

USE OF CLEARED RADIANCES IN 3D/4D VARIATIONAL DATA ASSIMILATION

E. Andersson, J. Pailleux*, J-N. Thépaut, J.R. Eyre,
A.P. McNally, G.A. Kelly and P. Courtier

European Centre for Medium-Range Weather Forecasts
Reading, U.K.

*Current affiliation, Météo-France, Toulouse, France

1. INTRODUCTION

In recent years interest has shifted towards retrieval schemes which use a NWP (Numerical Weather Prediction) forecast model to provide the background information (e.g. Eyre, 1989). The NWP model provides a better estimate of the atmospheric state than either a library of profiles or by pure statistical information. Such schemes are operational at ECMWF (Eyre *et al.*, 1992; McNally, 1993, in this volume), at U.K. Meteorological Office (Turner *et al.*, 1985) and are in pre-operational tests at NMC (National Meteorological Centre), Washington (Goldberg *et al.* 1993, in this volume). The work of Eyre *et al.* is very closely related to the work presented in this paper. Their scheme performs the retrieval in a variational formulation profile by profile, and can be seen as a one-dimensional analysis of TOVS radiances. Much of the development involved for TOVS is common between 3D/4D-Var and the one-dimensional scheme, including the radiative transfer model and the radiance monitoring/tuning system. To emphasize the link between the two projects, the one-dimensional scheme is known as "1D-Var".

The advantage of these variational schemes is the use of more accurate background information (a six-hour forecast, interpolated to the TOVS locations). For a one-dimensional scheme this introduces a correlation between the observation error and the background error, which may cause problems when the same six-hour forecast is used again as the background for the subsequent analysis (as discussed by Eyre *et al.*, 1992). The problem disappears in a three or four-dimensional variational (3D/4D-Var) scheme, where retrieval and analysis are combined. Radiances are then used directly together with all other observations and the background field.

In this paper we apply the adjoint technique to the variational retrieval/analysis problem in three/four dimensions. Global variational analyses at spectral resolution T63, 19 vertical levels, have been produced and compared with ECMWF OI analyses. We demonstrate the advantages of the 3D/4D variational approach to the assimilation of TOVS radiances and show the increased flexibility this method offers. The variational method is described briefly in section 2. We present results from a global three-dimensional analysis of TOVS radiances in section 3 and compare with an OI analysis which had used retrieved 1D-Var profiles. In section 4 we demonstrate that the four-dimensional formulation is able to infer additional information from the dynamics of the forecast model.

2. METHOD

2.1 Variational formulation

We follow the general variational approach to the assimilation of data into an NWP system (Lorenc, 1986; Talagrand, 1988) by minimizing the cost-function $J(\mathbf{x})$ with respect to the atmospheric state \mathbf{x} , where $J(\mathbf{x})$ measures the degree of mis-fit to the observations and to the background information. If the errors involved have Gaussian distributions, then the optimal penalty function is a sum of quadratic terms:

$$J(\mathbf{x}) = (\mathbf{x} - \mathbf{x}_b)^T \mathbf{B}^{-1} (\mathbf{x} - \mathbf{x}_b) + [\mathbf{y} - \mathbf{H}(\mathbf{x})]^T \mathbf{O}^{-1} [\mathbf{y} - \mathbf{H}(\mathbf{x})] \quad (1)$$

Where \mathbf{x}_b is the background with estimated error covariance \mathbf{B} , \mathbf{y} represents the observations with estimated error covariance \mathbf{O} , and \mathbf{H} is the observation operator (or "forward" operator) which computes model equivalents of the observed quantities at the observation points. The matrix \mathbf{O} should in addition to the observation error also include the representativeness error, i.e. the error in the forward operator.

Eq.(1) applies to a wide range of problems. It has the same form in one as well as three and four-dimensional applications. In the case of TOVS radiances, \mathbf{H} specifically represents the radiative transfer model that calculates radiances from the state vector of the forecast model. In 4D-Var, \mathbf{H} includes a model integration from the time of the background to the time of the observation (see Thépaut et al., 1992). 3D-Var is thus, in theory as well as in practice, equivalent to a 4D-Var without model integration.

