Simultaneous Non–linear Retrieval of Atmospheric Temperature and Absorbing Constituent Profiles from Satellite Infrared Sounder Radiances

Li Jun (李 俊), *Zhou Fengxian* (周凤仙) and *Zeng Qingcun* (曾庆存)
Institute of Atmospheric Physics, Academia Sinica, Beijing 100029
Received September 8, 1993; revised November 2, 1993

ABSTRACT

Based on Zeng's theory (1974), a successive linearized form of radiative transfer equation (RTE) is derived for simultaneous retrieval of atmospheric temperature and absorbing constituent profiles from satellite infrared observations. It contains the temperature component weighting function and absorbing constituent (H_2O, O_3, CH_4 etc.) component weighting functions. All these weighting functions reach maximum at their own "optimum information levels", and make the remote sensing equations well–conditional. Then the atmospheric profiles are derived by Newton's non–linear iteration method. Experiments of retrieval from both TIROS–N operational High Resolution Infrared Sounder (HIRS) and the simulated Atmospheric InfRared Sounder (AIRS) show an significant improvement.

Key words: Sounding, Weighting Function, Retrieval

I. INTRODUCTION

Satellite information will play an increasing role in Numerical Weather Prediction (NWP) and other operational uses. The current used TIROS–N Operational Vertical Sounder (TOVS) has 19 HIRS channels (Smith et al., 1979). Though TOVS data have been widely applied to NWP, weather analysis and climate change study, the accuracy of TOVS retrieval is limited due to its low vertical resolution. Recently the high resolution infrared sounders such as AIRS of the United States, IMG (Interferometric Measurements of Greenhouse gases) of Japan, IASI (Improved Atmospheric Sounding Interferometer) of France, MIPAS (Michaelson Interferometer for Passive Atmospheric Sounding) of Germany etc. are developed for flying on future satellite or polar orbiting platform. Each kind of these instruments has thousands of channels for single Field of View (FOV). It has been shown that the atmospheric temperature and absorbing constituent profiles can be achieved with improved vertical resolution and accuracy from these high resolution infrared sounders. However, a practical application of the new instrument observations requires the efficient retrieval method which leads to the optimal solution. The theory of remote sensing and retrieval has been described overall by Zeng (1974) and others. Some methods for the practical processing have also been developed for retrieval from TOVS data (Smith et al., 1985; Chedin et al., 1985; Li et al., 1993).

In this paper, a method based on Zeng's (1974) formulation for the simultaneous retrieval of atmospheric temperature and absorbing constituent profiles from infrared sounder data is developed. Retrieval results from both operational TOVS and simulated high resolution AIRS data show that this method has the potential application in the practical inversion of future satellite sounding system.

II. METHOD

In this section we develop a linearized form of the RTE which contains temperature and absorbing constituent mixing ratio weighting functions. In the equations that follow:

R = spectral radiance,

B = Planck radiance which is a function of temperature, i.e. an implicit function of pressure level p,

τ = the total transmittance of the atmosphere above the pressure level p,

$\delta(\ )$ = the difference between the true quantity and the initial value denoted by a superscript o,

$\sum(\ )_i$ = the summation of i quantities,

$\prod(\ )_i$ = the product of i quantities,

p_s = surface pressure,

τ_c = CO_2 component transmittance,

τ_i = i–th absorbing constituent component transmittance,

q_i = mixing ratio of ith absorbing constituent,

$T(p)$ = the true atmospheric temperature profile,

T_B = the brightness temperature,

k_i = absorbing coefficient of ith absorbing constituent,

T_s = surface skin temperature,

T_a = surface air temperature.

