The retrieval algorithm for a satellite-borne CO₂-sounder:

preliminary results in near infrared band

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Abstract: This study developed an inversion algorithm for the CO₂-sounder instrument to be launched on a Chinese satellite. By using the L1B spectral data of the Greenhouse gases Observing Satellite (GOSAT) as input, the simulation results of the column averaged CO₂ dry air mole fraction (XCO₂) retrieved from the CO₂-sounder algorithm were obtained and compared with the GOSAT L2 XCO₂ products for different seasons and geolocations. The simulation data showed a tendency to be less than the GOSAT L2 data, but the two data sets were generally in agreement with a global mean difference of -4.05 ± 6.06 ppm. For the matched data pairs, 51% had their relative differences less than 1% in absolute value, and 76% less than 2%. The seasonal and latitudinal variations of the XCO₂ differences were also investigated, and the largest discrepancy was found in the desert areas with the relative differences of about 3%~4%. These results suggested that better consistency between the two data sets could be achieved if more realistic observational parameters instead of model values were used in the simulation. These parameters included the a priori profiles of

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atmospheric temperature, concentrations of CO₂, O₂, and H₂O, surface reflectance, aerosol and cloud indices, etc.

Keywords: satellite-borne; XCO₂; retrieval algorithm; near infrared; spectrometer

1. Introduction

Atmospheric carbon dioxide (CO₂) is a well-known major greenhouse gas and has produced significant impact on the global climate. The concentration of CO₂ has increased from the global level of 280 ppmv in pre-industrial times to 379 ppmv in 2005 [1], most probably because of emissions from the burning of fossil fuels, clearing of forests and other human activities. It is necessary to accurately quantify the global distribution and variations of CO₂ sources and sinks for exactly predicting future atmospheric CO₂ concentrations and their impacts on climate. However, because of the sparseness of the observation sites for greenhouse gases, our understanding of global carbon cycle is spatially and temporally limited. The carbon fluxes of the atmosphere and the terrestrial ecosystem as well as the atmosphere and the ocean are not measured accurately, especially lacking of the observational data in the polar region, the desert area, the wide ocean and the plateau which sparsely populated. Satellite remote sensing provides an effective approach to monitoring the distributions of CO₂ at high spatio-temporal resolution on regional scales over globe. The column averaged CO₂ dry air mole fraction (XCO₂) which is sensitive to CO₂ variations near the surface [2] offers a new insight into the pattern of CO₂ mixing ratios. To improve the accuracy of source and sink estimates of CO₂, recent studies indicated that high precision on regional to global scales is required to resolve and

quantify the small (0.25% to 2%) variations [3] in XCO_2 .

The space-based measurements such as the Atmospheric Infrared Sounder (AIRS) [4], the Infrared Atmospheric Sounding Interferometer (IASI) [5], and the Scanning Imaging Absorption Spectrometer for Atmospheric Chartography (SCIAMACHY, which stopped working in April 2012) allow for the quantification of spatial, temporal and seasonal variations in CO_2 on global scales [6]. However, they are not the specific sensors designed to measure CO_2 . The Greenhouse gases Observing Satellite (GOSAT) was the first satellite designed specifically for monitoring CO_2 concentrations with high spatial resolution and geographic coverage. It was successfully launched on 23 January 2009 and equipped with two key instruments: the Thermal And Near infrared Sensor for carbon Observation-Fourier Transform Spectrometer (TANSO-FTS) and the Cloud and Aerosol Imager (TANSO-CAI) [7]. GOSAT has been returning global measurements of XCO_2 since June 2009 [8] and the precisions of the column abundances for single observations has been better than 1% in most cases [9]. The other satellite developed for CO_2 observations was Orbiting Carbon Observatory (OCO). After a launch failure, the replacement satellite, OCO-2, was successfully launched on 2 July 2014 (http://www.nasa.gov/mission_pages/oco2/index.html). The measurements collected by OCO-2 will be combined with data from the ground-based network such as Total Column Carbon Observing Network (TCCON) to provide scientists better understanding of the processes that regulate atmospheric CO_2 and its role in the global carbon cycle. The Chinese carbon dioxide observation satellite (TanSat) [10] and the Chinese scientific satellite (SciSat) are designed to monitoring

CO₂ and supported by the national high technology research and development program of China. They use the technique similar to those of the American OCO-2 and the Japanese GOSAT, respectively, to measure global distributions of CO₂ at high spatio-temporal resolution.

