INTERNATIONAL ATOVS PROCESSING PACKAGE: THE ALGORITHM DEVELOPMENT AND ITS APPLICATION IN REAL DATA PROCESSING

Jun Li, W. Wolf, W. P. Menzel, W. Zhang, H.L. Huang, T. H. Achtor, H. M. Woolf

Cooperative Institute for Meteorological Satellite Studies
Space Science and Engineering Center
University of Wisconsin-Madison
Madison, WI 53706

1. INTRODUCTION

The International ATOVS Processing Package (IAPP) is developed to retrieve the atmospheric temperature profile, moisture profile and other parameters in both clear and cloudy atmosphere from the ATOVS measurements. This algorithm contains three steps: 1) cloud detection, classification and screening; 2) regression retrieval processes; and followed by 3) a non-linear iterative physical retrieval. Nine (3 by 3) adjacent HIRS/3 spot observations together with AMSU footprints remapped to the HIRS/3 resolution, are used to retrieve the clear HIRS/3 radiances, temperature profile, moisture profile, total atmospheric ozone and microwave surface emissivity, etc. The algorithm is applied to the ATOVS data processing. Retrieval results are evaluated by the Root Mean Square (RMS) difference between retrieved and radiosonde sounding profiles. Case study shows that the accuracy of IAPP retrieval is near 2.0 K for temperature by using the HIRS/3 and AMSU-A measurements. The IAPP will be available to the worldwide users for processing the real time ATOVS data.

The Advanced Microwave Sounding Unit (AMSU), with a total of 20 channels in microwave, represents a dramatic improvement in microwave technology over the Microwave Sounding Unit (MSU) from the TIROS-N Operational Vertical Sounder (TOVS) (Smith et. al., 1979). The Advanced TOVS (ATOVS) which is comprised of AMSU and HIRS/3, are flying on the National Oceanic and Atmospheric Administration (NOAA) polar-orbiting satellite (NOAA-15). Two separate radiometers (AMSU-A and AMSU-B) comprise the AMSU platform. For the first time with AMSU, profiling of atmospheric temperature and moisture under all weather condition is possible. Figure 1 shows the AMSU-A sensitivity functions ($d\tau / d \ln p$); it can be seen that channel 9-13 have good sensitivity for the upper level temperature information. Another instrument of ATOVS is the High Resolution Infrared Radiation Sounder (HIRS/3) which is very similar to the HIRS/2 of TOVS (Smith et al., 1979). Data from the instrument are used in conjunction with the AMSU instruments to calculate the atmosphere's vertical