The true spectrum of radiance outgoing from the earth–atmosphere system is

$$R = B_s \tau_s - \int_0^{p_s} B d\tau \ . \tag{1}$$

Here and after we always omit the spectrum symbol ν in the equation. The first order variation of Eq.(1) yields

$$\delta R = \delta B_s \tau_s + B_s \delta\tau_s - \int_0^{p_s} \delta B d\tau - \int_0^{p_s} B d\delta\tau \ . \tag{2}$$

Integrating the last term by part yields, we have

$$\delta R = \delta B_s \tau_s - \int_0^{p_s} \delta B d\tau + [B(T_s) - B(T_a)]\delta\tau_s + \int_0^{p_s} \delta\tau dB \ . \tag{3}$$

If we ignore the deviation of the natural broading of absorbing coefficient of ith absorbing constituent relative to that associated with the "guess" atmospheric condition, we have

$$\tau_i = e^{-\int_0^p g^{-1} k_i q_i dp} \ , \tag{4}$$

$$\tau = \tau_c \prod_{i=1}^{L} \tau_i \ , \tag{5}$$

then

$$\delta\tau = \delta\tau_c \prod_{i=1}^{L} \tau_i + \tau_c \delta \prod_{i=1}^{L} \tau_i = \tau \sum_{i=1}^{L} \delta \ln\tau_i \tag{6}$$

for τ_c being a constant.

$$\delta\ln\tau_i = -\int_0^p g^{-1}k_i\delta q_i dp = \int_0^p \delta q_i \frac{d\ln\tau_i}{q_i dp}dp = \int_0^p \delta\ln q_i d\ln\tau_i \ . \tag{7}$$

Substituting Eq.(7) into Eq.(6), we obtain

$$\delta\tau = \tau\sum_{i=1}^{L}\int_0^p \delta\ln q_i d\ln\tau_i \ . \tag{8}$$

Substituting Eq.(8) into Eq.(3), we have

$$\delta R = \delta B_s\tau_s - \int_0^{p_s}\delta B d\tau + \sum_{i=1}^{L}\{\int_0^{p_s}[B(T_s)-B(T_a)]\tau_s\delta\ln q_i d\ln\tau_i + \int_0^{p_s}\tau(\int_0^p \delta ln q_i d\ln\tau_i)dB\}$$

$$= \delta B_s\tau_s - \int_0^{p_s}\delta B d\tau + \sum_{i=1}^{L}\{\int_0^{p_s}\delta\ln q_i[B(T_s)-B(T_a)]\tau_s d\ln\tau_i + \int_0^{p_s}\delta\ln q_i[\int_p^{p_s}\tau dB]d\ln\tau_i\} \ . \tag{9}$$

Using the first order variation $\delta B = \frac{\partial B}{\partial T}\delta T$, and $\delta R = \frac{\partial R}{\partial T_B}\delta T_B$ and denoting $\beta(p) = \frac{\partial B/\partial T}{\partial R/\partial T_B}$, then Eq.(6) can be written as

$$\delta T_B = \beta_s\tau_s\delta T_s - \int_0^{p_s}\beta\frac{\partial\tau}{\partial p}\delta T dp + \sum_{i=1}^{L}\int_0^{p_s}\delta\ln q_i[(T_s-T_a)\beta_s\tau_s + \int_p^{p_s}\beta\tau\frac{\partial T}{\partial p}dp]\frac{d\ln\tau_i}{dp}dp$$

$$= W_{T_s}\delta T_s + \int_0^{p_s}W_T\delta T dp + \sum_{i=1}^{L}\int_0^{p_s}W_{q_i}\delta\ln q_i dp \ , \tag{10}$$

where

$$W_{T_s} = \beta_s\tau_s \ , \tag{11a}$$

$$W_T = -\beta\frac{\partial\tau}{\partial p} \ , \tag{11b}$$

$$W_{q_i} = (T_s-T_a)\tau_s\beta_s\frac{d\ln\tau_i}{dp} + \left(\int_p^{p_s}\beta\tau\frac{\partial T}{\partial p}dp\right)\frac{d\ln\tau_i}{dp} = W^{*}_{q_i} + W^{**}_{q_i} \ . \tag{11c}$$

W_{T_s}, W_T, W_{q_i} are the weighting functions for the surface skin temperature, atmospheric temperature, and ith absorbing constituent mixing ratio weighting functions respectively, and can be easily calculated from the first guess profile condition.

