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Channel selection using information content analysis: A case study of CO_2 retrieval from near infrared measurements

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ABSTRACT

A major challenge in retrieving CO_2 concentrations from thermal infrared remote sensing comes from the fact that measurements in the 4.3 and 15 μm absorption bands (AIRS or TES) are sensitive to both temperature and CO_2 variations. This complicates the selection of absorption channels with maximum CO_2 concentration information content. In contrast, retrievals using near infrared (NIR) CO_2 absorption bands are relatively insensitive to temperature and are most sensitive to changes of CO_2 near the surface, where the sources and sinks are located. The Orbiting Carbon Observatory (OCO) was built to measure reflected sunlight in three NIR spectral regions (the 0.76 μm O_2 A-band and two CO_2 bands at 1.61 and 2.06 μm). In an effort to significantly increase the speed of accurate CO_2 retrieval algorithms for OCO, we performed an information content analysis to identify the 20 best channels from each CO_2 spectral region to use in OCO retrievals. Retrievals using these 40 channels provide as much as 75% of the total CO_2 information content compared to retrievals using all 1016 channels in each spectral region. The CO_2 retrievals using our selected channels have a precision better than 0.1 ppm. This technique can be applied to the retrieval of other geophysical variables (e.g., temperature or CH_4), or modified for other instruments, such as AIRS or TES.

1. Introduction

Understanding changes in the concentrations, global sources and sinks, dynamics and other processes that control the variability of atmospheric carbon dioxide (CO_2) has emerged as one of the principal challenges of 21st century Earth system science. Since ground-based measurements are sparse over the ocean, in the tropics and elsewhere in the developing world, satellite observations of atmospheric CO_2 are poised to revolutionize our understanding of global carbon cycle by providing unprecedented spatiotemporal resolution and coverage.

Carbon dioxide (CO_2) is one of the most important greenhouse gases, and the rapid increase in its concentration due to the anthropogenic sources in the atmosphere has great impact on the climate. The anthropogenic sources of CO_2 include fossil fuel combustion and other human activities. The natural sinks are the oceans and terrestrial plants. A better understanding of these sources and sinks is required to improve CO_2 flux estimates.

TCCON is a network of ground-based Fourier Transform Spectrometers (FTS) recording direct solar spectra in the near-infrared spectral region. The precise measurements of CO_2 column abundances, e.g., over Park Falls, Wisconsin and Lauder, New Zealand (http://www.tccon.caltech.edu/) [1], provide an essential validation resource for space-based estimation such as from the Atmospheric Infrared Sounder (AIRS) [2,3], the Tropospheric Emission Spectrometer (TES) [4], the Infrared Atmospheric Sounding Interferometer (IASI) [5], the Scanning Imaging

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Absorption Spectrometer for Atmospheric Chartography (SCIAMACHY) [6-8], the Orbiting Carbon Observatory (OCO) [9], and the Greenhouse gases Observing SATellite (GOSAT) [10,11].

Rayner and O'Brien [12] showed that space-based measurements could improve CO_2 flux estimates provided the measurements have a precision of better than about 2 ppm on regional scales. The observations from the thermal emission instruments such as AIRS, TES, and IASI have improved our understanding of the CO_2 seasonal variability and spatial distributions in the mid latitudes and tropics. These thermal infrared (TIR) observations have CO_2 weighting functions that peak in the middle and upper troposphere [2,4]. However, the near infrared (NIR) CO_2 measurements are very sensitive to the CO_2 near the surface (Fig. 1), where most of its sources and sinks are present [13]. Therefore, CO_2 retrieval using NIR measurements should improve the estimation of global CO_2 sources and sinks and provide complementary information to that from TIR estimations. It was found that a +0.1 K temperature error resulted in a +2.5 ppm CO_2 error in the TIR band retrievals [4]. However, the temperature uncertainty-induced CO_2 errors are much smaller in the NIR band retrievals. The target precision of the CO_2 column measurements from an OCO-like instrument is about 1 ppm for a single sounding on regional scales and monthly timescales [14].