Many algorithms have been developed to retrieve column abundances of trace gases. Buchwitz et al. [11] developed an algorithm based on Differential Optical Absorption Spectroscopy (DOAS) retrieval method for the inversion of SCIAMACHY data. Barkley et al. [12] proposed a Weighting Function Modified Differential Optical Absorption Spectroscopy (WFM-DOAS) inversion algorithm modifying the product from SCIAMACHY. Yoshida et al. [9] described a retrieval algorithm for CO₂ and CH₄ column abundances from short-wavelength infrared spectral observations by the GOSAT TANSO-FTS. Crisp et al. [13] developed the Atmospheric CO₂ Observations from Space (ACOS) retrieval algorithm for OCO-2 and GOSAT. Liu et al. [14] proposed a full physics retrieval algorithm for TanSat XCO₂ monitoring.

According to the requirements of scientific experiments and the features of CO₂-sounder aboard the Chinese scientific satellite, a retrieval algorithm was developed based on SCIATRAN model [15]. In Section 2 of this paper, a brief introduction of CO₂-sounder and the retrieval method are given. The preliminary results and discussion are presented in Section 3, and our conclusion is summarized in Section 4.

2. Methods and data

2.1. The CO₂-sounder

The CO₂-sounder is designed to measure atmospheric CO₂. It is a key instrument on the hyperspectral satellite. The CO₂-sounder detects short-wavelength infrared (SWIR) light reflected from the Earth's surface and scattered and absorbed by atmospheric molecules, aerosols, and clouds. It has four narrow bands in the SWIR region (0.76, 1.57, 1.65, and 2.05 μm) for monitoring gases O₂, CO₂ and CH₄ (Table 1). The satellite will fly in a sun-synchronous orbit and will use three observation modes. In nadir mode, the instrument detects the ground directly below the satellite. In glint mode, the instrument views the “glint” spot where solar radiation is directly reflected from the Earth's surface. In target mode, the instrument tracks the specific surface sites that the ground-based instruments observe atmospheric CO₂ as the satellite flies overhead.

Table 1
CO₂-sounder specifications

Band	Band 1	Band 2	Band 3	Band 4
Central wavelength [μm]	0.765	1.575	1.65	2.05
FWHM of the ILSF	0.6cm ⁻¹	0.27cm ⁻¹	0.27cm ⁻¹	0.27cm ⁻¹
SNR	>300	>300	>250	>250
Target species	O ₂	CO ₂	CH ₄	CO ₂

2.2. The retrieval method

The theoretical basis of retrieval algorithm is the Optimal Estimation method [16]. According to the method, the following equation has to be solved:

$$\mathbf{y} = \mathbf{F}(\mathbf{x}, \mathbf{b}) + \boldsymbol{\varepsilon} \quad (1)$$

where y is the measurement vector, $F(x, b)$ denotes the forward model that describes the physics of the measurement process, x is the state vector to be retrieved, b is a model parameter vector which describes the forward model and is assumed to be known, ε represents the measurement error and the forward model error. To obtain the optimal estimation of x , it is required to minimize the cost and penalty function, defined as

$$J(x) = [y - F(x, b)]^T S_\varepsilon^{-1} [y - F(x, b)] + (x - x_a)^T S_a^{-1} (x - x_a) \quad (2)$$

where x_a is the a priori state of x , S_a the variance covariance matrix of the a priori x_a , and S_ε the covariance matrix of the error ε . To account for the non-linearity of the inversion problem, the solution is found using the Levenberg-Marquardt [17] iterative approach:

$$x_{i+1} = x_i + (S_a^{-1} + K_i^T S_\varepsilon^{-1} K_i + \gamma D)^{-1} \{ K_i^T S_\varepsilon^{-1} [y - F(x_i, b)] + S_a^{-1} (x_i - x_a) \} \quad (3)$$

where the subscript i denotes the index of the i -th iteration; K is the weighting function (Jacobian) matrix, which is the derivative of the forward model as a function of the state vector x ; γ is a non-negative factor chosen at each step to minimize the cost function; and D is a diagonal scaling matrix.

The retrieval process starts with the forward model calculation using the input parameters selected for the radiative transfer model described below in Section 2.3. After the radiative transfer calculations are completed, the simulated radiance and appropriate weighting function are passed to the retrieval algorithm which estimates the desired atmospheric parameters appropriate to the measurement spectra. Due to non-linear of the retrieval problem, an iterative process is applied. Thus the forward

model and the inversion model are run subsequently until the convergence is reached.

