INVERSION OF MOISTURE PROFILES BY A NONLINEAR ITERATIVE PHYSICAL RETRIEVAL*

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Received August 13, 2003; revised November 12, 2003

ABSTRACT

The Advanced TIROS-N Operational Vertical Sounder (ATOVS) measurements are used to generate the atmospheric parameters, such as temperature and moisture profiles, under both clear and cloudy situations. This paper describes briefly the nonlinear iterative physical retrieval method. By using this retrieval scheme, an experiment has been carried out to retrieve the moisture profiles from ATOVS measurements on the NOAA-16 satellite for July of 2002. ATOVS profile retrieval results are evaluated by root mean square (RMS) differences with respect to RAdiosonde OBservation (RAOB) profiles. The accuracy of the retrieval is about 15%—23% for the relative humidity profile in this study.

Key words: ATOVS measurements, regression retrieval method, nonlinear iterative physical retrieval method, root mean square error

I. INTRODUCTION

Retrieving temperature and humidity profiles from satellite data started in the 1970s, the retrieval method has been improved greatly with the advanced techniques in remote sensing and computer. Many retrieval methods have been developed over the last three decades. These retrieval methods go into two categories: statistical regression technique and physical retrieval technique.

Statistical regression techniques are based on the relationship between atmospheric profiles and satellite observations. A set of historical satellite measurements and the collocated RAOB profiles are used to generate the regression coefficients for further application in the profile retrieval with real satellite data. The statistical regression based on the use of eigenvectors of statistical covariance matrices was widely used to interpret satellite sounding observations (Smith and Woolf 1976). Constraining the retrieval to be around the mean climate values prevents the result from an unrealistic profile. This kind of retrieval runs very fast since the regression does not deal with the forward calculation as

* Supported by the National Key Basic Research and Development Program granted by the Ministry of Science and Technology of China with a project number of 2001CB309402.

well as the weighting function.

Physical retrieval methods generate directly the atmospheric profiles from the satellite measurements. Therefore a fast radiative transfer model is exploited to calculate the synthetic spectral radiances from initial guess profiles. The best estimation is the one which minimizes the difference between the synthetic radiance and the real satellite observation. The physical retrieval is an iterative process achieved by adjusting the initial guess. Two physical retrieval schemes are widely used. These are the Simultaneous Physical Retrieval Method (SPRM, Smith et al. 1985) and the SPRM-based minimum variance simultaneous retrieval (Fleming et al. 1986). Their main characteristics are to retrieve simultaneously the atmospheric temperature profile, water vapor profile as well as the surface temperature. Chedin and Scott (1985) proposed the Improved Initialization Inversion (3I) method. At NSMC the statistical regression scheme was replaced by the physical retrieval scheme which itself has been updated several times (Li et al. 1993; Zhang et al. 1997). New retrieval methods have been developed since 1998 (Lavanant et al. 1999; Li et al. 2000; Wu et al. 2001). Different method may differ in the selection of initial guess, fast forward radiative transfer model, the cloud detection algorithm, etc. In contrast with temperature retrieval, humidity profile is more complicated due to its high nonlinearity with the observed radiance. This paper focuses mainly on the water vapor retrieval while many other articles focus on the temperature retrieval. The nonlinear iterative physical retrieval method is used to derive the moisture profile in our experiment. Those uncontaminated microwave channels are exploited to obtain the moisture profiles in many cloudy situations.

II. ATOVS MEASUREMENTS

In May of 1998, a new series of NOAA Polar-orbiting Operational Environmental Satellites commenced with the successful launch of NOAA-15. Its successors NOAA-16 & 17 were launched in 1999 and 2002 respectively. The onboard Advanced TOVS suite is comprised of two sounding instruments. One instrument is the twenty-channel High-resolution Infrared Radiation Sounder (HIRS/3). The other is the twenty-channel instrument of the Advanced Microwave Sounding Unit (AMSU). Two separate radiometers (AMSU-A for temperature sounding and AMSU-B for humidity sounding) comprise the AMSU instrument. The new generation satellite represents a dramatic improvement in microwave technology that will significantly enhance the atmospheric sounding capabilities in cloudy situation. The AMSU instrument has better atmospheric sounding capabilities in all weather conditions than the previous instrument mainly for atmospheric sounding in clear situation. AMSU-B built in U. K. is the first humidity sounding unit flown on the NOAA satellite. It was designed to mainly measure water vapor in five channels, one of which is located in the window region, another is in the weak water vapor absorption line, and the others are in the water vapor absorption band. AMSU-B is a cross-track radiometer with a swath of 2250 km. The instrument completes one scan line every 8/3 seconds with a total of 90 Earth fields-of-view. Spatial resolution at nadir is normally 16 km. Table 1 lists the AMSU-B channel characteristics.

