A new approach to HDO/H_2O ratio profile retrieval in the atmosphere from TANSO-FTS/GOSAT-2 spectrum data by using TIR and SWIR spectral ranges simultaneously: method and software

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Motivation

Satellite remote sensing of the isotopic composition of water vapor in the Earth's atmosphere is an actual problem, particularly HDO/H_2O isotope ratio retrieval. Condensation of the heavy water isotopologue HDO is faster, and the evaporation is slower, unlike the main isotopologue $H_2{}^{16}O$, and every evaporation and condensation process leads to a decrease in the relative HDO content in atmospheric water vapor. Thus, the isotope ratio is the tracer of hydrological cycle and contains information about origin and circulation of air masses in atmosphere **[Brenninkmeijer C.A.M. et al., 2003]**.

GOSAT/GOSAT-2

The Japanese satellite GOSAT (Greenhouse gases Observing SATellite) was launched in 2009 with TANSO sensor on board. TANSO sensor (Thermal And Near-infrared Sensor Observation) contains The TANSO-FTS high-resolution Fourier spectrometer, designed to simultaneously measure outgoing spectra in four IR ranges from 0.75 to 14.3 microns, and a four-channel TANSO-CAI radio-meter (Cloud and Aerosol Imager) for the detection of cloud and aerosol fields. To continue GOSAT project NIES (National Institute for Environmental Studies) and JAXA (Japan Aerospace Exploration Agency) developed and launched the new GOSAT-2 satellite with the upgraded TANSO-FTS-2 and CAI-2 in 2018.