The solution in the linear case, is given by:

$$\mathbf{x}_a - \mathbf{x}_b = \mathbf{B}\mathbf{H}'^T (\mathbf{H}'\mathbf{P}\mathbf{H}'^T + \mathbf{O})^{-1} [\mathbf{d} - \mathbf{H}(\mathbf{x}_b)] \quad (2)$$

where $\mathbf{x}_a - \mathbf{x}_b$ represents the analysis increment (analysis minus background). \mathbf{H}' is the Jacobian of \mathbf{H} and contains the partial derivatives of \mathbf{H} with respect to the elements of \mathbf{x} . In the nonlinear case, the solution can be found through e.g. Newtonian iteration (Rodgers, 1976; Eyre, 1989) or through the adjoint technique as described by Le Dimet and Talagrand (1986) and applied to the retrieval problem by Thépaut and Moll (1990). Details particular to the IFS/Arpège implementation of the adjoint technique have been documented in Pailleux et al. (1991).

At the minimum, the second derivative of the cost function. $\mathbf{J}''(\mathbf{x})$ represents the inverse of the analysis error covariance (omitting terms involving the gradient of $\mathbf{H}'(\mathbf{x})$):

$$\mathbf{J}''(\mathbf{x}) = \mathbf{A}^{-1} = \mathbf{B}^{-1} + \mathbf{H}'^T \mathbf{O}^{-1} \mathbf{H}' \quad (3)$$

2.2 3D/4D-Var as a retrieval scheme

The retrieval algorithm of 3D/4D-Var is to a large extent based on the operational 1D-Var algorithm. It uses the same fast radiative transfer model (Eyre, 1991), the same observation error statistics, the same bias correction (Eyre, 1992) and the same quality control (Eyre et al., 1992). The brightness temperatures used

are the global cloud-cleared data generated by NESDIS and disseminated as the so called "120 km BUFR TOVS" data set. These data have already undergone substantial pre-processing at NESDIS (see *Smith et al.*, 1979) followed by cloud-clearing (*McMillin and Dean*, 1982; *Reale et al.*, 1986).

The scheme is "physical" in that radiative transfer calculations are carried out at every TOVS point at every iteration. It is also "interactive" with the data assimilation cycle because it uses model data as background information. It retrieves temperature and humidity simultaneously. It is nonlinear and iterative.

Cloud-cleared radiances are used in the experiments reported here, although the scheme can in principle be applied to "raw" radiances to retrieve cloud parameters like fractional cloud cover and cloud height, as demonstrated in one dimension by *Eyre* (1989). However, this dramatically increases the nonlinearity of the inversion problem (*Eyre*, 1989; *Hoffman and Nehr Korn*, 1989).

In addition to these one-dimensional aspects, 3D-Var provides substantial new possibilities from its three-dimensional formulation. Primarily: *i*) Horizontal consistency is ensured, *ii*) All data types are used simultaneously and *iii*) Mass-wind balance constraints are imposed. These three points act as additional constraints on the inversion process. They introduce further redundancy to the estimation problem and will reduce the possibility of retrieval errors. Furthermore, in 4D-Var, the evolution in time of the background error covariances is taken into account implicitly through the dynamics of the forecast model and its adjoint.

2.3 TOVS observation operator

The computation of the TOVS observation cost function is organized like that for conventional data (*Vasiljević et al.*, 1992), with the addition that, for TOVS, horizontal observation error correlations are taken into account (*Pailleux*, 1989; 1992). However, data from different satellites are assumed to be uncorrelated. Data from different retrieval types are also assumed to be uncorrelated. Thus it has been possible to separate the observations in several de-correlated sets. With large numbers of TOVS it becomes necessary to split the sets further. Technical reasons limit the number of members in each set to a couple of hundred (currently we use 192). The radiance observation error correlation function is specified to be Gaussian with a length scale of 350 km.

The forward operator H , is the product of all the operations necessary to go from the control variable x to model radiances at observation points. The operator H is continuous in x . It may be linear or nonlinear and it ought to be differentiable in general but it does not have to be differentiable for *all* values of x . Linear interpolation is for example differentiable between model levels but not differentiable exactly *at* a model level.

