</td>
<td>(-87.42, 43.97)</td>
<td>2/11/04, 23:08</td>
<td>(-88.12, 44.47)</td>
<td>2/12/04, 00</td>
<td>(-87.48, 44.40)</td>
<td>2/11/04, 18:59</td>
<td>(0.70, 0.50)</td>
<td>5:01h</td>
</tr>
</tbody>
</table>

Due to the large time lag of AIRS data with respect to the ACE and rawinsonde data, one
might expect to see an offset in the AIRS soundings due to the diurnal cycle, perhaps resulting from radiative cooling following the daily maximum influx of solar radiation. Likewise, the large meridional shift of the Texas rawinsonde observation with respect to the related satellite data might lead to an overall shift in both pressure and temperature values.

4 The Soundings

After gathering all of the data, and determining the best way to extract a sounding of each type, I plotted all soundings on the same graph for each time and location. In figure 6, there are soundings for Alabama (left) and Wisconsin (right) that span the surface up to almost the top of the stratosphere. The balloon sounding, assumed to be the most accurate, is the (smoothed) solid black line. ACE and AIRS are the red and green lines, respectively. Interesting features are the smooth lapse rate shown in the Alabama sounding, and the lowered tropopause at the higher latitude of Wisconsin. Although the three profiles mostly match in the troposphere, that is largely expected, since the ACE-FTS data is not retrieved via absorption spectra there, but rather it is merely matched to atmospheric model output. Also, AIRS has sharply peaked weighting functions in the tropopause, so you would expect it to be quite accurate there, too, especially with all the spectral channels it uses.

In the next pair of images (figure 7), the pressure range is between 400hPa and 7hPa. Also, the ACE and AIRS soundings have been split into their error ranges over the course of each respective sounding. The error for the AIRS data was taken from the data source file, which contains a variable TAirStdErr, that serves as the absolute error in the temperature data. The error for the ACE data was assumed to be a constant 3K over the depth of the sounding, based on a similar comparison by Boone, et al. (4)

In the Alabama plot, the ACE data (in red) appears to encapsulate the balloon data except in two regions: 1) at the tropopause; 2) above 20 hPa. However, the AIRS data seems largely uncorrelated to the balloon sounding except below the tropopause. In the Wisconsin plot,
Figure 6: Profiles over Alabama, July 30, 2004, 19Z; Wisconsin Feb. 11, 2004, 19Z.

Figure 7: Margins of error around satellite temperature profiles.
both ACE and AIRS follow the balloon sounding up to about 40 hPa, where they both seem to diverge, though by different means.

The next two plots tell a different story, however (see figure 8). These plots indicate the vertical spatial resolution of each data type. Also, the balloon sonde data has been overlaid onto the ACE and AIRS data, which has been artificially separated over the temperature axis to allow comparison of the respective satellite resolutions.

In the Alabama plot, the ACE sounding disagrees with the balloon at the tropopause, though the AIRS sounding is quite in agreement, since, at the two pressure levels where AIRS has data near the tropopause, the two soundings match almost perfectly. Furthermore, higher in the soundings, the AIRS data either falls directly onto the balloon data at the corresponding pressure level, or renders an average of the balloon data over some spatial distance larger than the data resolution of the satellite. In contrast, the ACE data suggests disagreement with the balloon at two levels near the tropopause, though those points might be seen as overcompensations for the actual oscillatory nature of the sounding as seen in the balloon

Figure 8: Spatial resolution of each data source.
Higher up, the ACE data more or less mimics the averaging behavior of the AIRS data, though it is less believable, since the ACE weighting functions are so much narrower in this region than those of AIRS. For this reason, we expect the ACE averaging to be tighter, and for the ACE sounding to cross the balloon sounding in a more compensatory way, rather than the outright cooling bias that is shown between 20 hPa and 10 hPa.

Turning now to the Wisconsin sounding, the AIRS data again matches that of the balloon at all pressure levels that AIRS has a data point, and to within approximately 2K. Though, as above, the ACE data has several data points at lower altitudes that disagree with the respective balloon points. Worse, at higher altitudes, the ACE data seems to oscillate at a regular spatial period, with little relation to the actual profile.

The next series of plots (figure 9) shows the differences between the balloon soundings and the ACE and AIRS soundings for each case. Remarkable for the strong correlation between AIRS and ACE soundings is the case of Georgia, where the two satellites diverge from the balloon in the same manner for the entire illustrated region of the sounding. This strong agreement shows up in the middle part of the Alabama sounding, through much of the South Dakota sounding, and in the lowest portions of the Texas and Wisconsin soundings.

Such agreement from two vastly different data sources with different retrieval algorithms suggests that either the balloon sounding is partially inaccurate on those days, and the satellites have faithfully caught the actual profiles in tandem, or the satellites have common factors in their retrievals that lead to agreement in mutual error. A third possibility is that neither of the above is true.

A significant outlier in the ACE data is the cold spike over Louisiana at approximately 160 hPa. It looks as though, if the spike weren’t there, the sounding would roughly match that of AIRS, as it does over the same altitude range for Texas and Wisconsin. This spike is probably due to a phenomenon in the ACE interpolation algorithm that translates the original data from an irregular vertical grid to a regular 1 km vertical grid. According to Boone et al, the algorithm would occasionally produce a spike where two or more original data points were
Figure 9: Temperature differences between satellite and balloon data with window means.

found in the same interpolation segment. Unfortunately, the data used in this study is from version 1.0 of the algorithm, which still retained this bug.

