

## Measuring Stratospheric H<sub>2</sub>O with an Airborne Spectrometer

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### ABSTRACT

This study examines the ability of an infrared spectral sensor flying at the tropopause level for retrieving stratospheric H<sub>2</sub>O. Synthetic downwelling radiance spectra simulated by the line-by-line radiative transfer model are used for this examination. The potential of high-sensitivity water vapor retrieval is demonstrated by an ideal sensor with low detector noise, high spectral resolution, and full infrared coverage. A suite of hypothetical sensors with varying specifications is then examined to determine the technological requirements for a satisfactory retrieval. This study finds that including far infrared in the sensor's spectral coverage is essential for achieving accurate H<sub>2</sub>O retrieval with an accuracy of 0.4 ppmv (1-sigma). The uncertainties in other gas species such as CH<sub>4</sub>, N<sub>2</sub>O, O<sub>3</sub>, and CO<sub>2</sub> do not significantly affect the H<sub>2</sub>O retrieval. Such a hyperspectral instrument may afford an advantageous tool, especially for detecting small-scale lower-stratospheric moistening events.

### 1. Introduction

Stratospheric water vapor (H<sub>2</sub>O) radiatively cools the stratosphere but warms the troposphere. Previous studies have shown that stratospheric H<sub>2</sub>O is a contributor to Earth climate change. [Forster and Shine \(1999\)](#) show that, although the observed cooling of the lower stratosphere is thought to be due to the combination of stratospheric ozone (O<sub>3</sub>) loss and carbon dioxide (CO<sub>2</sub>) increase, the increase in stratospheric H<sub>2</sub>O may be capable of producing as much of the observed cooling as the O<sub>3</sub> loss does. [Solomon et al. \(2010\)](#) show that stratospheric H<sub>2</sub>O may even be an important driver for surface climate change. They argue that a 10% decrease of stratospheric H<sub>2</sub>O after the year 2000 acted to slow the rate of global surface warming from 2000–09 by 25% compared to what would have occurred due to only greenhouse gases. Moreover, [Anderson et al. \(2012\)](#) suggest that there is an increased risk of O<sub>3</sub> loss from lower-stratospheric moistening.

Various approaches have been adopted for measuring the stratospheric H<sub>2</sub>O. Before the 1990s the information was largely based on localized balloonborne measurements (e.g., [Oltmans et al. 2000](#)). It has been a concern as

to how well the changes in stratospheric H<sub>2</sub>O can be monitored due to calibration issues and limited spatial coverage ([Kley et al. 2000](#)). Although a variety of techniques—for example, the Harvard Lyman-alpha and Jet Propulsion Laboratory laser hygrometers—have been developed, the intercalibration between the instruments remains an issue (e.g., [Weinstock et al. 2009](#)). After the 1990s high-quality satellite observations, including the Stratospheric Aerosol and Gas Experiment II (SAGE II) ([Thomason et al. 2004](#)), the Halogen Occultation Experiment (HALOE) ([Russell et al. 1993](#)), the Microwave Limb Sounder (MLS)/Upper Atmosphere Research Satellite (UARS) ([Livesey et al. 2003](#)), and Atmospheric Chemistry Experiment–Fourier transform spectrometer (ACE-FTS) ([Bernath et al. 2005](#)), began to collect information about stratospheric H<sub>2</sub>O. Satellites have the capacity to cover the globe and measure multiple species simultaneously, which renders them efficient monitoring tools. However, limb and occultation sounders that are sensitive to stratospheric water vapor have large sampling footprints, which makes small-scale water vapor variation, for example, induced by convective moistening, hardly detectable ([Schwartz et al. 2013](#)). Moreover, satellite remote sensing relies on in situ measurements for calibration and validation. Improved stratospheric water vapor measurements remain much desired.

An airborne spectrometer can be deployed on an aircraft or a balloon. In fact, it is among the various techniques that have been applied for stratospheric

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H<sub>2</sub>O measurement. For example, an airborne far-infrared (FIR) interferometer was used to measure the stratospheric H<sub>2</sub>O (Harries 1973). Comparing the intensity radiated by pairs of adjacent H<sub>2</sub>O and O<sub>2</sub> lines, H<sub>2</sub>O mass mixing ratio can be estimated, although an isothermal stratosphere and constant H<sub>2</sub>O mixing ratio above the observer need to be assumed in the estimation. An airborne FIR radiometer was also used to measure the H<sub>2</sub>O injected into the stratosphere by thunderstorms under similar assumptions (Barrett et al. 1973). The assumptions made for the water vapor retrieval are known to be unrealistic. To accurately monitor stratospheric H<sub>2</sub>O, it is necessary to retrieve the vertical distributions of temperature and moisture altogether. This can be realized using a high-resolution infrared spectrometer (hyperspectrometer), which is capable of separating the two signals spectrally. Current state-of-the-art instruments include the Far-Infrared Spectroscopy of the Troposphere (FIRST) (Mlynchak et al. 2003), the Radiation Explorer in the Far Infrared (REFIR) (Palchetti et al. 2005), the Scanning High-resolution Interferometer Sounder (S-HIS) (Revercomb et al. 1998), and the Tropospheric Airborne Fourier Transform Spectrometer (TAFTS) (Canas et al. 1997). Among these hyperspectrometers, FIR coverage have been devised for TAFTS, REFIR, and FIRST [see Harries et al. (2008) for a review].

The H<sub>2</sub>O concentration is much lower in the stratosphere than in the troposphere, which makes it challenging to retrieve stratospheric H<sub>2</sub>O either from space or from on the ground. However, if an instrument is flown right below the stratosphere (at the tropopause), then by measuring the downward emission spectra of the stratosphere, the tropospheric obscuration is removed. In addition, in comparing to the occultation and limb sounding satellite measurements, an airborne measurement is of much smaller sampling volume and thus is advantageous of capturing small-scale variability. If such an instrument can operate in both uplooking and downlooking modes, then it can sound both the stratosphere and troposphere concurrently.

The goal of this paper is to examine the feasibility of retrieving the stratospheric H<sub>2</sub>O profile, using a hypothetical uplooking spectrometer flying at the tropopause level. In section 2, the spectral signature of stratospheric H<sub>2</sub>O in the tropopause downwelling longwave radiation is described. The simulation and retrieval methodology is described in section 3. In section 4, sounding of stratospheric temperature and H<sub>2</sub>O profiles with different instrument specifications are compared. Also examined is how well a hypothetical sensor can detect stratospheric moistening episodes. The limitations are discussed in the concluding section.

## 2. Spectral signature of stratospheric H<sub>2</sub>O

We first investigate the spectral signature of stratospheric H<sub>2</sub>O in comparison to those of other atmospheric state variables, which illustrates the information in spectral measurements. To generate the spectral signals corresponding to realistic H<sub>2</sub>O variability, we compare the spectrum simulated from the H<sub>2</sub>O data of Anderson et al. (2012) that capture elevated stratospheric H<sub>2</sub>O concentration caused by convective injection in summertime on the North America continent to the spectrum simulated from the standard midlatitude summer (MLS) profile (McClatchey et al. 1972). The MLS and Anderson profiles are shown in Fig. 1. The column H<sub>2</sub>O loading (integrated from 100 to 1 hPa) of the Anderson and MLS profiles are 0.0046 and 0.0041 kg m<sup>-2</sup>, respectively.

Downwelling radiance at 100 hPa is obtained by running the line-by-line radiative transfer model (LBLRTM, version 12.1) from Atmospheric and Environmental Research (AER) (Clough et al. 1992, 2005). The vertical resolution of the atmospheric profile input to LBLRTM is 2 hPa from 100 to 80 hPa, 5 hPa from 80 to 10 hPa, and 1 hPa from 10 to 1 hPa. High vertical resolution at 100–80 hPa is used to capture the highly variable water vapor concentrations around these levels. For molecular absorption, the Voigt profile is considered and all the H<sub>2</sub>O continua are considered. No aerosol or solar input at the top of the atmosphere (TOA) is considered. The model calculates the emission spectrum between 200 and 2200 cm<sup>-1</sup>, ignoring the scattering processes. Six molecular species are included in the calculation—namely, H<sub>2</sub>O, CO<sub>2</sub>, O<sub>3</sub>, N<sub>2</sub>O, CO, and CH<sub>4</sub>, which are active gas species in the infrared region. The zenith angle is set to zero for a zenith-uplooking instrument.

