

# Numerical Deviation Based Optimization Method for Estimation of Total Column CO<sub>2</sub> Measured with Ground Based Fourier Transformation Spectrometer: FTS Data

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**Abstract**—Numerical deviation based optimization method for estimation of total column CO<sub>2</sub> measured with ground based Fourier Transformation Spectrometer: FTS data is proposed. Through experiments with aircraft based sample return data and the ground based FTS data, it is found that the proposed method is superior to the conventional method of Levenberg Marquads based nonlinear least square method with analytic deviation of Jacobian and Hessian around the current solution. Moreover, the proposed method shows better accuracy and required computer resources in comparison to the internationally used method (TCCON method) for estimation of total column CO<sub>2</sub> with FTS data. It is also found that total column CO<sub>2</sub> depends on weather conditions, in particular, wind speed.

**Keywords**—FTS; carbon dioxide; methane; sensitivity analysis; error analysis

## I. INTRODUCTION

Greenhouse gases Observing SATellite: GOSAT carries TANSO CAI for clouds and aerosol particles observation of mission instrument and TANSO FTS<sup>1</sup>: Fourier Transformation Spectrometer<sup>2</sup> for carbon dioxide and methane retrieving mission instrument [1]. In order to verify the retrieving accuracy of two mission instruments, ground based laser radar and TANSO FTS are installed. The former is for TANSO CAI

and the later is for FTS, respectively. One of the other purposes of the ground-based laser radar and the ground-based FTS is to check sensor specifications for the future mission of instruments to be onboard future satellite with extended mission. Although the estimation methods for carbon dioxide and methane are well discussed [2]-[6], estimation method which takes into account measurement noise is not analyzed yet. Therefore, error analysis for additive noise on estimation accuracy is conducted.

In order to clarify requirement of observation noises to be added on the ground-based FTS observation data, Sensitivity analysis of the ground-based FTS against observation noise on retrievals of carbon dioxide and methane is conducted. Experiments are carried out with additive noise on the real acquired data of the ground-based FTS. Through retrievals of total column of carbon dioxide and methane with the noise added the ground-based FTS signals, retrieval accuracy is evaluated. Then an allowable noise on the ground-based FTS which achieves the required retrieval accuracy (1%) is reduced [7].

In the paper, Numerical Deviation Based Optimization Method for Estimation of Total Column CO<sub>2</sub> Measured with Ground Based Fourier Transformation Spectrometer: FTS Data is proposed. Through experiments with aircraft based sample return data and the ground based FTS data, it is found that the proposed method is superior to the conventional method of Levenberg-Marquardt: LM [8] based nonlinear least square method with analytic deviation of Jacobian and Hessian around the current solution [9]. Moreover, the proposed method shows

<sup>1</sup> [http://www.jaxa.jp/projects/sat/gosat/index\\_j.html](http://www.jaxa.jp/projects/sat/gosat/index_j.html)

<sup>2</sup> <http://ja.wikipedia.org/wiki/%E3%83%9E%E3%82%A4%E3%82%B1%E3%83%AB%E3%82%BD%E3%83%B3%E5%B9%B2%E6%B8%89%E8%A8%88>

better accuracy and shorter required computer resources in comparison to the TCCON<sup>3</sup> data [10],[11]) for estimation of total column CO<sub>2</sub> with FTS data. It is also found that total column CO<sub>2</sub> depends on whether condition, in particular, wind speed with aircraft based sample return data [12] and ground based FTS data. The following section describes the proposed method for total column CO<sub>2</sub> estimation with FTS data followed by some experiments with ground based and aircraft based sample return data. Then concluding remarks with some discussions is described.

## II. PROPOSED METHOD

### A. Ground-based FTS

Figure 1 shows schematic configuration of the ground-based FTS which is originated from Michelson Interference Measurement Instrument. Light from the light source divided in to two directions, the left and the forward at the dichotic mirror of half mirror. The left light is reflected at the fixed hold mirror and reaches to the half mirror while the forward light is reflected at the moving mirror and reaches at the half mirror. Then interference occurs between the left and the forward lights. After that interference light is detected by detector. Outlook of the ground-based FTS is shown in Figure2.

