Iteration Method for Simultaneous Estimation of Vertical Profiles of Air Temperature and Water Vapor with AQUA/AIRS Data

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Abstract—Iteration method for simultaneous estimation of vertical profiles of air temperature and water vapor with the high spectral resolution of sounder of AQUA/AIRS data is proposed. Through a sensitivity analysis based on the proposed method for the several atmospheric models simulated by MODTRAN, it is found that the proposed method is superior to the conventional method by 41.4% for air temperature profile and by 88.9% for relative humidity profile.

Keywords—Inversion; tropopause; AQUA; AIRS; Air temperature; sounder; MODTRAN

I. INTRODUCTION

Atmospheric sounding can be improved by using the high spectral resolution of sounder, such as AQUA¹/AIRS² onboard AQUA satellite, IASI³, instead of HIRS⁴, TOVS⁵ used in the past [1]. Estimation of air-temperature profile with AQUA/AIRS data on the tropospheric boundary is tried [2]. Meanwhile, water vapor and air-temperature profile estimation with AIRS data based on Levenberg-Marquadt is proposed [3]. On the other hand, a sensitivity analysis for air temperature profile estimation method around the tropopause using simulated AQUA/AIRS data is carried out [4]. Also, a method for water vapor profile retrievals by means of minimizing difference between estimated and brightness temperature derived from AIRS data and radiative transfer model is proposed [5].

These sensors have large number of channels, and have large amount of atmospheric sounding information in the measurement data. However, for the retrieval of air temperature profile, it is not practical nor an advantage to use all spectral points. Therefore, it is important for this work to eliminate those redundant channels whose information does not add to the final retrieval accuracy and even before for the sake of efficiency, those channels potentially contaminated by solar radiation or significantly affected by other gases (not required for temperature profiling). Because of the influence due to the thermal radiation from earth's surface and the sharp variation of air temperature at around tropopause⁶, on the other hand, the retrieval accuracies of air temperature at the surface and around the tropopause are not so high (~4 K) in the previous works⁷ even using the high spectral resolution of sounder. One of the factors for this result is caught by insufficient channels selection. Some of redundant channels have to be removed from the air temperature profile estimation.

In this paper, a simultaneous estimation of vertical profiles of air temperature and water vapor with AQUA/AIRS data is proposed. There is a relation between vertical files of air temperature and water vapor. For instance, when sea surface temperature is raised then water vapor in the atmosphere is increased accordingly. Vertical profiles estimation accuracies can be improved if the relation is used in the estimation method. In order to confirm the effect of simultaneous estimation, MODTRAN⁸ (Moderate Resolution Transmittance Code) is used for simulation.

The following section describes the theoretical background and related research works followed by the proposed method. Then, sensitivity analysis is described followed by simulation result. Finally, conclusion is described with some discussions and future research work.

II. PROPOSED METHOD AND RELATED STUDIES

A. Theoretical Background and Related Studies

The general forward model of the equation mapping the state (atmospheric profile) into measurement space (satellite-measured radiance or brightness temperature spectrum) is expressed as follows [6]:

$$y = F(x) + \varepsilon \tag{1}$$

Where, y is the measurement vector, F(x) is the forward model operator for a given state x, and ε is the measurement error.

The measurement error characteristics should be known, and the measurements *y* should be corrected before using them

¹ https://aqua.nasa.gov/

²https://ja.wikipedia.org/wiki/Aqua_(%E4%BA%BA%E5%B7%A5%E8%A1%9B%E6%98%9F)

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⁴https://www.eumetsat.int/website/home/Satellites/CurrentSatellites/Meto p/MetopDesign/HIRS/index.html

⁵ https://eosweb.larc.nasa.gov/content/tovs

⁶ https://en.wikipedia.org/wiki/Tropopause

⁷ https://climatedataguide.ucar.edu/climate-data/airs-and-amsu-

tropospheric-air-temperature-and-specific-humidity

⁸ http://modtran.spectral.com/

in the retrieval. Given a reasonable air temperature profile for x, equation (1) can be approximately linearized as follows:

$$y - y_0 = K_0 (x - x_0)$$
(2)

Where, $K_0 = \partial F(x) / \partial x$ is the weight function matrix with respect to x_0 , and x_0 is suitable reference state.

For the retrieval of air temperature profile from brightness temperature measurements y, the inverse problem associated with (1) is proposed by the concept of Bayesian optimal estimation⁹ described by Rodgers [6] as follows:

$$x = x_a + \left(K^T S_{\varepsilon}^{-1} K + S_a^{-1}\right)^{-1} K^T S_{\varepsilon}^{-1} \left(y - F(x_a)\right)$$
(3)

Where, x_a is a priori profile for air temperature, S_a is the a priori error covariance matrix and S_{ε} is the measurement error covariance matrix. *K* is the weighting matrix. $F(x_a)$ are the brightness temperatures from simulation with respect to x_a . Considered the problem is nonlinear, an iterative optimal estimation is selected as follows:

$$x_{i+1} = x_a + \left(K_i^T S_{\varepsilon}^{-1} K_i + S_a^{-1}\right)^{-1} K_i^T S_{\varepsilon}^{-1}((y - F(x_i)) + K_i(x_i - x_a))$$
(4)

Where, subscript *i* is the iteration index. The optimum can be obtained only by $2 \sim 4$ iterations because the problem is moderately nonlinear. This is the conventional method for vertical profile estimation with thermal infrared sounder data. Namely, vertical profile of air temperature is estimated separately with that of water vapor, independently.