Monochromatic radiance (output at a resolution of 0.001 cm<sup>-1</sup>) is calculated with LBLRTM for the unperturbed (MLS) and the perturbed (Anderson) cases. The results are then convolved with a triangular spectral response function with the half-width at half maximum (HWHM) equal to 0.01, 0.1, 1, and 10 cm<sup>-1</sup>. The results are shown in Fig. 2. Since H<sub>2</sub>O is the only difference between the MLS and Anderson profiles, the spectral difference occurs only at H<sub>2</sub>O absorption bands. The lower-stratospheric moistening affects the signal intensity in the water vapor rotational band (200–560 cm<sup>-1</sup>) and the vibrational–rotational band (1350–1850 cm<sup>-1</sup>). The 395–405 cm<sup>-1</sup> spectral interval from the water vapor rotational band and the 1555–1565 cm<sup>-1</sup> spectral interval from the vibrational–rotational band are enlarged for different HWHMs. These figures show that lowering the instrument spectral resolution (higher HWHM) will lower the signal intensity in the line center. The signal strength in the rotational band (FIR) is an order of magnitude

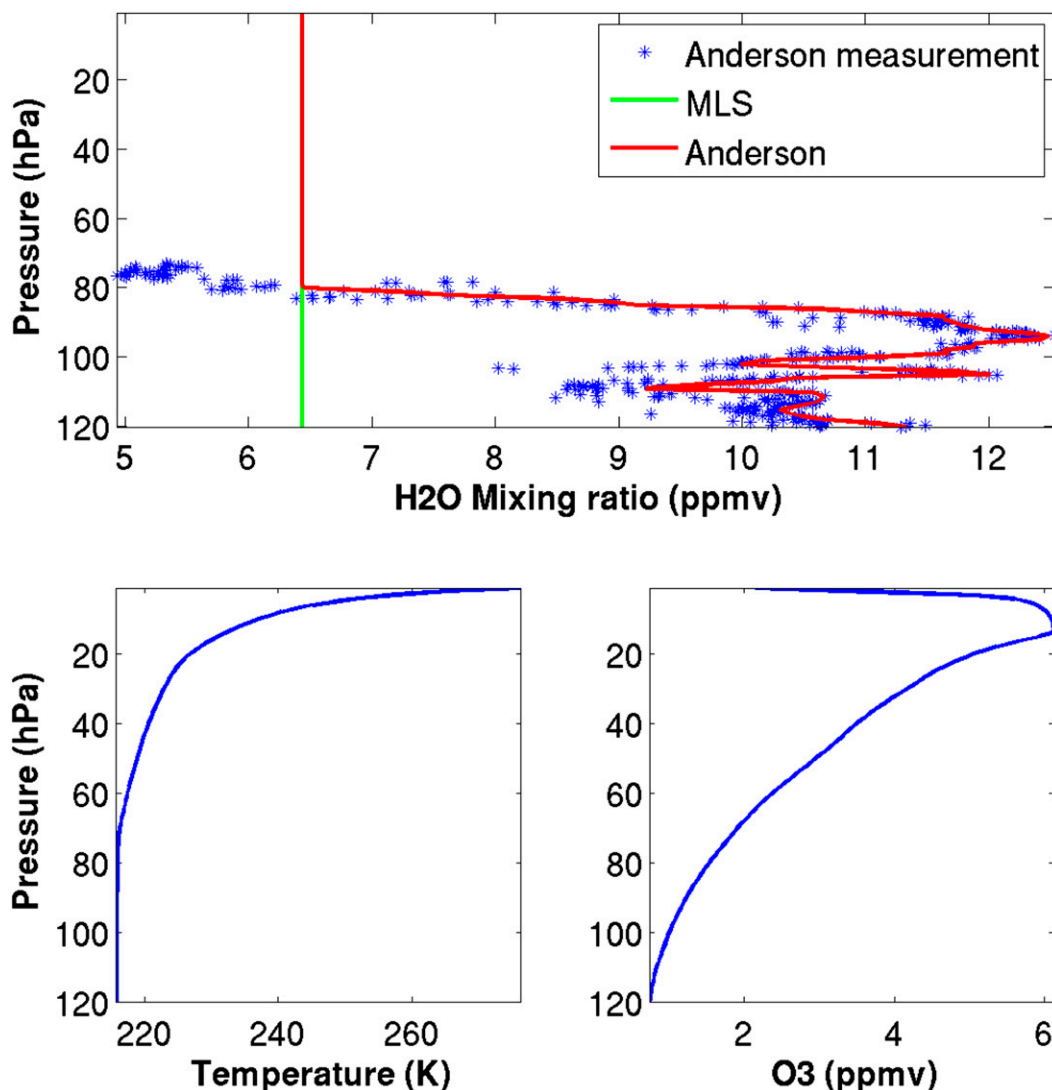


FIG. 1. H<sub>2</sub>O profiles for MLS and Anderson profiles, plus temperature and ozone profiles.

stronger than the vibrational–rotational band, which is coincident with the upwelling signals of H<sub>2</sub>O perturbation at the TOA (e.g., Harries et al. 2008). Given similar detector noise performance in the two bands, the rotational band is advantageous for measuring stratospheric H<sub>2</sub>O. In section 4, we discuss how the spectral coverage and noise level impact stratospheric H<sub>2</sub>O retrieval.

Other perturbation experiments are performed based on the MLS profile to examine the spectral signatures of temperature, CO<sub>2</sub>, and O<sub>3</sub>. The perturbations are prescribed as +1 K throughout the profile in temperature, +20 ppm in volume mixing ratio for CO<sub>2</sub>, and +10% in O<sub>3</sub>. The signal spectra from these experiments are compared with the H<sub>2</sub>O signal obtained above (Anderson minus MLS). As Fig. 3 shows, temperature perturbation affects the CO<sub>2</sub> absorption band (600–800 cm<sup>−1</sup>), the O<sub>3</sub>

absorption band (1000–1200 cm<sup>−1</sup>), and the H<sub>2</sub>O rotational band (200–580 cm<sup>−1</sup>). A change in CO<sub>2</sub> alters the radiance signal in the CO<sub>2</sub> absorption band, and O<sub>3</sub> modification mainly affects the O<sub>3</sub> absorption band. The comparisons here qualitatively show that the signal of H<sub>2</sub>O is spectrally distinct from those of the other variables.

Furthermore, we test whether the different signals calculated above are linearly additive. Figure 3 shows that the sum of the signals due to individual perturbations can well reproduce the signal when all the perturbations are prescribed simultaneously. The difference between these two spectra is generally two orders of magnitude less than the overall change signal itself.

The spectral distinction of the different signals suggests that stratospheric H<sub>2</sub>O and temperature may be retrieved simultaneously using an inverse method, such as the

