ON THE DIFFERENTIAL INVERSION METHOD FOR TEMPERATURE RETRIEVALS

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ABSTRACT

The differential inversion method (DIM) is reviewed in the context of the fundamental physics and mathematics governing the transfer of radiation for plane-parallel atmospheres in local thermodynamic equilibrium. In the Laplace inverse plane the Planck intensity is linearly related to upwelling radiance weighted by the weighting function. By applying the inverse transform, the local Planck intensity can be exactly expressed by a linear combination of the derivatives of upwelling radiances in the logarithmic pressure coordinate. Using seven HIRS channels, we perform numerical analyses of the DIM for temperature retrievals. Results based on distinct U.S. standard and tropical profiles show that the DIM converges to the true temperature solution with an accuracy of 1-2 K for tropospheric temperatures using a fifth-order polynomial function to fit seven HIRS radiances. The DIM is free from the need for a priori data basing and requires no constraints in the retrieval. Finally, it is pointed out that the key to the success of the DIM for practical applications appears to depend on whether an appropriate curve-fitting program can be developed for observed radiances.

1. INTRODUCTION

The sounding of temperature and moisture fields has been routinely performed from orbiting meteorological satellites in the last 15 years, with some success. However, the techniques and procedures used for inversion of the temperature profile, as well as atmospheric parameters from observed radiances, are mostly statistical in nature and are not based on the fundamental physics governing the transfer of radiation.

The upwelling radiance at the top of the atmosphere can be expressed by a Fredholm equation of the first kind involving the Planck intensity and weighting function. This equation is known to be mathematically ill-conditioned. If a suitable transform can be made, the integral may be removed and the ill-conditioned nature of the inverse problem may be resolved: that in the inverse space the inverse problem is linear and requires no specific constraint for retrieval. This is the basic concept that constitutes the so-called differential inversion method proposed by King (1985).

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In this paper, we explore the generalization and practicality of the DIM for temperature retrievals. In section 2, we review the fundamentals of the DIM. Applications of this method for practical temperature retrievals are then made using HIRS channels, and are given in section 3. Finally, a summary is presented in section 4.

2. THE PHYSICAL FUNDAMENTALS OF THE DIFFERENTIAL INVERSION METHOD

The upwelling radiance at the top of the atmosphere R_ν for a given channel may be derived from the basic radiative transfer equation for plane-parallel atmospheres in local thermodynamic equilibrium. In the pressure coordinate, we have

$$R_\nu = B_\nu(T_s)\, T_\nu(p_s) + \int_{p_s}^{0} B_\nu(p)\, \frac{\partial T_\nu(p)}{\partial p}\, dp \quad , \tag{1}$$

where B_ν is the Planck intensity, T_ν the transmittance, p_s the surface pressure, and T_s the surface temperature. The first and second terms represent, respectively, surface and atmospheric contributions.

We shall consider the pressure integration from p_s to $p \to \infty$ and write

$$\Delta R_\nu = \int_{\infty}^{p_s} B_\nu(p)\, \frac{\partial T_\nu(p)}{\partial p}\, dp \quad . \tag{2}$$

The layer below the surface may be viewed as an infinite isothermal emitter with a temperature T_s. Since $T_\nu(\infty) = 0$, ΔR_ν is exactly the same as the surface term $B_\nu(T_s)\, T_\nu(p_s)$ in the solution of the radiative transfer equation. In the band center $\Delta R_\nu \to 0$, whereas in the wing of a band, ΔR_ν could be an important source of upwelling radiance.

The weighting function, signifying the weight of the Planck intensity contribution to upwelling radiance, may be defined in the logarithm of pressure in the form

$$W_\nu(p) = - \frac{\partial T_\nu(p)}{\partial \ln p} \quad . \tag{3}$$

For each sounding channel ν, there must be a peak weighting function located at $p = \bar{p}$, which gives the maximum contribution of Planck intensity to the upwelling radiance. Since the spectral transmittance is related to an integration of the exponential function involving the optical depth, we may write $W_\nu(p) \equiv W(p/\bar{p})$. Over a small spectral interval, the Planck intensity does not vary significantly with the wavenumber ν. For simplicity of analysis, we may omit the wavenumber index in the Planck intensity. On the basis of the preceding discussion, the upwelling radiance may be rewritten in a simple mathematical form

$$R(\bar{p}) = \int_0^\infty B(p)\ W(p/\bar{p})\ dp/p \quad , \tag{4}$$

where $\bar{p}$ replaces the wavenumber index ν. Equation (4) is a well-known Fredholm equation of the first kind. The universal inversion problem is to derive a profile of $B(p)$, given $R(\bar{p})$ and $W(p/\bar{p})$ for finite $\bar{p}$ values. In practice, since only finite $\bar{p}$ values may be chosen, the solution of $B(p)$ from the forward radiative transfer equation is mathematically ill-conditioned. Constraints of one kind or another are required to obtain physically meaningful temperature profiles. However, if the integration can be removed by a proper inverse transformation, such constraints in the inversion problem are no longer required.