The chain of operators in the TOVS forward and adjoint calculations is shown schematically in Fig.1. It starts with a change of variable from the control variable to model spectral variables (*Heckley et al.*, 1992),

followed by the inverse spectral transforms to obtain grid-point data of temperature and specific humidity on the model's Gaussian grid. The model grid-point data are then interpolated in the horizontal with a 12-point bi-cubic interpolator and in the vertical to 40 pressure levels, assuming linearity of T and q in p . The radiative transfer model is formulated in terms of T and $\ln q$ on 40 fixed pressure levels from 1000 to 0.1 hPa. The calculations are carried out from $p = p(z_m)$ to 0.1 hPa, where z_m is the elevation of the TOVS locations, as given in the TOVS reports. The radiative transfer model also uses T_s and T_{2m} . As the control variable is currently limited to model level quantities we must either extrapolate the available information to 0.1 hPa or bring in auxiliary information from an external source. We have chosen to bring in the 1D-Var retrieved temperature at the surface (T_s) and in the stratosphere above the top of the model (7.3 hPa). We use the temperature at the lowest model level in place of T_{2m} .

For humidity we discard the model variables above 300 hPa. They are replaced with a constant value of q above 70 hPa and extrapolated according to an empirical power-law between 300 and 70 hPa.

Once model radiances have been computed, the cost function and its gradient with respect to radiances can be calculated. Then the adjoint operators are applied in the reverse order (Fig.1) to yield the gradient of the cost-function with respect to the control variable. The J_o computation is followed by the computation of J_b and its gradient (Heckley et al., 1992), and the whole procedure is repeated until the minimisation has reached convergence, or the maximum number of iterations has been reached.

3. RESULTS OF A THREE-DIMENSIONAL EXPERIMENT

In the following section, we will compare the result of a T63 three-dimensional variational analysis of TOVS radiances plus conventional data with our best estimate of the truth at the same resolution - a T63 OI analysis using all available data, including 1D-Var retrievals.

The 3D-Var analysis used radiances from 4,433 TOVS spots, in total 46,205 pieces of information from channels HIRS-1 to 7, 10 to 15 and MSU-2 to 4. In order to minimize the effect of forecast errors in surface temperature, only the seven most high-peaking channels were used over land (HIRS-1 to 4 and 12, MSU-3 and 4), and from cloudy spots only the cloud insensitive channels (HIRS-1 to 3, MSU 2 to 4) were used. The situation was 890209-12 UT, for which we had received "cloud-cleared" radiances from NESDIS, Washington, with nearly complete global data coverage.

We used the multi-variate J_b , assuming 10 % of the background error in the gravity modes and 90 % in the Rossby modes, as defined by a projection of the control variable onto the Normal Modes of the background. The control variable was in terms of the mass-variable P , vorticity, divergence and specific humidity, all in spectral space projected on the eigen-vectors of the vertical correlation matrix, as described

in Heckley *et al.* (1992). The OI forecast error variances on pressure levels were interpolated to model levels and used in 3D-Var as part of the matrix \mathbf{B} , Eq.1.

3.1 Convergence and control of gravity waves

The minimisation was continued for 50 iterations. Fig.2a shows the evolution of the two terms of the cost function. J_b is zero initially because the starting point of the minimisation is equal to the background (an initialized six-hour forecast). It appears that the convergence is saturated after about 35 iterations.

Fig.2b shows the evolution during the minimisation of the energy in the gravity waves of the first five vertical modes. The starting point contains very little gravity waves since it is an initialized six-hour forecast. As the minimisation draws to data, some of the information goes into the gravity part. However, it is clear from the diagram that the multi-variate balance formulation of J_b effectively controls the amount of gravity waves present in the analysis so that after an initial over-shoot (at about 10 iterations) a stable level is reached. No other means than J_b was used to control the amount of gravity waves in this experiment. Experience with the NMC scheme by Parrish and Derber (1992) showed that a separate initialisation step should not be needed.