Figure 3 (a) shows an example of the interferogram<sup>4</sup> (interference light detected by the detector of the ground-based FTS). By applying Fourier Transformation to the interferogram, observed Fourier spectrum is calculated as shown in Figure 3 (b). When the ground-based FTS observes the atmosphere, the observed Fourier spectrum includes absorptions due to atmospheric molecules and aerosol particles. By comparing to the spectrum which is derived from the radiative transfer code with atmospheric parameters, atmospheric molecules and aerosol particles are estimated.

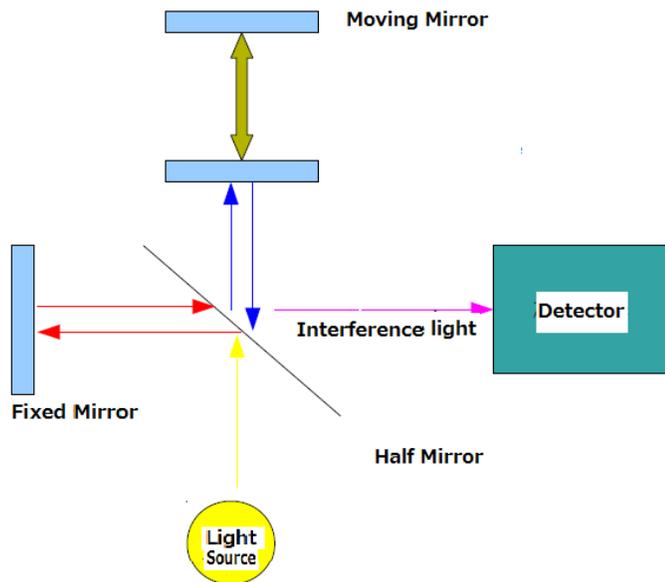


Fig. 1. Michelson Interference Measurement Instrument

<sup>3</sup> [https://tccon-wiki.caltech.edu/Network\\_Policy/Data\\_Use\\_Policy#References\\_and\\_Contact\\_Information](https://tccon-wiki.caltech.edu/Network_Policy/Data_Use_Policy#References_and_Contact_Information)

<sup>4</sup> <http://en.wikipedia.org/wiki/Interferometry>

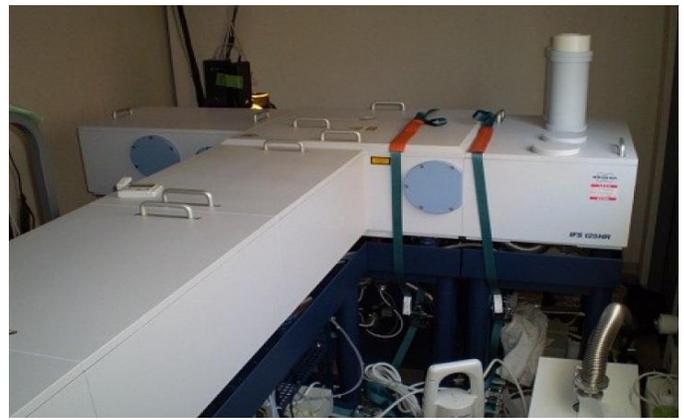
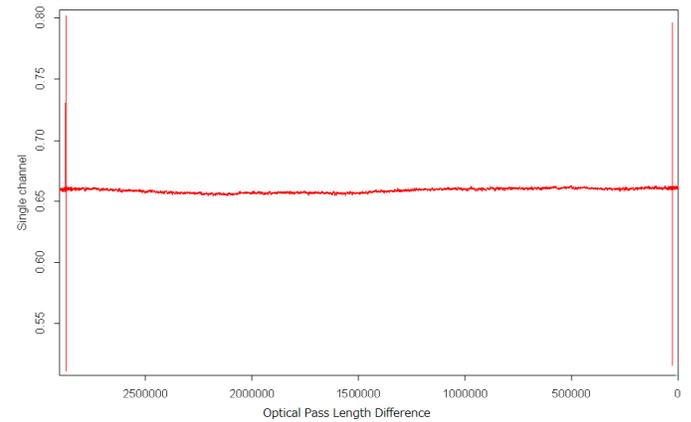
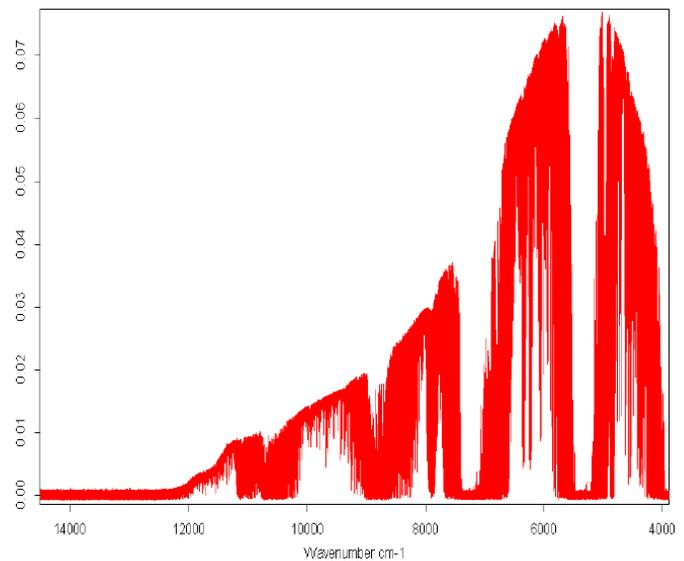