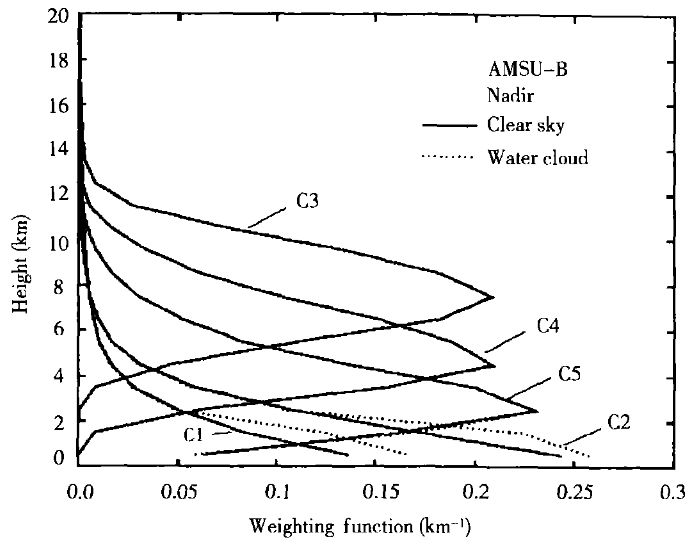

Fig. 1. The weighting functions of AMSU-B.

Table 1. AMSU-B Channel Characteristics and the Main Sounding Purposes

Channel number	Center frequency (GHz)	Bandwidth (MHz)	Major absorbing constituents	Peak altitude (hPa)	Main sounding purposes
1	89.0±0.9	1000	window	surface	surface characteristics, precipitation etc.
2	150.0±0.9	1000	H_2O	1000	precipitable water etc.
3	183.31±1.00	500	H_2O	400	atmospheric moisture
4	183.31±3.00	1000	H_2O	600	atmospheric moisture
5	183.31±7.00	2000	H_2O	800	atmospheric moisture

The weighting functions of AMSU-B are illustrated in Fig. 1. Each curve corresponds to certain channel's sensitivity for atmospheric information at different altitude. It can be seen that the radiance in Channel 1 comes mainly from surface, Channel 2 from the boundary layer, Channels 3—5 from the layer between 400 hPa and 800 hPa. In order to demonstrate the different impact of water cloud on window channel and water vapor channels, Fig. 1 also shows the weighting functions for both clear atmosphere (solid) and atmosphere with cloud water (dashed). It can be seen that water cloud has a significant impact on Channels 1—2 while having minor impact on Channels 3—5. Therefore the precipitation and cloud liquid water could be estimated from the radiances of Channels 1—2.

Moisture profiles had not been retrieved due to the severe interference of AMSU-B on-board NOAA-15 in our early study (Wu et al. 2001). However, this paper focuses on the moisture retrieval.

III. THE FUNDAMENTAL BACKGROUND OF PHYSICAL RETRIEVAL

It states that water vapor, carbon dioxide, ozone, and other gases are not only the absorbers, but also the emitters in the atmosphere. The absorbed energy is pertinent to the absorbers' amount as well as their characteristics. With the radiance measurement from satellite instruments in the absorption band, a sounding capability of deriving atmospheric temperature and moisture, and other constituent profile is assured. If we neglect scattering by the atmosphere in local thermodynamic equilibrium, the radiance emitted by the earth-atmosphere system is approximated by the following atmospheric radiative transfer equation:

$$R = \varepsilon B_s \tau_s - \int_0^{p_s} B \mathrm{d}\tau(0, p) + (1 - \varepsilon) \int_0^{p_s} B \mathrm{d}\tau^* + R', \tag{1}$$