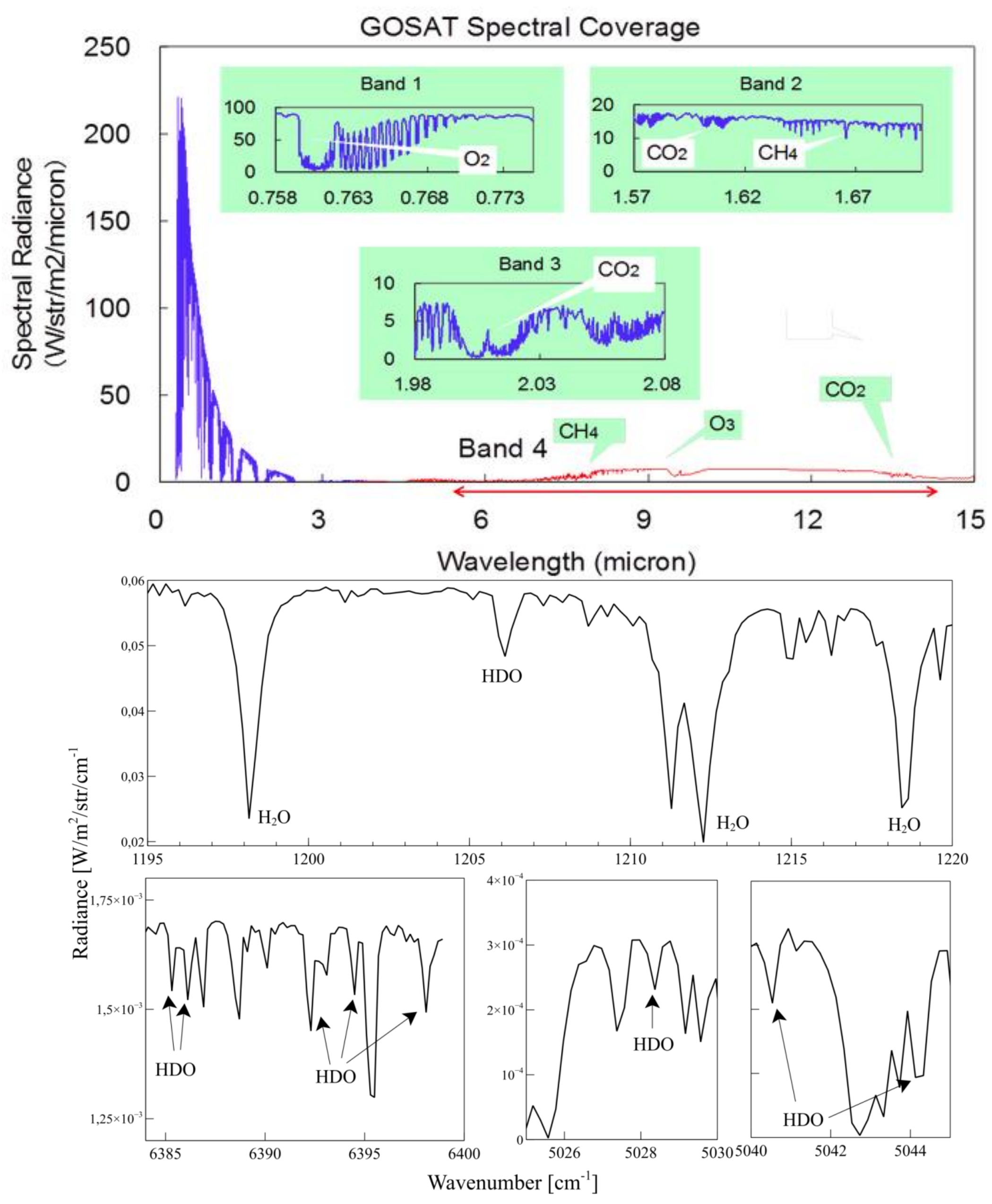

Fig. 1 – TANSO-FTS spectral bands **[https://www.eorc.jaxa.jp/GOSAT/mission.html]** and HDO spectral lines in TANSO-FTS: Band 4 (TIR), Band 2 and Band 3 (SWIR)

Method

The isotopic composition of the sample is usually expressed in delta values. The HDO/$H_2{}^{16}O$ ratio is commonly given in δD value:

$$\delta D=\left(\frac{(HDO/H_2O)_{sample}}{(HDO/H_2O)_{std}}-1\right)\cdot 1000$$

$(HDO/H_2O)_{sample}$ – relative concentration of sample, $(HDO/H_2O)_{std}$ = 3.1152×10^{-4} – Standard Mean Ocean Water (SMOW).

Following the **[Rodgers C.D., 2000]**, the forward problem in general form can be represented as:

$$\mathbf{y}=F(\mathbf{x})+\boldsymbol{\varepsilon}_{\mathbf{y}}$$

where **y** – measured spectrum, **x** – vector of atmospheric parameters, $\boldsymbol{\varepsilon}_{\mathbf{y}}$ – measurement error.
If we separate the forward model into TIR and SWIR, then equation can be written using the block representation of matrix-columns:

$$\begin{bmatrix}\mathbf{y}_{TIR}\\ \mathbf{y}_{NIR}\end{bmatrix}=\begin{bmatrix}\mathbf{F}_{TIR}(\mathbf{x})\\ \mathbf{F}_{NIR}(\mathbf{x})\end{bmatrix}+\begin{bmatrix}\boldsymbol{\varepsilon}_{yTIR}\\ \boldsymbol{\varepsilon}_{yNIR}\end{bmatrix}$$

$F_{TIR}(\mathbf{x})$, $F_{NIR}(\mathbf{x})$, $\boldsymbol{\varepsilon}_{yTIR}$, $\boldsymbol{\varepsilon}_{yNIR}$ – forward problems and measurement errors of TIR and SWIR ranges. Here, we used optimal estimation method to solve the inverse problem. This method is based on Bayesian estimates of atmospheric state, includes a priori information on atmospheric parameters in the form of multidimensional normal distribution and includes noise characteristics of the spectrometer. The cost function is minimized:

$$J(\mathbf{x})=[\mathbf{y}-\mathbf{F}(\mathbf{x})]^T\mathbf{S}_y^{-1}[\mathbf{y}-\mathbf{F}(\mathbf{x})]+[\mathbf{x}-\mathbf{x}_a]^T\mathbf{S}_a^{-1}[\mathbf{x}-\mathbf{x}_a]$$

$\mathbf{S_y}$ – covariance matrix of measurement errors, $\mathbf{S_a}$ – a priori covariance matrix of atmospheric parameters, $\mathbf{x_a}$ – a priori vector of atmospheric parameters. Minimization of cost function and vertical concentration profile retrieval is carried out according to the following iterative formula:

$$\mathbf{x}_{i+1}=\mathbf{x}_i+\left(\mathbf{K}_i^T\mathbf{S}_y^{-1}\mathbf{K}_i+\mathbf{S}_a^{-1}\right)^{-1}\left[\mathbf{K}_i^T\mathbf{S}_y^{-1}(\mathbf{y}-\mathbf{F}(\mathbf{x}_i))-\mathbf{S}_a^{-1}(\mathbf{x}_i-\mathbf{x}_a)\right]$$