With respect to high spectral resolution of sounder, thousands of measurements data are obtained in accordance with the channels. Air temperature profile (x) to only a few dozens of air temperatures at different altitude levels is usually dispersed. It is not practical nor an advantage to use all spectral points. Some of them, which information are not required for temperature profiling, even decrease the retrieval accuracies. Thus, it is important to sufficiently select channels suitable for the retrieval of air temperature profile.

B. Principle of Vertical Profile of Air Temperature and Water Vapor Estimations

Fig. 1 is spectral absorption characteristic in thermal IR region. The region $620 \sim 740 \text{ cm}^{-1} \text{ CO}_2$ absorption bands can be used for the retrieval of air temperature profile. More accurate reduction of the abundant channels is adopted the Information Content (IC) measure ¹⁰ as described by Rodger [7].

It, however, generally used in pre-process for the inverse scheme. It also means that the channels cannot be changed as the inverse scheme described as above to retrieve the air temperature profile after the pre-process for channels selection is performed. From the line-by-line computation for absorbance coefficient, on the other hand, absorbance coefficient is not only depended on the spectrum, but also associated with the air temperature [8]. Meanwhile, it is nonlinear between the absorbance coefficient and the air temperature. One channel which information can add best to the retrieval accuracies at the certain temperature may not be at the other temperature. This relation becomes more significant at around the tropopause of which the sharp equatorial structure with the sharp temperature changes. One of the factors, thus, that result in the difficulty to improve the retrieval accuracies of air temperature at around tropopause is that the channels cannot change in the inverse scheme with respect to the different retrieval temperature profile.

As mentioned before, there is cross link between air temperature and water vapor. Therefore, it may be possible to improve estimation accuracy by using the relation. Iteration method for simultaneous estimation of air temperature and water vapor profiles is then proposed.



Fig. 1. Spectral absorption characteristic in thermal IR region.

III. PROPOSED METHOD

A. Weighting Function

The weighting function is expressed as follows:

$$K = \partial T_{h} / \partial T \tag{5}$$

Where, T_b denotes brightness temperature while *T* denotes air temperature. At sensor brightness temperature, Tb and air temperature, T can be estimated with MODTRAN. Fig. 2(a) shows an example of the input parameters of MODTRAN while Fig. 2(b) shows the output of Tb and T come out from MODTRAN.

⁹ https://en.wikipedia.org/wiki/Bayesian_optimization

¹⁰ https://en.wikipedia.org/wiki/Information_criterion

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1489	6,716	0.4602	0.4771	0.9936	1.0000	1.0000	1.0000	0.9706	1.0000	1.0000	1.0000	1.0000	3,905	
1490.	6.711	0.2927	0.3037	0.9935	1.0000	1.0000	1,0000	0.9703	1.0000	1.0000	1.0000	1.0000	4.612	
1491.	6.707	0.2580	0.2677	0.9934	1.0000	1.0000	1.0000	0.9699	1.0000	1.0000	1.0000	1.0000	5.354	
1492.		0.8484						0.9695					5.506	
1493.	6.698	0.8629	0.8974	0.9923				0.9691					5.643	
1494.	6.693	0.8844	0.9193	0.9932	1.0000	1.0000	1.0000	0.9687	1.0000	1.0000	1.0000	1.0000	5.758	
1485.	6.689	0.7652	0.7958	0.9931	1.0000	1.0000	1.0000	0.9683	1.0000	1.0000	1.0000	1.0000	5.993	
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Fig. 2. Example of input parameters and output of MODTRAN.

Thus, atmospheric transparency can be estimated with MODTRAN followed by weighting function because the derivative of the transparency is weighting function. Fig. 3 shows an example of estimated atmospheric transparency and weighting function.

If the input parameter of certain wave number is selected for MODTRAN, then weighting function can be estimated accordingly as shown in Fig. 4.



Fig. 3. Example of estimated atmospheric transparency and weighting function.



Fig. 4. Example of atmospheric transparency.



Fig. 5. Weighting functions for the wave number, 1478、1483、1508、 1514、1519、1541、1544、1558、1585 cm⁻¹.

When the wave number of $1478 \times 1483 \times 1508 \times 1514 \times 1519 \times 1541 \times 1558 \times 1585 \text{ cm}^{-1}$ is selected, then the weighting functions are estimated as shown in Fig. 5.



0 0 0.005 0.01 0.015 0.02 0.025 0.03 0.035 0.04 0.045 0.05 (b) Air temperature

Fig. 6. Finding most appropriate wave number for estimation of water vapor and air temperature profiles.