where $\tau^* = \tau_s^2/\tau$, R is the spectral radiance in the infrared region or brightness temperature in the microwave region, B is the Planck radiance which is a function of temperature and pressure p, subscript s denotes surface, and τ is the atmospheric transmittance function of absorber coefficient and amount from level p to space. The moisture is implicitly taken into account in the transmittance term. R' represents the contribution of reflected solar radiation in the infrared region, ε is the surface emissivity assumed to be equal to 1.0 for infrared window channel. If the satellite observed radiance is known, then R can be considered a nonlinear function of the atmospheric temperature profile, water vapor profile, etc.

The calculation of weighting function or transmittance is the kernel in the physical retrieval of atmospheric parameters. For any channel, the distribution of the weighting function is related to the atmospheric layer interacting with the observed radiative intensity. In the medium absorption band, the emission from the lower atmosphere can hardly reach the satellite instrument due to the absorption from the atmosphere above. On the other hand, the emission from upper atmosphere has small contribution to satellite measurement due to the sparse atmosphere in upper layers. There exists a peak altitude for each weighting function. In the weak absorption band, the effective radiance comes from the lower atmospheric layer, weighting function peaks at a lower level. In the strong absorption band, the peak altitude of weighting function is high. With a given channel, the observed radiance is obtained from the atmospheric temperature, moisture, and the amount of other absorbing constituents. According to this radiation principle, several physical retrieval methods have been developed to derive the vertical profiles of temperature and moisture, etc. Mathematically, atmospheric parameter retrieval is to solve equation (1). But there is no unique solution for this kind of equation. A smaller error in the measurement can be greatly amplified in the retrieval result. Consequently, constrain must be set to insure accurate and meteorological meaningful retrieval results in the procedure for obtaining the solution.

IV. NONLINEAR ITERATIVE PHYSICAL RETRIEVAL

The nonlinear iterative physical retrieval method proposed by Li et al. (2000) of University of Wisconsin was implemented in the International ATOVS Processing Package (IAPP). It converges quickly to simultaneously derive the atmospheric temperature profiles, moisture profiles, surface temperature, total ozone amount, etc. If the satellite observed radiance R of each channel is known, then R can be considered as a nonlinear function of the atmospheric temperature profile, water vapor mixing ratio profile, surface temperature, microwave surface emissivity, etc. That is $R=R(T, q, T_s, \varepsilon, \cdots)$, or in general matrix form:

$$Y = F(X), \tag{2}$$

where the vector X contains 42 levels of atmospheric temperature, 42 levels of atmospheric water vapor mixing ratio, one surface temperature, one microwave surface emissivity, etc., and Y contains N satellite observed radiances. The linear form of Eq. (2) is

$$\delta Y = F' \cdot \delta X, \tag{3}$$

where F' is the linear or tangent model of the forward model F. F' is also called weighting function matrix and these weighting functions can be calculated by a differential scheme or perturbation method, especially for the water vapor mixing ratio and ozone mixing ratio components. However, an accurate and efficient way to calculate the weighting functions is necessary for real-time data retrieval processing. A general form of the minimum variance solution is to minimize the following penalty function (Rodgers 1976)

$$J(X) = [Y^m - Y(X)]^T E^{-1} [Y^m - Y(X)] + [X - X_0]^T H [X - X_0]. \tag{4}$$

The following quasi-nonlinear iterative form is obtained by using Newtonian iteration

$$\delta X_{n+1} = (F'^T_n \cdot E^{-1} \cdot F'_n + H)^{-1} \cdot F'^T_n \cdot E^{-1} \cdot (\delta Y_n + F'_n \cdot \delta X_n), \tag{5}$$

where $\delta X_n = X_n - X_0$, $\delta Y_n = Y^m - Y(X_n)$, X is the atmospheric profile to be retrieved, X_0 is the initial guess of the atmospheric profile, Y^m is the vector of the observed radiances or brightness temperatures used in the retrieval process, E is the observation error covariance matrix which includes instrument noise and forward model error, H is the a priori matrix which constrains the solution, and superscript T denotes the transpose. H can also be the inverse of the a priori initial guess error covariance matrix. If the statistics of measurement and a priori error covariance matrix is Gaussian, then the maximum likelihood solution is obtained.