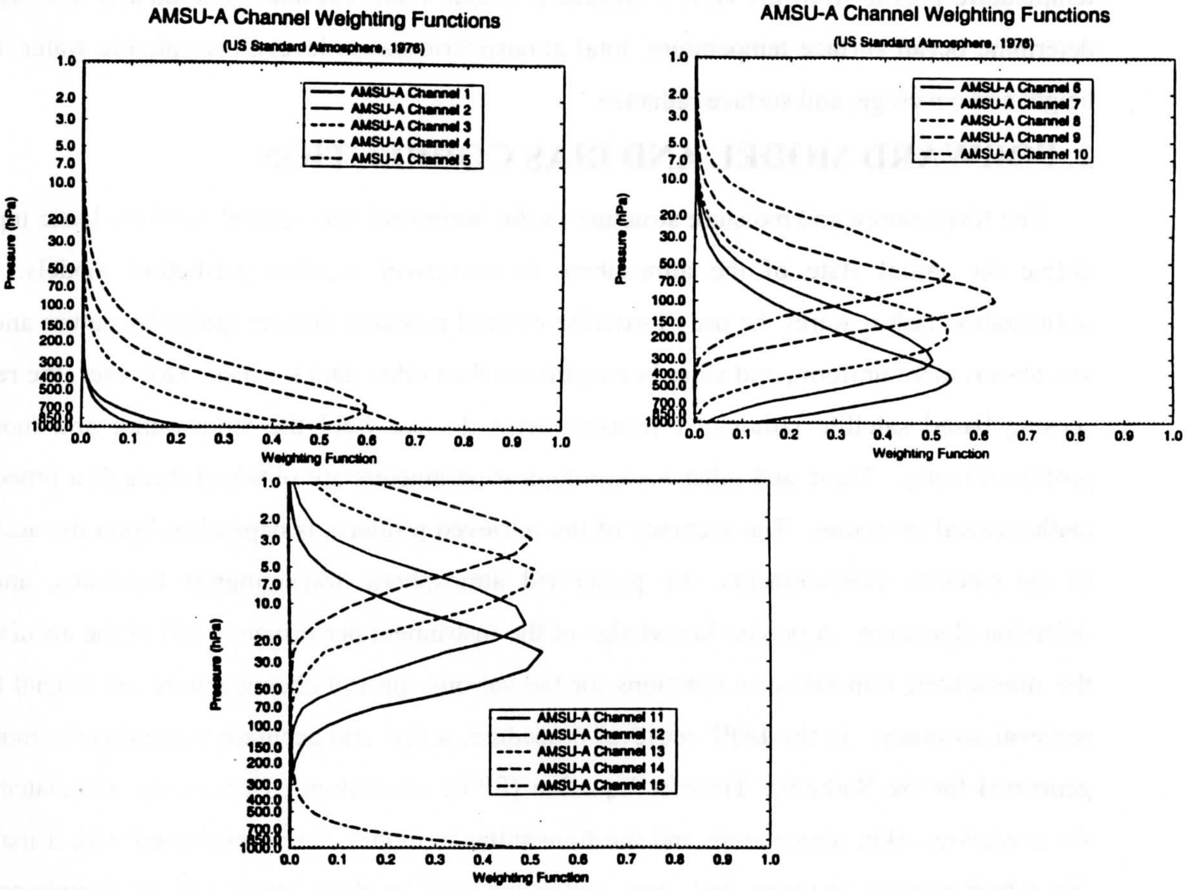

Figure 1, the AMAU-A sensitivity functions ($d\tau / d \ln p$), it can be seen that channel 9-13 have good sensitivity for upper level temperature information.

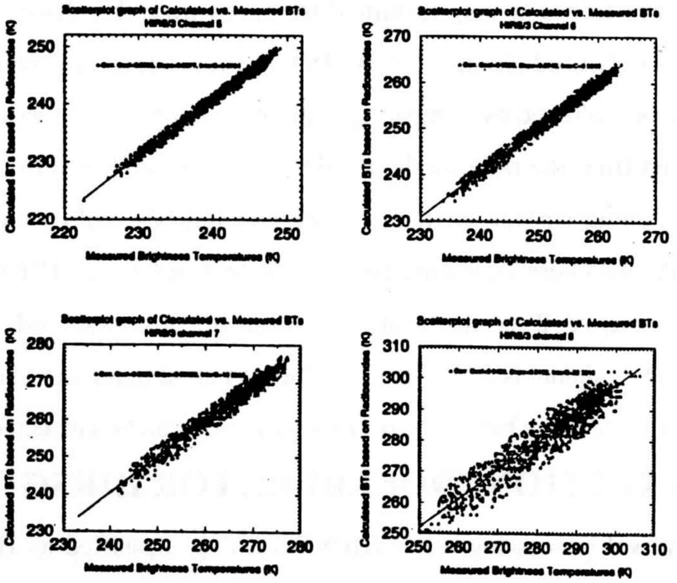

Figure 2, the scattering plot of observed and calculated brightness temperature for HIRS/3 channels 5, 6, 7 and 8.

temperature profile from the earth's surface to about 40km altitude. The data is also used to determine ocean surface temperature, total atmospheric ozone levels, precipitable water, cloud height and coverage, and surface radiance.

