TOVS RETRIEVALS AT THE U.K. METEOROLOGICAL OFFICE

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1. INTRODUCTION

The Meteorological Office has been processing data from the TIROS Operational Vertical Sounder (TOVS) routinely in real-time since 1983. Initial retrieval methods were conventional, using algorithms based on the International TOVS Processing Package (version 1) obtained from the University of Wisconsin-Madison. The inversion scheme used a statistical regression technique tuned to the TOVS local reception area of the U.K. (see Turner *et al.* 1985). Our recent research on TOVS data has been concerned mainly with more direct ways of applying radiance information in numerical weather prediction (NWP). Our motivation for pursuing this line of research arose from an awareness of the problems encountered with the original scheme and from an improved understanding of the error characteristics and information content of conventional retrieved profiles, leading to an appreciation of the difficulties in using such products optimally in NWP. These ideas are discussed in section 2.

A theoretical approach to the direct use of radiances in NWP analysis is presented in section 3. The formulation is quite general and could be applied as part of a 3- or 4-dimensional variational analysis scheme. However, at present we have only explored one-dimensional (vertical) methods. The theory for both a linear and nonlinear scheme is presented. Section 4 discusses the implementation of both these schemes. A linear scheme applied to cloud-cleared TOVS brightness temperatures is currently the method used in routine TOVS processing at the Meteorological Office. A nonlinear scheme applied to raw, potentially cloud-affected radiances has been demonstrated and is currently undergoing further development and testing.

The ideas for direct use of radiance translate easily to the next generation of operational sounders, the Advanced TOVS (ATOVS) system. Section 5 outlines recent work on simulating the potential of ATOVS for providing information to an NWP system. Special considerations relevant to ATOVS are discussed and some results of simulated performance are presented.

2. WHY DIRECT USE OF RADIANCES?

The satellite radiance inversion problem is mathematically ill-posed, and additional constraints are required to choose between the infinite number of atmospheric profiles which satisfy the measurements. This "prior information" has subtle but important effects on the retrieved profile. In the case of a linear inversion, the prior dependence can be assessed analytically (see Eyre 1987 or Eyre 1988). For a nonlinear inversion the effects are more complicated but no less important (see Rodgers 1988). The prior dependence leads to error characteristics in the retrievals which are difficult to handle properly in an NWP analysis. It leads to correlations of error in the horizontal and vertical which are nothing to do with the original radiance data (although these may contain biases which also contribute to correlated errors).

NWP background fields into which satellite observations are assimilated are now of such an accuracy that, if the satellite information is not assimilated carefully and with regard to its true error characteristics, it can easily degrade an otherwise good NWP field. This is particularly so in northern hemisphere mid-latitudes. When using retrieved profiles it is necessary to consider the effects of the correlations of error introduced by the retrieval process or, equivalently, to ask what is the status of the prior information which appears in the retrieval but is not true "observed" information. It is clear that satellite sounders do NOT measure temperature and humidity profiles – they measure radiances – but this obvious fact has not yet been adequately reflected in the way NWP analysis schemes treat satellite sounding data.

It is on the basis of these arguments that we have been led to move towards more direct ways of using radiance data in NWP and to seek methods by which they can be applied according to their true error characteristics and information content. For further discussion of these matters, see Eyre and Lorenc (1989).

3. THEORY OF DIRECT USE OF RADIANCES IN NWP

The problem of providing the best analysis for NWP may be expressed in terms of the minimisation of a cost function measuring the departure of the analysis from the observations and the background plus other constraints (see Lorenc 1986). The cost function $J(\mathbf{x})$ for NWP analysis field $\mathbf{x}$ may be written as:

$$
\begin{aligned}
J(\mathbf{x}) &= (\mathbf{x}-\mathbf{x}^b)^T \,.\, \mathbf{C}^{-1} \,.\, (\mathbf{x}-\mathbf{x}^b) \\
&+ (\mathbf{y}^m - \mathbf{y}\{\mathbf{x}\})^T \,.\, \mathbf{E}^{-1}.(\mathbf{y}^m - \mathbf{y}\{\mathbf{x}\}) \\
&+ J_3\,(\mathbf{x}) \qquad (1)
\end{aligned}
$$

where $\mathbf{x}^b$ is the background profile, $\mathbf{y}^m$ is the measured radiances, $\mathbf{y}\{\mathbf{x}\}$ is the forward model giving the radiances corresponding to $\mathbf{x}$, $\mathbf{C}$ is the expected covariance of background error and $\mathbf{E}$ is the expected covariance of measurement error (including forward model error). $J_3(\mathbf{x})$ includes terms added to impose additional physical or dynamical constraints. $\mathbf{x}$ is a "field" which may, in general, represent a 3- or 4-dimensional NWP model state. However, if the vertical and horizontal parts of the analysis are separated, it may be applied in one dimension to the problem of the vertical analysis of a set of observations (such as satellite radiances) at a single horizontal location. In the short term, the operational data assimilation at the Meteorological Office will follow this approach (see below).

