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# Impacts of spectroscopic errors on O<sub>2</sub> measurement requirements for the ASCENDS mission

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## Abstract

Remotely sensed observations of atmospheric composition require an estimate of surface pressure. This estimate can either come from an instrument with sensitivity in an O<sub>2</sub> absorption feature in the spectrum, or it can be provided by a numerical weather prediction (NWP) model. In this work, the authors outline a information-based methodology for setting measurement requirements for an active measurement of O<sub>2</sub> in the context of the Active Sensing of Carbon Emissions over Nights, Days and Seasons (ASCENDS) mission. The results indicate that the impacts of correlations in the spectroscopic errors between CO<sub>2</sub> and O<sub>2</sub> measurements are nontrivial, and actually tighten the requirement for the O<sub>2</sub> measurement by 5–10 %.

## 1 Introduction

The present surface based network of observing systems has been shown to be inadequate for reducing uncertainty in surface flux estimates of CO<sub>2</sub> at all but the coarsest spatial scales (Houweling et al., 2004). On the other hand, other experiments with pseudo-data (e.g. Rayner and O'Brien, 2001; Houweling et al., 2004; Hungershofer et al., 2010) suggest that column integrated CO<sub>2</sub> mixing ratio, denoted as XCO<sub>2</sub>, as retrieved from radiances measured by satellites with instruments that are sensitive to CO<sub>2</sub> absorption features, can provide enough observations with suitable precision to both improve current surface flux estimates and reduce their associated uncertainties.

Retrievals of XCO<sub>2</sub> require an estimate of surface pressure  $p^*$ , and at present, two options exist for providing it. The first is to use the collocated value of surface pressure derived from numerical weather prediction (NWP) models. The second is to employ a laser differential absorption spectrometer (LAS) to measure absorption in an O<sub>2</sub> band and utilize the near constant O<sub>2</sub> mixing ratio to retrieve a robust estimate of the local surface pressure. It is reasonable to ask whether the reduced errors in surface pressure

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provide improvements to the retrieved mixing ratios and resulting flux estimates that justify the cost.

Here we present a methodology to partially answer that question, by determining which observable contains the most information on the model profile of CO<sub>2</sub> mixing ratio, denoted  $q_{\text{CO}_2}(\rho)$ , and hence the most information on the surface fluxes in a transport model inversion. Specifically, we seek to provide an error constraint on the O<sub>2</sub> measurement, beyond which the cost of the measurement would not be justifiable. Section 2 defines the observations of interest and relevant terminology. In Sect. 3, the notion of Fisher information is introduced, and the relevant forms used in our methodology are discussed. The error components are defined in Sect. 4, and these together with the derivative of the observables with respect to the column concentration of CO<sub>2</sub> are used to calculate the information in each observable as a function of a few parameters related to observational error and NWP model surface pressure errors. Finally, a measurement requirement, in the form of an upper bound, is derived in Sect. 5 for the observational component of the O<sub>2</sub> error, and the value of this upper bound is computed for different magnitudes of surface pressure error.

## 2 Differential absorption lidar measurements

LAS instruments measure the difference in transmitted/received energies at two or more wavelengths (which for the two-line case we call “ $T_{\text{on}}$ ” and “ $T_{\text{off}}$ ”).  $T_{\text{on}}$  is a wavelength absorbed by CO<sub>2</sub> while  $T_{\text{off}}$  is not subject to absorption. We denote the logarithm of the ratio as  $\Delta\tau$ . That is,

$$\Delta\tau_{\text{CO}_2} := \log \left[ \frac{T_{\text{on}}}{T_{\text{off}}} \right] = \frac{1}{m_a g} \int_0^{\rho^*} q_{\text{CO}_2}(\rho) \Delta\xi_{\text{CO}_2}(\rho) d\rho \quad (1)$$

where  $m_a$  is the molar mass of air,  $g$  is the gravitational constant, and  $\Delta\xi_{\text{CO}_2}$  is the differential absorption cross section at pressure altitude  $\rho$ . This definition follows

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immediately from Beer's Law, which states that the transmission is given by

$$T = \exp \left[ - \int_{R_1}^{R_2} n_{\text{gas}}(r) \Delta \xi(r) dr \right]$$

with  $n_{\text{gas}}$  being the number density of the gas, and  $r$  denoting the path traversed by the laser. Since the actual quantities measured by the instrument are  $T_{\text{on}}$  and  $T_{\text{off}}$ , the quantity  $\Delta \tau_{\text{CO}_2}$  is the most direct link between the actual observation and the model profile  $q_{\text{CO}_2}(\rho)$ , assuming that  $\rho^*$  and  $\Delta \xi_{\text{CO}_2}$  are known.