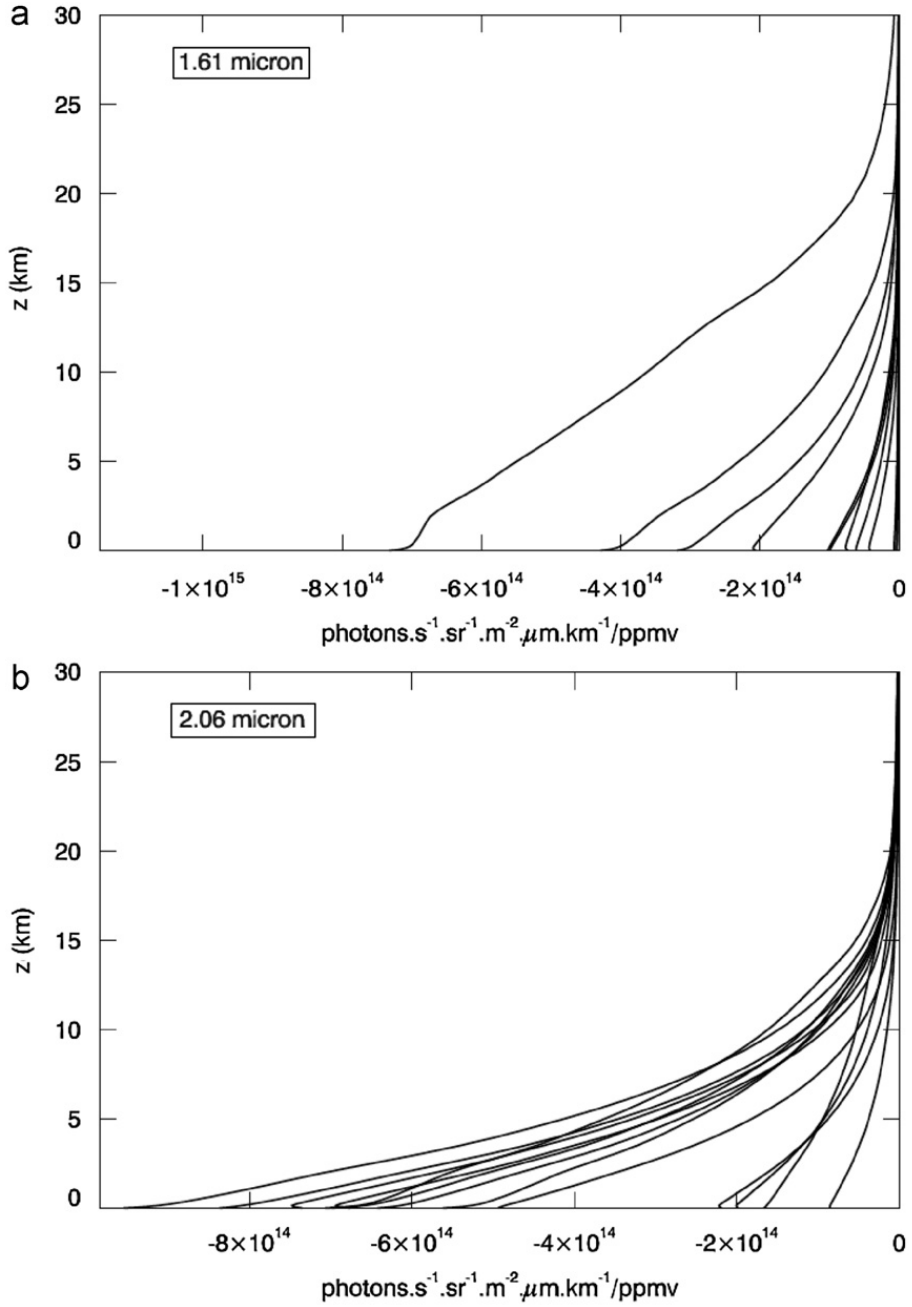

Fig. 1. Weighting functions for CO_2 peak near the surface: (a) 1.61 μm CO_2 band and (b) 2.06 μm CO_2 band.

For the first time, two satellites dedicated to CO_2 observations were launched in 2009—unfortunately, the NASA OCO experienced a launch failure. The JAXA GOSAT is providing space-based measurements in both NIR and TIR spectral regions. Both AIRS and TES provide measurements of the TIR CO_2 band at 15 μm. In addition, TES also uses two laser bands at 967–990 and 1070–1117 cm^{-1} for CO_2 retrieval [4]. An OCO-like instrument will measure the O_2 *A* band (0.76 μm), the CO_2 band at 1.61 μm and the CO_2 band at 2.06 μm. The GOSAT FTS covers a wide spectral range (0.76–15 μm).

