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# Upper-troposphere and lower-stratosphere water vapor retrievals from the 1400 and 1900 nm water vapor bands

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### Abstract

Measuring water vapor in the upper troposphere and lower stratosphere is difficult due to the low mixing ratios found there, typically only a few parts per million. Here we examine near infrared spectra acquired with the Solar Spectral Flux Radiometer during the first science phase of the NASA Airborne Tropical Tropopause EXperiment. From the 1400 and 1900 nm absorption bands, we infer water vapor amounts in the tropical tropopause layer and adjacent regions between 14 and 18 km altitude. We compare these measurements to solar transmittance spectra produced with the MODerate resolution atmospheric TRANsmission (MODTRAN) radiative transfer model, using in situ water vapor, temperature, and pressure profiles acquired con-10 currently with the SSFR spectra. Measured and modeled transmittance values agree within 0.002, with some larger differences in the 1900 nm band (up to 0.004). Integrated water vapor amounts along the absorption path lengths of 3 to 6 km varied from  $1.26 \times 10^{-4}$  to  $4.59 \times 10^{-4}$  g cm<sup>-2</sup>. A 0.002 difference in absorptance at 1367 nm results in a  $3.35 \times 10^{-5}$  g cm<sup>-2</sup> change of integrated water vapor amount, 0.004 absorp-15 tance change at 1870 nm results in  $5.5 \times 10^{-5}$  g cm<sup>-2</sup> of water vapor. These are 27 % (1367 nm) and 44 % (1870 nm) differences at the lowest measured value of water vapor  $(1.26 \times 10^{-4} \text{ g cm}^{-2})$  and 7 % (1367 nm) and 12 % (1870 nm) differences at the highest measured value of water vapor  $(4.59 \times 10^{-4} \text{ g cm}^{-2})$ . A potential method for extending this type of measurement from aircraft flight altitude to the top of the atmosphere (TOA) 20 is discussed.

#### 1 Introduction

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Water vapor in the stratosphere has important climatic (Forster and Shine, 2002; Solomon et al., 2010), dynamical (Joshi et al., 2006; Maycock et al., 2013), and chemical impacts (Stenke and Grewe, 2005). The long-term trends in water vapor have shown a general increase over the period of reliable measurements, starting in the



1970s with balloon borne hygrometer measurements (Oltmans et al., 2000; Rosenlof et al., 2001; Hurst et al., 2011). Later satellite measurements from, for example, the Halogen Occultation Experiment (HALOE), extended these measurements to global scales from the geographically limited balloon measurements (e.g. Remsberg et al.,

<sup>5</sup> 1996; Dessler and Kim, 1999). The record of stratospheric water vapor since 2000 has shown periods of both increasing and decreasing concentrations (Randel et al., 2004; Scherer et al., 2008; Fueglistaler, 2012; Nedoluha et al., 2013). The mechanisms driving changes in stratospheric water vapor concentrations are currently unresolved.

The transport of air from the troposphere to the stratosphere occurs mainly in the
 tropics (Brewer, 1949). Water vapor moving from the tropical troposphere to the stratosphere must pass through the so-called tropical tropopause layer (TTL) (Fueglistaler et al., 2009), characterized by very low temperatures. The TTL acts as a cold trap, "freeze drying" air as it passes through, limiting the entry of water vapor into the stratosphere (Brewer, 1949). Understanding the fate of water vapor as it encounters the TTL is one of the main science objectives of the NASA Airborne Tropical TRopopause EXperiment (ATTREX).

The first ATTREX science flights were conducted on the NASA Global Hawk (GH) aircraft from NASA Dryden Flight Research Center at Edwards Air Force Base in southern California during February and March of 2013. The GH carried instruments that

- <sup>20</sup> measured atmospheric state, composition, and radiation. Included in these were measurements of downwelling solar spectral irradiance, in situ water vapor mixing ratio, pressure, and temperature. In this work we examine the use of strong water vapor absorption bands in the near infrared (NIR) spectrum to infer water vapor amounts across the TTL, in the upper troposphere and lower stratosphere (UT/LS). Observed NIR wa-
- ter vapor absorptances are compared to model predicted absorptances using in situ profiles of water vapor, pressure, and temperature as input to the atmospheric radiative transfer model MODTRAN5 version 5.3.2 (Berk et al., 2006).