2. FORWARD MODEL AND BIAS CORRECTION

The temperature and moisture structure in the horizontal and vertical form the basic input to define the initial state of the atmosphere in numerical weather prediction models. The initialization task requires the use of satellite-derived products that are global by nature and that are denser, more uniform, and more homogeneous than other data sources. However, the remote sensing based satellite radiometer measurements do not yield the temperature and moisture profiles directly. These and other meteorological parameters are obtained through a process of mathematical inversion. The accuracy of the retrieved products is dependent upon the accuracy of the satellite measurements, the prescribed atmospheric transmittance functions, and the inversion algorithm. A precise knowledge of the instrument performance and of the accuracy of the atmospheric transmittance functions for the various spectral channels used are crucial to the retrieval accuracy. In the IAPP retrieval procedure, a fast and accurate transmittance model is generated for the Radiative Transfer Equation (RTE) calculation. Uncertainty associated with the emissivity, skin temperature and the transmittance model can be evaluated with a matchup file, which contains the time, and space collocated satellite observations and radiosonde profiles (Zhang et al., 1999). The empirical correction method for calculated discrepancies is to define a "bias" vector which can be added to the calculated brightness temperatures; if the forward calculations are shown to produce systematic differences from the observed, the bias correction method is more routinely used (Joiner, 1997). Before the retrieval procedure, the efficacy of the forward calculation is evaluated by comparing brightness temperatures observed for each channel with those calculated from the radiosonde profile. The skin temperature used in the calculation is obtained by combining surface air temperature and HIRS/3 multi-window channels. In the IAPP processing, the bias corrections are routinely calculated for all HIRS/3 channels and most AMSU channels. Figure 2 is the scattering plot of observed and calculated brightness temperature for HIRS/3 channels 5, 6, 7 and 8. There is good agreement between the calculation and observation, the systematic bias error of the calculation can be corrected in the retrieval.

3. CLOUD DETECTION PROCEDURE FOR HIRS/3 AND AMSU-A

Before the retrieval processing, each HIRS/3 FOV is classified as HIRS clear/cloudy and AMSU clear/cloudy. The AMSU scattering index and precipitating index based on Grody's approach (Grody, 1999) are used to identify the ice cloud and precipitating cloud. Only the

AMSU clear FOVs are used for retrieval calculation. For each AMSU clear FOV, a HIRS/3 cloud detection approach is applied to get the HIRS/3 clear/cloud index. This approach is separated into two steps: 1) if the HIRS/3 Channel 8 is too cold (<230K) then this FOV is cloudy, 2) use AMSU-A predicted HIRS brightness temperatures to check the HIRS/3 clear/cloudy. A regression relationship between AMSU-A channels 5-14 and HIRS/3 clear brightness temperatures is generated in advance, and this relationship is applied to the real observed AMSU-A observation to derive the predicted HIRS/3 brightness temperature. If there is a significant discrepancy between the HIRS/3 observed and predicted brightness temperatures for channels 5, 6, 7, 11, 12, 13, 14, 15 and 16, this FOV is HIRS cloudy. An accurate cloud detection is crucial for the following retrieval procedure.

4. FIRST GUESS FROM LINEAR REGRESSION RETRIEVAL

The IAPP retrieval is accomplished in two steps: 1) an initial temperature, water vapor, ozone profile and surface skin temperature is obtained by statistical regression based on the NOAA/NESDIS NOAA88 global radiosonde data set which has 8834 atmospheric profiles, and 2) an iterative physical solution of radiative transfer equation is conducted by using the results of step 1 as the initial profile to get the final measure of temperature profile, moisture profile and total atmospheric ozone. In the IAPP, a statistical regression model is generated for the first guess retrieval from ATOVS measurements under both clear and cloudy sky conditions, the regression performance is based on the HIRS/3 single FOV. The fast forward model calculation of AMSU and HIRS/3 radiance is performed for each radiosonde case of the NOAA88 data set to provide a radiosonde-ATOVS radiance pair for the statistical regression analysis. A regression equation is then generated based on these theoretical calculations of radiance and the related matching radiosonde temperature, moiture and ozone profiles. This regression equation can be applied to the real ATOVS radiance to allow the specification of an excellent initial profile of the atmospheric state, as needed for the physical solution of the RTE. In addition, the local satellite zenith angle of observation, the surface terrain elevation and the land/water index are also used as predictors to allow the direct use of non-limb adjusted radiance. The main advantage of regression equation using the theoretical calculation over the real observation is that it avoids the error due to the time and space difference between the satellite observation and radiosonde profile. In addition, surface temperature and moisture observations can also be used as additional predictors in the regression. This allows the use of surface observations as additional information to better constrain the statistical retrieval used as initial profile in the physical solution of the ATOVS RTE. Since the IAPP uses the 3 by 3 HIRS/3 FOV observations to obtain one retrieval profile, then either the clearest or the averaged clear radiance within the 9 FOVs is applied to the regression. Under clear sky condition, the HIRS/3 long-wave and medium-wave measurements plus the AMSU measurements are used to predict the atmospheric temperature and moisture profiles, total ozone, surface skin temperature and microwave surface emissivity, while under cloudy sky condition, only the AMSU and HIRS/3 stratospheric channel measurements are used to predict the above atmospheric parameters except the atmospheric ozone. The first guess of the microwave surface emissivity is obtained from the AMSU-A 50.3 GHz window channel brightness temperature (Huang and Li, 1998).