One of the major challenges to fast and accurate retrievals is the choice of channels used for the retrieval. We could of course use all the channels and retrieve all the parameters simultaneously. However, this results in complicated and slow retrievals. Further, it is very hard to eliminate biases due to correlations between the parameters. Clarmann and Echle [15] discussed the selection of the optimum microwindows with respect to their associated retrieval errors [15]. The sources of retrieval errors are random errors of the measurement, and errors of the forward model and its input parameters. One goal of channel selection is to make an optimum trade-off between random measurement errors and systematic errors. Adding more channels usually decreases random measurement errors but increases the systematic errors.

There has been some work on the optimization of retrievals from high spectral resolution measurements on the basis of information content (IC) analysis. Most of the earlier work has focused on choosing microwindows for retrieving temperature, humidity and other geophysical parameters. For example, Clarmann and Echle [15] and Dudhia et al. [16] developed the microwindow selection method for the Michelson interferometer passive atmospheric sounding (MIPAS) measurement; Chédin et al. [17] and Crevoisier et al. [18] used channel selection for CO_2 retrieval from AIRS spectra; Sofieva and Kyrölä [19] described channel selection for GOMOS measurements, Worden et al. [20] for TES, and Saitoh et al. (2009) [21] for GOSAT.

The selection of optimized microwindows by Clarmann and Echle [15] was applied to N_2O microwindows for measurements made by a Fourier transform spectrometer [15]. Another practical application of the microwindow selection that maximizes IC was demonstrated for the retrieval of methane profiles from MIPAS measurements by Dudhia et al. [16]. Crevoisier et al. [18] extended the methods to reduce the number of channels for the retrieval of CO_2 and other trace gases from AIRS. They compared a new method, the optimal sensitivity profile (OSP) method, with other methods based on IC and degrees of freedom (DOF) analysis and concluded that using the OSP method optimized the choice of channels for AIRS retrievals of CO_2 and other trace gases. The methods for the selection of measurement subsets using information theory were also examined by Sofieva and Kyrölä [19]. They developed a sequential deselecting procedure and proposed a fast algorithm for channel selection. These methods were applied to the selection of the most informative spectral channels for GOMOS measurements. GOMOS is a stellar occultation instrument for UV–visible spectra. Saitoh et al. developed an algorithm to retrieve CO_2 vertical profiles from the 15-μm band (700–800 cm^{-1}) for GOSAT [21]. They showed that separately selecting a subset of channels based on CO_2 IC for three vertical regions provided retrieval results equivalent to those using all channels in the 15-μm band. However, none of these studies considered the selection of CO_2 channels in the NIR. Our objective is to develop a general technique for channel selection using information analysis [22].

In this paper, we discuss the channel selection for retrieving the column abundance of CO_2 based on IC analysis. Nothing, however, precludes the use of this technique for retrieving any other geophysical parameter. Section 2 describes the forward model used for the radiative transfer simulations. Section 3 gives an introduction to the concepts of IC and DOF, and describes the channel selection technique. We compare a retrieval using the selected channels to one using all channels in Section 4. In Section 5, we derive some conclusions from our preliminary study and discuss the practical advantages of this technique.

2. Model

The radiances are computed using the OCO orbit simulator [23], which simulates a single orbit of an OCO-like instrument. The meteorological and cloud profiles are drawn from a static database of ECMWF profiles [24]. The surface properties are taken from MODIS and the CO_2 profiles are obtained from the parameterized chemical transport model [25]. The gas absorption cross sections are taken from HITRAN 2004 [26] with CO_2 line updates from 4300 to 7000 cm^{-1} provided by the work of Toth et al. [27]. This is done on a 0.01 cm^{-1} spacing high-resolution grid, which resolves individual O_2 or CO_2 lines in the near infrared with a minimum of two points per Doppler width [28]. The Rayleigh scattering properties are computed using the model of Bodhaine et al. [29]. The intensity and polarization calculations are performed using the successive orders of interaction [30] and the two orders of scattering [31] models, respectively. The radiative transfer computation time is dramatically improved using a low-streams interpolation technique [32]. The solar model [28] employs an empirical list of solar line parameters as well as a model for the solar continuum. The Jacobians are computed using finite differences (Fig. 1).