$J(\mathbf{x})$ is a minimum when its derivatives with respect to all elements of $\mathbf{x}$ are zero:

$$
J'(\mathbf{x}) = \mathbf{C}^{-1} \,.\, (\mathbf{x}-\mathbf{x}^b) - \mathbf{K}(\mathbf{x})^T \,.\, \mathbf{E}^{-1} \,.\, (\mathbf{y}^m - \mathbf{y}\{\mathbf{x}\}) + J_3'\,(\mathbf{x}) = 0 \qquad (2)
$$

where $\mathbf{K}(\mathbf{x}) = \mathbf{y}'\{\mathbf{x}\}$, the gradient of the radiative transfer model.

3.1 A linear approach

If $\mathbf{K}(\mathbf{x})$ can be taken as constant for all reasonable departures of $\mathbf{x}$ from $\mathbf{x}^b$, then the forward problem is linear:

$$
\mathbf{y}\{\mathbf{x}\} = \mathbf{y}\{\mathbf{x}^b\} + \mathbf{K} \,.\, (\mathbf{x}-\mathbf{x}^b) \qquad (3)
$$

If in addition we ignore $J_3'(\mathbf{x})$, then Eq. (2) may be solved analytically:

$$
\mathbf{x} = \mathbf{x}^b + \mathbf{W}.(\mathbf{y}^m - \mathbf{y}\{\mathbf{x}^b\}) \qquad (4)
$$

where $\mathbf{W} = \mathbf{C}.\mathbf{K}^T.(\mathbf{K}.\mathbf{C}.\mathbf{K}^T + \mathbf{E})^{-1}$. This is familiar as the minimum variance retrieval equation (see, for example, Rodgers 1976). Thus direct assimilation of radiances can be thought of as mathematically equivalent to a conventional minimum variance retrieval in which an NWP model field acts as the background for the inversion and its expected error covariance provides the constraint.

3.2 A nonlinear approach

If $\mathbf{K}(\mathbf{x})$ cannot be taken as constant, then there is in general no analytic solution; a numerical method must be found either to minimise $J(\mathbf{x})$ or to solve Eq.(2). One approach is to solve this equation iteratively using Newton's method:

$$\mathbf{x}_{n+1} = \mathbf{x}_n - J''(\mathbf{x}_n)^{-1} \,.\, J'(\mathbf{x}_n) \tag{5}$$

$$\mathbf{J}''(\mathbf{x}_n) \simeq \mathbf{S}(\mathbf{x}_n)^{-1} = \mathbf{C}^{-1} + \mathbf{K}(\mathbf{x}_n)^T \,.\, \mathbf{E}^{-1} \,.\, \mathbf{K}(\mathbf{x}_n) \tag{6}$$

or

$$\mathrm{S}(\mathbf{x}_n) = \mathbf{C} - \mathbf{C} \,.\, \mathbf{K}(\mathbf{x}_n)^T \,.\, (\mathbf{K}(\mathbf{x}_n).\mathbf{C}.\mathbf{K}(\mathbf{x}_n)^T + \mathbf{E})^{-1} \,.\, \mathbf{K}(\mathbf{x}_n) \,.\, \mathbf{C} \tag{7}$$

This is feasible for the one-dimensional case when $\mathbf{x}$ represents a vertical atmospheric profile (vector length ~60) but would not be practicable for the much longer vectors which occur in 3- or 4-dimensional analysis. An alternative minimisation technique would have to be found.