Usually $H = \gamma I$ is applied in Eq. (5), where γ is a smoothing factor, then

$$\delta X_{n+1} = (F'^T_n \cdot E^{-1} \cdot F'_n + \gamma I)^{-1} \cdot F'^T_n \cdot E^{-1} \cdot (\delta Y_n + F'_n \cdot \delta X_n). \tag{6}$$

While the smoothing factor γ is extremely important in the solution, but it is very difficult to determine. γ is dependent upon the observation, the observation error, and the initial guess of the atmospheric profile. It is often chosen empirically. The smoothing factor plays a critical role in the solution; if γ is too large, then the solution is over constrained and large biases could be created in the retrieval; if γ is too small, the solution is under-constrained and possibly unrealistic. The following formula is applied to determine the smoothing factor γ.

$$\| F(X(\gamma)) - Y^m \|^2 = \sigma^2, \tag{7}$$

where $\sigma^2 = \sum_{k=1}^{N} e_k^2$, e_k is the square root of the diagonal of E or the observation error of channel k, which includes instrument error and forward model error. Usually σ^2 can be estimated from the instrument noise and the validation of the forward radiative transfer model used in the retrieval. A simple numerical approach is adopted for solving Eq. (7), γ is changed in each iteration according to

$$\gamma_{n+1} = q_n \cdot \gamma_n, \tag{8}$$

where q is an increasing or decreasing factor for γ. Based on Eq. (7), q is obtained in each iteration by the following conditions:

$$q_0 = 1;$$
$$\text{If } \| F(X_n) - Y^m \| < \sigma^2, \text{ then } q_n = 1.5;$$
$$\text{If } \| F(X_n) - Y^m \| = \sigma^2, \text{ then iteration stops};$$
$$\text{If } \| F(X_n) - Y^m \| > \sigma^2, \text{then } q_n = 0.8.$$

The q factor has been found from empirical experience to insure that the solution is stable from one iteration to the next. γ will keep changing until the iteration stops.

To assure the retrieval accuracy, a precise knowledge of the instrument performance and the accuracy of the atmospheric transmittance functions for the various spectral channels is crucial. A fast and accurate transmittance model is utilized for the forward radiative calculation (Hannon et al. 1996), in which a 42 pressure level vertical coordinate is adopted from 0.1 to 1050 hPa.

V. MOISTURE PROFILE RETRIEVAL AND RESULT ANALYSIS

The nonlinear iterative physical retrieval method is implemented in our experiment of retrieving the moisture profiles from ATOVS measurements on the NOAA-16 satellite for July of 2002. Satellite measurements from two water vapor channels (CH11 − 12) of HIRS/3 and three water vapor channels of AMSU-B are mapped into a grid of approximately 50 km for retrieving the vertical moisture profiles. This grid corresponds to 2 by 2 HIRS fields of view.

1. *Determination of the Initial Guess*

Since the retrieval problem is ill-posed, additional information is needed to constrain the solution. Often this is accomplished by means of an initial guess profile obtained from a climatological library, regression retrieval from radiance, and numerical weather prediction (NWP) products. Usually it is easy to obtain the initial guess from a climatological library, but these historical profiles must be representative. Regression retrieval could be implemented conveniently as in our experimental study. NWP products are good resources for the initial guess in the physical retrieval, but the quality of NWP profile products is crucial. The access of NWP products must be guaranteed for the real-time data processing system. Our initial guess of temperature, water vapor, ozone profile and surface temperature is obtained by statistical regression based on the NOAA/NESDIS NOAA88 global radiosonde data set which has 8834 atmospheric profiles. The regression coefficients are generated by the forward calculation of AMSU-A and HIRS/3 radiances and the statistical regression analysis. The local satellite zenith angle of observation, the surface terrain elevation, and the land/sea tag are also used as predictors to allow the direct use of non-limb adjusted radiances. The advantage of the regression equation using the theoretical calculation over the real observation is that it avoids errors due to the temporal and spatial differences between satellite observation and radiosonde profile.