3. Channel selection

3.1. Methods: information content analysis

We apply information content analysis to choose channels that have the most information content for CO_2 and are at the same time insensitive to other parameters such as temperature, water vapor and surface pressure. In retrieval theory, there are two useful quantities that provide a measure of the information. Degree of freedom indicates the number of useful independent quantities in a measurement [33]. The Shannon information content is a scalar quantity that is defined qualitatively as the factor (in bits) by which knowledge of a quantity is improved by making the measurement [18]. The following equations show the relationship between information content (*H*),

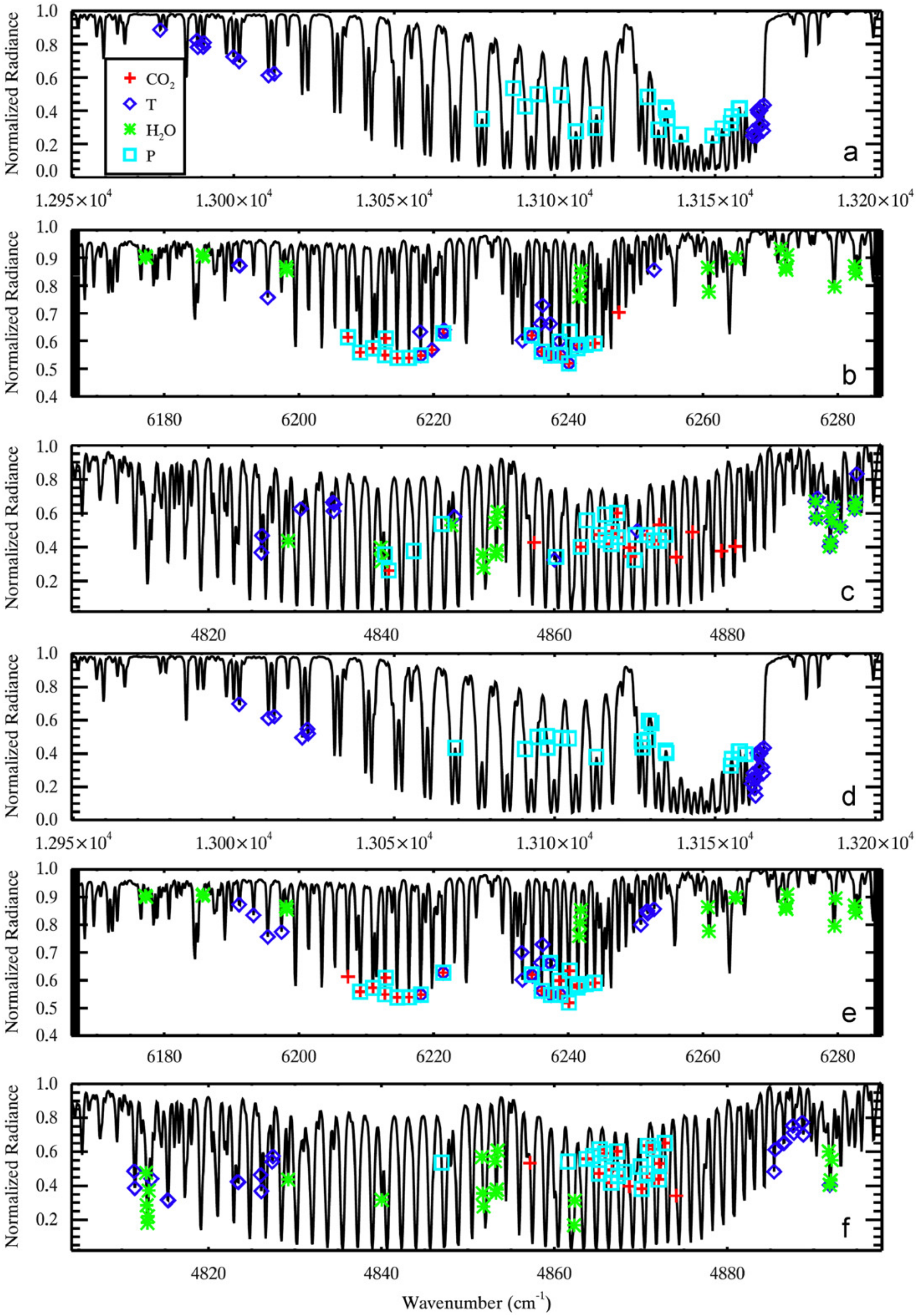

Fig. 2. Channels with highest IC for CO_2 (cross), temperature (diamond), H_2O (star) and surface pressure (square): (a–c) clear sky scenario and (d–f) cloudy sky scenario.

degrees of freedom (d_s), the singular values (λ_i) of the normalized Jacobian matrix ($\tilde{K}$) and the averaging kernel matrix (A) [33].