Once the "guess" atmospheric profiles are known, Eq.(10) is a linear form. This linear form contains the temperature and absorbing constituent weighting functions as known functions and δT and $\delta\ln q_i$ the functions to be solved. The weighting function has a maximum at a specific pressure level which is "the optimum information level" (Zeng 1974, 1979). Let us now consider the weighting function for the ith absorbing constituent mixing ratio, since

$|\tau| \leqslant 1$ and $\left|\frac{\partial B}{\partial p}\right| \leqslant \left|\frac{\partial B}{\partial p}\right|_{Maximum}$, it is obvious that

$$\lim_{p \to 0} W_{q_i}^{**} = 0 \ . \tag{12a}$$

and

$$\lim_{p \to p_s} W_{q_i}^{**} = 0 \ . \tag{12b}$$

Thus, there exists $P' \in (0, p_s)$, and $W_{q_i}(p') = \max W_{qi}(p)$, P' is so called "the optimum information level" of ith absorbing constituent radiance emission. Fig. 1 is the weighting functions of HIRS channels for water vapor component, where the numbers 10, 11 and 12 are for water vapor channels, 6 and 7 for temperature and water vapor joint channels.

Let us consider now a vector X which contains N (levels of pressure) atmospheric temperatures, N × L specific absorbing constituent mixing ratios (every absorbing constituent is expressed as the logarithm of mixing ratio according to Eq.(10) and one surface skin temperature. X is a vector of dimension N(L+1)+1. The Y vector containing k satellite brightness temperatures is related to X through Eq.(1) or Eq.(10). That is $X = (x_1, x_2, \cdots, x_{N(L+1)+1})^T = (T_1, T_2, \cdots, T_N, \ln q_{11}, \ln q_{12}, \cdots, \ln q_{1N}, \ln q_{21}, \ln q_{22}, \cdots, \ln q_{2N}, \cdots, \ln q_{L1}, \ln q_{L2}, \cdots, \ln q_{LN}, T_s)^T$. Then Eq.(10) can be written as

$$\delta y = \sum_{j=1}^{N(L+1)+1} w_j \delta x_j \ , \tag{13}$$

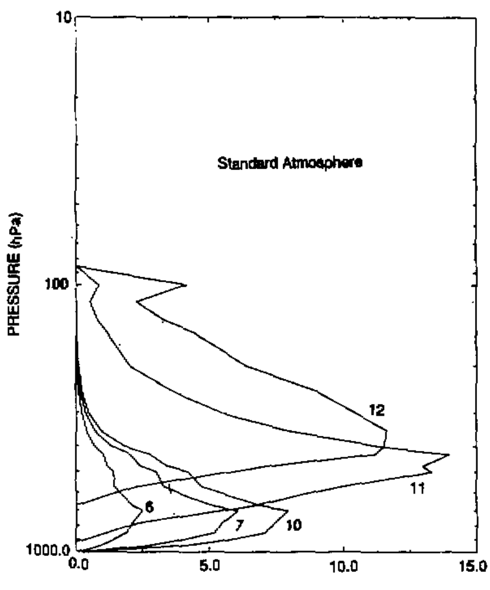

Fig. 1. NOAA-12 water vapor mixing ratio weighting function (see Eq.(10)).

where superscript T denotes matrix transposition, and

$$w_1 = 0.5W_{T1}(p_2 - p_1)$$

$$w_j = 0.5W_{Tj}(p_{j+1} - p_{j-1}) \qquad \text{when} \quad 1<j<N$$

$$w_N = 0.5W_{TN}(p_N - p_{N-1})$$

$$w_j = 0.5W_{q_i 1}(p_2 - p_1) \qquad \text{when} \quad j=Ni+1$$

$$w_j = 0.5W_{q_i j^*}(p_{j^*+1} - p_{j^*-1}) \qquad \text{when } Ni+1<j<N(i+1),\ j^* = \text{mod}(j, N)$$

$$w_j = 0.5W_{q_i N}(p_N - p_{N-1}) \qquad \text{when } j=N(i+1)$$

$$w_j = W_{T_s} \qquad \text{when } j=N(L+1)+1$$

i = 1,2,⋯, L. For a set of k channels:

$$\delta y_l = \sum_{j=1}^{N(L+1)+1} w_{lj}\delta x_j \qquad l = 1,2,\cdots,k \tag{14}$$