2. *Quality Control in Retrieving Procedure*

Several checks are made for quality control in the retrieving procedure.

(1) *Convergence check*

The following quantity is computed to check the convergence

$$\chi_i = |X_i - X_{i-1}|. \tag{9}$$

If $\chi_{i+1} > \chi_i$ within 2 iterations which means the iteration diverging, then the iteration stops, and the retrieval is set to be the initial guess; otherwise keeps iterating until $\chi <$ 0.25, or a maximum of 10 iterations is reached. Usually, more than 95% of solutions obtain convergence.

(2) *Saturation check*

Each level of the water vapor profile is checked for supersaturation in each iteration. If a level is supersaturated, 100% of relatively humidity is assumed.

(3) *AMSU-A cloud check*

The AMSU-A scattering index and discriminate functions (Grody 1999) are used to obtain the surface characteristics such as sea ice concentration, precipitation identification, and snow cover. The derived scattering index and rainfall index can be used to reject unreasonable retrievals. The scattering index (SI) is defined as

$$SI = \begin{cases} -113.2 + (2.41 - 0.0049 \times T23) \times T23 + 0.454 \times T31 - T89, & \text{water} \\ T23 - T89 & \text{land} \end{cases} \tag{10}$$

The above forms are valid for water and land respectively, where $T23$, $T31$ and $T89$ are the brightness temperatures for AMSU-A Channels 1, 2 and 15 respectively. These window channels are used to measure precipitation and cloud liquid water. They also play an important role in cloud detection. Mie theory predicts that scattering is negligible when the hydrometeor size is smaller compared to the wavelength for observations. In the presence of large hydrometeors or cloud, their absorption will become dominant at higher frequency (89 GHz). It decreases the microwave brightness temperature at 89 GHz, making the difference of $T23 - T89$ much larger. This microwave cloud detection is only used over land surface. Grody's scattering index serves as the criteria of cloud detection over ocean. If the scattering index is greater than 35, then the retrieval box is rejected for further processing.

3. *Validation of the Retrieval Results*

The RAOB data are used to evaluate the moisture retrieval. The primary validation strategies consist of: 1) vertical accuracy statistics, 2) comparison of vertical profile, and 3) horizontal field analysis. Each validation scheme is based on a match-up database of RAOB and retrieval result collocations with time and space.

(1) *Processing the match-up data*

The RAOB data were collected and collocated with moisture retrieval for the same period and area. The observing time for RAOB is at 00 and 12 Greenwich Mean Time (GMT) while the NOAA-16 observation time is around 06 and 18 GMT. The distance between two radiosonde stations is usually very large while the distance between two retrievals is about 50 km. Therefore the criteria for collocating the retrieval and RAOB are:

1) temporal difference is within 6 hours; and

2) spatial difference is within 1 degree of latitude/longitude.

Data meeting these two criteria serve as the collocation data for validation. The following vertical accuracy statistics and comparison of vertical profile are based on this match-up database.

(2) *Vertical accuracy statistics*

To illustrate the accuracy of ATOVS retrieval, all the retrieval results are compared with the RAOB profiles. These include the retrievals in clear and cloudy conditions, over sea and land. A total of about 10000 collocated samples are included in July of 2002. The mean bias and root mean square error (RMSE) are obtained by statistical analysis. RMSE is given by

$$\mathrm{RMSE} = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(X_{\mathrm{RAOB}} - X_{\mathrm{ATOVS}})^2}, \tag{11}$$

where X_{RAOB} and X_{ATOVS} are the RAOB observation and ATOVS retrieval respectively, and N is the total number of comparisons.

Figure 2 shows the mean bias and RMSE for relative humidity of the regression and physical retrieval for all clear and cloudy, land and ocean cases. The left panel is for mean bias, and the right for RMSE. Solid line is for physical retrieval, and dot-dashed line for regression guess. It can be seen that the RMSE for relative humidity is about 15%—23%. The results show the minor improvement of the physical retrieval over regression guess, indicating that regression retrieval could achieve good results with the use of sufficient sounding measurements for water vapor. Figures 3 and 4 show the mean bias and RMSE for relative humidity of the regression and physical retrieval for clear and cloudy cases, respectively.