5. RETRIEVAL ALGORITHM

If we neglect scattering by the atmosphere, the true clear spectrum of infrared radiance exiting the earth-atmosphere system is

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

where R is the spectral radiance in infrared region or brightness temperature in the microwave region, B is the Planck radiance or temperature in the microwave region which is a function of pressure p, τ is the atmospheric transmittance function, subscript s denotes surface, and R' represents the contribution of reflected radiation in the infrared region. If the satellite observed radiance or brightness temperature R of each channel is known, then R can be considered a non-linear function of the atmospheric temperature profile, water vapor mixing ratio profile, surface skin temperature, microwave surface emissivity etc. That is $R = R(T,q,T_s,\varepsilon...)$, or in general

$$Y = F(X), \qquad (2)$$

where the vector X contains L (levels of atmosphere) atmospheric temperatures, L atmospheric water vapor mixing ratios (the water vapor is expressed as the logarithm of the mixing ratio in practical applications), one surface skin temperature, one microwave surface emissivity etc., and Y contains N satellite observed radiances or brightness temperatures. The linearization form of Eq.(2) is

$$\delta Y = F' \cdot \delta X , \qquad (3)$$

where F' is the linear tangent model of the forward model F. The linear model uses the efficient analytical form (Li, 1994). A general form of the minimum variance solution is to minimize the following penalty function (Rodgers, 1976)

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

By using the following Newtonian iteration

$$X_{n+1} = X_n + J''(X_n)^{-1} \cdot J'(X_n), \qquad (5)$$

the following Quasi-Nonlinear iterative form (Eyer, 1989) is obtained

$$\delta X_{n+1} = (F_n'^T \cdot E^{-1} \cdot F_n' + H) \cdot F_n'^T \cdot E^{-1} \cdot (\delta Y_n + F_n' \cdot \delta X_n), \qquad (6)$$

where $\delta X_n = X_n - X_0$, $\delta Y_n = Y^m - Y(X_n)$, and X is the atmospheric profile to be retrieved, X_0 is the initial state of the atmospheric profile or the first guess, 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 be the inverse of the *a priori* first guess error covariance matrix or other type of matrix. If the statistics of both the measurement and *a-priori* error covariance matrix are Gaussian distribution, then the maximum likelihood solution is obtained. However, if the *a priori* error covariance matrix is not known or is estimated incorrectly, the solution will be suboptimal (Chahine et al., 1996). Usually $H = \gamma I$ is applied in the equation (6), where γ is the smoothing factor. Eq.(6) becomes

$$\delta X_{n+1} = (F_n'^T \cdot E^{-1} \cdot F_n' + \gamma I) \cdot F_n'^T \cdot E^{-1} \cdot (\delta Y_n + F_n' \cdot \delta X_n). \qquad (7)$$

While the smoothing factor γ is extremely important in the solution, it is very difficult to determine. It is dependent on the observations, the observation error, and the first guess of the atmospheric profile; often it is chosen empirically (Susskind, 1984; Smith et al., 1985; Hayden, 1988). The smoothing factor plays a critical role in the solution: if the γ is too large, then the solution is over constrained and large biases could be created in retrieval while if γ is too small, the solution is less constrained and an unstable solution will be obtained. In the IAPP retrieval procedure, following Li and Huang (1999), the Discrepancy Principal is applied to determine the smoothing factor γ :

$$\left\| F(X(\gamma)) - Y^m \right\|^2 = \sigma^2, \qquad (8)$$

where $\sigma^2 = \frac{1}{N}\sum_{k=1}^{N} e_k^2$, 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, that is $e_k^2 = \eta_k^2 + f_k^2$, η_k is the instrument noise of channel k while the f_k is the forward model error for the same channel. Usually, σ^2 can be estimated according to the instrument noise and the validation of the atmospheric transmittance model used in the retrieval. With Eq.(7) and Eq.(8), the atmospheric parameters and the smoothing factor can be determined together through the iterative form (Li and Huang, 1999).