Fig. 2. Outlook of the FTS used



(a)Interferogram

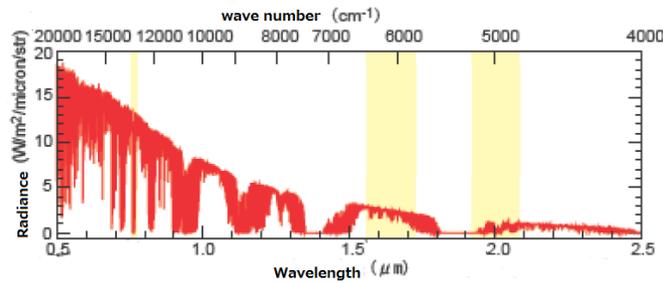


(b)Fourier spectrum

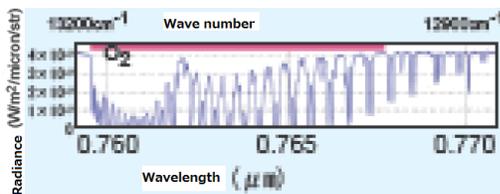
Fig. 3. Examples of interferogram and Fourier spectrum when FTS observes the atmosphere

### B. Principle for Carbon Dioxide and Methane Retrievals with TANSO FTS Data

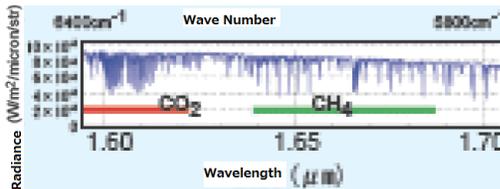
Figure 4 shows a principle of the retrieval method for atmospheric constituents using GOSAT/TANSO data. Figure 4 (a) shows Top of the Atmosphere: TOA radiance in the wavelength ranges from 500 to 2500nm (visible to shortwave infrared wavelength regions). There are three major absorption bands due to oxygen (760-770nm), carbon dioxide and methane (1600-1700nm), and water vapor and carbon dioxide (1950-2050nm) as shown in Figure 4 (b), (c), and (d), respectively. These bands are GOSAT/TANSO spectral bands, Band 1 to 3, respectively. In addition to these, there is another wide spectrum of spectral band, Band 4 as shown in Figure 4(e) which covers from visible to thermal infrared regions.