$\mathbf{x}_i$ – retrieved vector of atmospheric parameters, $\mathbf{K}_i$ –Jacobian matrix, which is the derivative of forward model as a function of the state vector: $\mathbf{K}_i=\partial F(\mathbf{x}_i)/\partial \mathbf{x}_i$

$$J(\mathbf{x})=J_{TIR}(\mathbf{x})+J_{NIR}(\mathbf{x})+[\mathbf{x}-\mathbf{x}_a]^T\mathbf{S}_a^{-1}[\mathbf{x}-\mathbf{x}_a],$$

$$J_{TIR}(\mathbf{x})=[\mathbf{y}_{TIR}-\mathbf{F}_{TIR}(\mathbf{x})]^T\mathbf{S}_{yTIR}^{-1}[\mathbf{y}_{TIR}-\mathbf{F}_{TIR}(\mathbf{x})]\ \text{and}\ J_{NIR}(\mathbf{x})=[\mathbf{y}_{NIR}-\mathbf{F}_{NIR}(\mathbf{x})]^T\mathbf{S}_{yNIR}^{-1}[\mathbf{y}_{NIR}-\mathbf{F}_{NIR}(\mathbf{x})]$$

minimization of cost function is carried out using the iterative formula taking into account the following block representation of its matrices and vectors:

$$\mathbf{y}_i=\begin{bmatrix}\mathbf{y}_{TIR}\\ \mathbf{y}_{NIR}\end{bmatrix},\quad \mathbf{F}(\mathbf{x})=\begin{bmatrix}\mathbf{F}_{TIR}(\mathbf{x})\\ \mathbf{F}_{NIR}(\mathbf{x})\end{bmatrix},\quad \mathbf{K}_i=\begin{bmatrix}\mathbf{K}_{iTIR}\\ \mathbf{K}_{iNIR}\end{bmatrix},\quad \mathbf{S}_y=\begin{bmatrix}\mathbf{S}_{yTIR} & \mathbf{0}\\ \mathbf{0} & \mathbf{S}_{yNIR}\end{bmatrix}$$

Software

The FIRE-ARMS software **[Gribanov K.G. et al., 2001]** (Fine Infrared Explorer for Atmospheric Radiation Measurements) is designed for retrieval of vertical profiles of temperature, humidity and content of various greenhouse gases from TIR spectra. This software was supplemented by VLIDORT procedures **[Spurr R., 2006]**. VLIDORT is vectorial linearized model of radiation transfer taking into account scattering in multilayer atmosphere, based on discrete ordinate method. The model includes single and multiple light scattering for various sensing geometry and various types of surface. VLIDORT also contains procedures for calculating profile Jacobians on a given grid of atmospheric layers. Model spectra are calculated line-by-line using precalculated look-up tables of cross sections.