The choice of observation determines an operator from the model state ( $q_{\text{CO}_2}$ ) to the space where the observations lie. The candidate observables in this document are the differential optical depth for  $\text{CO}_2$ ,  $\Delta \tau_{\text{CO}_2}$ , given in Eq. (1), and the ratio  $\frac{\Delta \tau_{\text{CO}_2}}{\Delta \tau_{\text{O}_2}}$ , which is written explicitly as

$$\frac{\Delta \tau_{\text{CO}_2}}{\Delta \tau_{\text{O}_2}} = \frac{\int_0^{\rho^*} q_{\text{CO}_2}(\rho) \Delta \xi_{\text{CO}_2}(\rho) d\rho}{\int_0^{\rho^*} q_{\text{O}_2}(\rho) \Delta \xi_{\text{O}_2}(\rho) d\rho}. \quad (2)$$

Note that the ratio  $\frac{\Delta \tau_{\text{CO}_2}}{\Delta \tau_{\text{O}_2}}$  resembles (modulo the different weighting functions) the ratio  $\frac{q_{\text{CO}_2}}{q_{\text{O}_2}}$ , and so can be thought of as a surrogate for  $X_{\text{CO}_2}$ , with appropriate scaling for the abundance of  $\text{O}_2$  in the atmosphere.

### 3 Information content

From (Rodgers, 2000), the Fisher information for the linearized retrieval problem with Gaussian error statistics is given by

$$\mathbf{I} = \mathbf{H}^T \mathbf{R}^{-1} \mathbf{H} + \mathbf{B}^{-1}, \quad (3)$$

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where  $\mathbf{R}$  is the observation error covariance matrix,  $\mathbf{B}$  is the prior error covariance matrix, and  $\mathbf{H}$  is the Jacobian of the observation operator  $\mathbf{h}$  that transforms model variables into observations. The Fisher information can be thought of as the information in the observation or retrieval about the input parameters, which compose the domain of  $\mathbf{h}$ .

For the observation operators in Eqs. (1)–(2), the predicted quantity is a scalar  $h$ , meaning that  $\mathbf{H}$  is a column vector. Assuming that the prior information on  $q_{\text{CO}_2}$  is the same for each candidate observable (i.e. they assume the same error statistics), this suggests that the scalar quantity

$$I_{q_{\text{CO}_2}} = \mathbf{H}_{q_{\text{CO}_2}}^T \mathbf{R}^{-1} \mathbf{H}_{q_{\text{CO}_2}} \quad (4)$$

provides a measure of a particular observable's information content on the model profile of  $\text{CO}_2$ . Here,  $\mathbf{H}_{q_{\text{CO}_2}}$  is the Jacobian of  $h$  with respect to the model layer mixing ratios  $[q_{\text{CO}_2}^1, \dots, q_{\text{CO}_2}^{n_{\text{layers}}}]$ , and so the quantity  $\sqrt{I_{q_{\text{CO}_2}}}$  has units  $\text{ppm}^{-1}$ , regardless of the units of  $h$ . This quantity thus provides a useful manner in which to compare the utility of very different observations. It should be noted that the Jacobian  $\mathbf{H}_{q_{\text{CO}_2}}$  is expensive to estimate for passive measurements (e.g. using a finite difference approximation), but quite simple to compute analytically in the case of a lidar measurement, by simply differentiating Eqs. (A1) and (A2) with respect to the layer mixing ratios  $q_{\text{CO}_2}^i$ , to yield Eqs. (A3) and (A4). It remains to compute  $\mathbf{R}$ .

## 4 Decomposition of errors

For the linear problem, the matrix  $\mathbf{R}$  characterizes the uncertainty present in the model's predicted value of the observable, as well as the observed value itself (Tarantola, 2005). As such,  $\mathbf{R}$  is a combination of observational uncertainty (in the signal to noise sense), the uncertainty in the simulated/retrieved external quantities (such as surface pressure,

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temperature and moisture), and the uncertainty from things that are not explicitly modeled. The first source is treated as random error with known statistics computed from the SNR. The second source includes surface pressure errors and errors in spectroscopy ( $\Delta\xi_{\text{CO}_2}$ ) due to misspecification of local temperature and water vapor, on which the spectroscopy strongly depends. The third category of errors is assumed to be negligible since we assume that transmission in nearby wavenumbers in the spectra differs only in the gas absorption, and so all other effects cancel out when we take the difference.