We shall approach the inverse problem by a transformation of variables. In view of the term $dp/p = d\ell np$ in Eq. (4), we may introduce the following variables: $\bar{\pi} = -\ell n\bar{p}$, $\pi = -\ell np$, and $v = \pi-\bar{\pi} = -\ell n(p/\bar{p})$. In the new coordinate $-\ell np$, Eq. (4) may be rewritten in the form

$$R(\bar{\pi}) = \int_{-\infty}^\infty B(\pi)\ W(-v)\ d\pi \quad . \tag{5}$$

This form allows us to perform the bilateral Laplace transform. By virtue of the convolution theory, we find (Widder, 1971)

$$r(s) = b(s)\ w(-s) \quad , \tag{6}$$

where s denotes the transform variable, and

$$r(s) = \int_{-\infty}^\infty e^{-s\bar{\pi}}\ R(\bar{\pi})\ d\bar{\pi} \quad , \tag{7}$$

$$b(s) = \int_{-\infty}^\infty e^{-s\pi}\ B(\pi)\ d\pi = \int_{-\infty}^\infty e^{-s\bar{\pi}}\ B(\bar{\pi})\ d\bar{\pi} \quad , \tag{8}$$

$$w(-s) = \int_{\infty}^{-\infty} e^{+sv}\ W(-v)\ dv \quad . \tag{9}$$

In Eq. (8), we may replace π by $\bar{\pi}$. This allows us to evaluate the Planck intensity at discrete local levels when an inverse transform is made. The term $1/w(-s)$ may be expanded into a Maclaurin series (Pearson, 1974) so that

$$\frac{1}{w(-s)} = \sum_{k=0}^\infty \lambda_k\ s^k \quad , \tag{10}$$

where the coefficient is related to the kth derivative of the function $1/w(-s)$ at $s = 0$ in the form

$$\lambda_k = \left[\frac{1}{w(0)}\right]^{(k)} / k! \quad . \tag{11}$$

It follows that the inverse Planck intensity defined in Eq. (6) may be expressed by an infinite power series in the form

$$b(s) = \sum_{k=0}^{\infty} \lambda_k s^k r(s) \quad . \tag{12}$$

In the inverse space, the Planck intensity may be related to the upwelling radiance by the function defined in Eq. (12): that an upwelling radiance defines a local Planck intensity. To get the Planck intensity, we shall perform the inverse Laplace transform using Eq. (8) so that

$$B(\bar{\pi}) = \mathcal{L}^{-1}[b(s)] = \sum_{k=0}^{\infty} \lambda_k \mathcal{L}^{-1}[s^k r(s)] \quad . \tag{13}$$

In the last expression, the inverse Laplace transform can be performed analytically. When $\pi \to -\infty$, i.e., $\bar{p} \to \infty$, the upwelling radiance does not exist in physical space. This allows us to set $R(\pi \to -\infty) = 0$. Thus, the inverse Laplace transform leads to

$$B(\bar{\pi}) = \sum_{k=0}^{\infty} \lambda_k R^{(k)}(\bar{\pi}) \quad . \tag{14}$$

The Planck intensity at a given level is now expressible in terms of the linear sum of radiance derivatives at that level. In the context of infinite summations, the solution is exact and no assumption is made. This solution requires no constraint and is self-limited to the highest order of recoverable derivatives.