To calculate the XCO_2 , the following equation is used:

$$XCO_2 = \frac{CO_2^{col}}{(O_2^{col}/O_2^{mf})} \quad (4)$$

where the CO_2^{col} and O_2^{col} are the CO_2 and O_2 column abundance, respectively; the O_2^{mf} is the dry air mole fraction of O_2 which equate to 0.2095. The CO_2 -sounder algorithm and the GOSAT algorithm are all based on the Optimal Estimation method, but in GOSAT algorithm XCO_2 is obtained as

$$XCO_2 = \frac{V}{h^T I} \quad (5)$$

where the V is the CO_2 column abundance, h is the dry air partial column, superscript T denotes the transpose operation, I is the n-form column-vector with elements of unity. In each iteration step, h is recalculated from the solved surface pressure and H_2O concentration profile. Details are described by Yoshida et al. [9].

Fig. 1. The differences of oxygen cross-section between HITRAN 2004, HITRAN 2008 and HITRAN 2012, taken from Moeini O[18].

2.3. The forward model data

The radiative transfer in the atmosphere is simulated using a model developed

based on the SCIATRAN model [15] and incorporated with the instrument characteristics and observation scenario of the CO₂-sounder. The a priori temperature profiles are obtained from the ERA-Interim (Jan 1979 – present) database of European Centre for Medium-Range Weather Forecasts (ECMWF) profiles (<http://apps.ecmwf.int/datasets/>). The altitude range of the temperature profiles for the algorithm is 0-60 km, but the highest of the ECMWF temperature profiles is only 48 km, so the US standard atmosphere models (Committee on Extension to the Standard Atmosphere, 1976) is combined with the ECMWF data. The temperature profiles are taken from US76 models above 48 km and linear interpolated from the both data at the border. The simulated results prove that the impact of the slight discontinuity of temperature at 48 km on the retrievals is small which is consistent with Tolton and Plouffe [19]. The surface is assumed to be Lambertian and the priori surface albedo products from the MCD43C3 data of Moderate Resolution Imaging Spectroradiometer (MODIS) [20] are interpolated. When the latitude and longitude of the observation in the 0.5°×0.5° grid data of MODIS, the surface albedo is linear interpolated from the four vertex of the region. Because the spectral change of O₂-A band with a maximum of about 15% for different version of HITRAN (Fig. 1)[18], the latest HITRAN 2012 [21] is used as the molecular spectroscopic parameter database. The gaseous absorption spectra are calculated by line-by-line model and a quite small integral step which is 0.005 nm is necessary to get a reasonable accuracy. Otherwise, the accuracy would be suspect according to our simulated results. The Rayleigh scattering properties are computed using the model of Bodhaine et al. [22]

with the refractive index [23] and weighted King factor [24] for air. The aerosol data are taken from LOWTRAN 7 model whose number and top altitudes of aerosol layers are fixed and the relative humidities are some discrete values including 0, 70%, 80% and 99%. The incident solar spectrum is obtained from the solar irradiance database reported by Dr. Kurucz (<http://kurucz.harvard.edu/sun/irradiance2008/>). The weighting function matrixes are computed using discrete-ordinate method.

3. The preliminary results

The GOSAT TANSO-FTS SWIR L1B data (version 161.160) on the 21th day of each month during June 2013 to May 2014 were selected for retrieval experiments. The L1B data were taken as the input to the CO₂-sounder retrieval algorithm, and XCO₂ values were retrieved for each day. The one day XCO₂ retrievals were used to represent individual months, from which the global distribution of XCO₂ for one year was produced. For comparison, our results were one-by-one matched with the corresponding GOSAT retrievals. The relative differences between the matched data pairs were calculated by $(\text{CO}_2\text{-sounder retrievals} - \text{GOSAT Data}) / \text{GOSAT Data}$. The matched data pairs were sorted by the absolute values of the relative differences with an interval of 1%. The number density was defined by the ratio of the paired numbers within each bin to the total data pairs.

The global XCO₂ distribution retrieved from the CO₂-sounder algorithm and from the GOSAT L2 products (version 02.21) are depicted in Fig. 2. For the entire period of the study, the retrieved results showed a tendency for CO₂-sounder retrievals to be smaller than GOSAT products. The global mean values are 390.42 ppm and

394.47 ppm for the CO₂-sounder retrievals and GOSAT products, respectively. Their global mean bias is -4.05 ppm and standard deviation is 6.06 ppm. The relative differences between the two data sets are less than 1% for 51% of the matched data pairs, and less than 2% for 76% pairs.

Fig. 2. (a) The global XCO₂ distribution retrieved from CO₂-sounder algorithm (red cross) and the corresponding GOSAT L2 products (green asterisk) for one day of each month during June 2013 to May 2014. The vertical straight lines represent their global mean values, respectively. (b) The number density distribution of the relative differences (in absolute value) between the CO₂-sounder and GOSAT retrievals.