$\mathbf{R}$  is treated as a diagonal matrix, whose entries are the sum of error variances arising from the three components described above. Assuming a single grid point in the retrieval (or spatially uncorrelated errors),  $\mathbf{R}$  can be considered to be a constant  $\sigma^2(h)$ , which is decomposed as

$$\sigma^2(h) = \sigma_{p^*}^2(h) + \sigma_{\Delta\xi}^2(h) + \sigma_{\text{obs}}^2(h) \quad (5)$$

The  $h$  dependence is included to emphasize the variability of the observable  $h$  due to errors in surface pressure, spectroscopy and instrument noise. Thus the information in a single measurement on the co-located model  $q_{\text{CO}_2}$  is  $\sigma^{-2}(h)|\mathbf{H}_{q_{\text{CO}_2}}|^2$ , which suggests that the  $i$ th component of  $\sigma^{-1}(h)\mathbf{H}_{q_{\text{CO}_2}}$  will represent the information in the observable about the model's  $i$ th layer CO<sub>2</sub> mixing ratio.

### 4.1 The surface pressure error contribution $\sigma_{p^*}^2(h)$

In order to determine the error variance contribution due to surface pressure misspecification, we make use of the uncertainty propagation formula, where if  $y = h(x)$  and  $\mathbf{H} = \nabla h$ , then

$$\mathbf{R}_y = \mathbf{H}^T \mathbf{R}_x \mathbf{H}, \quad (6)$$



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corrected to the observed station height using a standard lapse rate relationship. The resulting  $1\sigma$  value for the CONUS region was approximately 1.1 mbar and  $2\sigma$  value was 2.1 mbar. The global region exhibited a  $1\sigma$  value of 0.8 mbar and a  $2\sigma$  value of 1.7 mbar respectively. Globally these observations showed no significant biases, and only slight seasonal variation in standard deviations. The standard deviation varied as expected as a function of hemispheric region.

For the calculations that follow, we keep these values in mind, but treat  $\sigma^2(p^*)$  as a parameter whose value will partially determine the amount of O<sub>2</sub> error we deem cost-effective.

### 4.2 The environmental contribution $\sigma_{\Delta\xi}^2(h)$

The differential absorption cross section  $\Delta\xi$  is a function of the atmospheric state variables, and as such, the weighting functions in an automated retrieval will be dynamically estimated according to local temperature, water vapor and pressure. These atmospheric values will themselves be estimates, either taken from NWP models, satellite soundings or other proxies. In order to quantify the uncertainty in the observable due to uncertainty in spectroscopy,  $\sigma_{\Delta\xi}(h)$ , the uncertainty in  $\Delta\xi$  due to uncertainty in the atmospheric state must be quantified. To this end, sample sets of simulated weighting functions for both representative CO<sub>2</sub> absorption features at approximately 1.5711 and 2.0510  $\mu\text{m}$  (6364.92203 and 4875.59  $\text{cm}^{-1}$ ), and the O<sub>2</sub> absorption lines at 0.76468 and 1.2625  $\mu\text{m}$  (13 077.29386 and 7920.5976  $\text{cm}^{-1}$ ) were constructed from observed and modeled atmospheric profile data using a radiative transfer (RT) model to compute associated differential optical depths.

Similarly to the method described in Sect. 4.1, modeled and observed atmospheric state vectors were obtained for both surface and upper air temperature and moisture. The observed profiles were derived from RAwinsonde OBservation (RAOB) observations, while model data were taken from NWP model fields. The RAOBs were obtained from publicly available sources and the matching model data were extracted from GFS

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(NCEP, 2003) analysis fields. RAOBs provide a consistent measure that can be compared to NWP data for statistical purposes (Sun et al., 2010). The matching NWP profiles were selected using a nearest neighbor approach based on the RAOB station location, and contained vertical temperature/moisture (RH) profiles on a fixed pressure grid, and surface parameters (temperature, RH, surface pressure and station height). A conservative quality control scheme was used to screen out RAOB with missing data, and those in cloudy conditions based on the model cloud fraction and RAOB upper-air water vapor.