To obtain the inverse coefficient λ_k, we rewrite Eq. (9) in the form

$$w(-s) = \int_0^{\infty} (p/\bar{p})^{-s} W(p/\bar{p}) \, dp/p \quad . \tag{15}$$

In principle, if the weighting functions $W(p/\bar{p})$ are known, $1/w(-s)$ and its derivatives may be evaluated numerically. Subsequently, λ_k can be computed from Eq. (11). However, for the purpose of analysis, it is desirable to develop an analytic form that can approximate the shape of the weighting functions associated with sounding channels. A generalized weighting function was proposed by King (1985), viz.,

$$W_m = m^{m-1} \Gamma^{-1}(m) (p/\bar{p}) \exp\left[-m(p/\bar{p})^{1/m}\right] \quad , \tag{16}$$

where Γ is the Gamma function and m is an index controlling the sharpness of the weighting function. When m = 1 and 0.5, the weighting functions follow, respectively, the Goody-statistical and Elsaessor-regular band models. The weighting function so defined is normalized to unity. Figure 1 depicts the generalized weighting function for m = 0.5, 1, and 2. As m increases, it becomes broader.

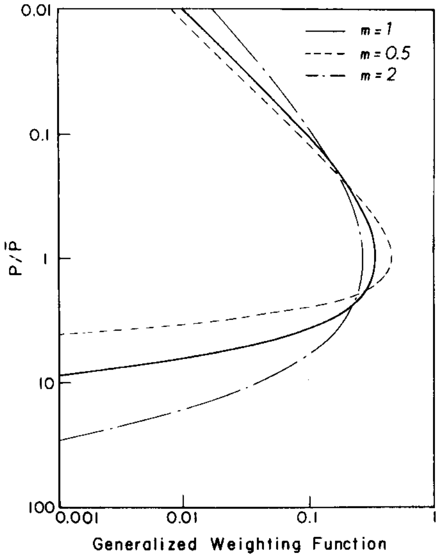


FIGURE 1. The generalized weighting function as a function of $p/\bar{p}$ for the parameter m of 0.5, 1, and 2.

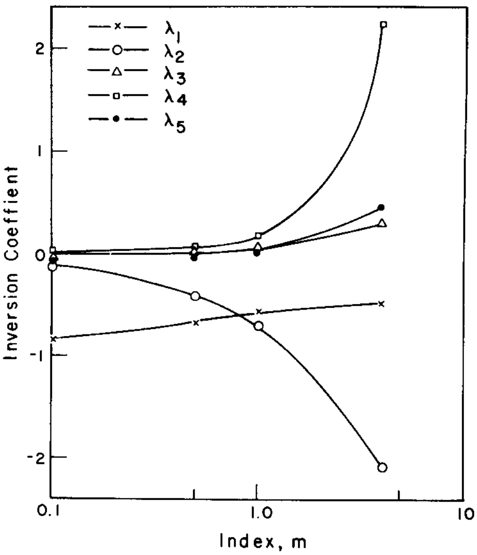


FIGURE 2. Inversion coefficients λ_i (i=1-5) as a function of the index m computed from Eqs. (11) and (17).

Using this weighting function, we can show from Eq. (15) that

$$w(-s) = \Gamma[m(1-s)] \,/\, [\Gamma(m)\, m^{-ms}] \quad . \qquad (17)$$

An evaluation of the inversion coefficient λ_k requires the derivations of Γ-functions, which are related to digamma and polygamma functions. Tables of these functions are given in Abramowitz and Stegun (1968). Figure 2 shows the inversion coefficients λ_k (k = 1-5) as functions of the index m. For any given m, λ_k may be obtained from this figure.

The foregoing discussions constitute our interpretation of the differential inversion method for temperature retrievals originally proposed by King (1985). In the next section, we shall perform synthetic analyses utilizing HIRS channels in the 15 μm CO_2 band in order to physically understand the generalization and determine the practicality of this method for temperature retrievals.

3. APPLICATIONS OF DIM FOR TEMPERATURE RETRIEVALS USING HIRS CHANNELS

In order to investigate the potential applicability of the DIM, we have used HIRS channels to perform the temperature retrieval. The

TABLE 1. HIRS CHANNEL CHARACTERISTICS

Channel	ν (cm^{-1})	ν_1	ν_2	$\Delta\nu$	Principal Absorbers	Level of W_{max}
1	668	666	670	4	CO_2	30
2	679	674	684	10	CO_2	60
3	690	685	697	12	CO_2	100
4	702	696	712	16	CO_2	250
5	716	708	724	16	CO_2	500
6	732	724	740	16	CO_2/H_2O	750
7	748	740	756	16	CO_2/H_2O	900