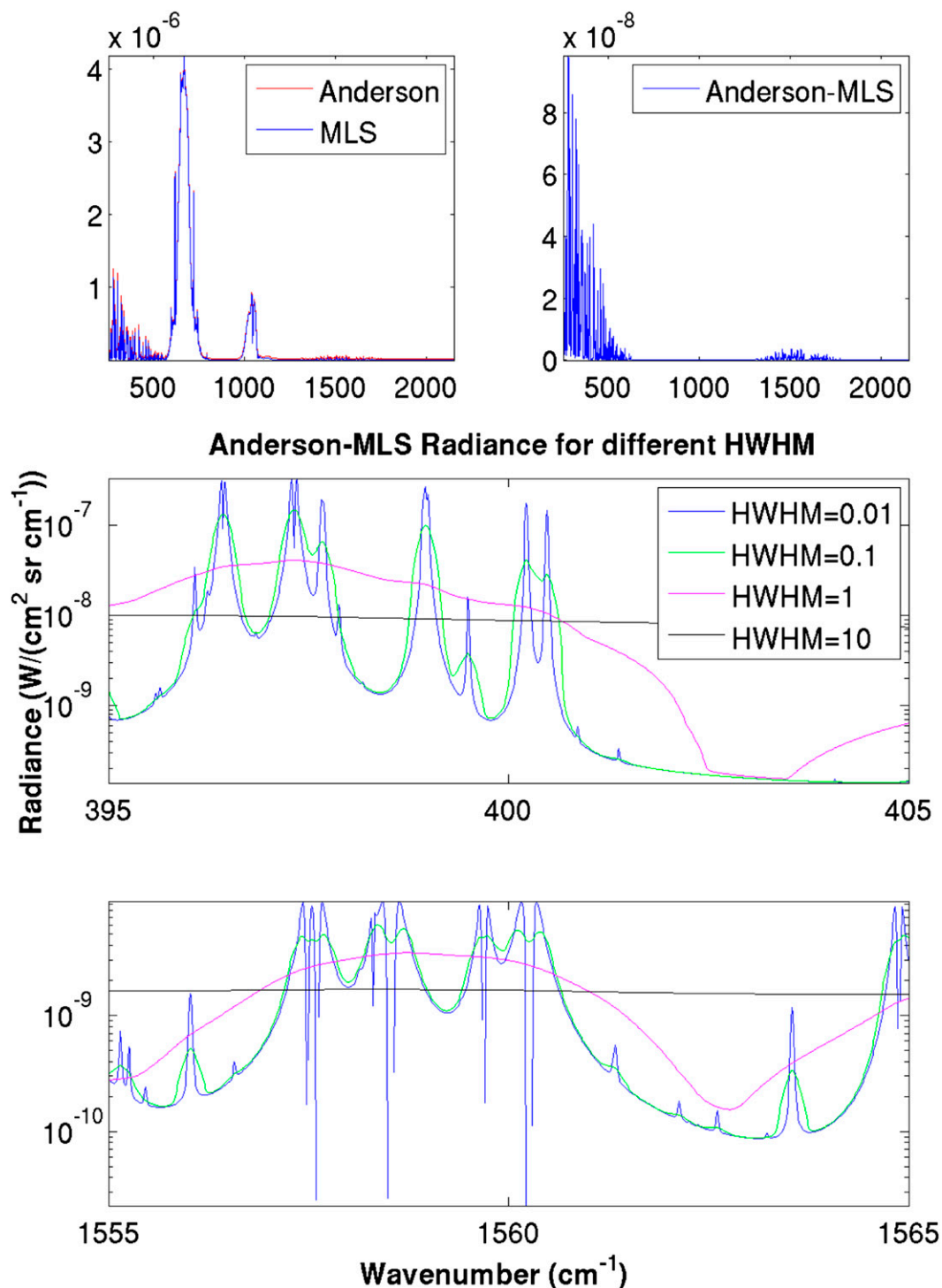


FIG. 2. Downwelling radiances at 100 hPa for MLS and convectively moistened (Anderson) profiles, and their difference at a spectral resolution of (top)  $\text{HWHM} = 1 \text{ cm}^{-1}$ , and at varied HWHMs ( $\text{cm}^{-1}$ ) for the spectral ranges of (middle) 395–405 and (bottom) 1555–1565  $\text{cm}^{-1}$ .

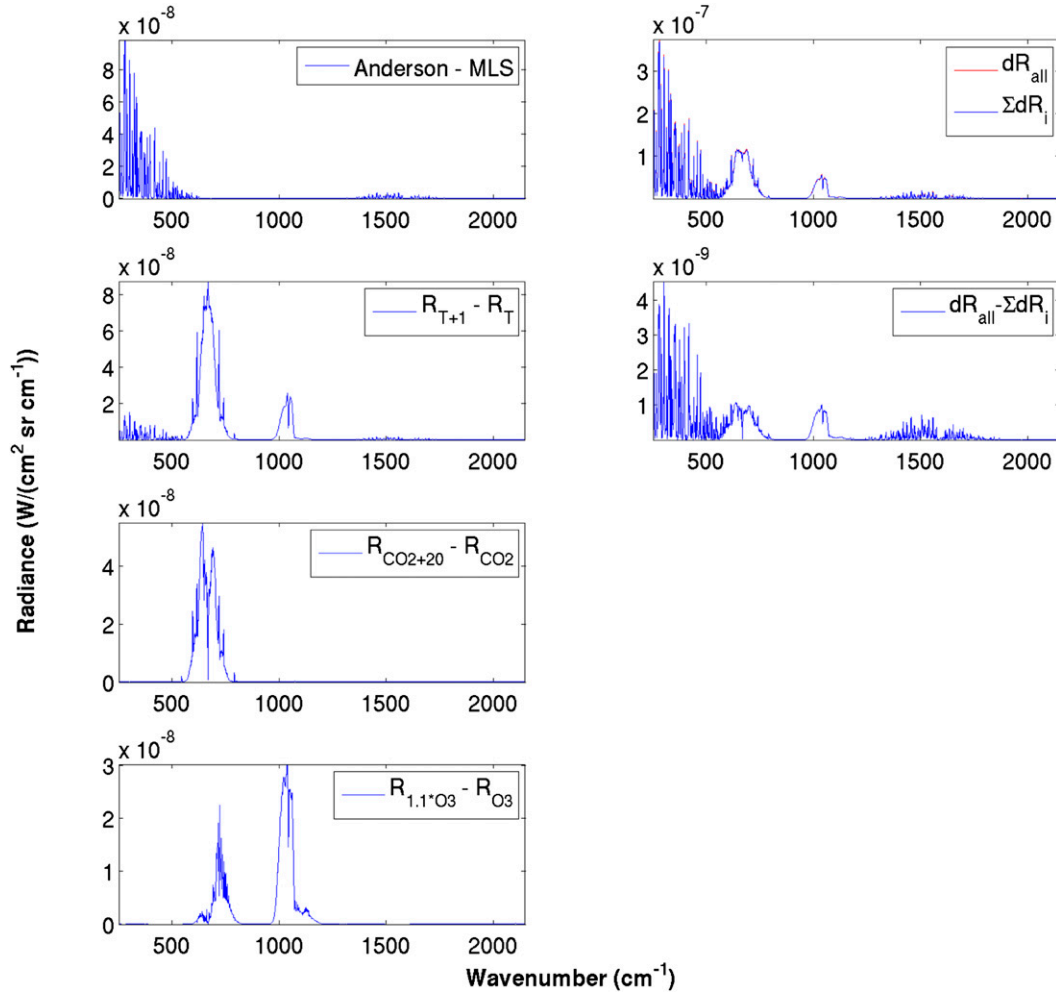


FIG. 3. (left) Comparison of spectral signature of the H<sub>2</sub>O signal with perturbations of (second) temperature (+1 K), (third) CO<sub>2</sub> (+20 ppmv), and (fourth) O<sub>3</sub> (+10%). (top right) Comparison of change in downwelling radiance due to simultaneous change in all the variables (red line) and the sum of changes induced by each variable (blue line). (bottom right) Difference between red and blue lines in (top right).

optimal estimation method described by Rodgers (2000). The results also suggest that there is likely an advantage to using the FIR region, at high spectral resolution, for H<sub>2</sub>O retrieval in particular.

### 3. Retrieval methodology

The retrieval methodology is based on the optimal estimation technique (Rodgers 2000). The linearized forward model can be described as

$$\mathbf{y} = \mathbf{y}_0 + \mathbf{K}_0(\mathbf{x} - \mathbf{x}_0) + \boldsymbol{\varepsilon} + \text{higher order terms}, \quad (1)$$

where  $\mathbf{x}$  is the state vector to retrieve and  $\mathbf{x}_0$  is the a priori (first guess) that is initially set to the mean of the climatology (training dataset). The elements of the state vector include temperature and the natural logarithm of water vapor mixing ratio at fixed vertical levels. Term  $\mathbf{y}$  is the

measurement (downwelling radiance measured at 100 hPa), and  $\mathbf{y}_0$  is the radiance corresponding to state vector  $\mathbf{x}_0$ . The quantity  $\mathbf{K}_0$  is the linearization of the forward model (Jacobian) computed at  $\mathbf{x}_0$ , and  $\boldsymbol{\varepsilon}$  is the measurement error vector. The forward model used for radiance and Jacobian calculation is the LBLRTM version 12.1.

The iteration method is the Gauss–Newton method, which is a least squares method that minimizes the sum of the squares of residuals in the solution. The iteration formula is

$$\hat{\mathbf{x}}_{i+1} = \mathbf{x}_0 + (\mathbf{K}_i^T \mathbf{S}_e^{-1} \mathbf{K}_i + \mathbf{S}_a^{-1})^{-1} \mathbf{K}_i^T \mathbf{S}_e^{-1} [\mathbf{y} - F(\hat{\mathbf{x}}_i) + \mathbf{K}_i(\hat{\mathbf{x}}_i - \mathbf{x}_0)], \quad (2)$$

which computes a new estimate for the state vector ( $\hat{\mathbf{x}}_{i+1}$ ) at each iteration. Term  $\mathbf{K}_i$  is the Jacobian at the current state vector estimate,  $\mathbf{S}_a$  is the a priori covariance of the

state vector, and  $\mathbf{S}_e$  is the covariance of the measurement error. Term  $F(\mathbf{x})$  is the forward model result, which is radiance. Terms  $\mathbf{K}^T$  and  $\mathbf{K}^{-1}$  are for matrix transpose and inverse operations applied to matrix  $\mathbf{K}$ , respectively. The iteration proceeds until the convergence criteria are met or the number of iteration reaches 10. The convergence criteria are defined as

$$\hat{\mathbf{S}}^{-1} = \mathbf{K}_i^T \mathbf{S}_e^{-1} \mathbf{K}_i + \mathbf{S}_a^{-1} \quad (3)$$

$$(\hat{\mathbf{x}}_{i+1} - \hat{\mathbf{x}}_i)^T \hat{\mathbf{S}}^{-1} (\hat{\mathbf{x}}_{i+1} - \hat{\mathbf{x}}_i) < \text{conv\_crit}, \quad (4)$$

where conv\_crit is the convergence critical value. It is calculated by setting  $(\hat{\mathbf{x}}_{i+1} - \hat{\mathbf{x}}_i)$  to the desired accuracy of 0.5 K for temperature and 0.05 ppmv for  $\text{H}_2\text{O}$ .