Writing in matrix form, Eq.(14) becomes:

$$\delta Y = K' \cdot \delta X\ , \tag{15}$$

K' is the tangent model of the original model $Y = K(X)$, which is a nonlinear one.

Let $Z = (X, Y)^T$. For a given first guess $Z^0 = (X^0, Y^0)^T$, we require

$$D(Z,Z^0) = \text{min}imum\ ,$$

where D is the distance between Z^0 and Z. It is found that the Mahalanobis Distance is a suitable distance in satellite data application (Li et al., 1990). Define a cost function $J(X)$ as follows;

$$\begin{aligned} J(X) &= D^2(Z,Z^0) \\ &= (Y - Y^0)^T E^{-1}(Y - Y^0) + \gamma(X - X^0)^T B^{-1}(X - X^0)\ , \end{aligned}$$

where X^0 is the first guess, Y the observed radiance, Y^0 the radiance calculated from the first guess by using Eq.(1), B the first guess error covariance matrix and E the satellite observation error covariance matrix. E includes the measurement errors of satellite and the model transmittance error. $J(X)$ contains two terms, one is the satellite observation contribution to the retrieval, the other is the first guess contribution. γ is a factor which balances the satellite observation and first guess contributions to the cost function.

According to Newton's nonlinear iteration method, we have

$$X_{n+1} = X_n - J''^{-1}(X_n) \cdot J'(X_n) \tag{16a}$$

and

$$0.5J'(X) = \gamma B^{-1} \cdot \delta X - K'^T \cdot E^{-1} \cdot \delta Y \tag{16b}$$

$$0.5J''(X) = \gamma B^{-1} + K'^T \cdot E^{-1} \cdot K'\ , \tag{16c}$$

where $\delta X_n = X_n - X^0$, $\delta Y_n = Y - K(X_n)$.

By Matrix manipulation, we arrive at the form

$$\delta X_{n+1} = (K_n'^T \cdot E^{-1} \cdot K_n' + \gamma B^{-1})^{-1} \cdot K_n'^T \cdot E^{-1} \cdot (\delta Y_n + K_n' \cdot \delta X_n)\ . \tag{17}$$

Since the effective information content of satellite observations is limited (Towmey, 1966; Zeng, 1974), and there are correlations among atmospheric variables, only a limited number of variables is needed to explain the vertical structure variation of atmospheric profiles. The number of independent variables can be obtained from a set of atmospheric profile samples, where as the structure functions can be defined from Empirical Orthogonal Functions (EOFs) analysis of the global TOVS Initial Guess Retrieval (TIGR) data set. Then the number of atmospheric variables for retrieval is significantly reduced. Assume that

$$\delta X = \Phi A \ , \tag{18}$$

where

$$A = (\alpha_1, \alpha_2, \cdots, \alpha_{\tilde{N}})^T$$

$$\Phi = \begin{bmatrix} \Phi_T & 0 & 0 & \cdots & 0 & 0 \\ 0 & \Phi_{\ln q_1} & 0 & \cdots & 0 & 0 \\ 0 & 0 & \Phi_{\ln q_2} & \cdots & 0 & 0 \\ & \cdots & \cdots & & & \\ 0 & 0 & 0 & \cdots & \Phi_{\ln q_L} & 0 \\ 0 & 0 & 0 & \cdots & 0 & \Phi_{T_s} \end{bmatrix}$$