3.3 The NWP interface

Equation (4) or its nonlinear equivalent may be considered as a conventional retrieval or as a vertical analysis at the observation point. The latter is consistent with the approach in the data assimilation scheme recently developed for operational use at the Meteorological Office (Lorenc *et al.* 1988), in which the horizontal and vertical aspects are separated. For all observation types, the datum is first interpolated to the vertical levels of the model at its own horizontal location, and then the information is spread in the horizontal to model grid points. For satellite radiances, the vertical stage is as described above. There is a problem of observational error correlation in the horizontal stage: because the background field is used in the inversion, retrieval errors are correlated with the background and hence with each other. However, since we can assess this correlation theoretically, we can allow for it in the horizontal analysis (see Lorenc *et al.* 1986). Thus, although our retrievals have correlated errors, the conceptual equivalence to the direct assimilation of radiance provides a theoretical framework for determining how the correlations of errors should be handled correctly within the horizontal stage of the assimilation.

4. IMPLEMENTATION FOR TOVS

4.1 The operational Local Area Sounding System (LASS)

The "forecast background" inversion scheme, which is based on the linear approach described in section 3.1, has been used in the operational LASS at Bracknell since 1987. In this scheme, the profile vector $\mathbf{x}$ includes the temperature and humidity profiles and the surface skin temperature, and the measurement vector $\mathbf{y}^m$ contains pre-processed, cloud-cleared TOVS brightness temperatures. $\mathbf{x}^b$ is a short-range (~12 hour) forecast interpolated in time and space to the location of the TOVS sounding. $\mathbf{y}\{\mathbf{x}^b\}$ is a forecast brightness temperature vector calculated in real time using a fast model based on the approach described by Weinreb *et al.* (1981). $\mathbf{W}$ is computed once per month using a $\mathbf{K}$ appropriate to a monthly mean profile for the European area. The effects on retrieval accuracy of errors in $\mathbf{C}, \mathbf{E}$ and $\mathbf{K}$ have been studied in detail (Watts and McNally 1988), and the values of $\mathbf{C}$ and $\mathbf{E}$ used in the inversion have been tuned through experiments with real data.

In addition to the development of the new inversion approach, it has been necessary to pay careful attention to many other aspects of the TOVS data processing. A new cloud-clearing scheme (Eyre and Watts 1987) was introduced into routine processing in 1987. Also considerable effort has gone into monitoring biases between retrieved, forecast and collocated radiosonde profiles and between the radiances calculated from them. On the basis of this monitoring, the biases applied to calculated radiances are tuned regularly (see Watts 1989).

4.2 Research on a nonlinear scheme

The scheme described above assumes a linear relationship between cloud-cleared brightness temperature and temperature/humidity profile. This is quite accurate for temperature but not really satisfactory for humidity. Also, in using pre-processed, cloud-cleared brightness temperatures, we are forced to tolerate errors in the radiances introduced by the cloud-clearing and pre-processing. In theory, it is preferable to use the raw, potentially cloud-affected radiances directly. This leads to a highly nonlinear problem, primarily because of the profound effect of clouds on infra-red weighting functions.

A scheme for inverting raw radiances has been developed using a Newtonian method to solve the nonlinear problem (Eyre 1989a). A "damped" version of the approach presented in section 3.2 has had to be adopted to overcome instability of the iteration (probably caused by the highly nonlinear nature of the problem). This involves, in the calculation of $J''(\mathbf{x})$, reducing the elements of $\mathbf{C}$ representing those variables which make the problem so nonlinear (i.e. the cloud parameters). When the iteration converges, a check is made on the fit of the measured to the calculated radiances in each channel. This is found to provide a powerful means of quality control. An important aspect for the practical implementation of this scheme has been the development of a fast method for computing $\mathbf{K}(\mathbf{x})$ in parallel with the calculation of $\mathbf{y}\{\mathbf{x}\}$. In this scheme, the variables cloud-top pressure, fractional cloud amount and microwave surface emissivity are added to the profile vector and are retrieved simultaneously with other profile parameters listed in section 4.1.

The scheme has been applied successfully to real data (Eyre 1989b). However it has not yet been shown to be consistently better than the linear scheme, and research continues. Recently, a joint experiment has begun with ECMWF in which this scheme is being applied to global TOVS radiances. In this way we hope to learn more about the characteristics of the scheme and study methods for tuning it effectively. The current version of the nonlinear scheme is rather expensive computationally. Although it converges in $\sim$4 iterations, it involves at each step the computation of $J''(\mathbf{x}_n)$ and a full radiative transfer calculation of $\mathbf{y}\{\mathbf{x}_n\}$ and $\mathbf{K}(\mathbf{x}_n)$. A more efficient scheme should be possible through a different approach to the minimisation of Eq. (2) and more economical use of the full radiative transfer model. Such developments would be essential if the scheme were to be extended from its present one-dimensional (vertical) form to an application in a 3- or 4-dimensional data assimilation system.