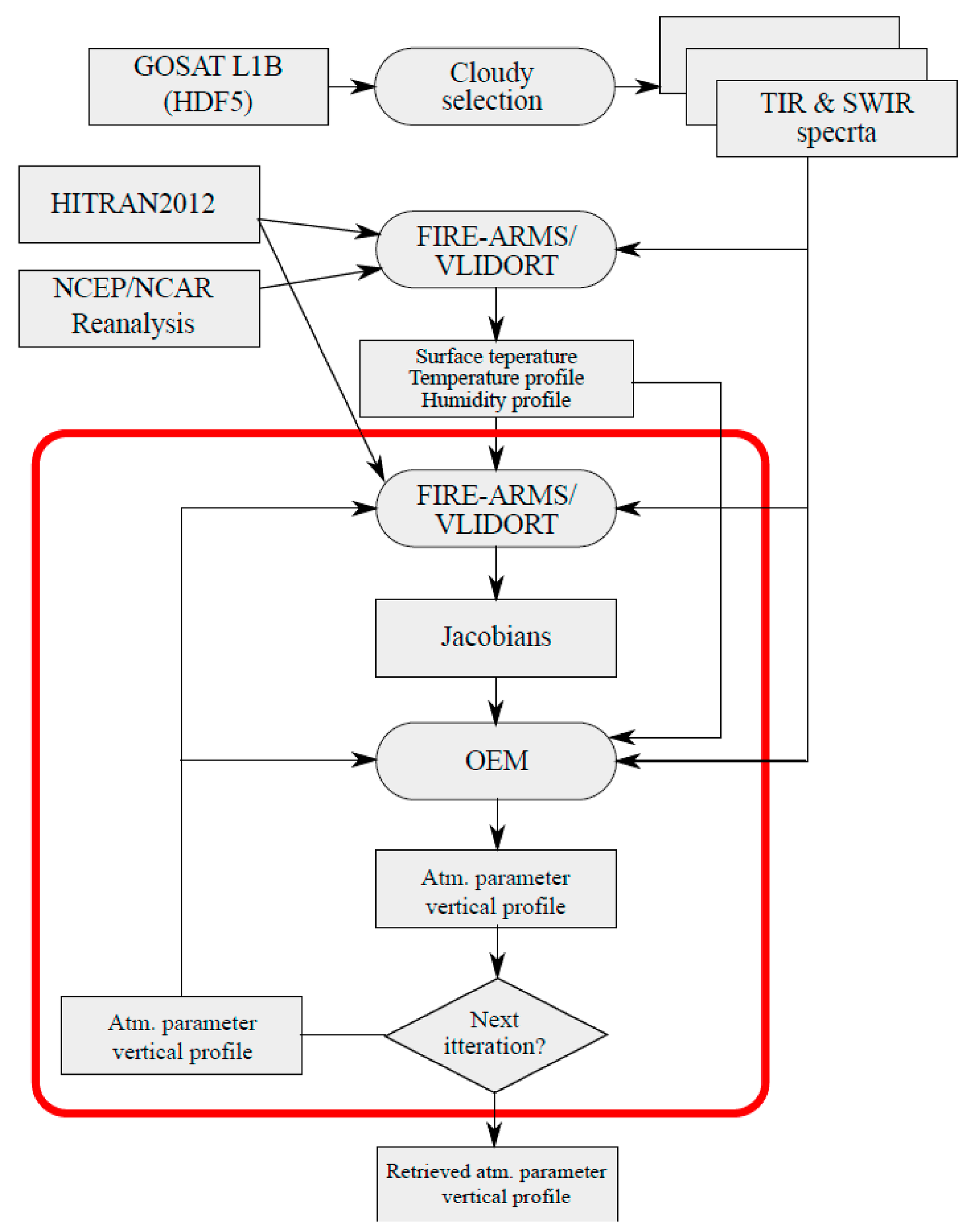

Fig. 2 – Rectangular blocks indicate data, rounded blocks indicate procedures; the fragment in the frame is the loop. The software also includes procedures for extracting GOSAT spectra from HDF5 files, calculating an initial guess of temperature and humidity vertical profiles from CAMS ECMWF reanalysis data

δD vertical profile retrieval

Here, we simultaneously retrieved logarithm of vertical profile concentration of main water isotopologue **[Schneider M. et al, 2006]** and vertical profile of δD, in this case vector of atmospheric parameters is presented as $\mathbf{x}=(ln(N_{H2O})_1,\ldots,\ ln(N_{H2O})_n,\delta D_{n+1},\ldots,\ \delta D_{2n})$, n – vertical mesh dimension. A priori covariance matrix is calculated using the isotopic version of general atmospheric circulation model ECHAM5-iso **[Werner M. et al, 2011].** The measured spectra were simulated with TANSO-FTS/GOSAT-2 parameters. A posteriori covariance matrix that characterizes retrieval error is calculated. The square root of diagonal elements has the dimension of desired value and practically represents the error in determining the atmospheric parameter.