Φ_T is the matrix of the first $\tilde{N}_T$ EOFs of temperature and, $\Phi_{\ln q_i}$ ($i=1,2,\cdots,L$) the matrix of the first $\tilde{N}_{q_i}$ EOFs of the ith absorbing constituent. $\Phi_{T_s} = 1$, $\tilde{N} = \tilde{N}_T + \sum_{i=1}^{L} \tilde{N}_{q_i} + 1$. It is obvious that

$$\Phi^T \Phi = I \ , \tag{19}$$

then the cost function becomes:

$$J(A) = \delta Y^T E^{-1} \delta Y + \gamma A^T B_A^{-1} A \tag{20}$$

where $B_A^{-1} = \Phi^T B^{-1} \Phi$ define $\tilde{K}' = K' \cdot \Phi$, follow Eq.(16), we get another iteration form

$$A_{n+1} = (\tilde{K}'^T_n \cdot E^{-1} \cdot \tilde{K}'_n + \gamma B_A^{-1})^{-1} \cdot \tilde{K}'^T_n \cdot E^{-1} \cdot (\delta Y_n + \tilde{K}'_n \cdot A_n) \ . \tag{21}$$

IV. CHOICE OF EOFs

Suppose the eigenvalues of temperature covariance matrix C_T are $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_{\tilde{N}} \geqslant 0$, then choice of the first $\tilde{N}_T$ EOFs of temperature should satisfy

$$\sum_{j=\tilde{N}_T+1}^{N} \lambda_i \leqslant N(\Delta T)^2 \ , \tag{22}$$

where ΔT is the maximum temperature error permitted.

Taking $\Delta T = 1.5$, the practical calculation shows that $\tilde{N}_T = 6$. Similarly, $\tilde{N}_{q_i} = 3$ provides humidity profile representations with an accuracy of about 20%. Thus the first 6 temperature and 3 water vapor EOFs can represent the atmospheric vertical structure variation within reasonable accuracy limits achievable with TOVS. Fig. 2 shows the cumulative explained variance based on the TIGR data set.

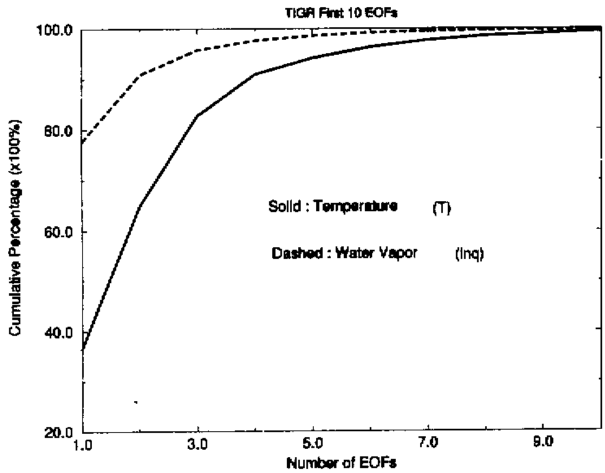

Fig. 2. Variance explained by temperature (T) and water vapor (lnq) EOFs of TIGR.

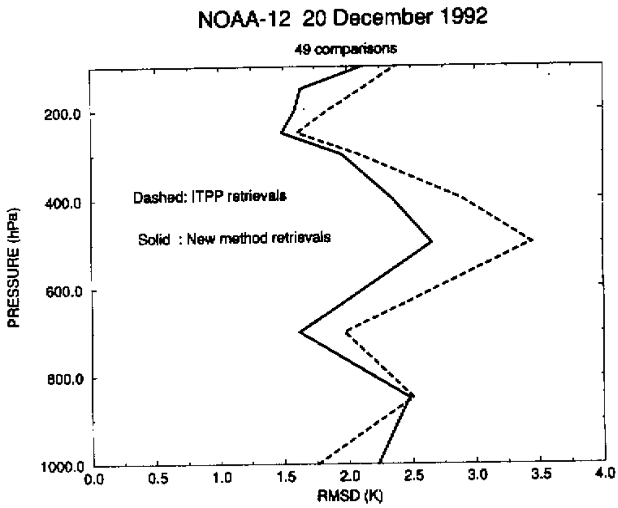

Fig. 3. A RMSD comparison of the temperature retrievals based on ITPP and new method on 20 December 1992 1338 GMT.