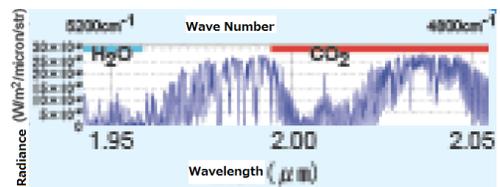
(a)TOA radiance



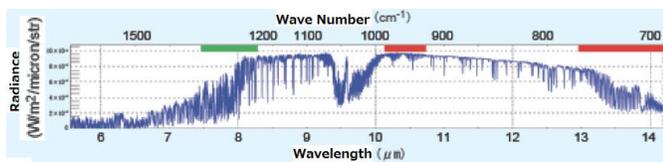
(b)Band 1



(c)Band 2



(d)Band 3



(e)Band 4

Fig. 4. Example of TOA radiance and absorption bands as well as spectral bands of GOSAT/TANSO instrument

### C. Estimation Algorithm Description

The conventional method for estimation of CO<sub>2</sub> is as follows, (1) Estimated spectrum derived from atmospheric simulator with atmospheric parameters including CO<sub>2</sub> and the actual FTS derived spectrum is compared, (2) then the initial atmospheric condition are updated for minimizing the square of difference between spectra derived from simulator and the actual FTS data iteratively. In order to minimize the square of difference, LM method is used in the conventional method as follows,

$$\min S = \sum_{i=1}^N (y_i - y(x_i; \mathbf{a}))^2 \quad (1)$$

where  $S$  denotes square difference,  $y_i$  and  $y(x_i, a)$  denote actual spectrum and simulated spectrum with atmospheric condition of  $a$ ,

$$\mathbf{a} = (a_1, a_2, \dots, a_M) \quad (2)$$

$A$  can be updated as follows,

$$\mathbf{a}_{k+1} = \mathbf{a}_k + \Delta \mathbf{a}_k \quad (3)$$

where  $\Delta \mathbf{a}_k$  is determined as the following equation is satisfied.

$$(\mathbf{H}(\mathbf{a}_k) + \lambda \mathbf{H}(\mathbf{a}_k)) \Delta \mathbf{a}_k = \mathbf{J}^T(\mathbf{a}_k) \Delta \mathbf{y}(x; \mathbf{a}_k) \quad (4)$$

where  $H$  and  $J$  denote Hessian and Jacobian, respectively.

$$\Delta \mathbf{y}(x; \mathbf{a}_k) = (y_1 - y(x_1; \mathbf{a}), y_2 - y(x_2; \mathbf{a}), \dots, y_N - y(x_N; \mathbf{a})) \quad (5)$$

$$\mathbf{J}(\mathbf{a}_k) = \begin{bmatrix} \frac{\partial S}{\partial a_1} & \frac{\partial S}{\partial a_2} & \dots & \frac{\partial S}{\partial a_M} \\ \frac{\partial S}{\partial a_1} & \frac{\partial S}{\partial a_2} & \dots & \frac{\partial S}{\partial a_M} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial S}{\partial a_1} & \frac{\partial S}{\partial a_2} & \dots & \frac{\partial S}{\partial a_M} \end{bmatrix} \quad (6)$$

$$\mathbf{H}(\mathbf{a}_k) = \begin{bmatrix} \frac{\partial^2 S}{\partial a_1 \partial a_1} & \frac{\partial^2 S}{\partial a_1 \partial a_2} & \dots & \frac{\partial^2 S}{\partial a_1 \partial a_M} \\ \frac{\partial^2 S}{\partial a_2 \partial a_1} & \frac{\partial^2 S}{\partial a_2 \partial a_2} & \dots & \frac{\partial^2 S}{\partial a_2 \partial a_M} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 S}{\partial a_M \partial a_1} & \frac{\partial^2 S}{\partial a_M \partial a_2} & \dots & \frac{\partial^2 S}{\partial a_M \partial a_M} \end{bmatrix} \quad (7)$$

where

$$\frac{\partial S}{\partial a_l} = -2 \sum_{i=1}^N \{y_i - y(x_i; \mathbf{a})\} \frac{\partial y(x_i; \mathbf{a})}{\partial a_l} \quad (8)$$