characteristics of these channels are listed in Table 1. To compute the transmittances, we have used the absorption coefficient sets derived by Chou and Kouvaris (1986) from line-by-line data (Rothman et al., 1983) based on the k-distribution method (Arking and Grossman, 1971). Over a small spectral interval, the order of absorption coefficients k has no bearing on the transmittance calculation. For a homogeneous path, we may express the spectral transmittance in the k-domain as follows:

$$T_{\bar{\nu}}(u) = \int_{\Delta\nu} e^{-k_\nu u} d\nu = \int_{k_{min}}^{k_{max}} e^{-ku} f(k)\, dk \quad , \qquad (18)$$

where $f(k) = (dk/d\nu)^{-1}$ is the probability density function, which can be obtained by ranking the absorption coefficients in the spectral interval $\Delta\nu$.

The absorption coefficients are available for each 0.002 cm^{-1} covering 540-800 cm^{-1} in the 15 μm CO_2 band. These values are calculated at 19 pressure levels. Temperature adjustments were also included using the following empirical equation:

$$\ell n\, k_\nu = a + b\,\Delta T + c\,\Delta T^2 \quad , \qquad (19)$$

where $\Delta T = T - 200$, and the empirical coefficients a, b, and c are pressure and wavenumber dependent.

Using the preceding absorption coefficients, the spectral transmittance for a given level p_i for each HIRS channel may be computed in inhomogeneous atmospheres in the form

$$T_{\bar{\nu}}(p_i) = \sum_{n=1}^{N} \exp\left(- \sum_{j=1}^{i} k_{nj}\, q_j\, \Delta p_j/g\right) \Delta\nu_n \quad , \qquad (20)$$

where q denotes the mixing ratio, g the gravitational acceleration,

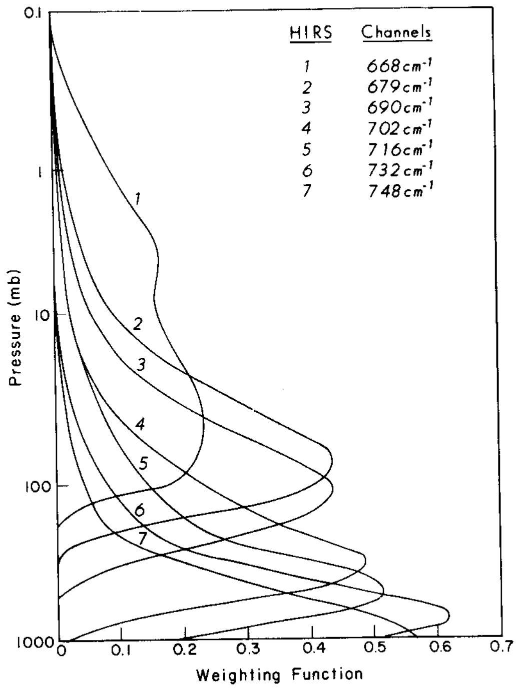


FIGURE 3. The weighting function of seven HIRS channels in the logarithmic pressure coordinate. The peaks of these weighting functions are listed in Table 1.

$\Delta\nu_i = 0.002$, and $N = \Delta\nu/\Delta\nu_i$. Figure 3 shows the computed weighting functions for seven HIRS channels. The peaks of these weighting functions are exactly the same as those listed in Table 1.

It is possible to compute λ_k directly from Eqs. (11) and (15) once numerical values for the weighting function are known. However, the computations could become very tedious. With the use of the generalized weighting function defined in Eq. (17), λ_k can be evaluated by known mathematical functions. We have developed a numerical method to fit HIRS weighting functions to the generalized weighting function to obtain the index m. We define the sum of the weighted square error at a given level i in the form

$$E = \sum_{i=1}^{M} \left[W_m(p_i/\overline{p}) - W(p_i/\overline{p}) \right]^2 \varepsilon_i \quad , \tag{21}$$

where M denotes the total atmospheric levels used in transmittance calculations, $\overline{p}$ the pressure level at which the weighting function W has a maximum value, and ε_i is a function defined by

$$\varepsilon_i = \begin{cases} \exp\left(-p_i/\bar{p}\right) & , \ p_i/\bar{p} > 1 \\ \exp\left(-\bar{p}/p_i\right) & , \ p_i/\bar{p} < 1 \end{cases} \tag{22}$$