3.2 Comparison of analysis increments

Fig.3a shows the 500 hPa height and wind increments of the 3D-Var analysis. Fig.3b shows the corresponding OI analysis. Conventional data dominate the analyses over land. In the southern oceans, where TOVS provides the dominant data source, 3D-Var (Fig.3a) picks up all the major features of the OI analysis (Fig.3b). The amplitude is somewhat larger in 3D-Var than in 1D-Var/OI. The agreement is very good with one exception: a 95 metre height increment in the 3D-Var analysis at (-2,-50), which corresponds to a 24 metre increment in the OI.

This increment is in the baroclinic area of a 956 hPa cyclone. A closer look at the 3D-VAR temperature increments level by level (not shown) indicates that the cold air in the lower troposphere in the 3D-Var analysis has advanced further than in the first-guess. Positive increments aloft indicate that the warm occluded air ahead of the surface warm front is warmer and has reach further around the low (towards the pole) than in the first-guess. Qualitatively this amounts to a displacement of the front by the analysis. Kelly (1978) suggested the zero contour of 500 hPa vorticity as an objective indicator of the position of upper-air fronts. A comparison of vorticity maps for the analysis and the background indeed showed that the 3D-Var had moved the front forward a distance of 70 to 100 km. The radiances have cooled the lower part of the troposphere by up to 7 degrees (at 750 hPa) and warmed the lower part of the stratosphere, in so doing lowered the tropopause from 250 to 400 hPa. The change in upper troposphere humidity is also consistent with a colder air-mass. In summary, it seems that the unusually large 3D-VAR increment has occurred in an area were there has been a slight phase error in the first-guess. The analysis increments are consistent with moving the frontal system forward. This gives us some confidence that the large 3D-Var analysis

increment in this area can be realistic. However, there is necessarily little vertical structure in the increments, and they have a tendency to be barotropic by design of J_b .

The results presented indicate that the 3D-Var retrieval/analysis of TOVS radiances works as anticipated. The analysis increments in general agree with those produced by 1D-Var/OI. The size of the increments are somewhat larger in 3D-Var, which partly reflects the high degree of confidence we put on measured radiances relative to SATEM retrievals. The 1D-Var retrievals are also given a lower weight in OI to account for their correlation with the background error. In addition, 3D-Var assumes larger temperature forecast errors than 1D-Var, a discrepancy that needs to be reconciled.

4. RESULTS OF A FOUR-DIMENSIONAL EXPERIMENT

A 4D-Var experiment was carried out in order to find out to what extent the dynamics of the forecast model, in the absence of J_b , could provide wind increments in response to TOVS information solely on the mass field. The background information is generally much less important in 4D-Var than in 3D-Var. The three-dimensional analysis problem is under-determined unless background information is provided. In four dimensions, a strong constraint is posed by the evolution of the forecast model; the model trajectory has to stay close to the observations over a period of time, which makes it possible to ignore J_b at low resolutions.

The experiment presented here used TOVS from 18,208 locations over a 24 hour period as well as most conventional data (SYNOP-SHIPs, DRIBU, TEMP, PILOT, AIREP and SATOB). The resolution of the spectral model was T42-L19 (140 000 degrees of freedom). The model was used in its adiabatic version, and a combination of a weak constraint term on the tendencies of the energy in the gravity components of the model solution and a normal mode initialisation scheme was applied in the assimilation process in order to control noise.

A second assimilation was run with only conventional data so that the difference between the two assimilations would show the impact of TOVS in the presence of all other data.

The J_o computation was split into one-hour time slots, but is otherwise as described in section 2.3 and Fig.1. The forward operator in the 4D case involves a model integration to the time of the observations, and in the adjoint part there is the corresponding adjoint integration to obtain the gradient of the cost function with respect to the initial time. The minimisation was terminated at 30 iterations, although the cost function was still decreasing. Previous experiments had shown that in the absence of a background there was a tendency to draw to the data too much at the final stages of the minimisation and noise was generated. After 30 iterations the cost function had been divided by a factor of six.