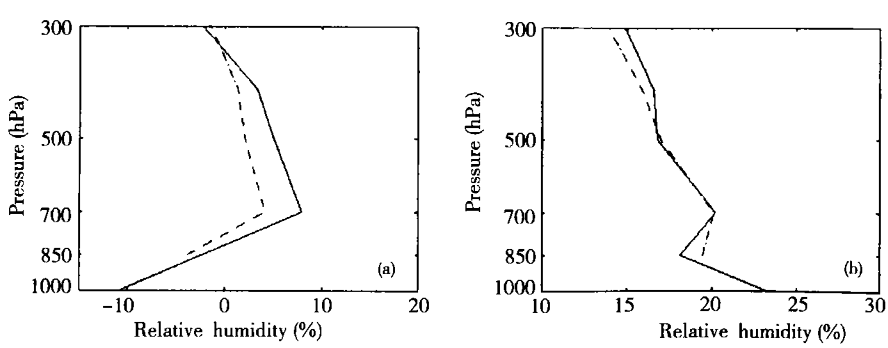

Fig. 2. The comparison of physical and regression retrieval with RAOB profile. The left panel (a) is for mean bias, and the right (b) for RMSE. Solid line is for physical retrieval, and dot-dashed line for regression guess (a total of about 10000 collocated samples are included in July of 2002).

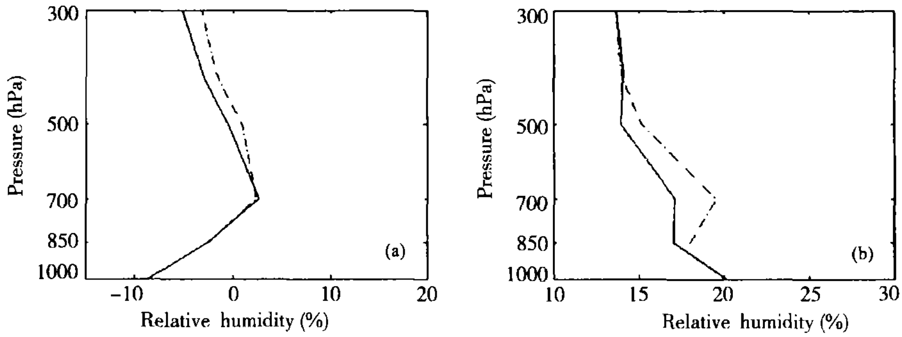

Fig. 3. As in Fig. 2, but for clear cases.

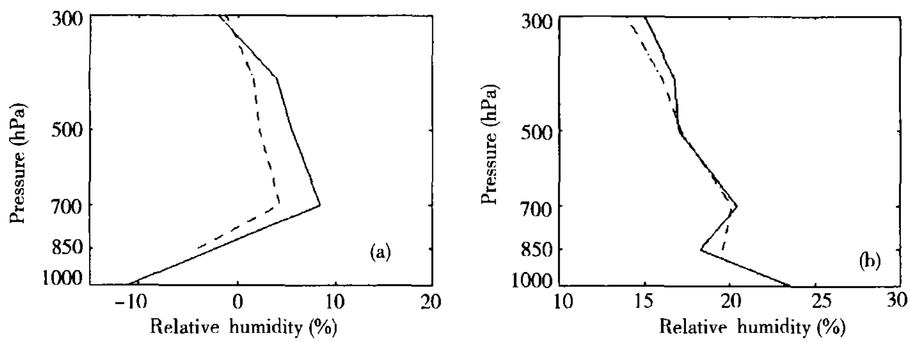

Fig. 4. As in Fig. 2, but for cloudy cases.

(3) *The comparison of vertical profiles*

Two RAOB stations were selected to carry out the case study for ATOVS humidity physical retrieval and regression guess at 18 GMT 23 July 2002. Figure 5 illustrates the comparisons of relative humidity of physical retrieval and regression guess with RAOB for a northern station near Beijing and a southern station near Wuhan, respectively. The left panel is for Beijing, and the right for Wuhan. It can be clearly seen that both results are close to RAOB observations while physical retrieval has substantial improvement over regression guess, especially for Beijing Station.