The associated optical depths for the desired wave numbers, at standard layer heights between the surface and 100 km above the surface, were computed by combining the atmospheric state vectors with a nominal CO<sub>2</sub> profile with a constant vertical mixing ratio of 385 ppm to construct appropriate input parameters for the Line-By-Line Radiative Transfer Model (LBLRTM) (Clough et al., 2005). LBLRTM computes optical depths from Voigt line shape functions and a continuum model that includes self- and foreign-broadened water vapor as well as continua for carbon dioxide, oxygen, nitrogen, ozone and extinction due to Rayleigh scattering. The version employed in this study included 2012 updates to the CO<sub>2</sub> line parameters and coupling coefficients based on the work of Devi et al. (Devi et al., 2007a, b) the O<sub>2</sub> line parameters based on HITRAN (Rothman et al., 2009) and additional quadrupole parameters between 7571–8171 cm<sup>-1</sup>.

Each of 2500+ pairs of observation and model-based weighting functions were constructed by dividing the discrete optical depth for each layer by the layer thickness given as a function of layer height or difference in atmospheric pressure. The top panel of Fig. 1 shows the average for the ensemble set of weighting functions at each selected wavelength, and the bottom panel illustrates the ensemble variance due to variations in vertical temperature and moisture. The weighting functions were created for –10 pm offset for the CO<sub>2</sub> absorption features at 1.571 μm and the off-line center position for the 2.051 μm CO<sub>2</sub> feature and the two selected O<sub>2</sub> absorption lines at 0.76 μm and 1.26 μm.

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Assuming that the differences in optical depths derived from NWP and observed environments have the same distribution as the true errors, the sample error covariance  $\mathbf{R}_{\Delta\xi}$  is computed, and transformed into  $\sigma_{\Delta\xi}^2(h)$  using the error propagation formula Eq. (6), with the relevant partial derivatives are given by Eqs. (A7)–(A9). This matrix has dimensions  $(2n_{\text{layers}}) \times (2n_{\text{layers}})$ , where  $n_{\text{layers}}$  is the number of atmospheric layers in the model. The differences are binned into layers, and the variance for CO<sub>2</sub> and O<sub>2</sub> is computed, in addition to the in-layer covariance between CO<sub>2</sub> and O<sub>2</sub>. Between-layer error correlations are assumed to be zero.

Sample error variances for the 1.571 μm + 10 pm and 2.051 μm CO<sub>2</sub> instruments and the 0.76468 μm and 1.2625 μm O<sub>2</sub> instruments as a function of height are shown in Fig. 2, and the covariances are shown in Fig. 3. Note that the sign of the correlation for each CO<sub>2</sub>–O<sub>2</sub> varies with height and by instrument. For example, the covariance 1.571 μm + 10 pm and 1.26 μm instruments is negative near the surface and positive above the boundary layer, while the opposite pattern is observed for the 2.051 μm and 1.2625 μm instruments. The layer thickness for the displayed error covariances is 25 mb, and varying this parameter showed that the impact of this choice on the covariances was minimal.

Applying Eq. (6) with the profiles in Figs. 2 and 3 and Eqs. (A7)–(A9) yields Table 1. The values between the  $\Delta\tau_{\text{CO}_2}$  and  $\frac{\Delta\tau_{\text{CO}_2}}{\Delta\tau_{\text{O}_2}}$  observables are not directly comparable, since they represent different quantities, but converting these values to percentages of a nominal measurement with a constant CO<sub>2</sub> mixing ratio of 400 ppm yields a variability of about 0.04 % for the  $\Delta\tau_{\text{CO}_2}$  measurements, and 0.06 % for the ratio observables.

It is important to note that these computations assume a perfect radiative transfer model, and as such do not contain systematic errors in the spectroscopic characterizations themselves. Quantifying the impact of such errors is beyond the scope of this paper, and we assume that the state of the art radiative transfer models will be used in any operational retrievals.