$$\tilde{K} = S_{\xi}^{-1/2} K S_a^{1/2}, \tag{1}$$

$$I_n - A = (K^T S_{\xi}^{-1} K + S_a^{-1}) S_a^{-1} = \hat{S} S_a^{-1}, \tag{2}$$

$$H = \frac{1}{2}\sum_i \ln(1+\lambda_i^2) = -\frac{1}{2}\ln|I_n - A|, \tag{3}$$

$$d_s = \sum_i \lambda_i^2/(1+\lambda_i^2) = tr(A), \tag{4}$$

where S_a is the covariance matrix for the a priori and S_ε is the measurement error covariance matrix.

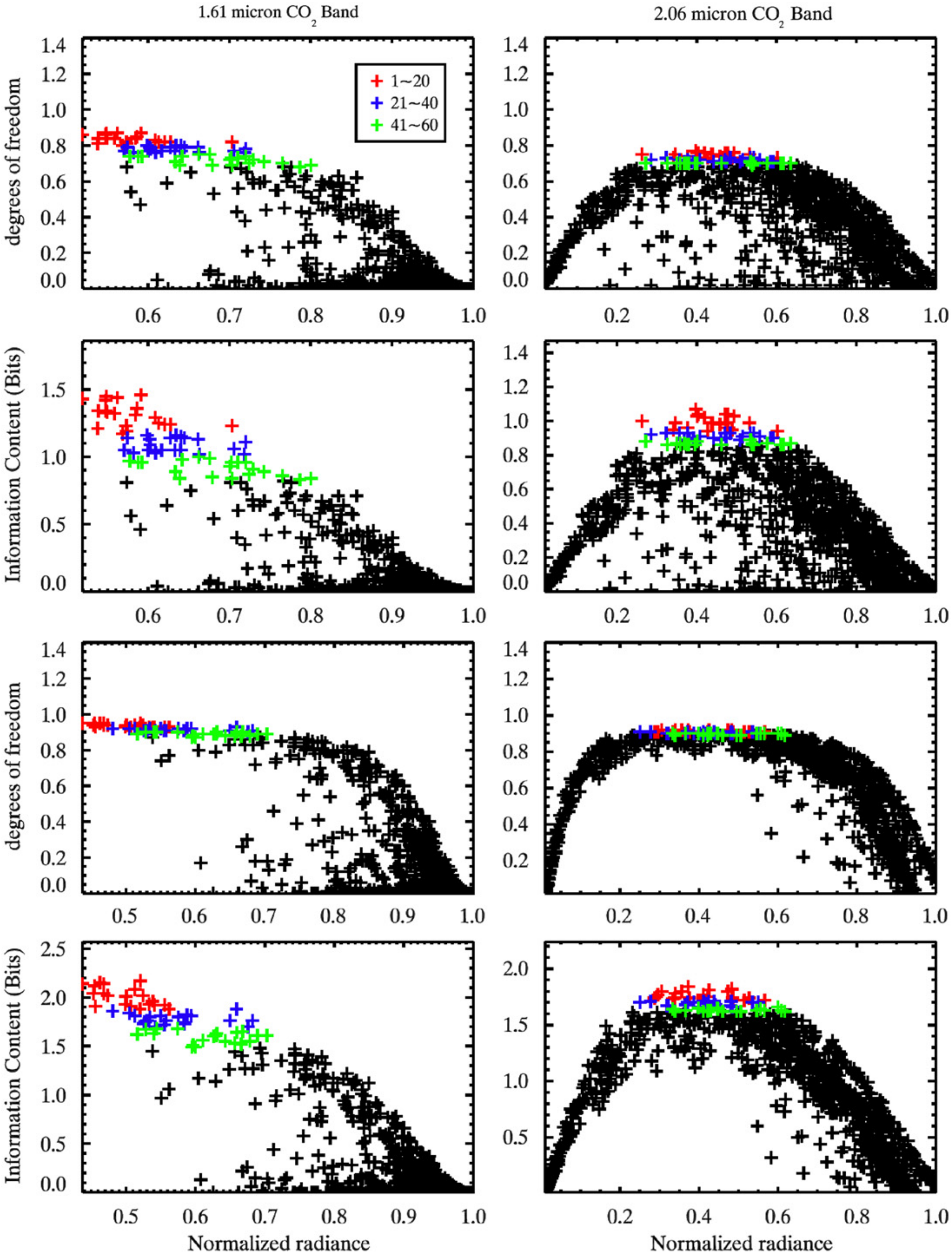

Fig. 3. Channels with highest IC for CO_2 are those with intermediate absorption. (red) channels ranked 1–20; (blue) channels ranked 21–40; (green) channels ranked 41–60. (top 4) clear sky scenario; (bottom 4) cloudy sky scenario; (left column) 1.61 µm band; (right column) 2.06 µm band.