The comparisons above show that the mean structure of atmospheric moisture profiles can be achieved from ATOVS measurements. However, due to some uncertainties, such as the failure of detecting low-level cloud, surface type uncertainty, surface emissivity error etc., the retrieval may be subject to large error especially in the low atmospheric levels. In order to improve the retrieval in low-level atmosphere, more investigations are needed which focus on the cloud check, surface temperature and the surface emissivity.

(4) *The analysis of horizontal fields*

Horizontal field analysis provides better meteorological context concerning the characteristics of the derived satellite products than the vertical accuracy statistics (Reale 2001). Figures 6 illustrates the NOAA-16 ATOVS retrieved moisture field for 500 hPa at 18 GMT 23 July 2002. Figure 7 displays the water vapor image of AMSU-B Channel 3

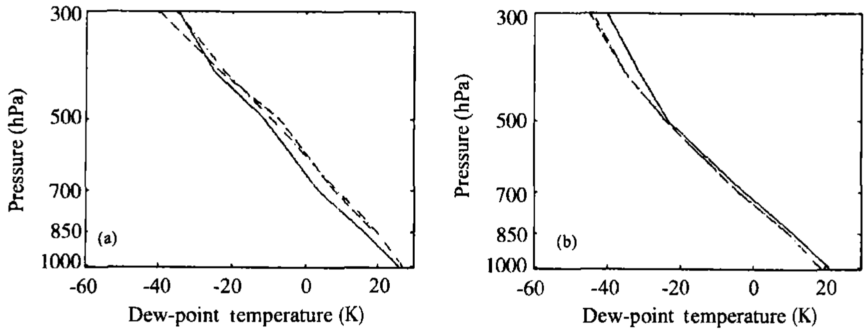

Fig. 5. The comparisons of physical and regression retrieval with RAOB profile. The left panel (a) is for Beijing Station (54511), and the right (b) for Wuhan Station (57494). Solid line is for RAOB profile, dashed line for regression guess, and dot-dashed line for physical retrieval (at 18 GMT 23 July 2002 for ATOVS onboard NOAA-16).

(183 ± 1 GHz) with weighting function peaking at 400 hPa. Good consistency is observed in these two figures, illustrating the robust derived ATOVS products on a regional scale.

4. *Error Analysis*

RAOB observation is often used as "truth" in the statistical analysis of satellite sounding products. Their difference is regarded as "error" in a sense of statistics. However, Their physical meaning is different due to the different measurement means in satellite and conventional sounding. RAOB measures the instantaneous state while the satellite sounding product denotes an average in a column of atmosphere. Moreover,

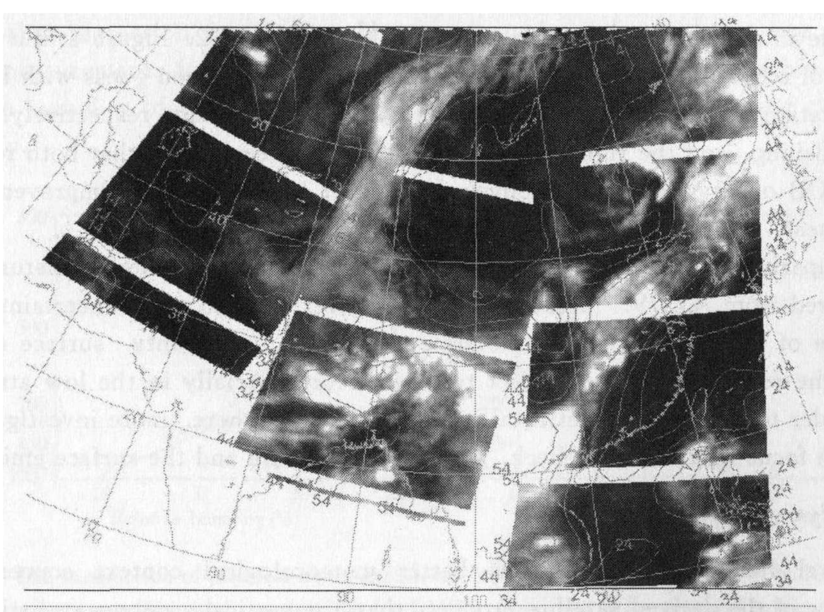

Fig. 6. NOAA-16 ATOVS retrieved moisture field for 500 hPa at 18 GMT 23 July 2002. The brightness temperature of HIRS/3 Channel 10 is displayed in the background.