V. RETRIEVAL EXPERIMENTS

1. *Retrievals from Operational TOVS Data*

The TOVS data for our retrieval experiments consist of two NOAA−12 satellite passes over mid−U.S., and the first guess fields for the retrievals are based on the NWP with interpolation to the times of satellite passes. The new scheme and the current operational International TOVS Processing Package (ITPP) (Smith et al., 1985) are then run for each satellite pass using the same TOVS observations and first guesses as input. The γ is set to 0.1 and two iterations are applied in the new retrieval procedure in correspondence with ITPP. Fig. 3 shows the Root Mean Square Deviation (RMSD) comparison between retrievals and radiosonde data for temperature on 20 December 1992 1338GMT, where dashed line is ITPP retrievals and solid line is new retrievals. Fig. 4 is the same but for the dewpoint temperature. Figs. 5 and 6 are the same as Figs. 3 and 4 but on 19 February 1993 0116 GMT. As can be

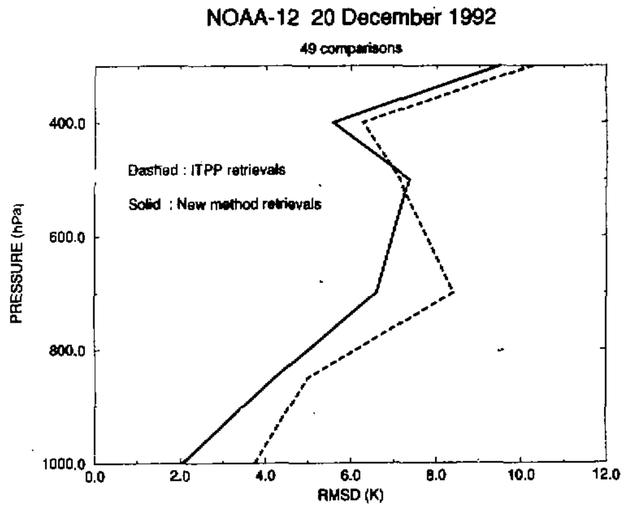

Fig. 4. A RMSD comparison of the dewpoint temperature retrievals based on ITPP and new method on 20 December 1992 1388 GMT.

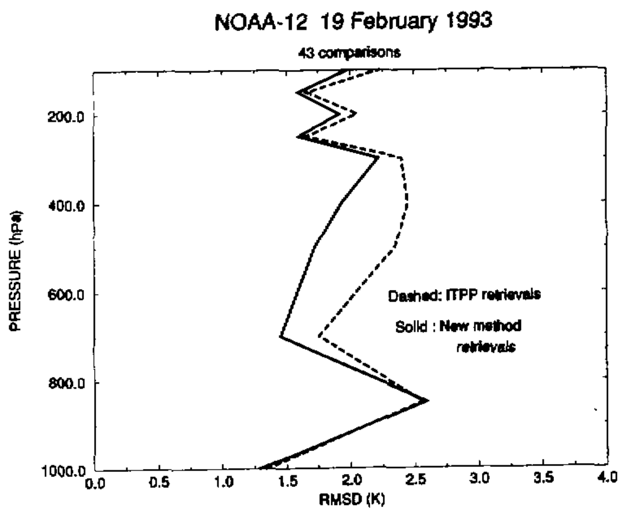

Fig. 5. A RMSD comparison of the temperature retrievals based on ITPP and new method on 19 February 1993 0116 GMT.