In addition to the sensitivity to even very small amounts of water vapor, these bands have the additional benefit of being virtually free of molecular (Rayleigh) scattering and



aerosol extinction. This can be a substantial source of error when using, for example, the 940 nm water vapor band as in the case of the POAM III (Lumpe et al., 2002) or SAGE II (Chu et al., 1993; Thomason et al., 2004) satellite instruments. However, clouds remain a potential source of interference in these wavelength bands.

<sup>5</sup> We also explore the potential use of these bands to infer the column stratospheric water vapor amounts from aircraft altitude to the top of the atmosphere (TOA) based on solar irradiance measurements from the GH and other high flying aircraft.

#### 2 Background – water vapor absorption in the solar spectrum

Water vapor is the strongest and most prevalent absorber of solar radiation in the Earth's atmosphere (Goody and Yung, 1989). The three fundamental water vapor bands occur at 2.66, 2.74, and 6.3 µm (~ mid infrared). Their combination and overtone bands in solar wavelengths extend from the very weakly absorbing bands in the visible to the relatively strong bands in the NIR centered near 1400 and 1900 nm; these are nearly always saturated at sea level.

- <sup>15</sup> In the troposphere, the concentration of water vapor decreases rapidly with height. At the tropopause, 16–18 km in the tropics, the mixing ratios are very small, typically a few ppmv, as compared to the surface where tropical water vapor mixing ratios are 20 000–25 000 ppmv. The vertical mixing ratio profile of water vapor used in the MODTRAN5 model for a tropical type atmosphere is shown in Fig. 1.
- Figure 2 shows the water vapor transmittance spectrum in the solar wavelength range for the entire atmosphere (black spectrum), from sea level to the top of the atmosphere (TOA; defined here as 100 km altitude). The input water vapor profile is the default tropical model that has a column-integrated amount of 4.11 g cm<sup>-2</sup>. Also plotted on the left panel of Fig. 2 are modeled transmittances from 18 km (red spectrum),
- the greatest height that the tropical tropopause reaches, to TOA and from 14 km (blue spectrum) to TOA. These are the approximate maximum and minimum heights that the GH reached during its vertical profiling. At this height the only remaining appreciable



water vapor absorption in the solar spectrum occurs at the two strongest bands centered near 1400 and 1900 nm and amounts to less than 0.03 in absorptance (1 minus transmittance). This is shown in an expanded view on the right hand side plot of transmittance of Fig. 2. Nevertheless, an instrument with sufficient signal-to-noise ratio (SNR) can make accurate measurements of water vapor even for absorptances over

(SNR) can make accurate measurements of water vapor even for absorptances over this small range, as will be demonstrated. The 1400 and 1900 nm water vapor bands are the focus of this paper.

#### 3 Instrumentation

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Measurements from three instruments were used for the present analysis work: the Solar Spectral Flux Radiometer (SSFR), the NOAA Water instrument (NW), and the Meteorological Measurement System (MMS). Each of these instruments is briefly described.

The SSFR (Pilewskie et al., 2003) is comprised of a pair of Zeiss monolithic spectrometers connected by fiber optics to a miniature integrating sphere that produces the cosine weighted response required for measurements of irradiance. One integrating sphere measures the downwelling irradiance from the top of the aircraft, the other the upwelling irradiance from the bottom of the aircraft. The visible-near infrared, 256 pixel silicon detector array, covers the wavelength range 350–1000 nm with 3 nm sam-

- pling and 8 nm full-width half maximum (FWHM) resolution. The 1000–2200 nm range is measured by a 256-pixel element InGaAs array. This portion of the spectrum has 4.5 nm sampling and 12 nm FWHM resolution. The instrument records a complete spectrum every second (1 Hz). The absolute radiometric uncertainty is approximately 5%; it is wavelength dependent with greater uncertainty with increasing wavelength. The absolute radiometric accuracy is limited by the NIST traceable standards of irradi-
- <sup>25</sup> ance used to calibrate instrument. The precision of the spectrometers is much better, about 0.1 % with averaging, as shown by the repeatability of the measurement and



discussed in detail in Sect. 6. The work described in this paper relies solely on the precision of the spectrometers to derive atmospheric transmittance in the NIR.