4.1 Impact on the mass field

Fig.4 represents the 500 hPa height field difference between the 4D-Var experiment using conventional and

TOVS data and the 4D-Var analysis using conventional observations only. This level roughly corresponds to the peak of HIRS channels 4, 5 and 15 and MSU channel 2. The impact of TOVS radiances is mainly located in the mid-latitudes of the southern hemisphere, and more particularly over the oceans where the differences reach more than 100 m. Bearing in mind the lack of conventional data in the southern hemisphere, the horizontal distribution of the impact is as expected.

4.2 Impact on the wind field

It is more interesting to look at the wind increments inferred by the use of the radiances (Fig.5). When comparing with Fig.4, one can notice that in the mid-latitudes the wind differences are geostrophically related to the geopotential differences, as expected from balanced fields. This shows that the information brought by the additional observations is dynamically consistent with the model solution. In other words, the mass-wind equilibrium information, mainly enforced by the presence of a constraint term on the gravity wave tendency and a normal mode initialisation before the model integration, has been properly transferred by the dynamics.

Wind differences are also noticeable in the tropics. The location of the largest wind difference patterns correspond quite well to the locations of the humidity increments (not shown). This raised the question whether there had been an impact on the wind analysis from the humidity information in the radiances.

To investigate this wind-humidity coupling, a 4D-Var experiment using TOVS data had to be rerun but excluding TOVS humidity channels HIRS-11 and 12. The new resulting 500 hPa wind difference is shown in Fig.6. A large part of the wind increments has been wiped out, both in the tropics and in the mid-latitudes.

Channels HIRS-11 and 12 are rather sensitive to temperature which is very variable in the mid-latitudes. In the tropics where the temperature field is fairly flat, the comparison between Fig.6 and Fig.5 clearly confirms that a large part of the wind increments is due to radiance measurements in the humidity channels. Since in our experiments the humidity field behaves like a passive tracer, this result, intrinsically linked to the four-dimensional nature of the assimilation, shows a nice example of how the dynamics of the model is able to infer information on an un-observed component of the flow (the wind) from remotely sensed information on the humidity field.

5. CONCLUSION

A three/four-dimensional variational analysis scheme, which uses radiances directly, has been developed. The scheme has been validated and shown to work well. It successfully combines retrieval and analysis, and produces balanced fields.

The first results show a good agreement with OI analyses in oceanic areas. We expect improvements in

the near future from the introduction of SSU (Stratospheric Sounding Unit) and a refined specification of forecast error statistics.

Future work will show whether or not there is a significant positive impact on forecast quality from the direct use of radiances. Experiments will also be carried out to determine which sub-set of channels to use over land and sea, and to study the impact of the radiances on the tropical wind-field. TOVS data in the tropics are currently not used in ECMWF operational analysis. With a more appropriate tropical mass/wind balance imposed in 3D-Var, we can expect improvements. There is also a positive impact expected from the use of HIRS channels 11 and 12 on the humidity analysis. Statistics of TOVS minus forecast differences have shown systematic biases in the current ECMWF analyses (Eyre, 1992), especially in the sub-tropics, which the radiance data should be able to correct.

The 4D-Var experiments have shown that the evolution of the model over a 24-hour period acts as an additional constraint on the retrieval/analysis. It was shown that 4D-Var is able to infer information on the tropical wind field from the use of the humidity sensitive TOVS channels in an adiabatic experiment.

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TOVS J_o Calculation - direct and *adjoint*