With the factor ε_i, E is particularly dominated by error near the maximum weighting function. We then proceed to minimize E, viz.,

$$\frac{\partial E}{\partial m} = \sum_{i=1}^{N} 2\left[W_m(p_i/\bar{p}) - W(p_i/\bar{p})\right] \varepsilon_i \left\{(1-1/m) - (p_i/\bar{p})^{1/m}\left[1 - \ell n(p_i/\bar{p})/m\right] + \ell n m - \psi(m)\right\} = 0 \ , \tag{23}$$

where $\psi(m)$ is the digamma function. The bisection method is subsequently used to solve for m (Hamming, 1973). Table 2 lists the values of the parameter m for each HIRS channel, RMS error, and error near the peak of the weighting function. Also listed are values for the peak weighting function. The RMS errors are sufficiently small to have a significant effect on the upwelling radiance calculation. For channel 1, a large m is found since it has a broad weighting function. For other channels, m ranges between 0.2 and 0.7. It is apparent that neither the random model nor the regular model can fit HIRS transmittances well. Once the parameter m is known, the inversion coefficient λ_k may then be evaluated for each channel (see Fig. 2).

It is necessary to develop a curve-fitting method to fit the seven upwelling radiance values since high-order derivatives are required to calculate the Planck intensity. We have used a fifth-order polynomial function as a first approach to fit seven HIRS radiances, i.e.,

$$R(\bar{\pi}) = \sum_{n=0}^{5} a_n \bar{\pi}^n \ , \tag{24}$$

TABLE 2. VALUES OF PARAMETER m, RMS ERROR, AND ERROR NEAR THE PEAK WEIGHTING FUNCTION FOR THE HIRS CHANNELS

Channel	m	RMS error	W_{max}*	error near peak
1	2.8370	0.0141	0.234	-0.0036
2	0.6410	0.0137	0.433	0.0073
3	0.6668	0.0107	0.436	0.0017
4	0.4570	0.0237	0.487	-0.0129
5	0.4273	0.0137	0.517	-0.0048
6	0.2305	0.0159	0.614	0.0076
7	0.3160	0.0118	0.566	-0.0004

*W_{max} denotes the maximum value of the weighting function.

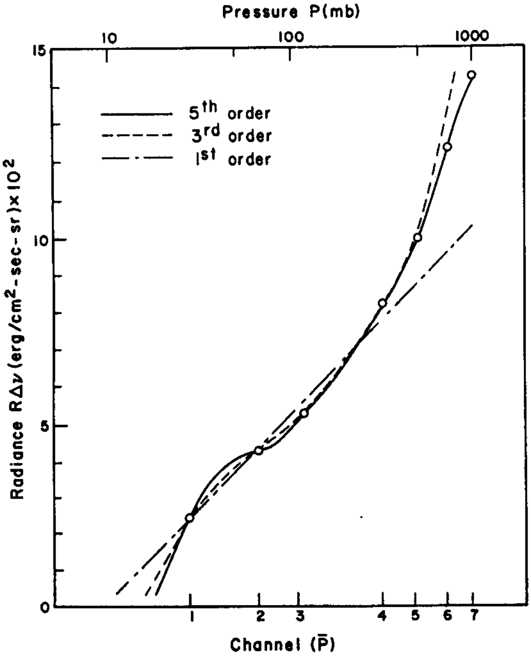
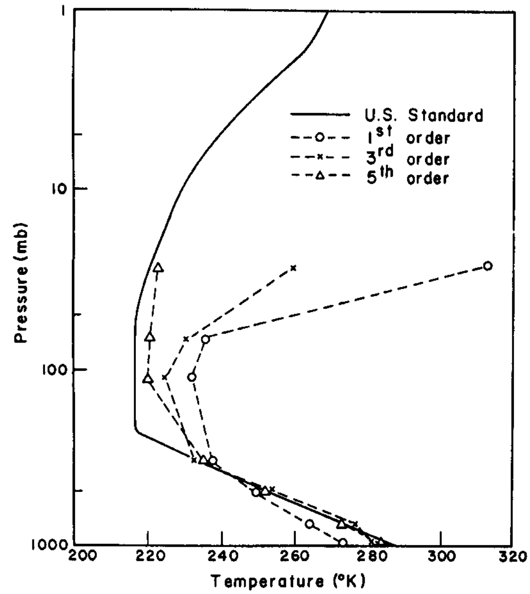


FIGURE 4. The computed upwelling radiances (circles) for seven HIRS channels in the logarithmic pressure coordinate, and curve fittings to the computed values using first-, third-, and fifth-order polynomials. The U.S. standard temperature is used in the computation.

where $\bar{\pi} = -\ln\bar{p}$. Derivatives up to the fifth-order may then be carried out. Newton's interpolation formula (Hamming, 1973) was used to obtain the coefficients a_n. Figure 4 shows the fitting of seven HIRS spectral radiances using first-order (straight line), third-order, and fifth-order polynomials. The U.S. standard temperature profile was used in the radiance calculation. The fifth-order fitting shows fluctuations for channels 1-3. This suggests that a smooth curve-fitting method could be advantageous in the inversion exercises because high-order derivatives of the curve are required.