The NOAA water vapor instrument is a two channel, closed-path, tunable diode laser absorption spectrometer. Different inlet geometries for the two channels allow for sam-

- <sup>5</sup> pling of only water vapor into one channel, and sampling of total water (the sum of water vapor, liquid and water ice) into the second channel. In each channel a 2.7 μm tunable diode laser and an InAs detector are used to measure absorption over a mirror folded absorption path of 79 cm. The laser scans over strong (2693.82 nm) and weak (2694.06 nm) water vapor absorption features (or lines). The strong line provides
- high sensitivity for measurement of low water vapor mixing ratios, while the weak line provides dynamic range for measurement at higher mixing ratios. The detection cells are operated at constant temperature and pressure to reduce the measurement uncertainty associated with line parameter changes. The overall measurement uncertainty is 5 % + 0.23 ppmv with a detection limit of 0.5 ppmv. The precision at 1 Hz is typically
  near 0.17 ppmv.

The MMS instrument measures aircraft position, altitude, attitude, winds, and, importantly for this work, pressure and temperature. Pressure is measured with a Paroscientific 6015A laboratory grade sensor. The static temperature is measured with a Rosemount 102E4AL immersed open platinum wire. After a thorough systematic calibration process, including aerodynamic compensation from induced aircraft maneuvers, final

static pressure accuracy is 0.3 hPa and static temperature accuracy is 0.3 K. The 1 Hz sampled MMS data were used in this study. Both sensors are NIST traceable and are periodically recalibrated by a certified laboratory.

#### 4 Measurement technique

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<sup>25</sup> During the ATTREX 2013 field campaign, the GH flew southwest from NASA Dryden-Edwards Air Force Base in southern California. After transit to the tropical Pacific, the aircraft began a series of vertical profiles through the UT/LS, between 14 and 18 km.



From these profiles, those performed during daylight (11 total during the experiment period) were selected for analysis. Figure 3 shows the first two profiles from the first science flight on 2 February 2013.

The derivation of atmospheric transmittance from the vertical profiles of solar spectral irradiance was straightforward. Five to ten minutes (300–600 spectra) of zenith SSFR data immediately prior to and after the descent from 18 km were averaged to give a robust measurement of the downward spectral irradiance at this altitude. The averaging both increases the SNR of the measurement and reduces the effects of attitude (pitch and roll) changes that are unavoidable during flight. The same averaging was performed during the period of level flight at the bottom of the profile near 14 km. These time periods are over-plotted in red (~ 18 km) and blue (~ 14 km) in Fig. 3. Transmittance spectra (*T*) were created from these averaged spectra by dividing the low altitude average zenith downwelling irradiance (*F*<sub>14km</sub>) by the high altitude average zenith

 $T = \frac{F_{14\,\text{km}}}{F_{18\,\text{km}}}$ 

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downwelling irradiance at ( $F_{18 \text{ km}}$ ):

The total absorption path length, denoted with the letter *H* in the Fig. 6 depends on the altitude change of the aircraft profile ( $\Delta Z$ ) and the solar zenith angle (SZA) during the profile; *H* increases with increasing SZA. The vertical profiles during ATTREX were 3–4 km in *Z*; the range of solar zenith angles during the profiles produced values for *H* up to 5.93 km.

Figure 4 shows the resultant measured transmittance spectra from the first two profiles. The water vapor bands are shaded in gray, the  $CO_2$  bands in green, and the oxygen band in red.  $CO_2$  and  $O_2$  absorption features in the near infrared are of little interest to this work other than to note their presence in the spectra. Figure 5 shows the

NW measurement of the water vapor number density and integrated H<sub>2</sub>O amount over the vertical profile. The measured integrated water vapor for the second profile was approximately three times greater (Fig. 5, right hand panel) than the first profile (Fig. 5)



(1)

left hand panel). In Fig. 4 the differences in the integrated water vapor paths are clearly indicated in the transmittances derived from the SSFR irradiances. The second profile, with the higher water vapor amount had a significantly lower relative transmittance in the water vapor bands than the first profile.