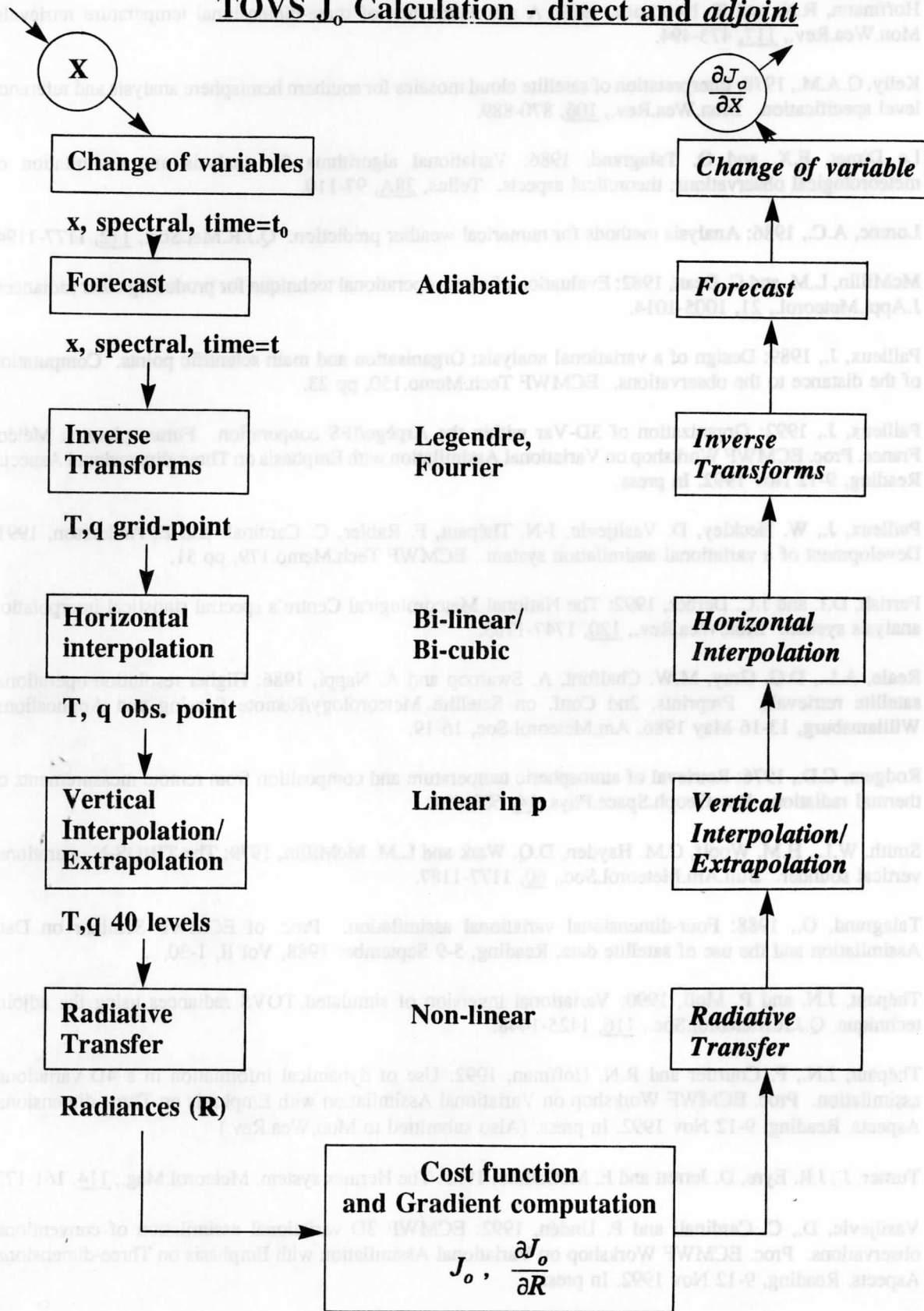
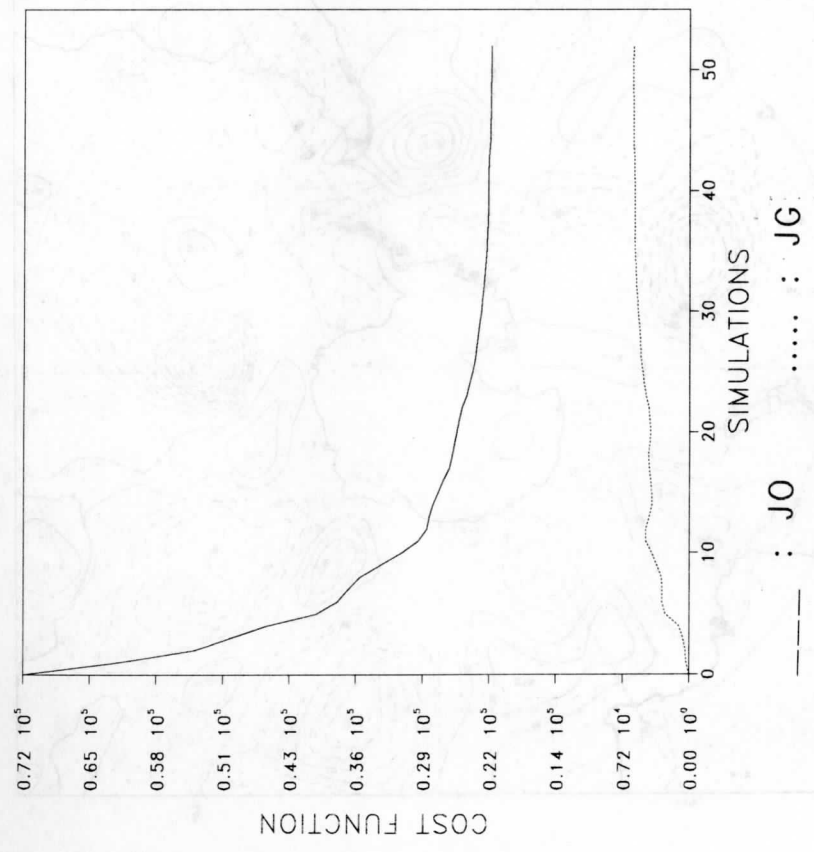