$$\frac{\partial^2 S}{\partial a_l \partial a_m} = 2 \sum_{i=1}^N \left[ \frac{\partial y(x_i; \mathbf{a})}{\partial a_l} \frac{\partial y(x_i; \mathbf{a})}{\partial a_m} - \{y_i - y(x_i; \mathbf{a})\} \frac{\partial^2 y(x_i; \mathbf{a})}{\partial a_l \partial a_m} \right] \quad (9)$$

when the current solution is reached to one of minima,  $y_i - y(x_i; \mathbf{a}) \approx 0$  so that the following approximation becomes appropriate,

$$\frac{\partial^2 S}{\partial a_l \partial a_m} = 2 \sum_{i=1}^N \frac{\partial y(x_i; \mathbf{a})}{\partial a_l} \frac{\partial y(x_i; \mathbf{a})}{\partial a_m} \quad (10)$$

In the solution space, the updated solution can be determined with relatively small step size for all directions in isotropic manner in the LM method as shown in Figure 5.

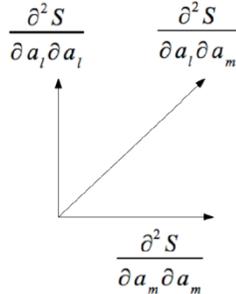


Fig. 5. Solution update directions for LM method

The method proposed here is the solution update direction can be determined arbitrary as shown in Figure 6.

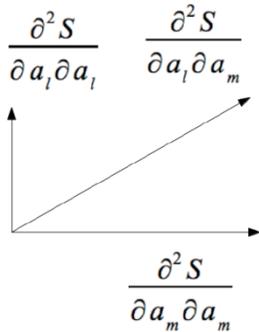


Fig. 6. Solution update directions for the proposed method

### III. EXPERIMENTS

#### A. Ground-based FTS Data Used

The ground-based FTS data used for experiments are acquired on November 14 and December 19 2011. Figure 7 shows the interferograms derived from the acquired the ground-based FTS data.

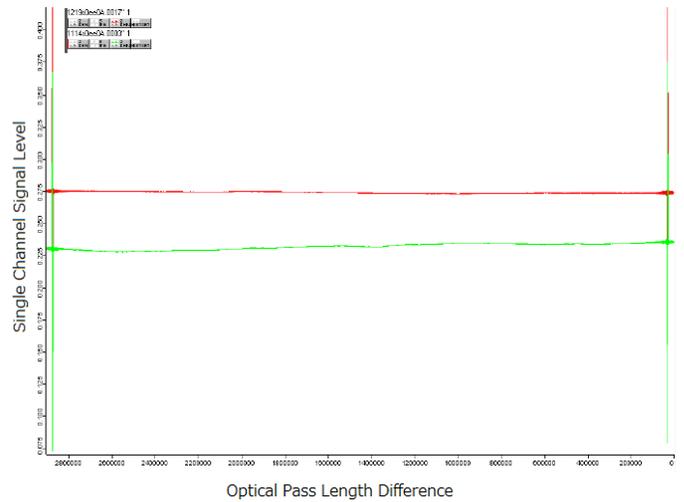


Fig. 7. Example of interferograms used for experiments

#### B. Experimental Method

Observation noise is included in the observed interferograms. In addition to the existing noise, several levels of additional noises which are generated by random number generator of Messene Twister with zero mean and several standard deviations is added on to the iterferograms as shown in Figure 8.