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Fig. 7. Relation between CO_2 transparency and altitude while weighting function of CO_2

This is the same thing for estimation of weighting functions at arbitrary wave numbers as shown in Fig. 6. When the wave number is selected at the water vapor absorption bands, then weighting function for water vapor profile estimation can be selected as shown in Fig. 6(a). That is the same thing for air temperature profile estimation. When the wave number is selected at the air temperature absorption bands, then weighting function for air temperature profile estimation can be selected as shown in Fig. 6(b).

As shown in Fig. 4, atmospheric transparency due to carbon dioxide of air temperature is calculated with MODTRAN. Fig. 7(a) shows the relation between CO_2 transparency and altitude while weighting function of CO_2 is shown in Fig. 7(b).





Fig. 8. Relation between H_2O transparency and altitude while weighting function of H_2O .

On the other hand, Fig. 8(a) shows the relation between H_2O transparency and altitude while weighting function of H_2O is shown in Fig. 8(b).

B. Relation between Water Vapor and Air Temperature

It is possible to calculate air temperature and precipitable water, or water vapor content in the atmosphere by using MODTRAN. Fig. 9(a) shows the relation for Mid-Latitude Summer in day time model while Fig. 9(b) shows the relation for Mid-Latitude Winter in night time model, respectively.



Fig. 9. Relation between air temperature and water vapor.



(b) Mid-latitude winter (day time) Fig. 10. Relation between air temperature and water vapor.

Meanwhile, Fig. 10(a) shows the relation for Mid-Latitude Summer in night time model while Fig. 10(b) shows the relation for Mid-Latitude Winter in day time model, respectively.

As shown in Fig. 9 and 10, it is obvious that there is relation between air temperature and water vapor. Therefore, it may be possible to improve estimation accuracy by using the relation. Iteration method for simultaneous estimation of air temperature and water vapor profiles is then proposed.

The proposed method is an iteration method. Firstly, initial value of air temperature and relative humidity is selected. Then, air temperature profile is estimated with the initial value of relative humidity by the conventional method. After that, relative humidity is estimated with the estimated air temperature profile just mentioned above by the conventional method. These processes are repeated iteratively until the residual error reaches to the convergence radius.

IV. ACCURACY EVALUATION

A. Preliminary Results

When the wave number of $1478 \\ 1483 \\ 1508 \\ 1514 \\ 1519 \\ 1541 \\ 1544 \\ 1558 \\ 1585 \\ cm^{-1}$ is selected, then the weighting functions are estimated as shown in Fig. 5. Fig. 11 shows water vapor (Relative Humidity) profile estimated with the conventional method. In the figure, solid line shows MODTRAN derived profile while dotted line shows the estimated profile with the conventional method. There are some differences as shown in Fig. 11 clearly.



TABLE I. EXAMPLE OF THE ESTIMATION ACCURACY EVALUATION RESULT FOR RELATIVE HUMIDITY PROFILE FOR MID-LATITUDE SUMMER MODEL

Wave number -1 cm	Peak (km)	Correct Rh (%)	Estimated R h(%)	Diff.
1585	4	39.049	42.640	3.591
1402	5	31.417	33.380	1.963
1602	6	29.980	22.828	7.152
1608	7	30.310	32.359	2.049
1567	8	29.630	22.573	7.057
1650	10	29.440	35.553	6.113
1671	11	19.480	18.332	1.148
1700	12	10.694	9.329	1.365

Estimation accuracy is calculated through comparisons between the estimated relative humidity and the MODTRAN derived humidity. An example of the estimation accuracy evaluation result is shown in Table I.

B. Results for the Proposed Method

Fig. 12(a) and (b) shows air temperature (a) and relative humidity (b) profiles of MODTRAN derived and the estimated by the conventional method as well as the estimated by the proposed method, respectively.

TABLE II. RMSE: ROOT MEAN SQUARE ERROR OF THE CONVENTIONAL AND THE PROPOSED METHODS FOR ESTIMATION OF AIR TEMPERATURE (T) AND RELATIVE HUMIDITY (RH) PROFILES

Profile	Conventional	Proposed		
(T)	1.031(K)	0.607(K)		
(RH)	1.779(%)	0.197(%)		



Fig. 12. Air temperature (a) and relative humidity (b) profiles of MODTRAN derived and the estimated by the conventional method as well as the estimated by the proposed method.

Table II shows RMSE: Root Mean Square Error of the conventional and the proposed methods for estimation of air temperature (T) and relative humidity (RH) profiles. It is obvious that the proposed method is superior to the conventional method by 41.4 % for air temperature profile and by 88.9 % for relative humidity profile.

V. CONCLUSION

Iteration method for simultaneous estimation of vertical profiles of air temperature and water vapor with the high spectral resolution of sounder of AQUA/AIRS data is proposed. Through a sensitivity analysis based on the proposed method for the several atmospheric models simulated by MODTRAN, it is found that the proposed method is superior to the conventional method by 41.4 % for air temperature profile and by 88.9 % for relative humidity profile.

Further study is highly required for another experiment with a variety of dataset and atmospheric conditions.

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