Since there are correlations among atmospheric variables, only a limited number of variables are needed to explain the vertical structure variation of an atmospheric profile (Smith, 1976). The number of independent structure functions can be obtained from a set of global atmospheric profile samples. Assume

$$X - X_0 = \Phi A \ , \tag{9}$$

where $A = (\alpha_1, \alpha_2, ..., \alpha_M)$, and $\Phi = \begin{bmatrix} \Phi_T & 0 & 0 & 0 & 0 \\ 0 & \Phi_q & 0 & 0 & 0 \\ 0 & 0 & \Phi_o & 0 & 0 \\ 0 & 0 & 0 & \Phi_{T_s} & 0 \\ 0 & 0 & 0 & 0 & \Phi_\varepsilon \end{bmatrix}$, Φ_T is the matrix of the first $\widetilde{N}_T$ EOFs of the temperature profile, Φ_q is the matrix of the first $\widetilde{N}_q$ EOFs of the water vapor mixing ratio profiles, Φ_o is the matrix of the $\widetilde{N}_o$ ozone mixing ratio profiles, $\Phi_{T_s} = \Phi_\varepsilon = 1$, and $M = \widetilde{N}_T + \widetilde{N}_q + \widetilde{N}_o + 1 + 1$. It is obvious that $\Phi^T \Phi = I$. Defining $\widetilde{F}' = F' \cdot \Phi$, Eq.(7) and Eq.(8) become

$$A_{n+1} = (\widetilde{F}_n'^{T} \cdot E^{-1} \cdot \widetilde{F}_n' + \gamma I) \cdot \widetilde{F}_n'^{T} \cdot E^{-1} \cdot (\delta Y_n + \widetilde{F}_n' \cdot A_n) \ , \tag{10}$$

where A_0=0, and

$$\left\| F(A(\gamma)) - Y^m \right\|^2 = \sigma^2 \ . \tag{11}$$

Eq.(10) and Eq.(11) are applied to derive the solution from ATOVS observations.

6. RETRIEVAL RESULT VALIDATION AND ANALYSIS

The algorithm was tested by using the real ATOVS measurements. To illustrate the capability of the algorithm, a case study of Nov.16, 00Z NOAA-15 orbit ATOVS data was carried out for detail comparison between radiosonde profiles and ATOVS sounding profiles. In the current retrieval procedure, AMSU-B measurements are not used for the time being due to the AMSU-B bias problem. HIRS/3 channels and AMSU-A channels are used in both regression and physical retrieval procedures in clear sky while only HIRS/3 stratosphere channels and