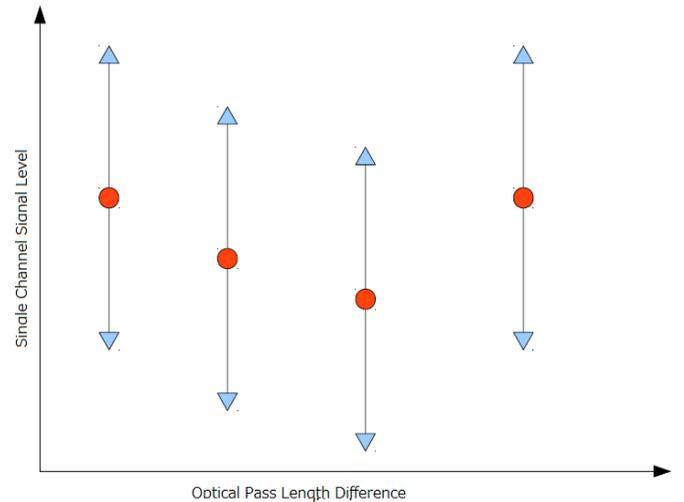


Fig. 8. Method for adding the noises to the acquired interferograms

C. Aircraft Based Sample Return Data Derived Total Column CO<sub>2</sub>

Aircraft based sample return data is acquired with aircraft altitude of 500 m and 7km. Therefore, CO<sub>2</sub> for the atmosphere between two altitude can be retrieved. Using GlovalView-CO<sub>2</sub> model, CO<sub>2</sub> for the atmosphere above 7km is estimated. Also, it is assumed that CO<sub>2</sub> for the atmosphere below 500m can be the same CO<sub>2</sub> at 500m.

The conventional method utilizes the vertical profile model of GlobalView-CO<sub>2</sub>. The profile can be estimated with the following equation,

$$c_s = \gamma c_a + \left( \frac{VC_{G,ak}^{aircraft} - \gamma VC_{G,ak}^{apriori}}{VC_{air}} \right) \quad (11)$$

where  $c_s$  denotes averaged column density of the dried atmosphere,  $VC_{G,ak}$  denotes total column gas amount which is calculated with Rogers and Connor equation and vertical profile derived from the aforementioned model. Also,  $VC_{G,ak}^{aircraft}$  denotes total column gas amount at the aircraft altitude.

D. Aircraft Based Sample Return Data Used

Aircraft based sample return data which are acquired on January 9 2012, January 13 2012 and January 15 2013 are used together with match-upped data of ground based FTS data. The number of data for each day is 116, 52, and 200 files, respectively.

E. Experimental Results

Total column CO<sub>2</sub> for three days of experiments is estimated with the proposed method and compared to the TCCON data, Ohyama (LM method based retrieval) as well as actual aircraft based sample return data derived total column CO<sub>2</sub>. Figure 9 shows the results.

As shown in Table 1, it is found that the proposed method is superior to the other conventional methods in terms of estimation accuracy and the required computer resources. One of the reasons for this is that the proposed method allows update the next solution to the arbitrary directions with relatively large steps.

Table 2 shows weather conditions, atmospheric pressure, air temperature on the ground, Relative Humidity (RH), irradiant flax and the averaged wind speed on the ground. It was cloudy on January 9 and 13, 2012. In particular on January 13 2012, it was poor sun shine time period. Therefore, there are so many data missing.

On the other hand, it was fine on January 15 2013. Therefore, the number of data points is greater than the other two days.