5. A POSSIBLE APPROACH FOR ATOVS

From about 1993, starting with the satellite NOAA-K, the combination of sounding radiometers known as TOVS will be replaced by the ATOVS set. TOVS consists of the High-resolution Infrared Radiation Sounder (HIRS2), the Microwave Sounding Unit (MSU) and the Stratospheric Sounding Unit (SSU). For ATOVS, HIRS2 will be retained but MSU and SSU will be replaced by the new Advanced Microwave Sounding

Unit (AMSU). The characteristics of these instruments are summarised in Table 1. HIRS2 is a 20-channel instrument with a horizontal resolution of about 40 km. AMSU is in fact 2 instruments: a low-frequency part, AMSU-A (channels 1–15 from 23–89 GHz) with a horizontal resolution of about 50 km, and a high-frequency part, AMSU-B (channels 16–20 from 89–183 GHz) with a horizontal resolution of about 17 km. AMSU-A will be the primary temperature sounding instrument and will represent a considerable improvement in horizontal and vertical resolution over MSU. HIRS will still yield valuable and complementary information, particularly in the absence of clouds, mainly through narrower weighting functions in channels sounding the lower troposphere. AMSU-A will contain channels sounding temperature from the surface almost to the stratopause, and it will have improved vertical resolution compared to SSU. AMSU-B will provide information on water vapour profiles and will extend useful coverage into some (but not all) cloudy areas.

The inversion approach presented in section 3 is very flexible (particularly the nonlinear method) and can in principle be applied to many types of remote measurement. Research has begun on adapting the method to the special characteristics of ATOVS. A simulation study has been performed to examine the information content of ATOVS data in the context of a NWP system. This study is reported fully elsewhere (Eyre 1989c) and so only the major features and a summary of the results are given here.

The basic approach to the inversion problem is the same as for TOVS, through minimisation of Eq. (1) or solution of Eq. (2). At present only the one-dimensional (vertical) problem has been explored. In addition to those variables used with TOVS to specify the atmospheric profile vector $\mathbf{x}$, it is necessary to extend the list for the ATOVS problem, particularly with regard to the treatment of microwave surface emissivity and absorption by cloud liquid water. It is proposed to treat the variation of microwave surface emissivity with frequency, $\varepsilon(\nu)$, using a parametric model which is applicable to a wide range of natural surfaces. Grody (1987) has suggested the model

$$\varepsilon(\nu) \;=\; \frac{\varepsilon_o \;+\; \varepsilon_\infty\,(\nu/\nu_o)^k}{1 \;+\; (\nu/\nu_o)^k} \tag{8}$$

where the 4 parameters – ε_o, ε_∞, ν_o and k – take different values for different surfaces. More extensive measurements of the emissivities of natural surfaces may lead to an improved formulation. However some parameterisation of this type will be needed if we are to exploit fully the multi-spectral measurements from AMSU. For the simulation

Table 1. Summary of instrument characteristics

Instrument	Horizontal resolution (km)	Channels number (total)	Channels number	Channels wavelengths/ frequencies	Purposes
HIRS/2[1]	~ 40		7	13–15μm	Temperature profile
			1	11.1μm	(troposphere and
			1	9.7μm	lower stratosphere)
		20	3	6.5–8.4μm	Humidity profile
			4	4.2–4.6μm	(troposphere)
			2	3.6-4.1μm	Surface temperature
			1	0.7μm	Total ozone
MSU	~170		4	50–57 GHz	Temperature profile (troposphere and lower stratosphere)
SSU	~200		3	15μm (pressure modulation)	Temperature profile (mid-upper stratosphere)
AMSU-A	~ 50		1	23 GHz	Temperature profile
			1	37 GHz	(troposphere, stratosphere)
		15	12	50–58 GHz	Total column water vapour
			1	89 GHz	Cloud liquid water
					Surface parameters
AMSU-B	~ 17		1	89 GHz	Humidity profile
		5	1	157 GHz	(troposphere)
			3	183 GHz	Cloud water/ice
					Precipitation
					Surface parameters
AMRIR	~0.5[2]		1	13.55μm	Temperature profile
		11	2	10.8, 12.0μm	(lower troposphere)
			2	4.4–4.6μm	Surface temperature
			2	3.72, 4.01μm	Cloud parameters
			4	0.6–1.6μm	Imagery for many other applications

Notes

(1) HIRS/2I on NOAA-11 replaces channels centred at 8.16 and 4.24 μm by ones at around 12.7 and 4.1μm respectively. HIRS/2 values have been used throughout this study.