The atmospheric temperature and water vapor at 12 fixed pressure levels (10 hPa—spaced between 100 and 10 hPa, and then at 5 hPa and at 1 hPa) are considered for the retrieval here. In Eq. (2), the state vector has 24 elements with elements 1–12 corresponding to temperature and elements 13–24 corresponding to the logarithm of the water vapor mixing ratio. Stratospheric temperature and  $\text{H}_2\text{O}$  profiles obtained from the ACE-FTS instrument (Bernath et al. 2005) are used for testing the retrieval here. Only the North American profiles are selected. These profiles are selected in the region of  $30^\circ\text{N} < \text{latitude} < 60^\circ\text{N}$  and  $70^\circ\text{W} < \text{longitude} < 130^\circ\text{W}$ , between years 2004 and 2009. The temperature and  $\text{H}_2\text{O}$  profiles are interpolated to the 12 pressure levels. Overall, 286 temperature and  $\text{H}_2\text{O}$  profiles are retained after removing unrealistic profiles (those with high fluctuations in temperature/ $\text{H}_2\text{O}$  profiles, or decreasing temperature with altitude above the tropopause level). Out of the 286 profiles, 246 are randomly chosen and used to build the training dataset. The remaining unused 40 original ACE-FTS profiles are used as test cases and are referred to as the measurement dataset.

ACE-FTS is a solar occultation instrument, which measures infrared radiation at high spectral resolution ( $0.02 \text{ cm}^{-1}$ ) and spectral bandwidth from  $750$  to  $4400 \text{ cm}^{-1}$ . The satellite instrument samples atmospheric volumes that extend a few kilometers vertically and hundreds of kilometers horizontally (Bernath et al. 2005); thus, it does not capture smaller-scale atmospheric variability. To overcome this limitation of the dataset, we amend the dataset with artificially moistened profiles. To do so, each  $\text{H}_2\text{O}$  profile is perturbed by adding  $x \times \text{STD}(\text{H}_2\text{O})$  to a randomly selected 20-hPa-thick segment of the profile, where  $x$  is a random value drawn from the standard uniform distribution on the interval (0, 5) and  $\text{STD}(\text{H}_2\text{O})$  is the  $\text{H}_2\text{O}$  standard deviation of the prior in that 20-hPa-thick segment. The perturbed  $\text{H}_2\text{O}$  profiles are then added to the original training dataset. The mean of all the training dataset is used as the a priori (first guess) in the retrieval tests. An a priori covariance matrix  $\mathbf{S}_a$  is built using the

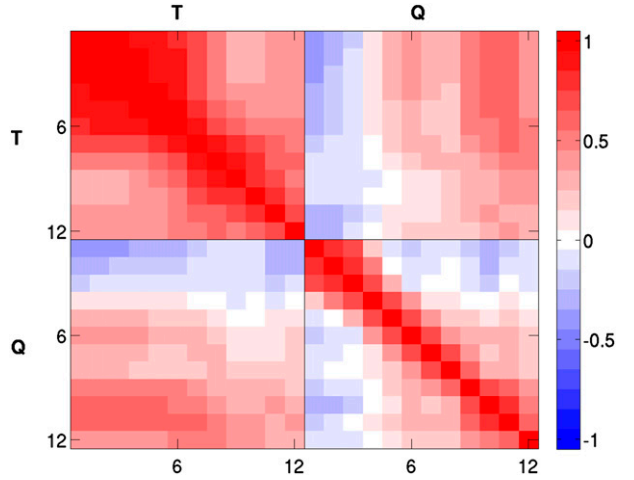


FIG. 4. Prior correlation matrix. The T–T and Q–Q portions show the corresponding temperature and log( $\text{H}_2\text{O}$ ) correlations, respectively; the T–Q portions show the temperature and  $\text{H}_2\text{O}$  correlation. The tick labels on the axes correspond to the 12 vertical pressure levels used.

enlarged training dataset (492 profiles). Figure 4 shows the correlation matrix of the training dataset. Figure 5 shows a subset of the measurement dataset chosen from the  $45^\circ$ – $50^\circ\text{N}$  latitudinal band as an example. The right panel shows the  $\text{H}_2\text{O}$  profiles that are artificially moistened. Note that the moistening prescribed here is very modest compared to the magnitude measured by Anderson et al. (2012).

The sensor noise covariance  $\mathbf{S}_e$  is assumed to be a diagonal matrix (uncorrelated noise). We start the analysis using a uniform noise magnitude equal to  $0.25 \times 10^{-7} \text{ W cm}^{-2} \text{ sr}^{-1} \text{ cm}$ , which represents a very low noise detector. The magnitude of the noise will be varied to show the dependence of retrievals on the noise level. For every noise level, the random noise vector is generated and added to the synthetic radiance signal computed from the truth profile to mimic the sensor noise.

To account for the effect of spectral resolution on the retrieval outcome, all of the line-by-line calculations of radiance and Jacobian are performed with a monochromatic resolution of  $0.001 \text{ cm}^{-1}$ . Then they are convolved with the triangular scan function to spectral resolutions with the desired HWHM. The convolved radiance and Jacobian are used as input in the retrieval algorithm. Two spectral intervals are studied:  $650$ – $2200$  and  $200$ – $2200 \text{ cm}^{-1}$ . The first one represents the midinfrared (MIR), while the second one covers the full thermal infrared spectrum, including the FIR (below  $650 \text{ cm}^{-1}$ ). The merit of each spectral interval for the retrieval of temperature and  $\text{H}_2\text{O}$  is examined and compared.

The quality of the retrieval is determined by a basic error statistic, the root-mean-square (RMS) of the errors.

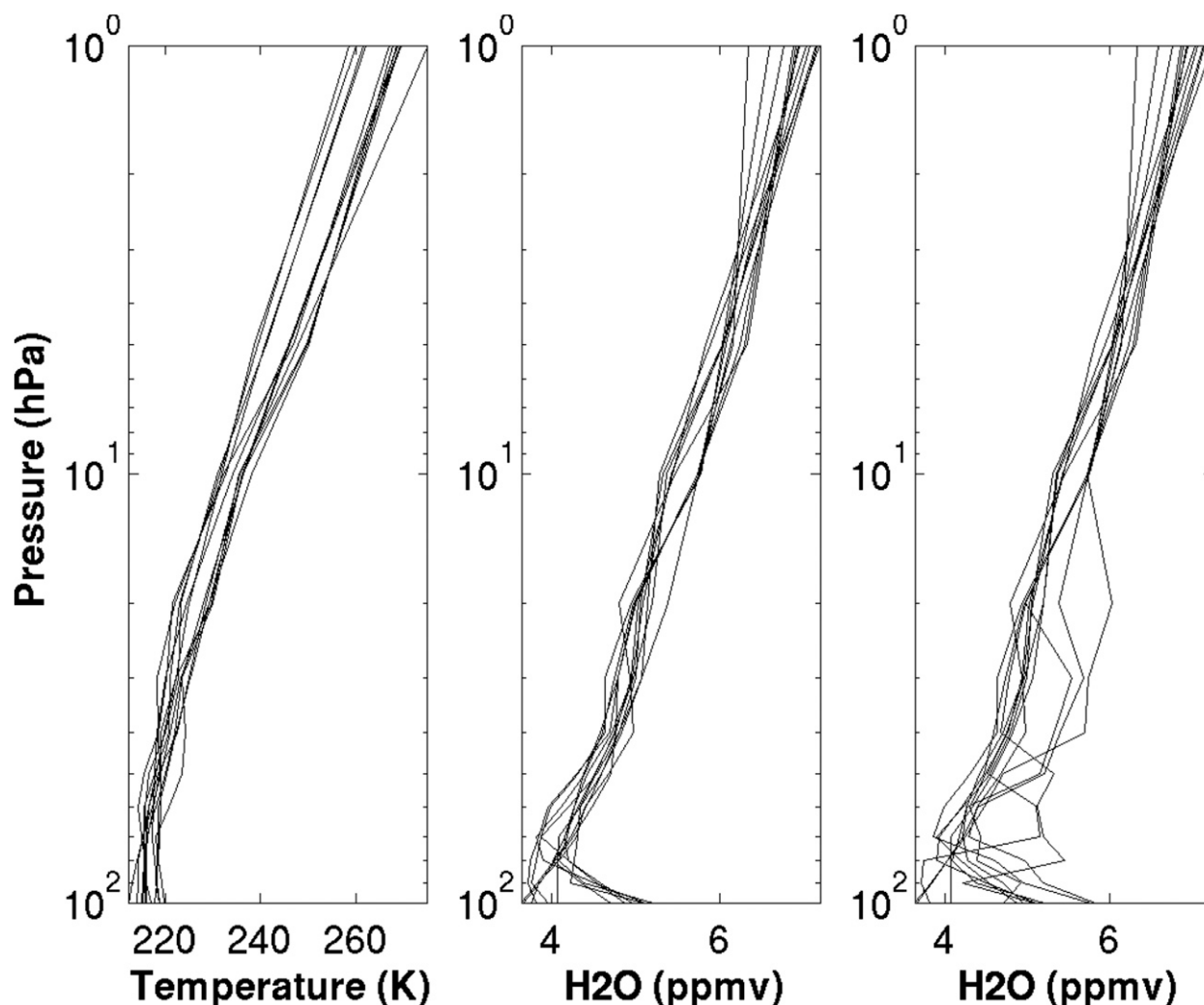


FIG. 5. Subset of (left) temperature and (middle)  $\text{H}_2\text{O}$  profiles for the  $45^\circ$ – $50^\circ\text{N}$  latitudinal band. (right) Artificially moistened  $\text{H}_2\text{O}$  profiles.