At this point, since the inversion coefficients λ_k are known, as are the derivatives, the Planck intensity at the peak of the weighting function $\bar{p}$ can be computed from Eq. (14). From the Planck intensity for each channel, the temperature can be evaluated. Figure 5 shows retrieval results for the first-, third-, and fifth-order polynomial fittings to synthetic HIRS radiances using the U.S. standard temperature profile. It is quite encouraging to find that the retrieval results converge to the true solution as high-order radiance derivatives are incorporated in the calculation. For the fifth-order approximation, errors in the retrieved temperatures in the lower atmosphere corresponding to channels 4-7 are within about 2 K.



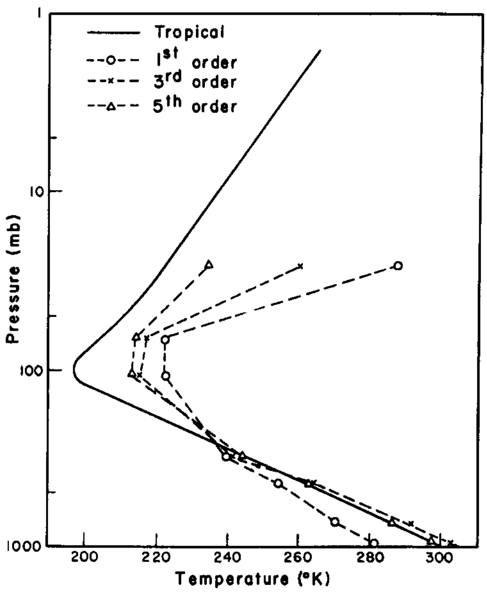


FIGURE 5. Results of DIM temperature retrievals using first-, third-, and fifth-order expansions for the U.S. standard temperature profile.

FIGURE 6. Same as Fig. 5, except for the tropical temperature profile.

Retrieved temperatures associated with channels 1-3 show larger deviations from true values. These deviations are due to the unsatisfactory fitting described previously. We have also used the tropical temperature profile to perform the retrieval. As shown in Fig. 6, the shape of this profile differs significantly from that of the U.S. standard profile. Again, the retrieved solution converges to the true profile when higher-order radiance derivatives are included in the inversion calculation. The retrieved temperatures are within about 1 K for channels 4-7. However, large errors are found in the upper levels corresponding to channels 1-3. The large retrieval errors are in part caused by the large curvature occurring at about 100 mb, and by the unsatisfactory fitting of radiances for these channels.

Finally, we perform retrieval analyses by adding random errors in the radiance values. Maximum random errors of 2 and 5% were used. The resulting temperature errors are shown in Fig. 7. Except for channel 1, the addition of random errors does not produce significant errors in temperature retrievals. This is particularly evident for channels 4-7, where peaks of the weighting function are in the lower atmosphere. The inability to perform retrievals for channel 1 when random errors are added is due to the nature of the broad weighting

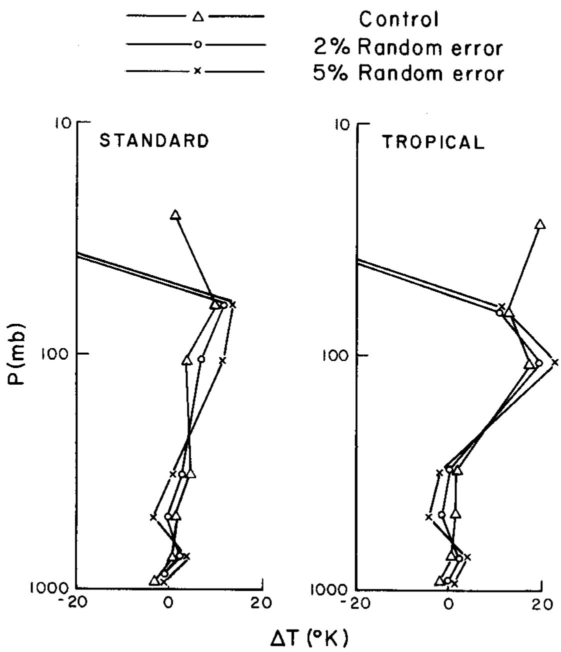


FIGURE 7. Analyses of errors for DIM temperature retrievals with and without random errors. Maximum random errors of 2 and 5% are used in the calculation.