The seasonal XCO₂ distribution of the CO₂-sounder retrieved and the GOSAT products are described in Fig. 3 and Fig. 4. For the four seasons, the global mean values are 393.16 ppm, 388.70 ppm, 389.00 ppm and 391.01 ppm for the CO₂-sounder retrievals, and are 396.95 ppm, 392.45 ppm, 393.38 ppm and 395.25 ppm for the GOSAT products. In the spring and summer, 77% to 82% CO₂-sounder retrieval results are in close proximity to GOSAT and fell in the 2% deviation region (Fig. 4), and the mean biases are about -3.7 ppm and smaller than 1% (Fig. 3). In contrast, the mean biases of the CO₂-sounder values in the autumn and winter are

about -4.3 ppm, slightly more than 1%, and the standard deviations are also slightly larger than those of spring and summer.

Fig. 3. Same as Fig. 2 (a), but for four seasons represented by one day of each month.

Fig. 4. Same as Fig. 2(b), but for four seasons represented by one day of each month.

The latitude-longitude distributions of the differences between the CO₂-sounder retrievals and GOSAT products are presented in Fig. 5(a), and the zonal means of the differences averaged within a latitudinal interval of 10° are exhibited in Fig. 5(b). As shown in Fig. 5(a), the CO₂-sounder retrieval results of the Southern Hemisphere are especially close to GOSAT products and the large biases of the differences are found at the desert areas such as the Sahara Desert, the Arabian Desert and the Australian Desert, those form the low values center of XCO₂ and the differences between the CO₂-sounder retrievals and GOSAT results are fell in the 3%~4% region. The zonal mean biases of the differences as well as their standard deviation are all smaller than 1% except for the regions of latitude bands of 10°-30°N (Fig. 5(b)) which is consistent with described in Fig. 5(a). The zonal fluctuations of the differences over the Southern Hemisphere are also smaller than those over the Northern Hemisphere (Fig. 2, Fig. 5(b)).

4. Discussions and Conclusions

The radiative transfer model and inversion algorithm have been developed for the CO₂-sounder instrument to be launched on a Chinese satellite. The simulation results of XCO₂ were retrieved from the CO₂-sounder algorithm by using GOSAT L1B spectral data and compared with the GOSAT L2 XCO₂ products to examine the accuracy of the retrieval software.

The CO₂-sounder retrievals for the GOSAT L1B spectra globally observed during June 2013 to May 2014 were generally in agreement with the GOSAT L2 products, with a tendency of the CO₂-sounder retrievals smaller than the GOSAT data. The global mean difference was -4.05 ± 6.06 ppm and the relative differences between the two data sets were less than 1% (in absolute value) for 56% of the matched data pairs, and less than 2% for 83% pairs.

Fig. 5. (a) The global distribution of the XCO₂ differences between the CO₂-sounder retrievals and GOSAT data and (b) the latitudinal distributions of the zonal mean bias and the standard deviation.

The mean biases are about -3.7 ppm within the 1% region in spring and summer. In contrast, the mean biases of the CO₂-sounder values in the autumn and winter are about -4.5 ppm, slightly more than 1%. The seasonal difference is thought to be partly

due to the different vegetation photosynthesis and climate conditions in spring/summer and autumn/winter. Another possible reason could be attributed to the mismatch between the LOWTRAN 7 model used in the simulation calculations and the realistic state of aerosols and clouds during the GOSAT observations. This mismatch could enlarge the uncertainty of the CO₂ retrievals since the clouds and aerosols are the important factors [25] which affect the accuracy of XCO₂ retrievals, especially for the state in autumn and winter.

The CO₂-sounder retrievals and GOSAT products were found in better agreement in the Southern Hemisphere than in the Northern Hemisphere. Also the zonal fluctuations of the differences between the two data sets were smaller over the Southern Hemisphere than over the Northern Hemisphere. This is consistent with the larger bias in the Northern Hemisphere described by Qu et al. [26], and is believed to be associated with the frequent human activities and CO₂ sources in Northern Hemisphere.

The major error source is the uncertainty of the simulation results in the desert area. If the retrieval results of the Sahara Desert and the Arabian Desert were removed from the statistics, the global mean difference could be improved to -2.50 ± 5.21 ppm. It suggests that the estimation and the real properties of the desert were significantly mismatched.

The relative differences between the CO₂-sounder retrievals and GOSAT products were less than 2% (in absolute value) for 76% of the matched data pairs. Recent studies indicated that high precision on regional to global scales is required to

resolve and quantify the small (0.25% to 2%) variations [3] in X_{CO_2} to improve the accuracy of source and sink estimates of CO_2 . The simulation results are generally within the 2% upper limit and suggest the feasibility of the CO_2 -sounder retrieval software, though further refinement is required to improve its accuracy.

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