The larger pattern of disagreement between ACE and AIRS is the oscillatory behavior of ACE that seems to have a spatial period of a few km. This pattern is seen most prominently in the soundings above Louisiana, Texas and Wisconsin. This pattern has also been recognized by others, such as Sica et al, in a comparison of ACE soundings with another limb sounder called Sounding of the Atmosphere using Broadband Emission Radiometry (SABER). This comparison is illustrated in figure 10. According to the authors, the oscillations were due to other problems in the interpolation scheme mentioned above. These oscillations were reportedly fixed in later versions of the retrieval algorithm, though they still exist in new data sets to a small extent. (11) One final feature of the grid of plots shown in figure 9 are the colored vertical lines. They are the mean values of the temperature differences for AIRS and ACE over the pressure domain shown in the plots. One can see that the largest mean difference for ACE is about 1.5K (Wisconsin), and that for AIRS is about 2K (Louisiana).
5 Difficulties in this Study

There were several issues that arose in the course of this study that originally represented limiting factors in the process of obtaining accurate and parallel soundings worthy of focused comparison. The first of these is the peculiar lack of lat/lon definitions in the AIRS data file. In short, the temperature data was defined over three dimensions: latitude, longitude, and pressure. However, the latitude and longitude dimensions weren’t defined in the file. Instead, their projections were defined as 2D variables. The issue led to some difficulty in extracting coordinates from the AIRS files to match those in the ACE data, though eventually, a beneficial method arose.

Another issue involved my own interpolation scheme. In order to calculate differences between the satellite and balloon data sets, it was necessary to interpolate all the data onto the same regular grid. However, this procedure introduced large-scale changes in the shape of the ACE temperature profile, to the degree that, at some pressure level in the stratosphere, the interpolated temperature value was several degrees warmer than the actual, unaltered value. This represents a limitation, or bug in the interpolation software, and was dealt with by
truncating the data to the window limits of the plots shown in the above study (400 hPa - 7 hPa), and then interpolating within the window.

A third issue, outstanding without adding a fourth data set, is the condition that the temperature and pressure data of the satellites is entirely dependent on the assumption that the $CO_2$ profile is constant in the region of study. The $CO_2$ profile is not a variable returned in the ACE retrieval algorithm, so it cannot be analyzed to check for variations corresponding to anomalies found in the P, T data.

Lastly, all retrieval idiosyncrasies are not known to the casual user of remote sensing data. In the course of this study, it became clear that there were idiosyncrasies involved with the ACE data, though, had I not been focused on the question of the accuracy of the data itself, I might not have ever considered the issue. It seems that these details arise over the course of validation studies and are slowly disseminated to the community as they are discovered, but they cannot be explained by a study of this scope, except to claim that there seems to be trouble with the retrieval algorithm.

6 Conclusions

The following conclusions arise from the above study. AIRS soundings have mean error $\Delta T = 2K$ in the region (1000 hPa < P < 7hPa). They closely match in situ data below the tropopause, and seem to approximate it in stratosphere, perhaps as a result of the averaging nature of the wide weighting functions in the region. They have rare maximum anomalies of $\Delta T = 7K$ with respect to collocated balloon soundings.

ACE-FTS soundings have mean error $\Delta T = 2K$ in the region (1000 hPa < P < 7hPa) and often follow AIRS soundings with the exception of a few outliers.

Furthermore, the ACE soundings exhibit wild spatial oscillations (usually averaging to zero) above the tropopause for some cases but not others. Sica et al suggest that this occurs when
the retrieval algorithm precedes version 2.0 and also when there is a temperature minimum
above 30 km. However, the latter condition wasn’t true for any of the cases in which I found
the oscillations.

Sica et al also found a cold bias near 35 hPa, but I didn’t see any good evidence of this
with the exception of the Texas sounding. However, in that case, the cold spike at 35 hPa
seems more a part of the high altitude oscillations described above, rather than an isolated,
systematic cold bias.

Due to the above issues regarding ACE, Kerzenmacher et al recommend using temperature
profiles that are averaged over 4 days, rather than using a single sounding. They claim
this eliminates most of the unphysical oscillations (though not all), and gives soundings that
closely match the balloon soundings. Furthermore, they give an estimate of the accuracy of
the time-averaged soundings of $\Delta T < 2.5K$ for 10 km to 30 km in altitude. (7)

The trouble with the above suggestion regarding averaged time-series of ACE data is that
there simply isn’t very much ACE data to average. According to the map of ACE observations
above (figure 5), any 4 day series would have to be spatially separated by (at least) tens of
degrees of latitude or longitude, which wouldn’t make much sense if one wants a sufficiently
localized sounding. On the other hand, there doesn’t seem to be any pattern between the
amount of accuracy of an observation and the corresponding amount of simultaneity or
colocation between the balloon and the satellite; though, in the above study, these are both
quite small, and thus are effectively unstudied.

Bernath et al found an accuracy in ACE retrievals of within 1K - 2K below 50 km, and, as
mentioned above, Boone et al found a mean accuracy of 3K above 300 hPa. (2)

Lastly, according to the AIRS QuickStart document, we should expect an accuracy of within
1K in the troposphere. Above the tropopause, the error values provided in the data file were
1 K - 2K. My conclusions are consistent with each of these estimates. (8)
References