The retrieval accuracy is indicated by the RMS of the differences between the retrieved and truth quantities at each level for all of the test profiles; such an RMS profile, in comparison to the standard deviation (STD) of the training dataset (i.e., the *a priori*), also shows how the retrieval reduces the uncertainty in the atmospheric state. The retrieval precision is indicated by the STD of an ensemble of repeated retrievals of the same profile, where the simulated spectrum has been perturbed at a given noise level (the “measurement error”; Rodgers 2000).

#### 4. Sounding of stratospheric temperature/ $\text{H}_2\text{O}$

##### a. Ideal and realistic instruments

The goal is to retrieve each truth profile by using the noise-added synthetic radiance spectrum computed from

them. In other words, assuming that the synthetic radiance signal is sensed by the sensor, we examine how precisely the iteration technique can reproduce the truth profile. First, we restrict our retrieval test to the 40 unmoistened original ACE-FTS profiles.

To examine the potential of retrieving stratospheric  $\text{H}_2\text{O}$  and temperature simultaneously, we first analyze an “ideal” instrument, which has full IR coverage ( $200$ – $2200\text{ cm}^{-1}$ ), a high spectral resolution ( $0.1\text{ cm}^{-1}$ ), and a very low noise level ( $0.25 \times 10^{-7}\text{ W cm}^{-2}\text{ sr}^{-1}\text{ cm}$ ). The noise level mimics the desired performance of the Climate Absolute Radiance and Refractivity Observatory (CLARREO) instrument (Wielicki et al. 2013), similar to what is used by Merrelli and Turner (2012).

Figure 6 shows the spectral Jacobian for  $\text{H}_2\text{O}$  ( $\mathbf{K}_q$ ) and temperature ( $\mathbf{K}_T$ ). For information content assessment,

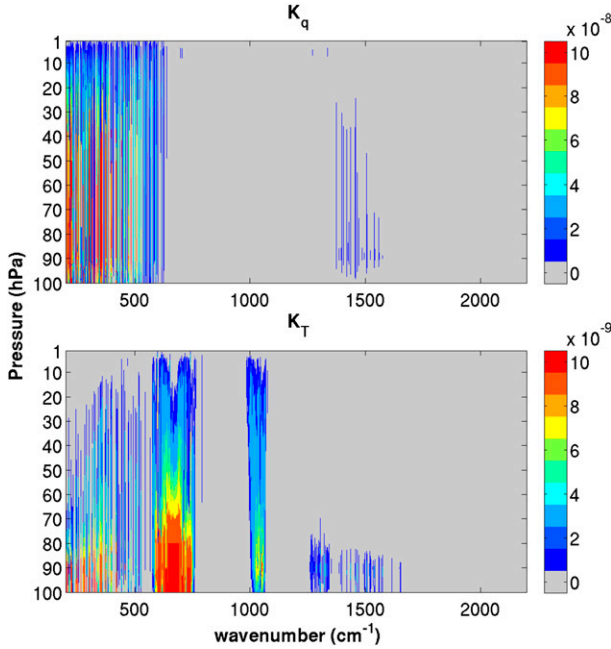


FIG. 6. Spectral Jacobian of (top)  $\text{H}_2\text{O}$  [ $\text{W cm}^{-2} \text{sr}^{-1} \text{cm log}(\text{H}_2\text{O})^{-1}$ ] and (bottom) temperature ( $\text{W cm}^{-2} \text{sr}^{-1} \text{cm K}^{-1}$ ).

the degrees of freedom for signal (DFS) is used, similar to the studies of the TOA spectra (e.g., Worden et al. 2004; Merrelli and Turner 2012). DFS is defined as the trace of averaging kernel matrix  $\mathbf{A}$ , which, following Rodgers (2000), is formulated as

$$\mathbf{A} = (\mathbf{K}_i^T \mathbf{S}_e^{-1} \mathbf{K}_i + \mathbf{S}_a^{-1})^{-1} \mathbf{K}_i^T \mathbf{S}_e^{-1} \mathbf{K}_i. \quad (5)$$

Figure 7 shows the averaging kernel for temperature and  $\text{H}_2\text{O}$ . The rows 2, 5, 7, and 10 (out of 12), corresponding to different pressure levels, of the averaging kernels are shown. The total DFS is 1.8 and 4.4 for  $\text{H}_2\text{O}$  and temperature, respectively. The cumulative DFS (CDFS) normalized by the total DFS (Fig. 7c) shows that 100–40 and 100–10 hPa vertical segments contain 80% of the information for  $\text{H}_2\text{O}$  and temperature, respectively. The rows of the  $\mathbf{A}$  matrix in Eq. (5) are the smoothing kernel that acts at each level in the retrieved state estimate, which indicates the vertical resolution in the retrieval results. The relatively low DFS and the broad shapes of  $\mathbf{A}$  of the  $\text{H}_2\text{O}$  results from the relatively smaller magnitude of the  $\text{H}_2\text{O}$  Jacobian smoothing term ( $\mathbf{K}_i^T \mathbf{S}_e^{-1} \mathbf{K}_i$ ) compared to the inverse of the apriori covariance  $\mathbf{S}_a^{-1}$ .

Numerous tests are performed to examine the effects of changing the spectral resolution, spectral coverage, and noise level on the quality of the retrievals, and the results were compared to the retrieval by the above-mentioned

ideal instrument. For example, in order to investigate the impact of the instrument noise, we adopt another noise level of  $0.75 \times 10^{-7} \text{ W cm}^{-2} \text{sr}^{-1} \text{cm}$  which, together with the lower noise level, encompasses the noise magnitude of the CLARREO instrument throughout the spectrum, to compare to the ideal case. These tests facilitate recommending a realistic sensor configuration that gives the desired retrieval results. Table 1 outlines a subset of the experiment cases that are investigated; Fig. 8 shows the corresponding results. Case 1 represents the ideal sensor setting. It has the highest DFS for temperature and  $\text{H}_2\text{O}$  (Table 1) and the lowest RMS error (red line in Fig. 8) among cases 1–5. Case 2 examines the impact of removal of FIR from case 1. The RMS error in the  $\text{H}_2\text{O}$  retrieval increases drastically and  $\text{H}_2\text{O}$  DFS drops to 0.6. The results here show that the FIR (below  $650 \text{ cm}^{-1}$ ) is critical for the  $\text{H}_2\text{O}$  retrieval. This corroborates with the results from analysis of the spectral signature of stratospheric  $\text{H}_2\text{O}$  (section 2). Case 3 examines the impact of the increase in noise level of case 1. Case 4 verifies the effect of lower spectral resolution on the quality of the retrievals. Case 4 has a similar performance to case 3 for  $\text{H}_2\text{O}$  retrieval, but the temperature retrieval quality degrades compared to case 3, as shown by the temperature DFS value. Case 5 examines the impact of the combined effect of lower spectral resolution and higher noise level. The  $\text{H}_2\text{O}$  RMS error increases compared to cases 2–4, and  $\text{H}_2\text{O}$  DFS drops below one. Comparing case 5 to case 3, the finer spectral resolution appears to generate better temperature retrievals, especially in the upper stratosphere. Among all the cases with a noise level of  $0.75 \times 10^{-7} \text{ W cm}^{-2} \text{sr}^{-1} \text{cm}$ , case 3 has an agreeable performance for both  $\text{H}_2\text{O}$  and temperature retrievals. Given these results, for further examination below, we focus on an instrument specified as case 3 and designate it as the “realistic sensor.”