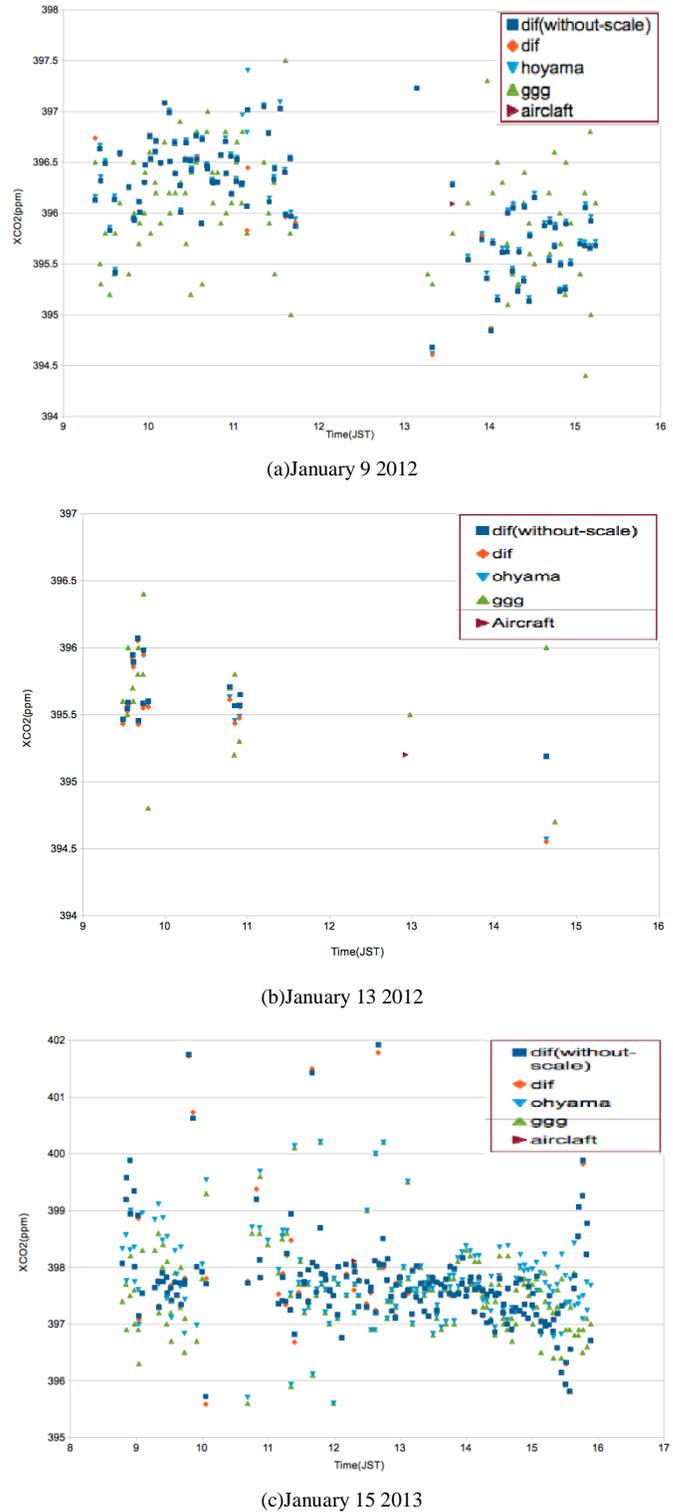


Fig. 9. Comparison among the estimated total column CO<sub>2</sub> derived from the proposed method, the conventional methods, TCCON and LM method based retrievals

TABLE I. COMPARISON OF THE RESIDUAL RMS ERROR AGAINST TRUTH DATA DERIVED FROM AIRCRAFT WITH VERTICAL PROFILE MODEL AMONG THE PROPOSED, LM METHOD AND TCCON DATA

Date	Proposed	LM	TCCON
2012/1/9	0.429	0.438	0.467
2012/1/13			
2013/1/15	0.315	0.32	0.986

TABLE II. WEATHER CONDITIONS OF THE DATES FOR EXPERIMENTS

Date	Pressure (hPa)	Temp. (°C)	RH(%)	Irradiant Flux(MJ/m <sup>2</sup> )	Wind(m/s)
2012/1/9	1022.8	7	66	9.23	2.7
2012/1/13	1020.1	4.8	65	4.99	1.8
2013/1/15	1019	6.7	55	12.39	4.2

#### IV. CONCLUSION

Numerical deviation based optimization method for estimation of total column CO<sub>2</sub> measured with ground based Fourier Transformation Spectrometer: FTS data is proposed. Through experiments with aircraft based sample return data and the ground based FTS data, it is found that the proposed method is superior to the conventional method of Levenberg Marquads based nonlinear least square method with analytic deviation of Jacobian and Hessian around the current solution. Moreover, the proposed method shows better accuracy and required computer resources in comparison to the TCCON data for estimation of total column CO<sub>2</sub> with FTS data. It is also found that total column CO<sub>2</sub> depends on weather conditions, in particular, wind speed.

Through the experiments with aircraft based sample return data (as the truth data) together with ground based FTS data, it is found that the proposed method is superior to the other conventional methods in terms of estimation accuracy and the required computer resources. One of the reasons for this is that the proposed method allows update the next solution to the arbitrary directions with relatively large steps.

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