(2) To be averaged to ~4 km to reduce noise on sounding channels.

studies conducted so far, Eq. (8) has been assumed, and its 4 free parameters have been included in the profile vector, to be retrieved simultaneously with the other parameters listed in section 4.1 and 4.2. Total column cloud liquid water has also been added.

It has also been necessary to adjust the specification of the measurement vector $\mathbf{y}^m$ to refer to the set of ATOVS channels and to construct a corresponding forward model $\mathbf{y}\{\mathbf{x}\}$ and its gradient with respect to all the profiles parameters $\mathbf{K}(\mathbf{x})$. The models developed for TOVS (see Eyre 1987a) have been adapted accordingly. The microwave models do not represent any scattering processes within cloud. Where these effects are significant – and they will be where large ice particles or precipitation are present – it is assumed that these conditions will be detected by some pre-processing stage and that no inversion will be attempted here.

It can be shown that the expected covariance of error in retrievals obtained by solving Eq. (2) is

$$\mathbf{S}(\mathbf{x}) \ = \ \mathbf{C} \ - \ \mathbf{C}.\mathbf{K}(\mathbf{x})^T.(\mathbf{K}(\mathbf{x}).\mathbf{C}.\mathbf{K}(\mathbf{x})^T + \mathbf{E})^{-1} \ . \ \mathbf{K}(\mathbf{x}).\mathbf{C} \ . \qquad (9)$$

This is exact for the linear case and a good approximation under most circumstances of interest for the nonlinear case. If an adequate numerical method can be found for solving Eq. (2), then the solution will have error characteristics described by Eq. (9). The optimal performance of the system under different conditions may therefore be explored by evaluating $\mathbf{S}(\mathbf{x})$ over a range of values of $\mathbf{x}$, $\mathbf{C}$ and $\mathbf{E}$; it is not necessary to perform numerous retrievals from simulated radiances. Also, by comparing the retrieval error covariance $\mathbf{S}$ with the prior (background) error covariance $\mathbf{C}$, the amount of information which the satellite data can add to the NWP system may be assessed in a very economical way.

It has been assumed that the background values for the temperature and humidity profiles and the surface pressure and temperature are taken from a short-range forecast, and so the corresponding elements of $\mathbf{C}$ represent the typical error covariance of such a forecast. Cloud and surface emissivity parameters have been assumed not to be available from the forecast model. Their prior values take some reasonable average figures and their prior uncertainties have been assumed large, such that the retrieved values of these variables are effectively unconstrained by the background. In constructing the matrix $\mathbf{E}$, the effects of both radiometric noise and errors in the forward model have been simulated.

Retrieval error covariances and related quantities have been calculated for various combinations of channels representing both TOVS and ATOVS, for various atmospheric profiles representing different latitude zones, for different cloud conditions, for different microwave surface emissivities representing land and sea, for different assumptions regarding the prior information including the characteristics of forecast error, and for different levels of radiometric noise and forward model error. The results are reported in detail elsewhere (Eyre 1989c) but Fig. 1 gives an example of them. It shows the expected r.m.s. retrieval errors (square roots of the diagonal elements of **S**) for different radiometer combinations compared with the r.m.s. prior error (square roots of the diagonal elements of **C**). In addition to expected errors in the profiles of temperature and ln (water vapour mixing ratio), errors in the related quantities of thickness (from 1000 mb to other levels) and layer water vapour content (from 300 mb to other levels) are shown. Prior errors are typical of a 12h forecast in the European and N. Atlantic areas. Calculations shown for each combination of radiometers have been performed under the same conditions: assuming a mean mid-latitude profile, no cloud (but also no prior knowledge of the cloud), surface emissivities typical of a calm sea and sounding at nadir.

Figure 1 demonstrates that the potential ability of MSU alone to improve on a short-range temperature forecast is usually very limited, and the potential of AMSU is considerably greater. It also shows that, under cloud-free conditions, the addition of HIRS to either microwave system improves the performance significantly. This and other results confirm the value of retaining a combined infra-red and microwave sounding system and the considerable improvement theoretically obtainable from the ATOVS system compared with the TOVS system. The simulations also confirm that, although the potential to improve on forecast temperatures at fixed pressure levels is rather limited for all systems, the potential impact on thicknesses of broad layers is much greater.