#### 5 S Radiative transfer modeling

To assess the ability of SSFR measurements to infer water vapor across these relatively small absorption path lengths (3–6 km) and small water vapor amounts, radiative transfer modeling of the vertical profile transmittance was performed for comparison with the measured transmittances. The atmospheric radiative transfer model, MOD-

- <sup>10</sup> TRAN5, was run using the profiles of water vapor concentration from the NW instrument and the profiles of temperature and pressure from MMS as input. MODTRAN5 was used to calculate the solar spectral irradiance at the altitudes of the top and bottom of each GH profile. The ratio of the two yields the transmittance spectrum in an identical manner to the SSFR measurements (Eq. 1).
- <sup>15</sup> MODTRAN5 uses a correlated-k model for gaseous absorption (Lacis et al., 1991). This MODTRAN version of the band model includes updated line parameters from the HITRAN 2008 line database (Rothman et al., 2009). The water vapor continuum is modeled using the Clough–Kneizys Water Vapor Continuum version 2.4. (Mlawer et al., 2012). The CO<sub>2</sub> mixing ratios were set to 392 ppmv.
- The MODTRAN5 atmospheric profiles over the range of the GH profiles were modified to include the measurements of water vapor from NW and pressure and temperature from MMS. Altitudes above and below the aircraft flight level were set to the default tropical profile values. Over the range of the aircraft profile, the model atmospheric levels were set to every 250 m resulting in about 12 levels for each profile. The water vapor number densities were linearly interpolated to the model levels (e.g., 14.250, 14.500, 14.500).
- 14.750 km...) and were scaled to ensure that the integrated water vapor amount in the model (lower vertical resolution) matched that of the integrated NW measurements



(higher vertical resolution). The downwelling spectral irradiance was calculated for the mean of the high altitude and low altitude legs of the GH profile and the ratio of the two resulted in the atmospheric transmittance over the absorption path length.

To estimate the effects of the water vapor variability on the calculated transmittance spectra, water vapor measurement variation was propagated into the model by including plus and minus one standard deviation of NW water vapor number densities in the model profiles. The model was run at 1 cm<sup>-1</sup> sampling and 2 cm<sup>-1</sup> resolution. Computed spectra were convolved with the slit function of the SSFR for direct comparison with the measurements.

#### 10 6 Results

In Figs. 6–8 the measured and modeled transmittance spectra for all eleven profiles included in this study are plotted. The individual profiles are labeled SF (Science Flight) followed by the science flight number and the profile number. For example, SF-2-2 corresponds to science flight number two (9 February 2013) and the second profile during that flight. There were two daylight profiles per flight with the exception of the

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third flight, which had only one profile.

The mean SSFR spectra are plotted in black and the model spectra in blue. The modeled spectra at plus/minus one standard deviation of measured water vapor are shown in red. In general, the spatial variation in the water vapor profiles has little effect

<sup>20</sup> on the computed transmittance spectra, 0.001 or less, and indeed it is difficult to distinguish the mean spectra in blue from the standard deviation spectra in red in most of the plots.

The right-hand columns in Figs. 6–8 show the measured-modeled residual spectra. In general, measured and modeled transmittances agree to within 0.002 in the 1400 nm water band and 0.003 to 0.004 in the 1900 nm band. Figure 9 shows the mean and standard deviation difference spectrum for the eleven cases. The MODTRAN5 computed absorptance is slightly greater than that measured by SSFR in both the 1400



and 1900 nm bands. The largest consistent discrepancy occurs at 1849 nm, where the mean difference of all cases is nearly 0.004 (see Fig. 9). Most of the 1900 nm band agrees to within 0.002 or better, as does the entire 1400 nm band. Note that the measurements fall very close, to within 0.001 of unity in the spectral regions free of molecu-

- lar absorption, for example around 1300 nm (Fig. 9). The atmosphere at these heights 5 and wavelengths is essentially transparent. This confirms the radiometric precision of the instrument is about 0.1% with averaging of the spectra. At longer wavelengths, the differences become slightly greater (~ 0.002) due to the lower SNR of the measurement. Solar irradiance rapidly decreases with wavelength in the NIR.
- The results of the MODTRAN5 and SSFR water vapor transmittances and absorp-10 tances are summarized in Fig. 10. The top two plots show model calculations of the water vapor transmittance spectrum at SSFR resolution. The positions of the strongest absorption wavelength in each band, at 1367 nm (left) and 1870 nm (right), are indicated with a red line. In the second row, the values of absorptance from SSFR and MODTRAN5 at these wavelengths are plotted against each other for the eleven cases.
- 15 In the bottom row, the absorptance is plotted against the LOS integrated water vapor amount for both the MODTRAN and SSFR absorptances. The correlation between MODTRAN modeled and SSFR measured absorptances is quite good. The agreement for the higher water vapor amounts is better, this is to be expected; the higher the water
- vapor amount the greater the absorptance and the larger the signal. 20