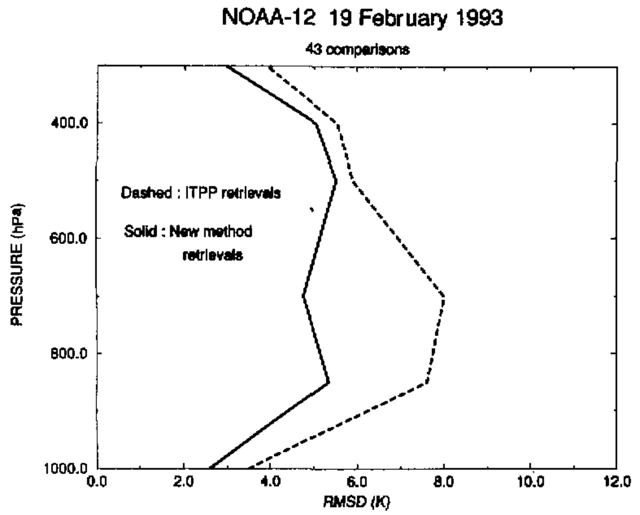

Fig. 6. A RMSD comparison of dewpoint temperature retrievals based on ITPP and new method on 19 February 1993 0116 GMT.

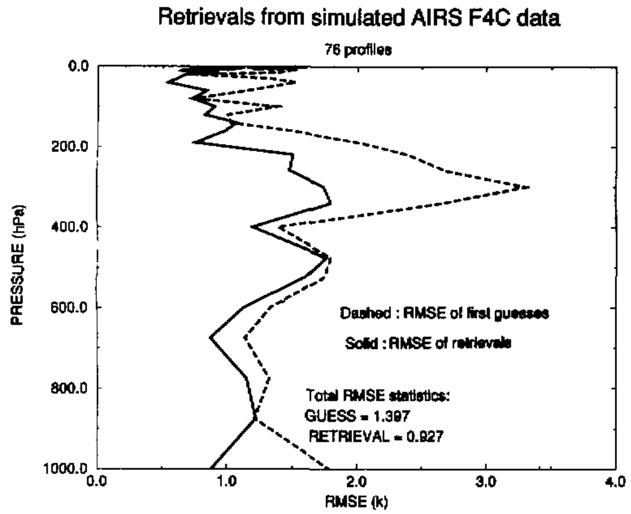

Fig. 7. ARMSE comparison of temperature retrievals and first guesses from F4C simulated AIRS data.

seen that, the accuracy of retrievals of both temperature and water vapor profiles are improved by using the new method.

2. Retrievals from Simulated AIRS Data

In these experiments, we use statistical regression results as first guess, and the procedure described above is performed to AIRS simulated data sets F4C and F4D. The γ now is set to 0.01 because less first guess contribution is needed in the cost function due to the high resolution of AIRS data, and maximum 5 iterations are applied in the retrieval procedure. Figs. 7 and 8 are the Root Mean Square Error (RMSE) of retrievals and first guesses for temperature and water vapor mixing ratio from F4C data sets, where dashed line is RMSE of the first guesses and solid line is RMSE of retrievals. Figs. 9 and 10 are the same as Figs. 7 and 8 but from F4D. Results show that the accuracy of temperature retrieval is better than 1 degree, also the water vapor retrieval error approaches only 10%.

VI. CONCLUSION

We have developed a new retrieval method for satellite infrared sounding data based on RTE successive linearization and Newtonian iteration based on Zeng's theory (1974). The scheme described has been applied successfully to operational TOVS data. The improvement to the current retrieval method used in the ITPP is obvious. Retrievals from simulated high resolution AIRS data also show that the accuracy of temperature retrieval is better than 1 degree and water vapor retrieval accuracy is better than 10%.

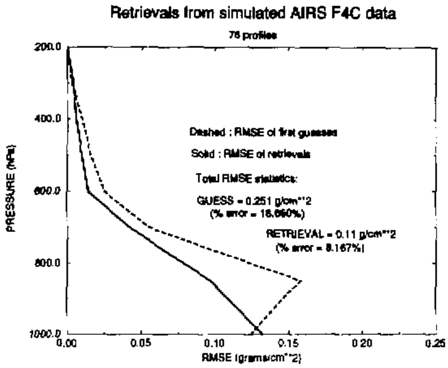

Fig. 8. A RMSE comparison of water vapor mixing ratio retrievals and first guesses from F4C simulated AIRS data.