Besides the baseline measurement strategy (zenith uplooking at 100 hPa), a few additional instrument deployment strategies are examined. These include taking measurements at different zenith angles, taking measurements at multiple vertical levels, and taking multiple measurements under each atmospheric condition and conducting multiple retrievals and then averaging for the same condition. Our examination shows that changing the observation angle does not noticeably affect the RMS error statistics. Also, taking 10 measurements and averaging the retrievals under the same condition renders an equal performance compared to making one retrieval from the averaged spectral measurement, and neither shows significant improvement as judged by the RMS statistics. However, we find that adding measurement at an additional vertical level may considerably improve the retrieval performance; this is especially true for the  $\text{H}_2\text{O}$

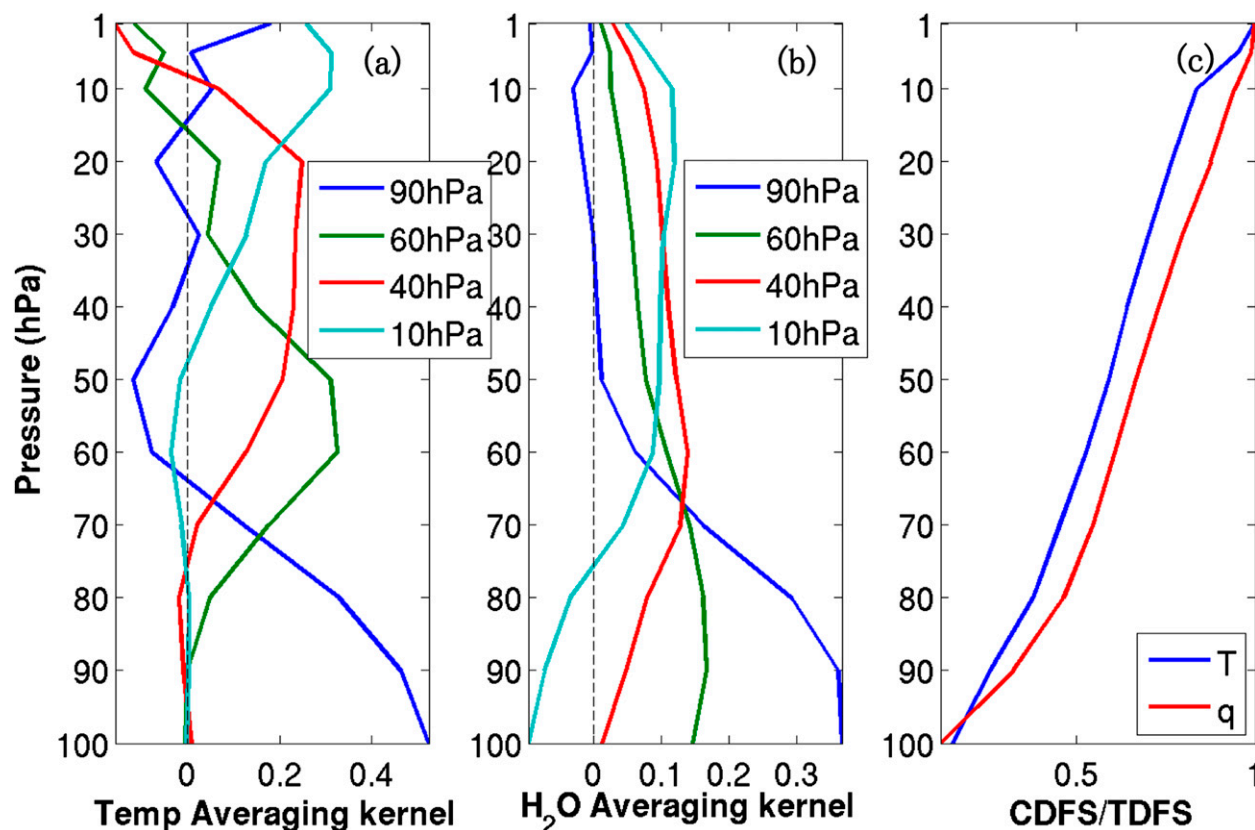


FIG. 7. Different rows of the averaging kernel matrix (corresponding to different pressure levels) for (a) temperature and (b) H<sub>2</sub>O. (c) CDFS normalized with the total degree of freedom for signal (TDFS) for temperature and H<sub>2</sub>O.

retrieval. Case 6 in Table 1 and Fig. 8 shows the information content increase for both temperature and H<sub>2</sub>O when downwelling radiance spectra are obtained at both 100 and 90 hPa. This suggests that the retrieval can be optimized by flying the instrument to multiple altitudes at the same location.

In summary, we find that an infrared hyperspectrometer with a 200–2200 cm<sup>−1</sup> spectral coverage, a 0.1 cm<sup>−1</sup> spectral resolution, and a  $0.75 \times 10^{-7}$  W cm<sup>−2</sup> sr<sup>−1</sup> cm noise level can generally achieve a retrieval accuracy of 0.2 ppmv

for H<sub>2</sub>O and 2 K for temperature up to about 20 hPa, and a precision of 0.02 ppmv for H<sub>2</sub>O and 0.2 K for temperature. Such an IR spectrometer can afford a valuable in situ instrument for sounding the lower to midstratosphere.

#### b. Forward model error

The retrieval above only considers temperature and water vapor in each level; other trace gas species are set to fixed values and are not retrieved. If the trace gas profile

TABLE 1. Different test scenarios in Fig. 8.

RMS	Spectral resolution (cm <sup>−1</sup> )	Spectral coverage (cm <sup>−1</sup> )	Noise level (W cm <sup>−2</sup> sr <sup>−1</sup> cm)	Observer levels (hPa)	DFS temperature	DFS H <sub>2</sub> O
Case 1 (ideal sensor)	0.1	200–2200	$0.25 \times 10^{-7}$	100	4.40	1.76
Case 2 (without FIR)	0.1	650–2200	$0.25 \times 10^{-7}$	100	4.32	0.60
Case 3 (higher noise)	0.1	200–2200	$0.75 \times 10^{-7}$	100	3.53	1.19
Case 4 (lower resolution)	1	200–2200	$0.25 \times 10^{-7}$	100	3.11	1.02
Case 5 (higher noise and lower resolution)	1	200–2200	$0.75 \times 10^{-7}$	100	2.36	0.87
Case 6 (multialtitude)	0.1	200–2200	$0.75 \times 10^{-7}$	100 and 90	4.47	2.06

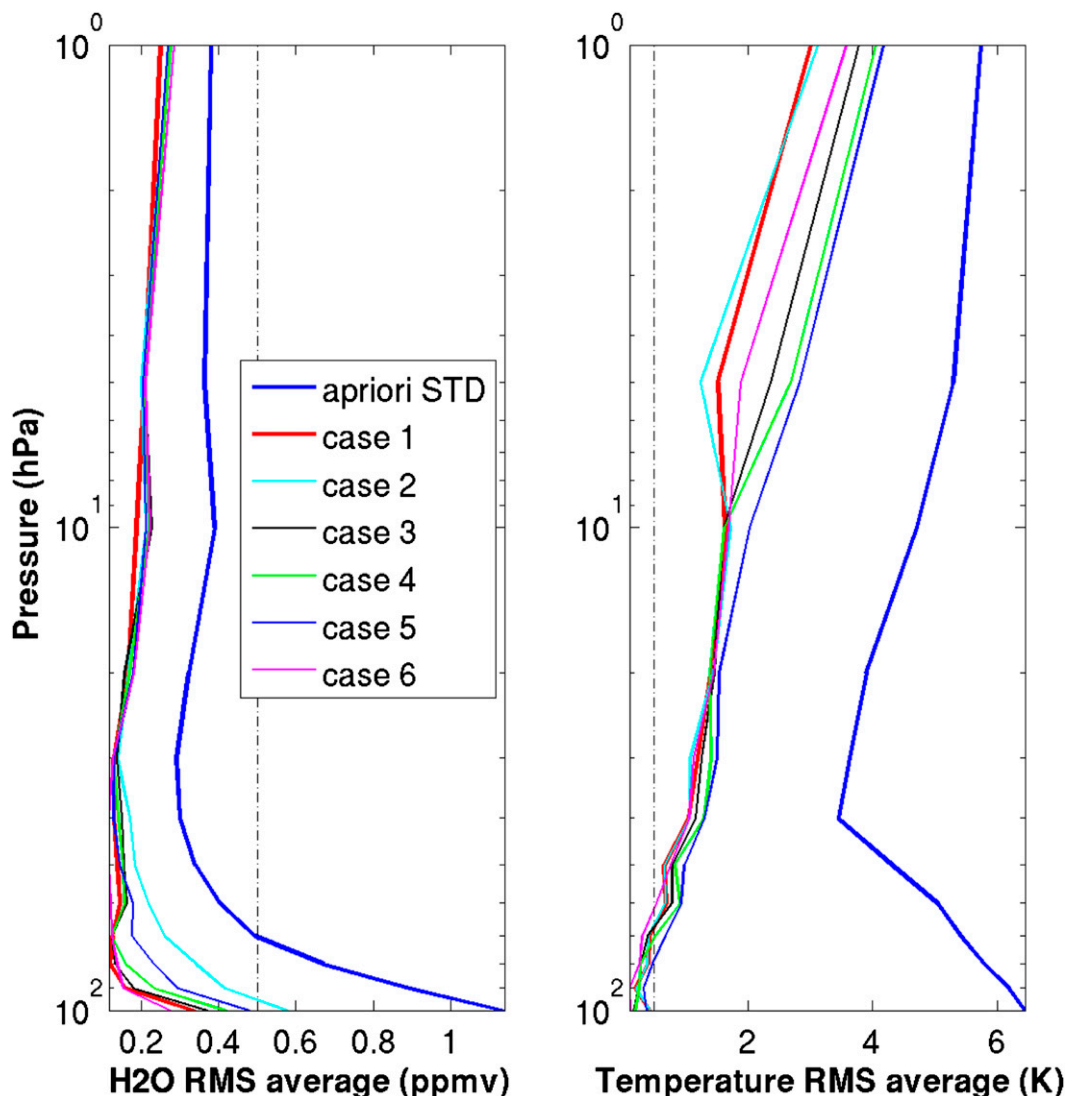


FIG. 8. Comparison of STD of a priori and retrieval RMS, for different sensor specifications. See Table 1 for a complete description of all cases.

is different from the assumed values, then the difference creates a forward model error. The effect of forward model error is examined here.