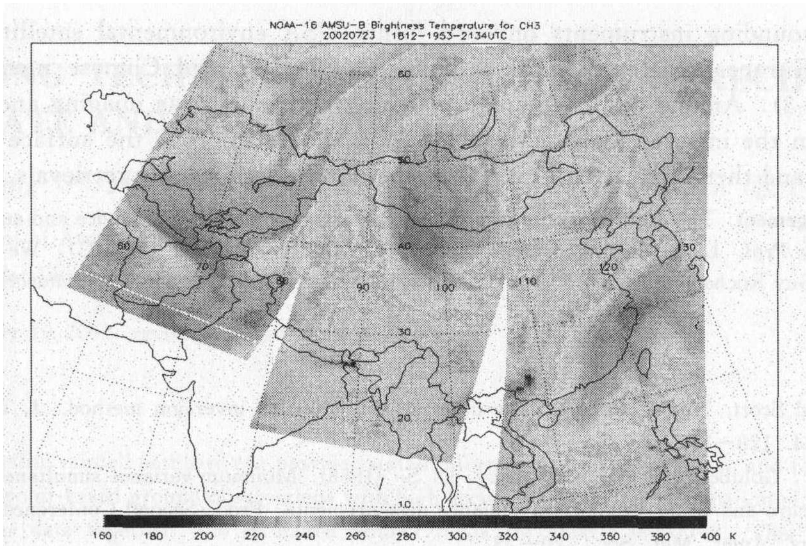

Fig. 7. The water vapor image of NOAA-16 AMSU-B Channel 3 (183 ± 1 GHz) at 18 GMT 23 July 2002. Dark grey represents dry atmosphere, Light grey for wet one.

RAOB itself has a few percent of error. Recently, "error" is replaced by "bias" in the accuracy analysis of the satellite sounding products. The error of satellite sounding product is caused by many factors, i. e.

• Temporal difference between RAOB and ATOVS observations: This is an important factor in causing large errors. For example, the observation time for ATOVS of NOAA-16 is around 06 GMT and 18 GMT while RAOB is at 00 GMT and 12 GMT. They are 6 hours apart. Atmospheric moisture may change greatly in the course of 6 hours.

• Spatial difference between RAOB and ATOVS observations: This is another important factor in causing large errors. One degree of latitude/longitude is the matching distance. Atmospheric moisture may change greatly over such a long distance, especially for complicated topography.

• Error in the guess and retrieval: The quality of initial guess has a direct impact on the accuracy of retrieval product. The retrieving error is also from the radiative forward model which is only a simplified model.

• Error in the satellite observation: Satellite instrument noise and calibration errors are main factors causing radiance error. They could not completely eliminated from the radiance even though corrections have been made in the satellite data preprocessing.

VI. CONCLUSION

By comparing the retrieval with RAOB data, the accuracy of the retrieval is about 15%— 23% for the relative humidity profile. Using ATOVS measurements, the atmospheric humidity can be derived with good accuracy especially in many cloudy conditions. This is the significant improvement over the previous TOVS measurements. Therefore ATOVS measurements have the global accurate moisture sounding capability in nearly all weather conditions. In the future, such retrievals could be improved over China by using the high spectral resolution infrared observation on EOS-Aqua platform, and by using other sounding instruments onboard future USA environmental satellites (NPP, NPOESS), European meteorological satellite (METOP), and Chinese meteorological satellite (FY-3). Among improvements, matching instruments as imaging and sounding radiometers in the infrared and microwave region should improve the surface and cloud information, and then improve the quality of the atmospheric profile retrievals.

Acknowledgement: The authors would like to acknowledge the penetrating advice and suggestions of this research by Prof. LI Guangqing (NSMC) and Prof. DONG Chaohua (NSMC). We owe special thanks to Dr. Guy Rochard of Meteo France/CMS for his thoughtful reviews of the manuscript.

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