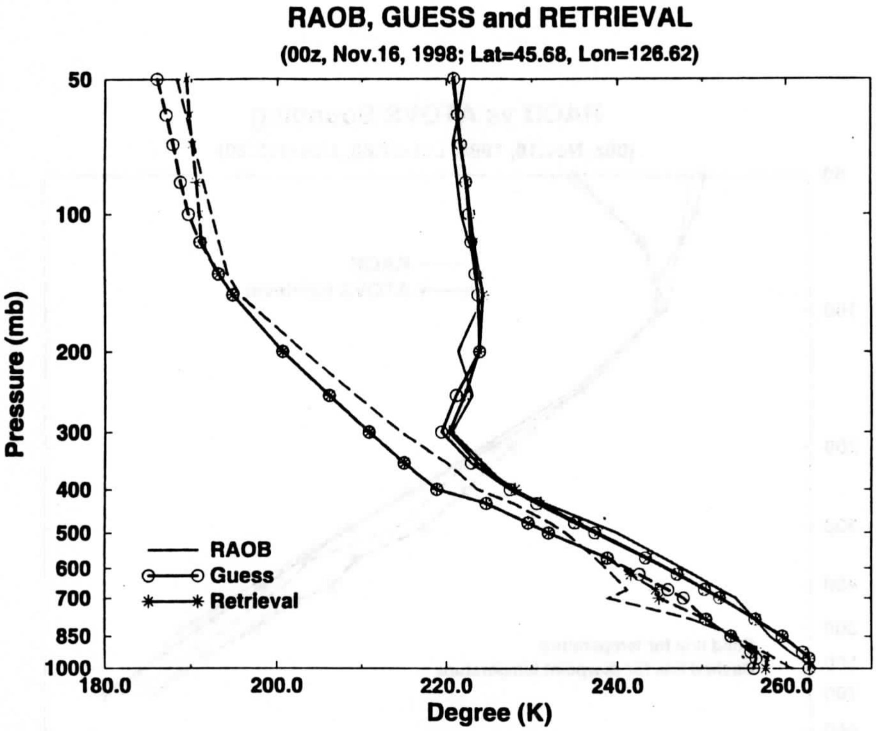

Figure 3, a clear HIRS/3 and AMSU-A physical retrieval comparing with the regression first guess and RAOB observation.

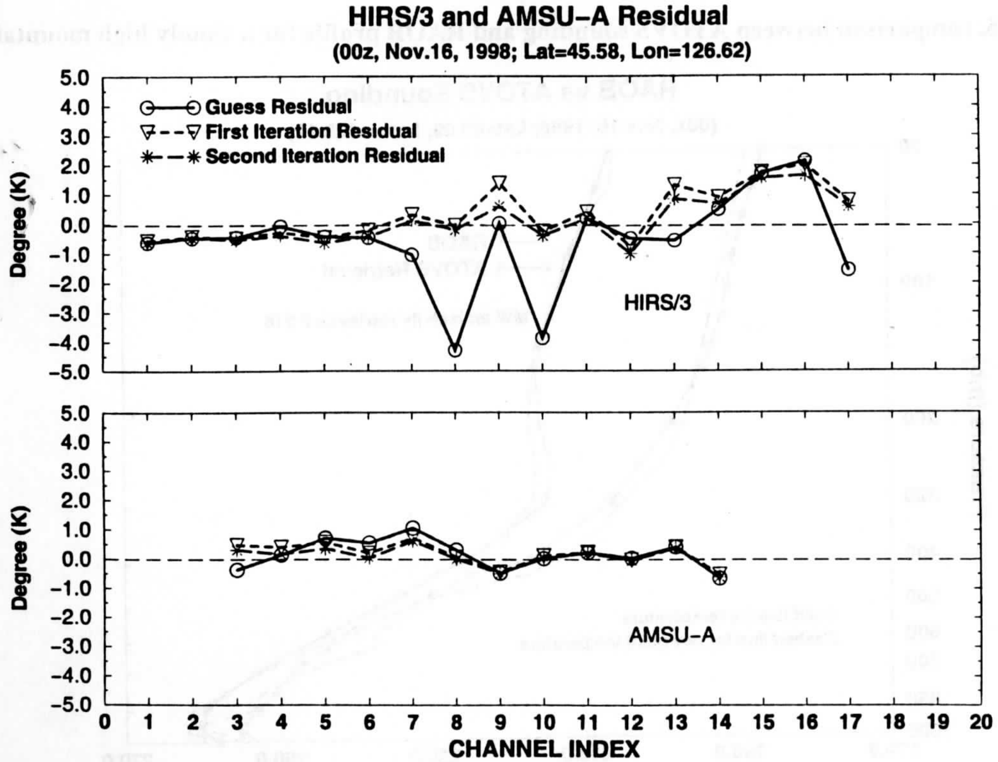

Figure 4, the HIRS/3 and AMSU-A brightness temperature residual for the same case of figure 3.