### 4.3 The observational error variance $\sigma_{\text{obs}}^2(h)$

The observed differential absorptions  $\Delta\tau$  contain an instrument specific level of precision, which we refer to as  $\sigma_{\text{obs}}^2(h)$ . This is typically quantified by the scientists that build and test the instrument in a controlled environment. The ratio observable has “noise” defined as the propagation of the noise from the CO<sub>2</sub> and O<sub>2</sub> instruments:

$$\sigma_{\text{obs}}^2 \left( \frac{\Delta\tau_{\text{CO}_2}}{\Delta\tau_{\text{O}_2}} \right) = \Delta\tau_{\text{O}_2}^{-2} \sigma_{\text{obs}}^2(\Delta\tau_{\text{CO}_2}) + \Delta\tau_{\text{CO}_2}^2 \Delta\tau_{\text{O}_2}^{-4} \sigma_{\text{obs}}^2(\Delta\tau_{\text{O}_2}) \quad (8)$$

By controlling the size of the individual lidar instruments’ noise, we control the contribution to the overall error, and thus we would expect that a smaller error in one of the instruments would allow a more relaxed requirement on the other, keeping the error budget for XCO<sub>2</sub> fixed.

### 5 An information-based O<sub>2</sub> requirement

In Sect. 4, an algorithm for computing  $\sigma^{-1}(h)$  for two particular observation operators  $h$  from errors in temperature, water vapor and pressure is described. In the case of differential absorption lidar observables, we have simple analytical expressions for  $h$ , assuming knowledge of the surface pressure  $p^*$  and the weighting function, and so the Jacobian  $\mathbf{H}_{q_{\text{CO}_2}}$  can be calculated directly using Eqs. (A3) and (A4). Using these two pieces, we can now compute the aforementioned quantity  $I_{q_{\text{CO}_2}}$  for assumed values of the three parameters:  $\sigma^2(p^*)$ ,  $\sigma_{\text{obs}}^2(\Delta\tau_{\text{CO}_2})$  and  $\sigma_{\text{obs}}^2(\Delta\tau_{\text{O}_2})$ . A minimum requirement for the O<sub>2</sub> lidar investment to be cost effective is that the information in the ratio observable in Eq. (2) is larger than the CO<sub>2</sub> only observable, stated as:

$$\sigma^{-1}(\Delta\tau_{\text{CO}_2}) \frac{\partial \Delta\tau_{\text{CO}_2}}{\partial q_{\text{CO}_2}^i} \leq \sigma^{-1} \left( \frac{\Delta\tau_{\text{CO}_2}}{\Delta\tau_{\text{O}_2}} \right) \frac{\partial}{\partial q_{\text{CO}_2}^i} \frac{\Delta\tau_{\text{CO}_2}}{\Delta\tau_{\text{O}_2}} \quad (9)$$

for every layer  $i$ . Squaring both sides of Eq. (9) and expanding the error variances yields the requirement

$$\sigma_{\text{obs}}^2(\Delta\tau_{\text{O}_2}) \leq \frac{\Delta\tau_{\text{O}_2}^2}{\Delta\tau_{\text{CO}_2}^2} \left[ \sigma_{p^*}^2(\Delta\tau_{\text{CO}_2}) + \sigma_{\Delta\xi}^2(\Delta\tau_{\text{CO}_2}) - \sigma_{p^*}^2 \left( \frac{\Delta\tau_{\text{CO}_2}}{\Delta\tau_{\text{O}_2}} \right) \Delta\tau_{\text{O}_2}^2 - \sigma_{\Delta\xi}^2 \left( \frac{\Delta\tau_{\text{CO}_2}}{\Delta\tau_{\text{O}_2}} \right) \Delta\tau_{\text{O}_2}^2 \right] \quad (10)$$

Note the lack of the observational error term for  $\Delta\tau_{\text{CO}_2}$  on the right hand side of Eq. (10). The remaining terms depend solely on the expected error in surface pressure that arises from using an NWP estimate of  $p^*$  in place of an observed value, denoted  $\sigma^2(p^*)$ . The upper bound given by Eq. (10) was computed for different values of  $\sigma(p^*)$ , and the results are displayed as percentages of the corresponding  $\Delta\tau_{\text{O}_2}$  observations in Table 2.