The forward model error analysis is performed separately for the primary gas species  $\text{CH}_4$ ,  $\text{N}_2\text{O}$ ,  $\text{O}_3$ , and  $\text{CO}_2$ . To apply a forward model error, the gas species concentration is perturbed with an additive error vector, randomly generated for each profile (the amplitude of the perturbation is 20 ppm for  $\text{CO}_2$  and the STD of their variation is given by the ACE-FTS dataset for the other gases). The comparison for RMS error statistics of retrievals with and without forward model error implementation for different trace gas species is shown in Fig. 9. We find that although the errors in  $\text{O}_3$  and  $\text{CO}_2$

affect the quality of the temperature retrievals, the  $\text{H}_2\text{O}$  retrieval is largely unaffected.

Interestingly, we find that forward errors degrade the retrieval results more noticeably at the lower noise level ( $0.25 \times 10^{-7} \text{ W cm}^{-2} \text{ sr}^{-1} \text{ cm}$ ), as the higher noise ( $0.75 \times 10^{-7} \text{ W cm}^{-2} \text{ sr}^{-1} \text{ cm}$ ) acts to block out the impact of the forward errors prescribed here. This is confirmed by comparing the spectral signals due to each forward model error factor to the noise levels.

It is important to note that the impact of the forward error shown here represents the error one would get if naively ignoring the uncertainty in these gases, and that it can be minimized if these gases are simultaneously considered in the retrieval. Simultaneous multispecies

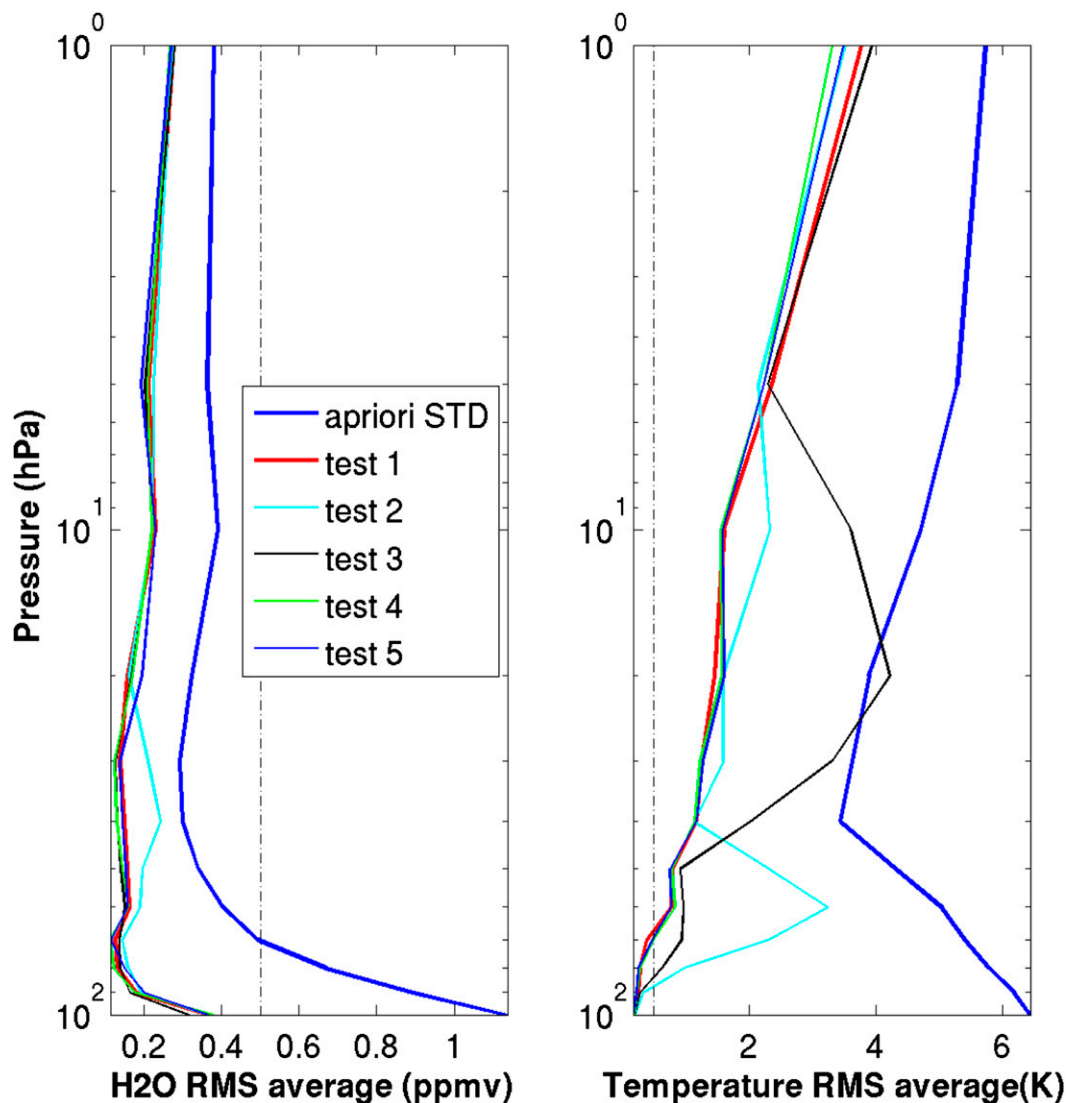


FIG. 9. Effect of forward model error on the retrieval RMS, for different gas species—test 1: realistic sensor with no forward model error, test 2: realistic sensor with  $\text{CO}_2$  forward model error, test 3: realistic sensor with  $\text{O}_3$  forward model error, test 4: realistic sensor with  $\text{N}_2\text{O}$  forward model error, and test 5: realistic sensor with  $\text{CH}_4$  forward model error.

retrieval is beyond the scope of this paper, but we are interested in investigating this in future work.

### c. Detection of moistening

Last, we test how well the stratospheric moistening episodes as identified by Anderson et al. (2012) can be detected using the recommended sensor. To conduct this test, we include in the retrieval the  $\text{H}_2\text{O}$  profiles that are artificially moistened from the 40 ACE-FTS test profiles, which extend the test to a total of 80 profiles.

The retrieval algorithm is performed using the *realistic* sensor configuration (case 3). The RMS error in the retrieval of truth profiles with and without moistened profiles is shown in Fig. 10. Although the RMS

error in the moistened case is larger than the unmoistened case, it is considerably less compared to the uncertainty in the a priori guess. In general, a reduction in the uncertainty of more than 50% is achieved for the vertical distribution of water vapor; the retrieval accuracy is better than 0.4 ppmv for water vapor and 1 K for temperature up to 40 hPa. The RMS of the fractional error between the retrieved and truth  $\text{H}_2\text{O}$  loadings is 1.3% (unmoistened: 1.2%; moistened: 1.4%), which indicates that the measurement technique is very proficient at detecting moistening events. As an example, Fig. 11 demonstrates the retrieval of an arbitrarily selected profile, with and without moistening in the layer of 100–80 hPa. The results show that the retrieval