#### 7 Stratospheric water vapor

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The results of this work thus far have focused on aircraft measurements during vertical profiles of a few kilometers in the UT/LS. The radiative transfer modeling using in situ measured profiles of water vapor amount has demonstrated that absorptance in the strong bands of water vapor at 1400 and 1900 nm can be used to infer water vapor amounts over short path lengths (3-6 km) and small water vapor concentrations (a few ppmv). Here we investigate the potential of using SSFR measurements to infer the



column water vapor amount from downwelling irradiance from aircraft altitude to the top of the atmosphere.

The proposed technique relies on the transparency of the atmosphere at wavelengths surrounding the water vapor bands. A transmittance spectrum is created by fitting a model TOA solar spectrum to wavelengths near, but outside of the water vapor bands at 1400 and 1900 nm. An example is shown in Fig. 11.

MODTRAN5-modeled solar irradiances at 20, 18, 16 and 14 km are shown in the top left panel of Fig. 11, along with the TOA solar spectrum (Kurucz, 1995). The sun is directly overhead, creating the shortest possible absorption path lengths at these altitudes. In the top right panel, the transmittance spectrum for the path from the TOA

- altitudes. In the top right panel, the transmittance spectrum for the path from the TOA to each altitude is plotted. To produce these transmittance spectra, first the TOA solar spectrum was scaled to match downwelling irradiance spectrum at the wavelengths 1301, 1516, and 1756 nm, indicated by the three black vertical lines in the transmittance spectra, where the transmittance is very close to unity. The ratio of the scaled TOA so-
- lar spectrum to the downwelling irradiance produces a transmittance spectrum. The scaling of the TOA spectrum is a simple gain across all wavelengths; no wavelength dependent (shape) changes were made. The mean deviation from a transmittance of unity for all altitudes at the three wavelengths is 0.001, which is approximately equivalent to the measurement uncertainty. Thus the impact on the retrieval of water vapor is negligible.

In the lower right panel of Fig. 11 the integrated water vapor amount is plotted against the absorptance for the 1367 and 1870 nm bands. Over this small range of water vapor amount, the absorptance is very nearly linear. A linear fit to the absorptance and integrated water vapor amount for this range of water vapor gives the following two equations for the two wavelengths:

$$H_2O_{g \, cm^{-2}} = 1.76 \times 10^{-2} \cdot (Absorptance_{1367 \, nm}) - 1.70 \times 10^{-6}$$
  
 $H_2O_{a \, cm^{-2}} = 1.49 \times 10^{-2} \cdot (Absorptance_{1870 \, nm}) - 4.56 \times 10^{-6}$ 

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(2)

(3)

The intercepts of these equations are very near zero ( $\sim 10^{-6}$ ) as expected; zero absorptance should correspond to zero water vapor amount. These linear fits provide a simple method for estimating the uncertainty of the SSFR absorptance measurement in terms of water vapor amount. For instance, an uncertainty of 0.002 in the SSFR absorptance at 1367 nm (the mean difference between the model and the measurements) corresponds to a  $3.35 \times 10^{-5}$  g cm<sup>-2</sup> integrated water vapor change. Similarly, a 0.004 change in absorptance at 1870 nm results in a  $5.51 \times 10^{-5}$  g cm<sup>-2</sup> change in water vapor amount.