To first order, one would expect that the  $\text{O}_2$  measurement error requirement should match the pressure requirement, e.g. for a pressure error of 1 mb we should have an  $\text{O}_2$  measurement error of about 0.1 %. Table 2 shows that the impact of including the spectroscopic errors as part of the calculation is to make the measurement requirements more stringent. For example, in order for the  $\text{O}_2$  measurement to add information in the presence of a 1 mb NWP pressure error, the  $\text{O}_2$  measurement must be made with a higher degree of precision, about 0.09 %. This is quite different from the case of passive measurements where the joint measurement of  $\text{CO}_2$  and  $\text{O}_2$  can remove joint scattering effects (O'Brien and Rayner, 2002). Such effects are already handled by the DIAL measurement itself. This impact, while seemingly small, adds an extra burden to the design and implementation of an  $\text{O}_2$  instrument. As higher values of  $\sigma(p^*)$  become acceptable, the upper bound on  $\frac{\sigma_{\text{obs}}(\Delta\tau_{\text{O}_2})}{\Delta\tau_{\text{O}_2}}$  approaches the value of  $\frac{\sigma(p^*)}{p^*}$ , which indicates the diminishing importance of spectroscopic errors as surface pressure errors get large. However, in the range discussed in Sect. 4.1, spectroscopic errors are non

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trivial, and comprise between 5–10% of the upper bound value. Thus when stating measurement requirements, the simple scaling of surface pressure will not be enough to ensure that the O<sub>2</sub> measurement is cost effective.

## 6 Conclusions

5 The preceding work defines an information based requirement for an O<sub>2</sub> instrument to provide additional information on column CO<sub>2</sub> above and beyond a CO<sub>2</sub> measurement taken together with an NWP prediction of surface pressure. The requirement includes the impacts of environmentally induced spectroscopic error correlations between the O<sub>2</sub> and CO<sub>2</sub> measurements, as well as the expected variability of each due to sur-  
 10 face pressure errors. Tests were performed using proxies for errors in the atmospheric state taken from NWP predictions and RAOBs for two different candidate CO<sub>2</sub> and O<sub>2</sub> spectral lines. The major result is that for reasonable surface pressure errors a measurement of O<sub>2</sub> needs to be better (in percentage terms) than the surface pressure estimate to contribute useful information to CO<sub>2</sub> retrievals.

## 15 Appendix A: Discretized operators and their derivatives

Equations (1)–(2) above are two examples of **h**. In the discrete case (i.e. in a numerical model), these observation operators are expressed using sums:

$$\Delta\tau_{\text{CO}_2} = \frac{1}{m_a g} \sum_{i=1}^{n_{\text{layers}}} q_{\text{CO}_2}^i \Delta\xi_{\text{CO}_2}^i \Delta p^i \quad (\text{A1})$$

$$\frac{\Delta\tau_{\text{CO}_2}}{\Delta\tau_{\text{O}_2}} = \frac{\sum_{i=1}^{n_{\text{layers}}} q_{\text{CO}_2}^i \Delta\xi_{\text{CO}_2}^i \Delta p^i}{\sum_{i=1}^{n_{\text{layers}}} q_{\text{O}_2}^i \Delta\xi_{\text{O}_2}^i \Delta p^i} \quad (\text{A2})$$

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The derivatives of the discrete observation operators with respect to  $q_{\text{CO}_2}^i$  are given by

$$\frac{\partial \Delta \tau_{\text{CO}_2}}{\partial q_{\text{CO}_2}^i} = \frac{\Delta \xi_{\text{CO}_2}^i \Delta \rho^i}{m_a g} \quad (\text{A3})$$

$$\frac{\partial}{\partial q_{\text{CO}_2}^i} \frac{\Delta \tau_{\text{CO}_2}}{\Delta \tau_{\text{O}_2}} = \frac{\Delta \xi_{\text{CO}_2}^i \Delta \rho^i}{\sum_{j=1}^{n_{\text{layers}}} q_{\text{O}_2}^j \Delta \xi_{\text{O}_2}^j \Delta \rho^j}. \quad (\text{A4})$$

5 Assuming sigma coordinates, i.e.  $\rho = b\rho^*$ , the derivatives with respect to  $\rho^*$  are

$$\frac{\partial \Delta \tau_{\text{CO}_2}}{\partial \rho^*} = \frac{1}{m_a g} \sum_{i=1}^{n_{\text{layers}}} q_{\text{CO}_2}^i \Delta \xi_{\text{CO}_2}^i \Delta b^i, \quad (\text{A5})$$

$$\frac{\partial}{\partial \rho^*} \frac{\Delta \tau_{\text{CO}_2}}{\Delta \tau_{\text{O}_2}} = 0. \quad (\text{A6})$$