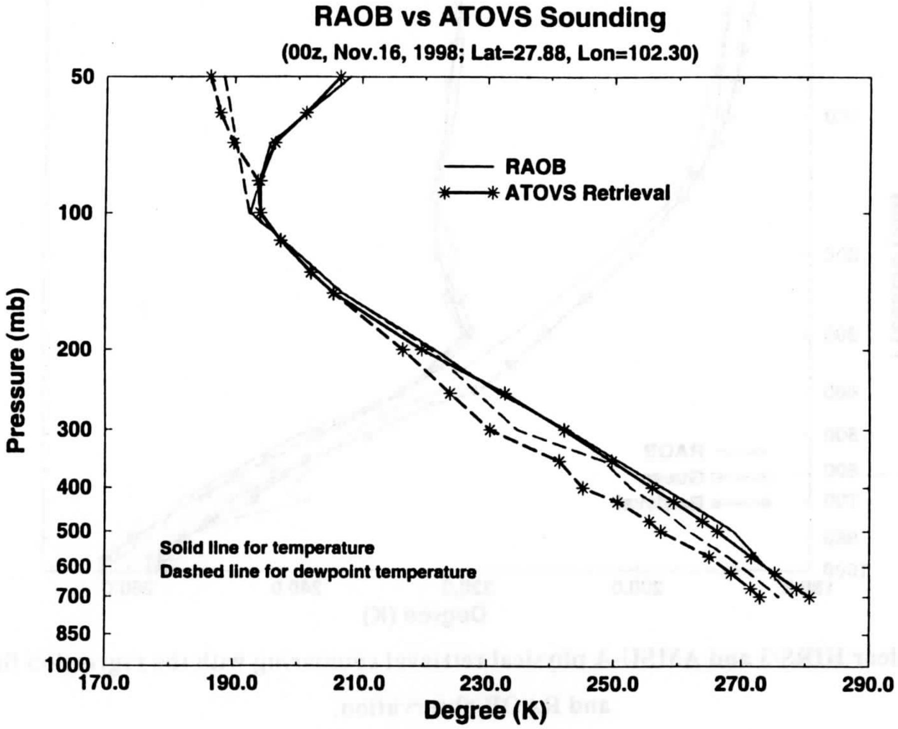

Figure 5, comparison between ATOVS sounding and RAOB profile for a cloudy high mountain case.

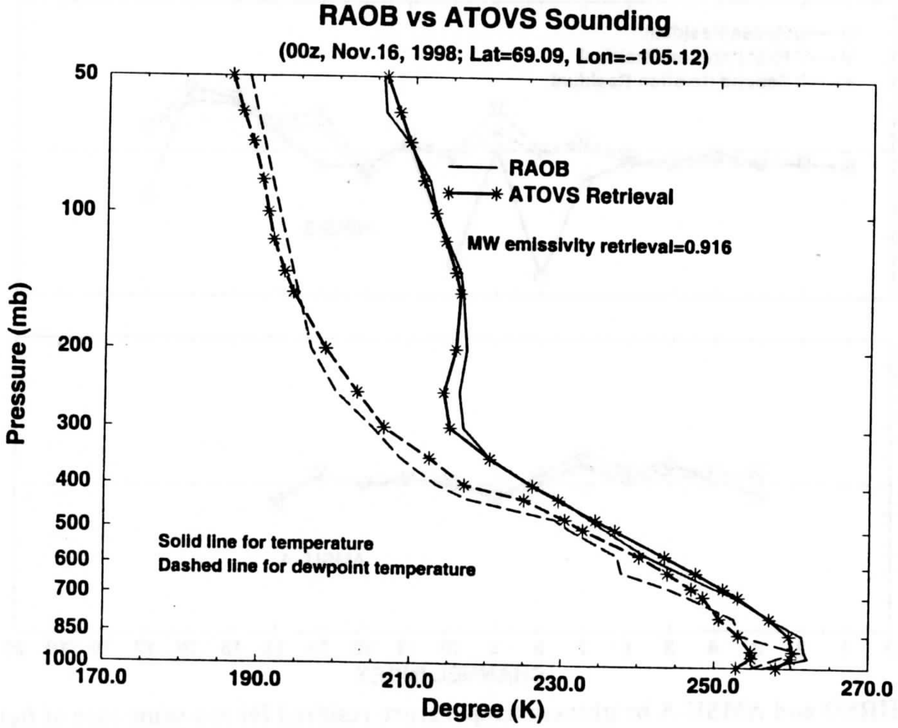

Figure 6, same as figure 5 but for another clear land retrieval.