It should be stressed that these are simulations of optimal performance. They assume that the conditions implied in the inversion (e.g. the prior error and the radiance error characteristics) actually occur in practice. It is also assumed that all aspects of the data processing – the calibration, pre-processing, radiative transfer calculation, etc. –

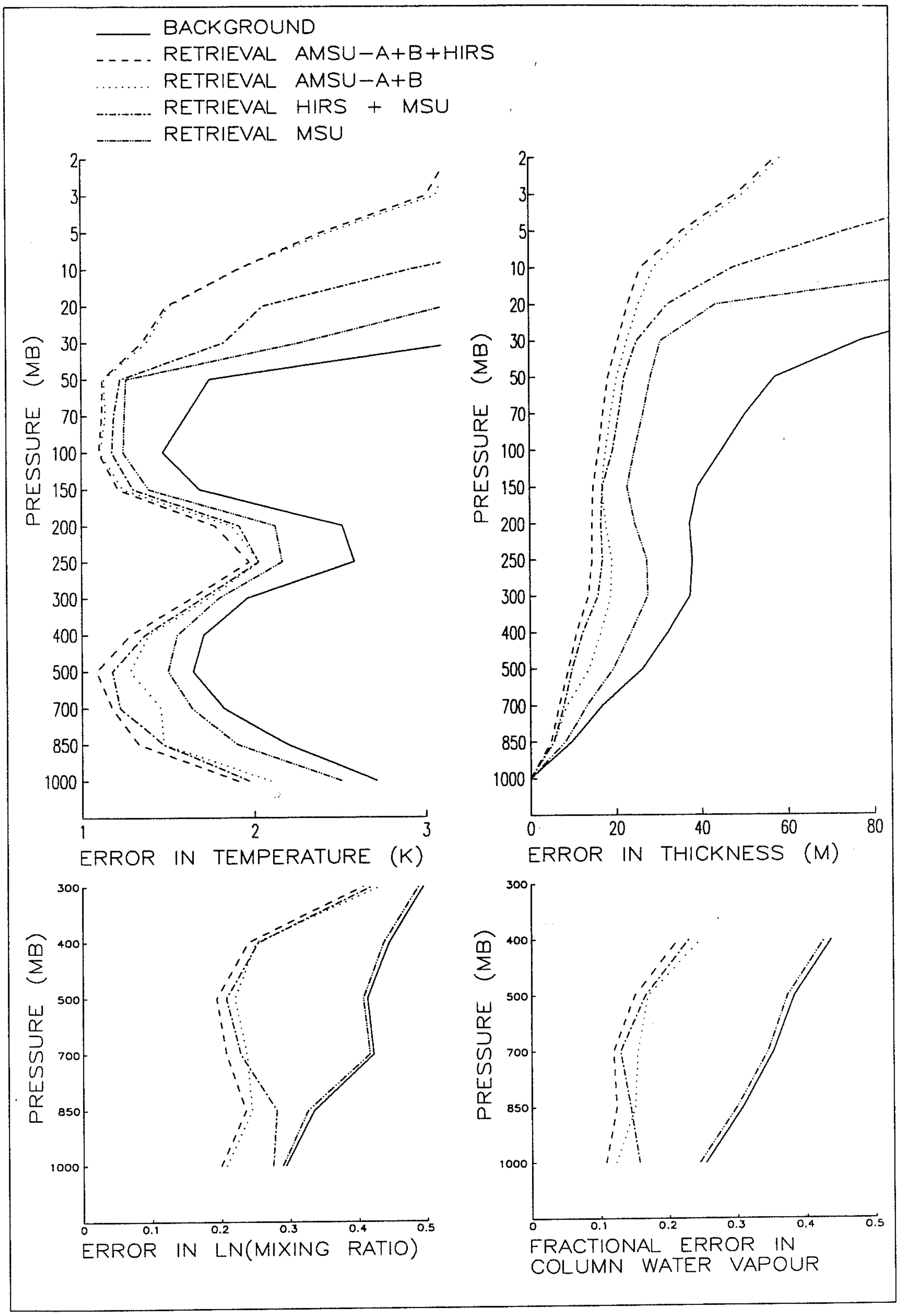

Figure 1. Simulated retrieval performance for some combinations of TOVS and ATOVS radiometers.

are of high quality. It still remains a major challenge to exploit satellite sounding data in such a way that we come close to obtaining from the data the information content achievable in theory.

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