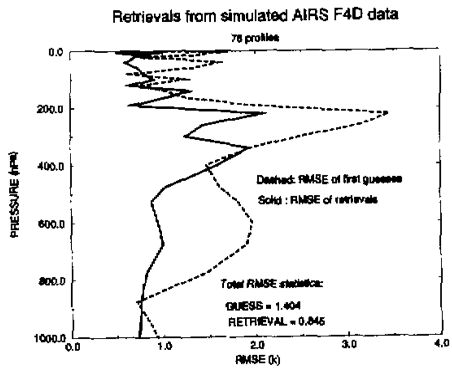

Fig. 9. A RMSE comparison of temperature retrievals and first guesses from F4D simulated AIRS data.

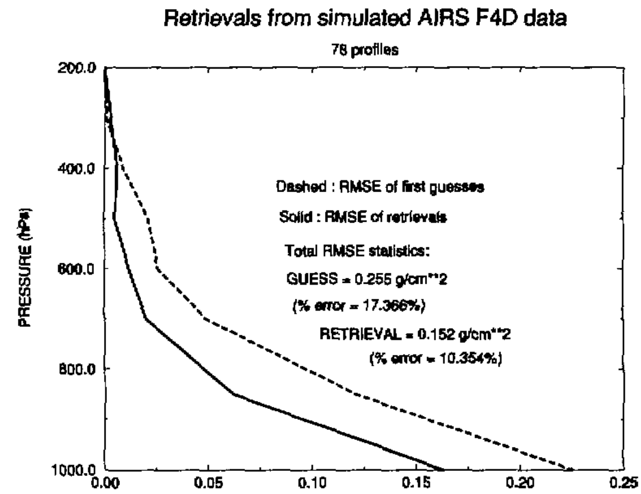

Fig. 10. A RMSE comparison of water vapor mixing ratio retrievals and first guesses from F4D simulated AIRS data.

This study was done during one of the authors (Li Jun), as a visiting scientist working, at the Cooperative Institute for Meteorological Satellite Studies (CIMSS), University of Wisconsin-Madison. He wishes to thank Professor Smith for his support and many valuable discussions. Also thanks to Dr. H.-L. Huang for providing simulated AIRS data and the guess data for AIRS retrievals.

REFERENCES

Chedin, A., N. A. Scott, C. Wahiche and P. Moulinier (1985), The improved initialization inversion method: a high resolution physical method for temperature retrievals from the TIROS-N series, *J. Climate Appl. Meteorol.*, **24:** 128-143.

Li, J. and W. L. Smith (1993), Simultaneous inversion of satellite soundings using adjoint technique. Part I. Thoery. (to be published.)

Li, J. and F. X. Zhou (1990), Computer indentification of multispectral satellite imagery, *Adv. in Atmos. Sci.* **7:** 366-375.

Smith, W. L. and J. Li (1993), Simultaneous inversion of satellite soundings using adjoint technique. Part II. Application to TOVS data. (to be published.)

Smith, W. L., H. M. Woolf, C. M. Hayden, D. Q. Wark and L. M. McMillin (1979), TIROS-N operational vertical sounder, *Bull, Amer. Meteor, Soc.*, **60:** 1177-1187.

Smith, W. L., H. M. Woolf, C. M. Hayden and A. J. Schreiner (1985), The Simultaneous export retrieval package, pp. 224-253 in *Tech. Proc. 2nd International TOVS Study Conf.*, Igls, Austria, 18-22 February 1985, report of CIMSS, University of Wisconsin-Madison.

Zeng, Q. C. (1974), Principle of atmospheric Infrared remote sensing, Science Press, Beijing, 174 pp. (in Chinese).

Zeng, Q. C. (1979), The theoretical problems of infrared remote sensing of the atmosphere, *Scientia Sinica*, **22:** No.5.

Twomey, S. (1966), Indirect measurements of atmospheric temperature profiles from satellites, II. Mathematical aspects of the inversion problem, M. W. R. **94:** No.6.