3.2. Channel selection

First, we apply IC analysis to each channel to determine the DOF and IC for CO_2. Then the channels (in each band) are ranked in decreasing order of IC. It is found that the channels with high IC for CO_2 are those with intermediate absorption (Fig. 2). This is because, for very weak channels, there is too little CO_2 absorption to give a useful signal, while for the saturated channels the absorption is too high to have any sensitivity to the CO_2 concentration. We apply the same procedure for other parameters, such as temperature, water vapor and surface pressure, and then rank the channels in a similar fashion. The 20 channels with highest IC for CO_2, temperature, water vapor and surface pressure are plotted, respectively, in Fig. 2. The O_2 A-band channels are only sensitive to temperature and pressure. Fig. 2 also shows that the channels with high IC for CO_2 are mostly different from those for temperature, water vapor and surface pressure.

The order of the channels (in terms of IC) for clear sky is very similar for high aerosol optical depth (AOD) and high cloud optical depth (COD) scenarios. This implies that the channel selection procedure is robust and could be applied to retrieval under different scenarios. It is evident that more channels have DOF close to 1 in the high AOD scenario (see last four panels of Fig. 3). This is probably due to backscattering by aerosols.

Fig. 4 shows the 40 channels (20 each in the 1.61 and 2.06 μm CO_2 bands) with highest IC for CO_2 and the corresponding IC for temperature, water vapor and surface pressure. Most of the channels have high IC for CO_2 and surface pressure but low IC for temperature and water vapor. We use the following procedure to choose the channels for CO_2 retrieval. First, channels with CO_2 IC more than 0.8 bits are selected. Within the selected channels, those that have more than 0.2 bits temperature IC are removed. Among the remaining channels, 40 (20 each in the 1.61 and 2.06 μm CO_2 bands) that have least sensitivity to surface pressure and water vapor are selected for the CO_2 retrievals (see Table 1 for a list of chosen channels).

A simultaneous retrieval using all 2032 channels in both the 1.61 and 2.06 μm CO_2 bands provides 1.67 DOF and 5.9 bits of IC. Fig. 5 shows that a retrieval using the first 200 channels (ranked in order of decreasing IC) in each band would have 1.55 DOF and 5.35 bits of IC. This represents about 90% of the IC provided by a retrieval using all channels. If we use just the top 20 channels in each band, we still retain around 75% of the IC.