The derivatives of the observation operators with respect to the differential optical depth  $\Delta \xi^i$  are

$$\frac{\partial \Delta \tau_{\text{CO}_2}}{\partial \Delta \xi_{\text{CO}_2}^i} = \frac{1}{m_a g} q_{\text{CO}_2}^i \Delta \rho^i, \quad (\text{A7})$$

$$\frac{\partial}{\partial \Delta \xi_{\text{CO}_2}^i} \frac{\Delta \tau_{\text{CO}_2}}{\Delta \tau_{\text{O}_2}} = \frac{q_{\text{CO}_2}^i \Delta \rho^i}{\sum_{j=1}^{n_{\text{layers}}} q_{\text{O}_2}^j \Delta \xi_{\text{O}_2}^j \Delta \rho^j}, \quad (\text{A8})$$

$$\frac{\partial}{\partial \Delta \xi_{\text{O}_2}^i} \frac{\Delta \tau_{\text{CO}_2}}{\Delta \tau_{\text{O}_2}} = - \frac{q_{\text{O}_2}^i \Delta \rho^i \sum_{j=1}^{n_{\text{layers}}} q_{\text{CO}_2}^j \Delta \xi_{\text{CO}_2}^j \Delta \rho^j}{\left( \sum_{j=1}^{n_{\text{layers}}} q_{\text{O}_2}^j \Delta \xi_{\text{O}_2}^j \Delta \rho^j \right)^2}. \quad (\text{A9})$$

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**Table 1.**  $\sigma_{\Delta\xi}(h)$  for  $h = \Delta\tau_{\text{CO}_2}$  (first row) and  $h = \frac{\Delta\tau_{\text{CO}_2}}{\Delta\tau_{\text{O}_2}}$  (second and third rows) from spectroscopic errors computed using Eqs. (A7)–(A9) and the profiles in Figs. 2 and 3.

	1.571 $\mu\text{m}$	2.051 $\mu\text{m}$	
	$1.646 \times 10^{-4}$	$3.827 \times 10^{-4}$	$\Delta\tau_{\text{CO}_2}$
0.76 $\mu\text{m}$	$4.127 \times 10^{-8}$	$9.213 \times 10^{-8}$	$\frac{\Delta\tau_{\text{CO}_2}}{\Delta\tau_{\text{O}_2}}$
1.2625 $\mu\text{m}$	$5.390 \times 10^{-7}$	$1.279 \times 10^{-6}$	$\frac{\Delta\tau_{\text{CO}_2}}{\Delta\tau_{\text{O}_2}}$

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**Table 2.** Upper bounds on  $\sigma_{\text{obs}}(\Delta\tau_{\text{O}_2})$  expressed as percentages of  $\Delta\tau_{\text{O}_2}$ , computed as a function of the expected surface pressure error  $\sigma(p^*)$ .

$\sigma(p^*)$	1.571 $\mu\text{m}$		2.051 $\mu\text{m}$	
	0.76 $\mu\text{m}$	1.2625 $\mu\text{m}$	0.76 $\mu\text{m}$	1.2625 $\mu\text{m}$
0.5000	0.0293	0.0200	0.0203	0.0190
1.0000	0.0914	0.0889	0.0889	0.0887
1.5000	0.1444	0.1428	0.1429	0.1427
2.0000	0.1959	0.1947	0.1947	0.1946
2.5000	0.2467	0.2458	0.2458	0.2457
5.0000	0.4984	0.4979	0.4979	0.4979
10.0000	0.9992	0.9989	0.9990	0.9989