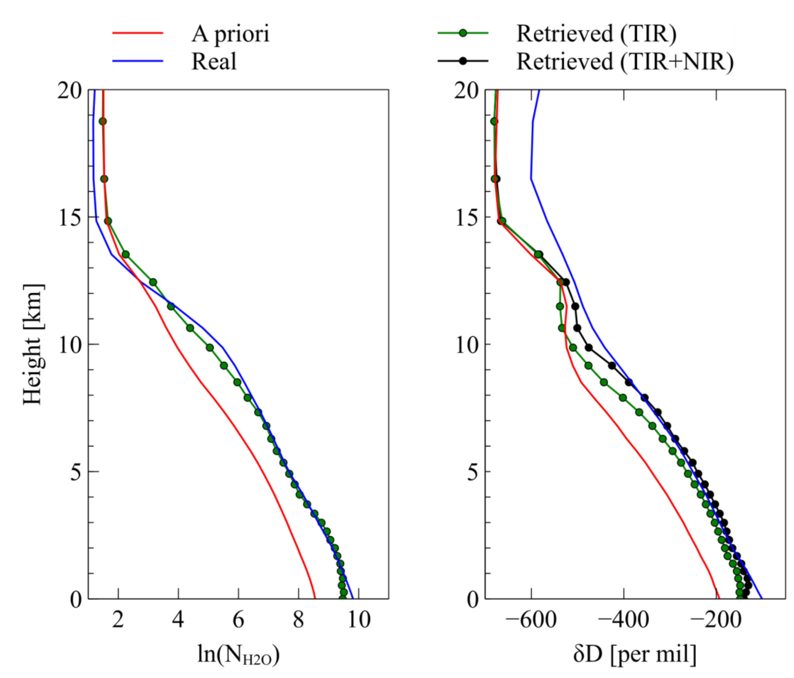

Fig. 3 – A priori (red), real (blue) and retrieved profiles of $log(H_2O)$ and δD from TIR (green) and SWIR (black) simulated spectra of TANSO-FTS/GOSAT-2

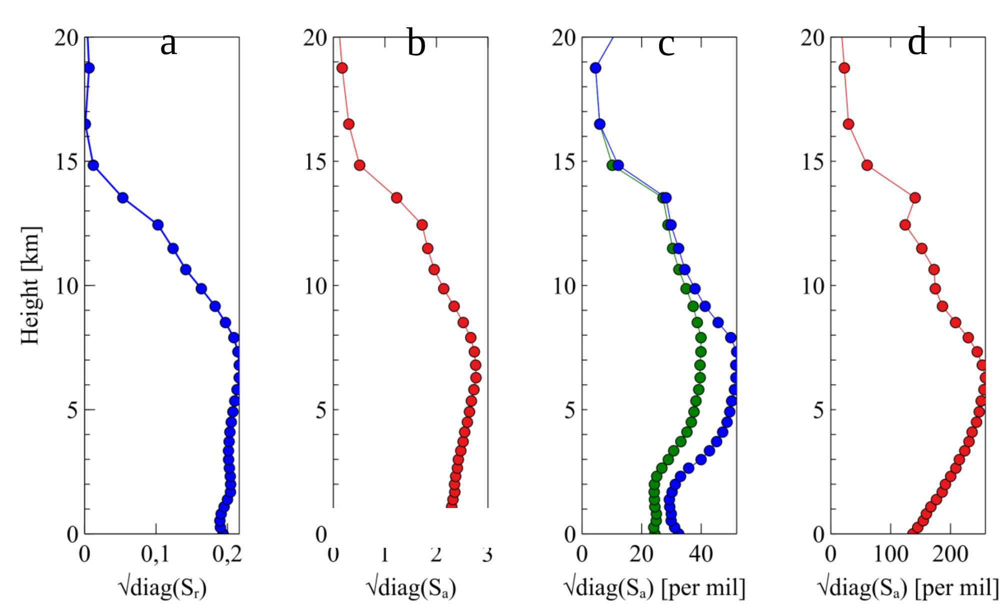

Fig. 4 – A posteriori standard deviations for vertical profiles $log(H_2O)$ (a,b) and δD (c,d) retrieval; TIR (blue) and SWIR (green) in comparison with a priori error

Conclusion

A software version has been created that allows joint use of TIR and SWIR spectral ranges to retrieve vertical profiles of HDO/$H_2{}^{16}O$ ratio in the atmosphere by optimal estimation method. A priori statistical ensemble was calculated using output data of ECHAM5-iso general atmospheric circulation model. In model experiments using model spectra, we have shown that simultaneous use of both spectral ranges (thermal and shortwave IR) to retrieve vertical profiles of δD in the atmosphere can improve accuracy compared to using each of ranges separately.

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