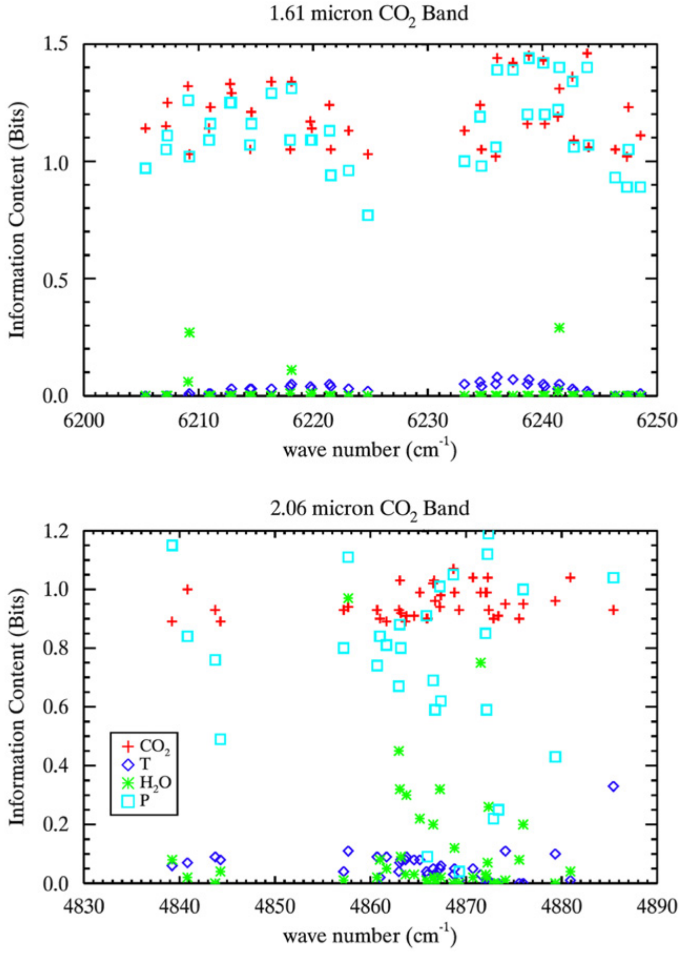

Fig. 4. IC for (cross) CO_2; (diamond) temperature; (asterisk) H_2O; (square) surface pressure for 40 channels with highest CO_2 IC.

4. CO_2 retrievals

For the retrieval study, we assume a constant CO_2 concentration of 370 ppmv (parts per million by volume). The signal to noise ratio (SNR) is set to be 300 for all channels. This is a reasonable value for an OCO-like instrument. The (constant) *a priori* and initial guess for CO_2 are set at 375 and 380 ppmv, respectively. The diagonal values of the a priori covariance matrix are set to be 1% of the initial value. The off diagonal elements are calculated assuming exponential decay with a scale height of 8 km [33].

In the lower atmosphere, the temperature, water vapor, and aerosol profiles are well determined by the measurement; they are strongly constrained by the *a priori* at higher altitudes [34]. With this in mind, we retrieve the CO_2 concentrations at seven levels between 2 and 5 km, where we expect maximum sensitivity from NIR measurements. Table 2 presents the retrieval results for six cases. Case 1 is the ideal case where the measurements have no random noise. The column averaged dry air mole fraction of CO_2 (X_{CO_2}) from a full-channel retrieval is 370.007 ppmv, in excellent agreement with the true X_{CO_2}. Case 2 is the same as case 1 except that random noise has been added to the pseudo-measured spectrum. Case 3 considers what happens if we average 100 retrievals with different sets of random noise. This is to simulate a retrieval of several contiguous soundings from real space-based measurements. The X_{CO_2} precision is comparable to the case with no noise. Cases 4–6 are the same as cases 1–3 except that we use only the 40 channels selected by IC analysis. In the case with no random noise, the X_{CO_2} precision is 0.048 ppmv (case 4). The precision when we average 100 retrievals with different random noise (case 6) is only 0.057 ppmv, which is comparable to case 4. Fig. 6 shows very good agreement between the retrieved CO_2 profiles and the truth.

Table 1

1.61 μm (cm^{-1})	2.06 μm (cm^{-1})
6212.76	4872.26
6209.1	4880.93
6207.28	4872.05
6211.04	4872.15
6247.51	4875.98
6207.17	4869.29
6205.37	4872.36
6210.92	4873.39
6248.55	4872.88
6244.03	4875.57
6246.34	4832.21
6209.21	4874.63
6247.38	4874.74
6205.26	4874.01
6216.24	4842.02
6245.18	4878.08
6212.64	4872.77
6245.06	4895.52
6203.48	4875.46
6243.77	4876.09

In the above study, CO_2 is the only unknown parameter. The other atmospheric variables are assumed to be perfectly known. However, in a real retrieval, uncertainties in these atmospheric parameters would introduce a bias in the CO_2 retrieval. For the purposes of this work we only consider the clear sky scenario; cloudy scenarios will be discussed in a subsequent paper. A 1 K uncertainty in the temperature profile resulted in a 0.5 ppmv bias in the retrieved X_{CO_2}. A similar 10 hPa perturbation to the surface pressure or 1% uncertainty in the water vapor profile caused a similar X_{CO_2} bias (Table 3).

Table 2

Case	Random noise	Channels	ΔX_{CO_2} (ppmv)
Case 1	No	2032	0.01
Case 2	Yes	2032	0.17
Case 3	Yes (averaging 100 cases)	2032	−0.01
Case 4	No	40	0.05
Case 5	Yes	40	0.62
Case 6	Yes (averaging 100 cases)	40	0.06

5. Conclusions

OCO-like instruments typically have thousands of detector channels. However, it is unnecessary to use all the channels to retrieve CO_2 since only some of them are