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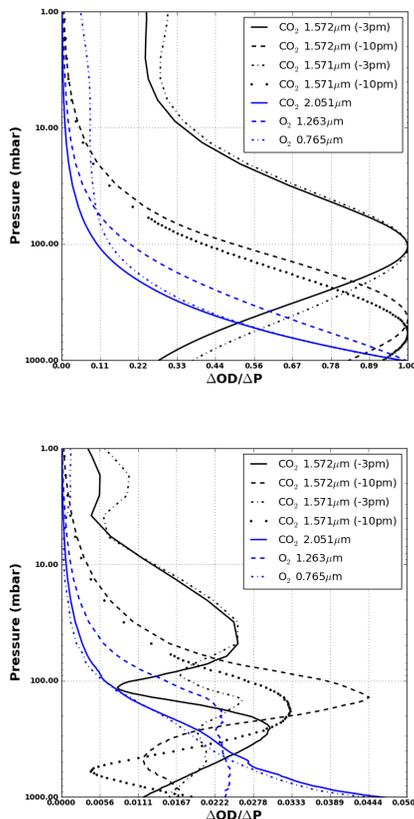
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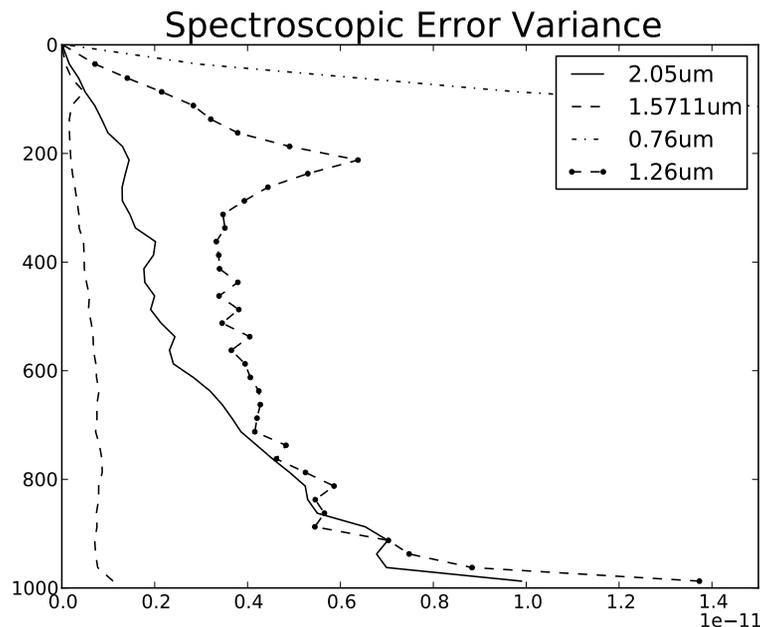
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**Figure 1.** Normalized ensemble weighting functions derived from global vertical temperature and moisture profiles. The upper panel shows the average weighting function for each selected wavelength, and the lower plot illustrates the variability in the weighting functions due to differences in temperature and moisture as a function of vertical height. The variability shown in the lower plot is given as the standard deviations of the difference between the average weighting function values and the ensemble members.

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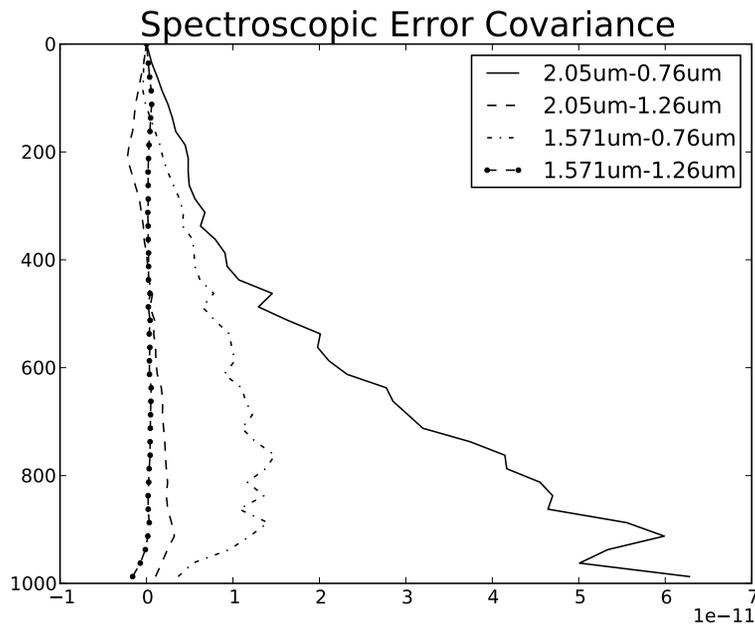


**Figure 2.** The variance of the differences between differential optical depths derived from observed and modeled atmospheric soundings, as a function of pressure. The 0.76 μm instrumental variance is approximately 2 orders of magnitude larger at its largest value (not shown).

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**Figure 3.** The in-layer covariance of the differences between differential optical depths derived from observed and modeled atmospheric soundings, as a function of pressure.

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