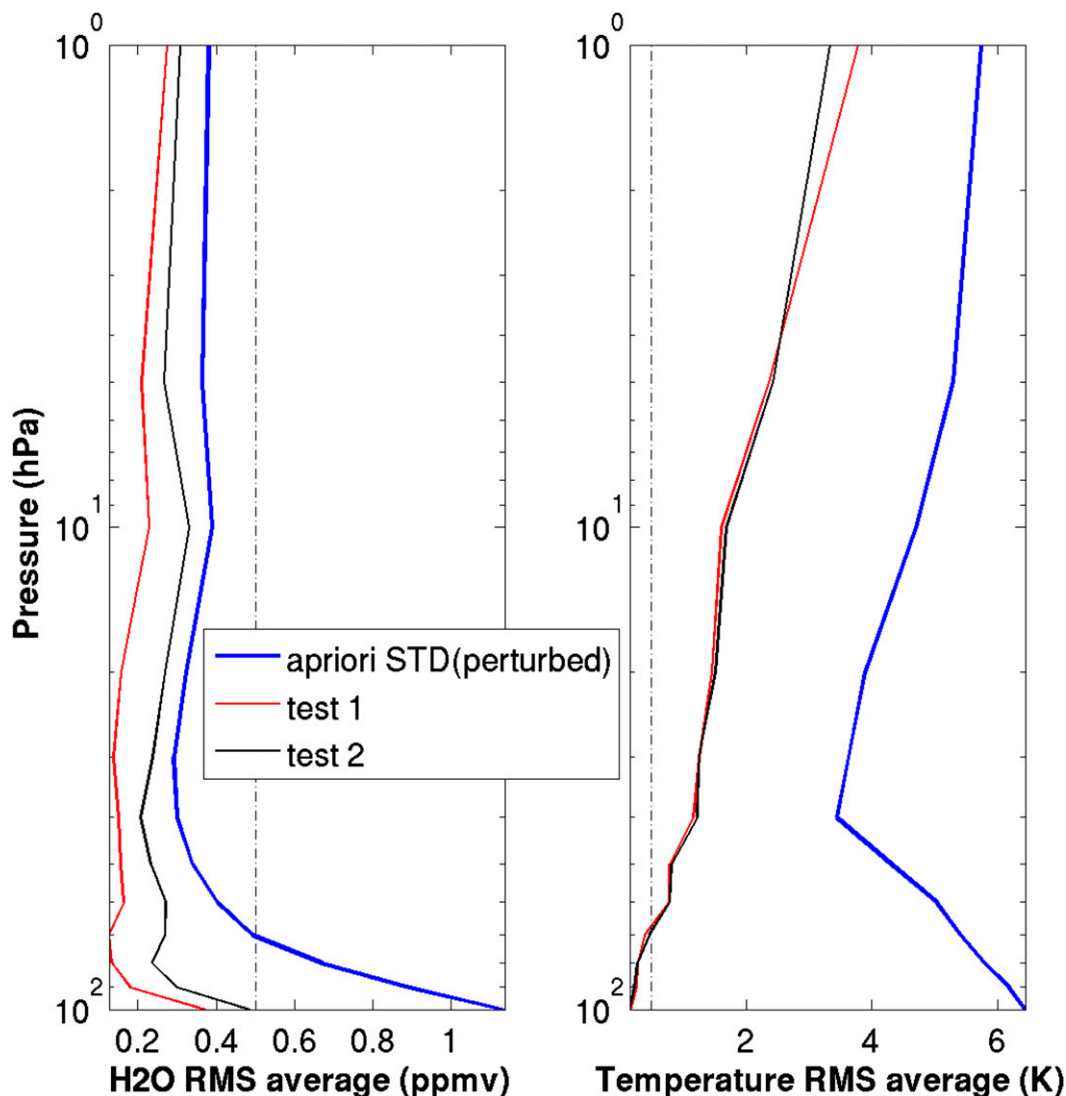


FIG. 10. Ability of realistic sensor to retrieve dry and moistened profiles—test 1: RMS of dry profiles retrievals and test 2: RMS of moistened profiles retrievals.

algorithm can well capture the  $\text{H}_2\text{O}$  concentration in both dry and moist cases.

## 5. Conclusions

Stratospheric  $\text{H}_2\text{O}$  is an important factor that affects climate change. Airborne infrared spectrometers are useful observational tools that may augment existing in situ and satellite observations. This study examines the feasibility of flying such a spectrometer at tropopause level to monitor stratospheric  $\text{H}_2\text{O}$ .

Observational data derived from the ACE-FTS satellite are used for testing this hypothetical instrument. Synthetic downwelling radiance is obtained by the LBLRTM radiation code. The Gauss–Newton iterative

technique is used to obtain a solution from the retrieval algorithm. This study shows that a sensor with  $200\text{--}2200\text{ cm}^{-1}$  spectral coverage,  $0.1\text{ cm}^{-1}$  spectral resolution, and a noise level of  $0.75 \times 10^{-7}\text{ W cm}^{-2}\text{ sr}^{-1}\text{ cm}$  is able to reach the accuracy of  $0.4\text{ ppmv}$  and  $1\text{ K}$  for simultaneous retrieving  $\text{H}_2\text{O}$  and temperature in the lower to midstratosphere. The retrievals become unreliable above 10 and 40 hPa for temperature and the  $\text{H}_2\text{O}$ , respectively. The results indicate that FIR, compared to MIR, is critical for profiling stratospheric  $\text{H}_2\text{O}$ , and a practical sensor needs to include this portion of the spectrum to successfully retrieve stratospheric  $\text{H}_2\text{O}$ . The forward model errors arising from uncertainties in  $\text{CH}_4$ ,  $\text{N}_2\text{O}$ ,  $\text{O}_3$ , and  $\text{CO}_2$  do not significantly affect the  $\text{H}_2\text{O}$  retrieval, although there is a larger impact on

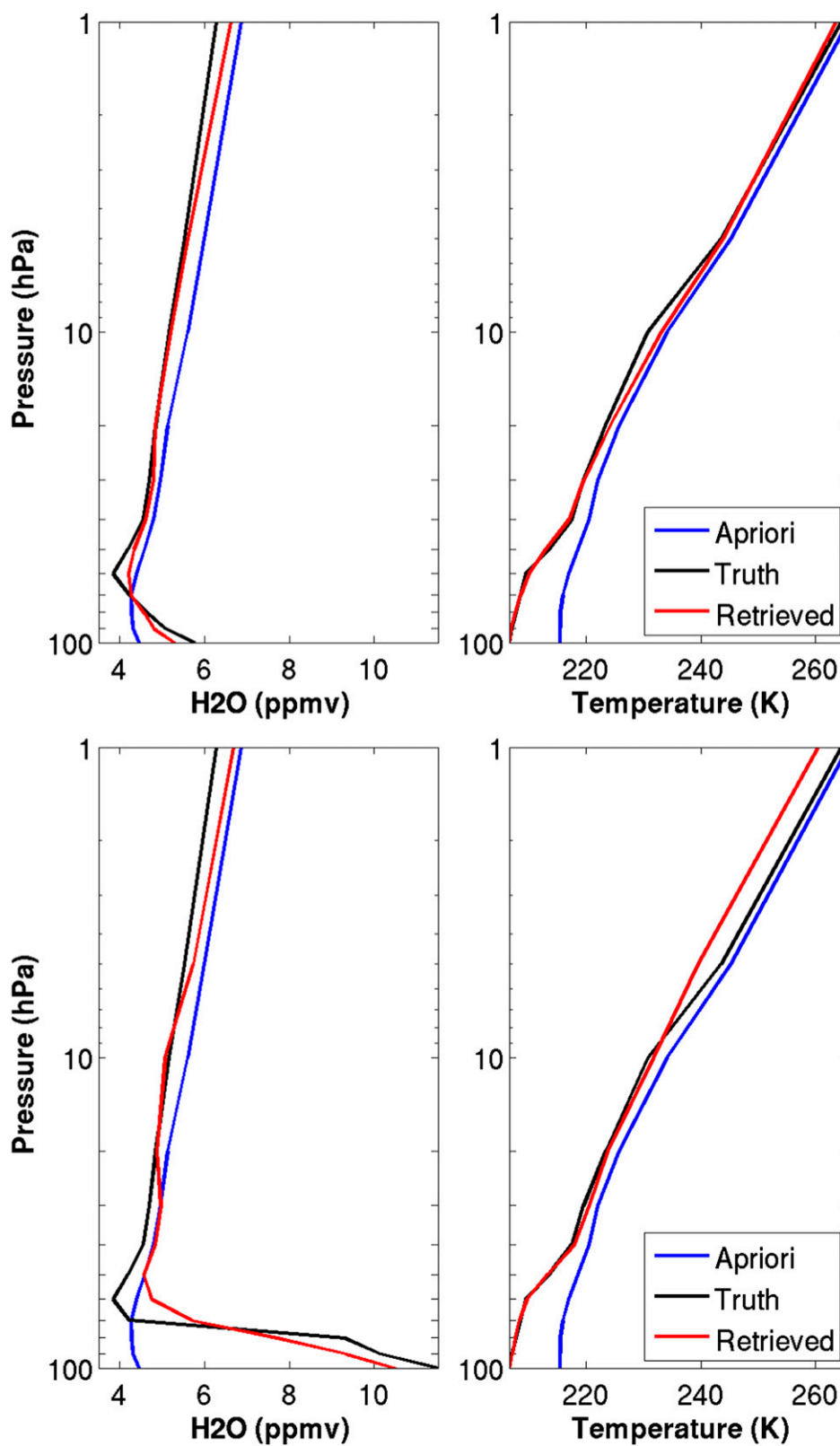


FIG. 11. Comparison of retrieval ability of realistic sensor for (top) dry and (bottom) moistened profiles for one case. The moistening is 2 times the original profile from 100 to 80 hPa.

the temperature results, especially for O<sub>3</sub> and CO<sub>2</sub> perturbations.

An airborne spectrometer has a fast response time and thus can capture the variability of water vapor on small temporal and spatial scales. This makes it an advantageous instrument for monitoring such lower-stratospheric moistening events, as documented by Anderson et al. (2012). The tests here show that the water vapor loading within the stratosphere can be detected to be within 1.3% uncertainty.

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