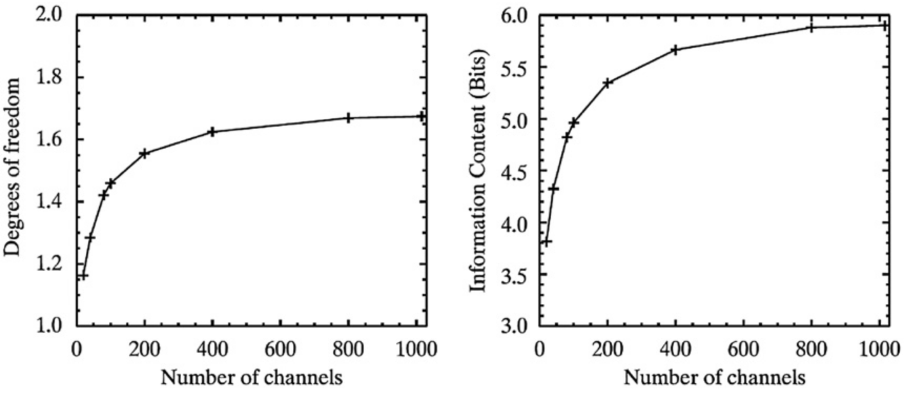

Fig. 5. IC increases with the number of channels selected. The increase in IC is very little from 200 channels to 1016 (all) channels.

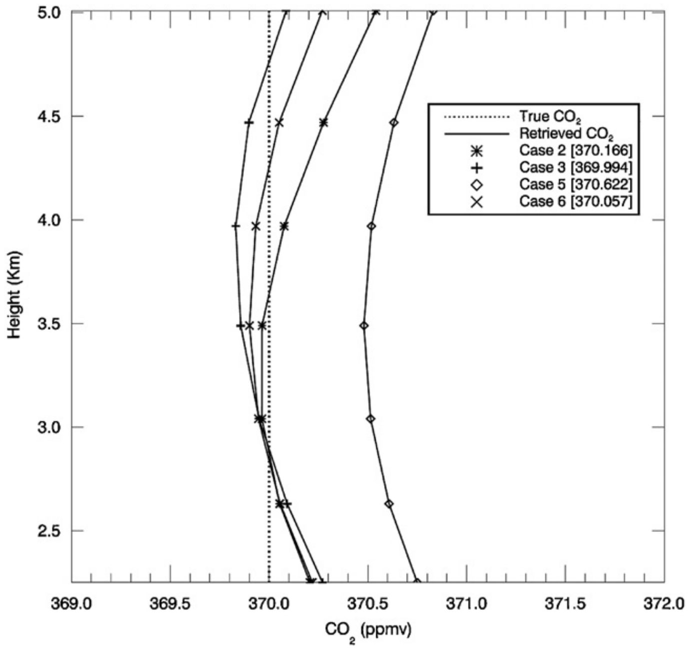

Fig. 6. CO_2 retrieval comparison. Case 2: all channel retrieval; Case 3: average of 100 all-channel retrievals; Case 5: 40-channel retrieval; Case 6: average of 100 40-channel retrievals. The *a priori* is 375 ppm (constant) for all cases. Random noise is included in the pseudo-measurements.

Table 3

	Uncertainty	Bias in X_{CO_2} (ppmv)
Temperature	1 K	0.46
Surface pressure	10 hPa	0.55
Water vapor	1%	0.44

sensitive to CO_2. Further, many channels are sensitive to other variables such as temperature and surface pressure. We have developed a technique based on IC analysis to select channels for CO_2 retrievals using NIR measurements. It was found that the channels have high CO_2 IC are those with intermediate absorption. We selected 40 channels with high sensitivity to CO_2 and low sensitivity to other parameters. The channel selection was found to be independent of the scattering scenario (clear vs. cloudy sky). Retrieval using the 40 channels was also shown to retain 75% IC.

Retrievals using the selected channels have comparable error characteristics to the all-channel retrievals. The precision of the 40-channel retrieval after averaging over several pseudo-soundings is about 0.05 ppmv. Even with the uncertainties of 1 K in temperature, 10 hPa in surface pressure, or 1% in water vapor, the X_{CO_2} bias would be about 0.5 ppmv.

The same technique can be applied to select channels most sensitive to *T*, surface pressure, water vapor or any other parameter. In this way, it is possible to retrieve them one by one. This introduces the possibility of an iterative retrieval to account for uncertainties in relevant geophysical parameters. The channel selection technique allows us to use optimal sets of channels to retrieve atmospheric variables. We intend to apply this method to CO_2 retrievals from GOSAT measurements.

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