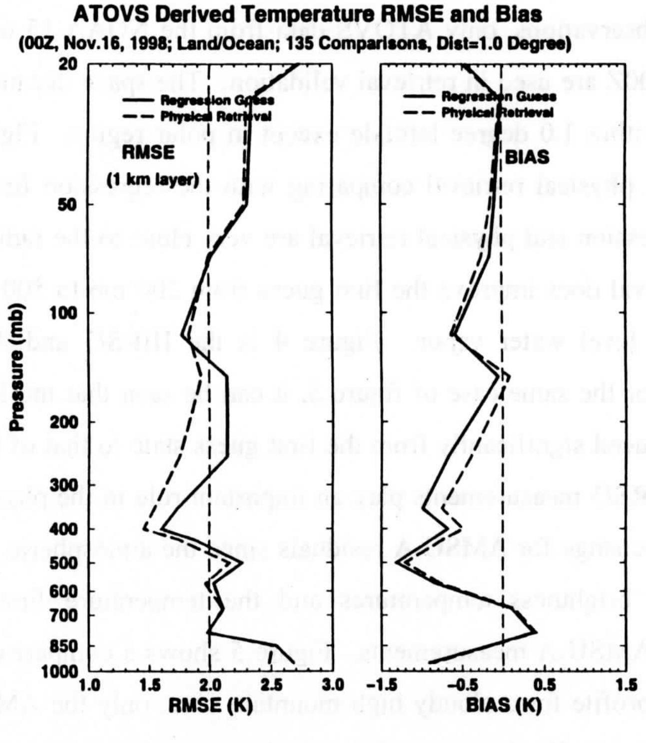

Figure 7, 1 km layer temperature RMSE and bias of the regression and physical retrieval of the

Figure 8. same as figure 7 but for 2 km layer dewpoint temperature RMSE.

AMSU-A channels are used in cloudy sky condition. In order to compare the retrieval profiles with the radiosonde observations, only ATOVS data from the NOAA-15 orbit within 1.5 hour difference of 12 Z or 00Z are used in retrieval validation. The space distance between ATOVS and RAOB must be within 1.0 degree latitude except in polar region. Figure 3 shows a clear HIRS/3 and AMSU-A physical retrieval comparing with the regression first guess and RAOB observation, both regression and physical retrieval are very close to the radiosonde observation, and the physical retrieval does improve the first guess from 200 mb to 500 mb for temperature and also for the low level water vapor. Figure 4 is the HIRS/3 and AMSU-A brightness temperature residual for the same case of figure 3, it can be seen that the HIRS/3 residuals for some channels are reduced significantly from the first guess state to that of the second iteration, suggesting that the HIRS/3 measurements play an important role in the physical retrieval, while there is no significant change for AMSU-A residuals since the atmospheric temperature is more linear to the AMSU brightness temperatures and the temperature first guess takes more information from the AMSU-A measurements. Figure 5 shows a comparison between ATOVS sounding and RAOB profile for a cloudy high mountain case, only the AMSU-A channels and HIRS/3 1-3 channels are used in this retrieval, result shows good agreement between the ATOVS sounding and RAOB suggesting that the AMSU-A measurements can provide good atmospheric information under the cloudy sky condition. Figure 6 is same as figure 5 but for another clear land retrieval, from the RAOB observation, low-level temperature inversion is observed, and the ATOVS sounding has the same inversion structure, which illustrates the capability of ATOVS remote sensing the atmosphere. Figure 7 is 1 km layer temperature RMSE and bias of the regression and physical retrieval of the whole orbit for all clear and cloudy, land and ocean cases, results show the significant improvement of physical retrieval over the first guess especially from 100 mb to 500 mb, and the average RMSE of temperature retrieval is less than 2 K. Figure 8 is same as figure 7 but for 2 km layer dewpoint temperature RMSE and bias, there is still improvement of the physical retrieval over the guess. With the AMSU-B measurement in future, the improvement will be even more significant.

7. CONCLUSION

The IAPP algorithm designed for real time ATOVS data processing, is described in this paper. Retrieval results from real ATOVS measurements show that the algorithm is reliable under both HIRS/3 clear and cloudy conditions. With AMSU data, the atmospheric parameters can be derived in all weather conditions, which is an advantage over the TOVS measurements.

The IAPP will be improved by including the AMSU-B measurement for water vapor profiling in the near future.

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