function. In this case, the parameter $m \cong 2.8$, and λ_k have large negative and positive values as shown in Fig. 2. As a result, small errors in radiance values are amplified and propagate onto the retrieved Planck intensity, leading to unstable results for this channel.

4. SUMMARY

The DIM for temperature retrievals has been reviewed in terms of the theory of radiative transfer. It is shown that in the Laplace transform space the Planck intensity is directly related to the upwelling radiance weighted by the weighting function. After expanding the transformed weighting function in a Maclaurin series and performing the inverse transform, the Planck intensity in real space can be exactly expressed by a linear combination of the derivatives of radiances.

Using seven HIRS channels in the 15 μm CO_2 band, numerical analyses for temperature retrievals have been carried out. These involve the curve-fitting of seven radiance values. We demonstrate that a fifth-order polynomial fitting to radiance values is adequate to yield correct retrieval results for temperature and that the DIM converges to the true temperature solution. In retrieval exercises, two distinct U.S. standard and tropical temperature profiles were used. The retrieved temperatures in the troposphere corresponding to channels 4-7 are accurate within 1-2 K. In general, an addition of random errors with a maximum value of 5% to radiance values does not introduce instability in the inversion exercises. One exception is channel 1, corresponding to the center of the 15 μm CO_2 band, which has a broad weighting function. This appears to suggest that the DIM is particularly useful and practical for sharp weighting functions. Our preliminary conclusion is that the DIM is a powerful retrieval method with no constraints required. Future research will involve an improved fitting program for upwelling radiances, an objective error analysis, and tests of the method using observed radiances and temperature profiles.

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DISCUSSION

Smith: I think it is an exciting approach especially if you are dealing with a near continuum of radiance observations as future instruments are going to be doing. I have a comment though. First of all, you denoted the radiance as a function of P or pressure. Since its structure is directly related to the temperature structure as a function of pressure, the higher order the radiance information, the better off you are as far as temperature profile information content. However, in looking at the results that you've shown for a very limited number of measurements, it didn't appear that you are conserving energy. I was wondering what was causing that.

Liou: What do you mean by conserving energy?

Smith: Well, if you integrate the radiative transfer equation over your temperature profile it didn't appear that you would end up with the observed radiance being equal to that. You would calculate from your solution profiles. They are fitting very well in the troposphere and then systematically off in the stratosphere. If you integrate the difference between your solution and the truth using the weighting functions for those channels it does not appear that you would end up with zero.

Liou: Well, there is some deviation of temperatures by about a degree here. And perhaps the deviation here can make up for the loss there. Well, I don't understand the meaning of conservation of energy. You performed the radiance calculation using the profile plus the weighting function. Do you mean that the radiance should not deviate that much from this profile because that is where most of the energy comes from?

Rodgers: I wondered if you would like to try on your retrieval method the set of diagnostics I presented yesterday.

Liou: I must apologize, I just got in last night so I didn't attend your talk. Some sort of statistical analysis? I'll get with you later.

Yee: The energy conservation may not exactly apply to this particular problem. Maybe we didn't pay much attention to what you mentioned about localization of this particular method. In other words this may not rely on the entire profile. That means the interference of one particular layer of the retrieval is not inferenced by the other layers very heavily. Because of this differentiation, I have some questions though. For the fifth order of differentiation, you may have to rely on many layers away but I would suspect that their weight would decrease very fast from the first order. So essentially you still rely on a very local point of the radiance. And also that particular layer of temperature. So this problem is very different.

Liou: Right. But Bill mentioned that when you perform integrations over the radiative transfer equation, the retrieved profile used in the radiance calculation, if the retrieval is good, should approximate the overall observed profile. That is the energy conservation principle, if I understand it correctly.

Gille: Is the answer to the point that Bill brought up, that although it appears that your fit suggests low temperatures at the top when you integrate over that broad weighting function you are incorporating only a small part of the low temperature?