In practice, a model TOA spectrum would be fit at these wavelengths to a SSFR spectrum and the ratio calculated. A pre-calculated lookup table of absorptances generated from a range of water vapor amounts, solar zenith angles, and altitudes would be used to determine the integrated water vapor amount above the aircraft. This retrieval could be undertaken in near real-time from aircraft equipped with high bandwidth downlinks. This type of real-time retrieval is becoming more common with the introduction

- of such satellite downlinks to the NASA ER-2 and Global Hawk aircraft. In the lower 15 left panel of Fig. 11, the water vapor amounts corresponding to the transmittances are plotted as a function of altitude. The values for the transmittances plotted in the top left panel are color-coded. The range of water vapor amounts fall within the same range as those measured in the UT/LS during ATTREX, indicating that stratospheric water vapor
- amounts are within the capability of the SSFR to measure. However, this will require 20 that radiometric calibration of the instrument be modified to remove the water vapor surrounding the laboratory setup. The water vapor bands can have significant (1-2%)absorption) even over the path length (50 cm) from the NIST irradiance standard to the light collector (Kindel et al., 2001). The absorption by water vapor in the laboratory radiometric calibration of the SSFR has likely masked the small absorption in previous

SSFR measurements.

## Discussion Paper AMTD 7, 10221-10248, 2014 UT and LS water vapor retrievals from the 1400 and 1900 nm **Discussion** Paper water vapor bands B. C. Kindel et al. **Title Page** Introduction Abstract Conclusions References Tables Figures Back Close Full Screen / Esc Printer-friendly Version Interactive Discussion

Discussion Paper

**Discussion** Paper

#### 8 Summary and conclusions

Water vapor in the upper atmosphere has important climatic, dynamical and chemical impacts on the Earth's atmosphere. The accurate measurement of water vapor in the upper troposphere and stratosphere is important in quantifying these impacts. In this

- work we have examined the use of the strong water vapor bands in the solar spectrum to infer water vapor amount in the UT/LS. This work, unlike most previous work using solar transmittance type retrievals, used aircraft in situ measurements of water vapor vertical profiles over very small mixing ratios, a few ppmv, to predict the transmittance and compare with measurements. Most solar transmittance type retrievals have little
  if any independent validation of water vapor amount, vertical distribution, pressure, or
- temperature profile (Schwab et al., 1996; Harries et al., 1996).

Comparisons of modeled and measured transmittance spectra for eleven cases resulted in spectra that agreed to generally 0.002 in transmittance with deviations up to 0.004 in some channels of the 1900 nm band. The measurement uncertainly is ap-

proximately 0.001 as demonstrated by the repeatability of the measurements in nonabsorbing wavelengths (e.g. 1300 nm). This increases to 0.002 at longer wavelengths where the SNR is not as high.

A technique for inferring water vapor from zenith viewing aircraft solar spectral irradiance has been outlined. This technique relies on the use of wavelengths surrounding <sup>20</sup> the strong NIR water vapor bands where the atmosphere is essentially transparent. Radiative transfer modeling of water vapor transmittance from altitudes of 14 to 20 km, indicate that integrated water vapor amounts, and thus the transmittances from these altitudes to the TOA fall in a similar range to the shorter path lengths examined in this work. This technique could potentially produce near real-time retrievals of aircraft to

the TOA water vapor amounts. Work is required to modify the radiometric calibration to remove the effects of water vapor in the laboratory as well as forward radiative transfer modeling to determine the integrated water vapor amounts from the measurement of transmittance.



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the tropopause, the mixing ratio is only a few ppmv.



**Figure 2.** (left) Water vapor transmittance in a tropical atmosphere is shown from the surface (black), 14 km (blue) and 18 km (red) to the top of the atmosphere. (right) An expanded plot of the water vapor absorption high in the atmosphere at 1400 and 1900 nm.















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**Figure 5.** Water vapor number density profiles from the NOAA Water instrument. The red points correspond to the in situ water vapor number densities during the descent and ascent for the two profiles. The blue line is the mean of the ascent and descent number densities. The green line is the integrated water vapor amount (scale at the top of the plot). Note the large difference in the horizontal axis ranges and the integrated water vapor amounts between the two profiles.





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**Figure 6.** (left) Measured (black) and modeled (blue) transmittances for vertical profiles during the first and second ATTREX science flights are plotted. The red traces show plus and minus one standard deviation of the modeled transmittance. (right) Difference between the measured and modeled transmittances. The vertical profile distance Z, the solar zenith angle SZA, the absorption path length H, and the integrated water vapor amounts are given in the left hand plots.





Figure 7. Same as Fig. 5 for profiles during the third and fourth ATTREX science flights.









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spectra are plotted for the eleven profiles.