Fig.1 Schematic of the calculation of the observation cost function (J_o) for TOVS radiances - direct (on the left) and adjoint (on the right).

a) 3D Variational analysis
Experiment: TOVO



b) 3D Variational analysis
Experiment: TOVN

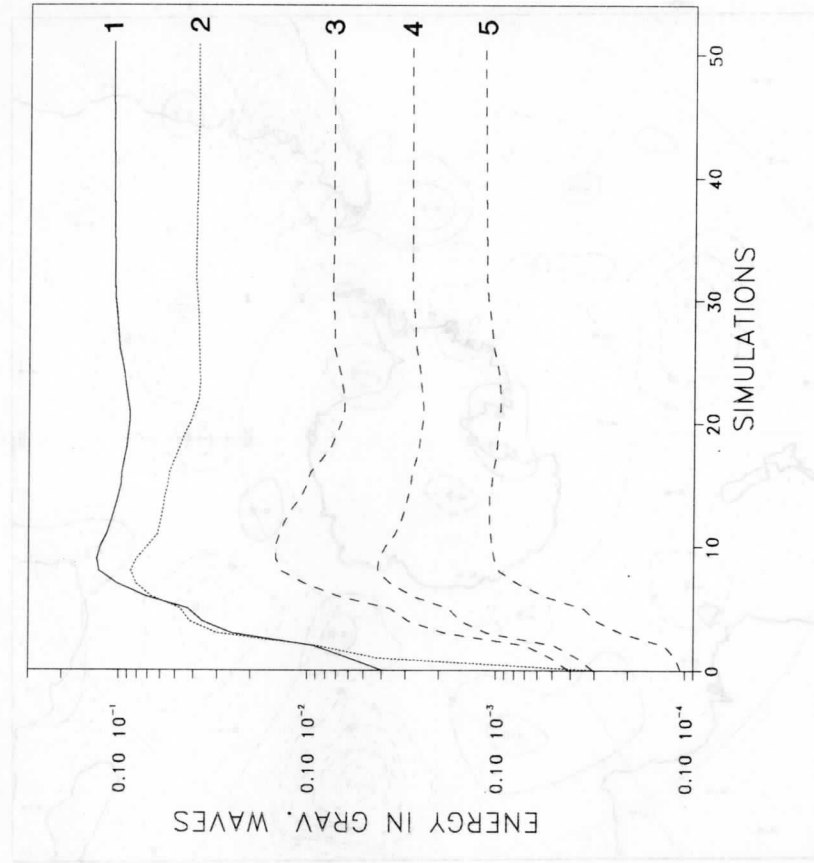


Fig. 2 Evolution during the minimisation of (a) the cost functions (J_0 , full line and J_G , dotted) and (b) energy in gravity modes 1 to 5, as indicated.

1989_0209-12 UTC 500hPa wind and height

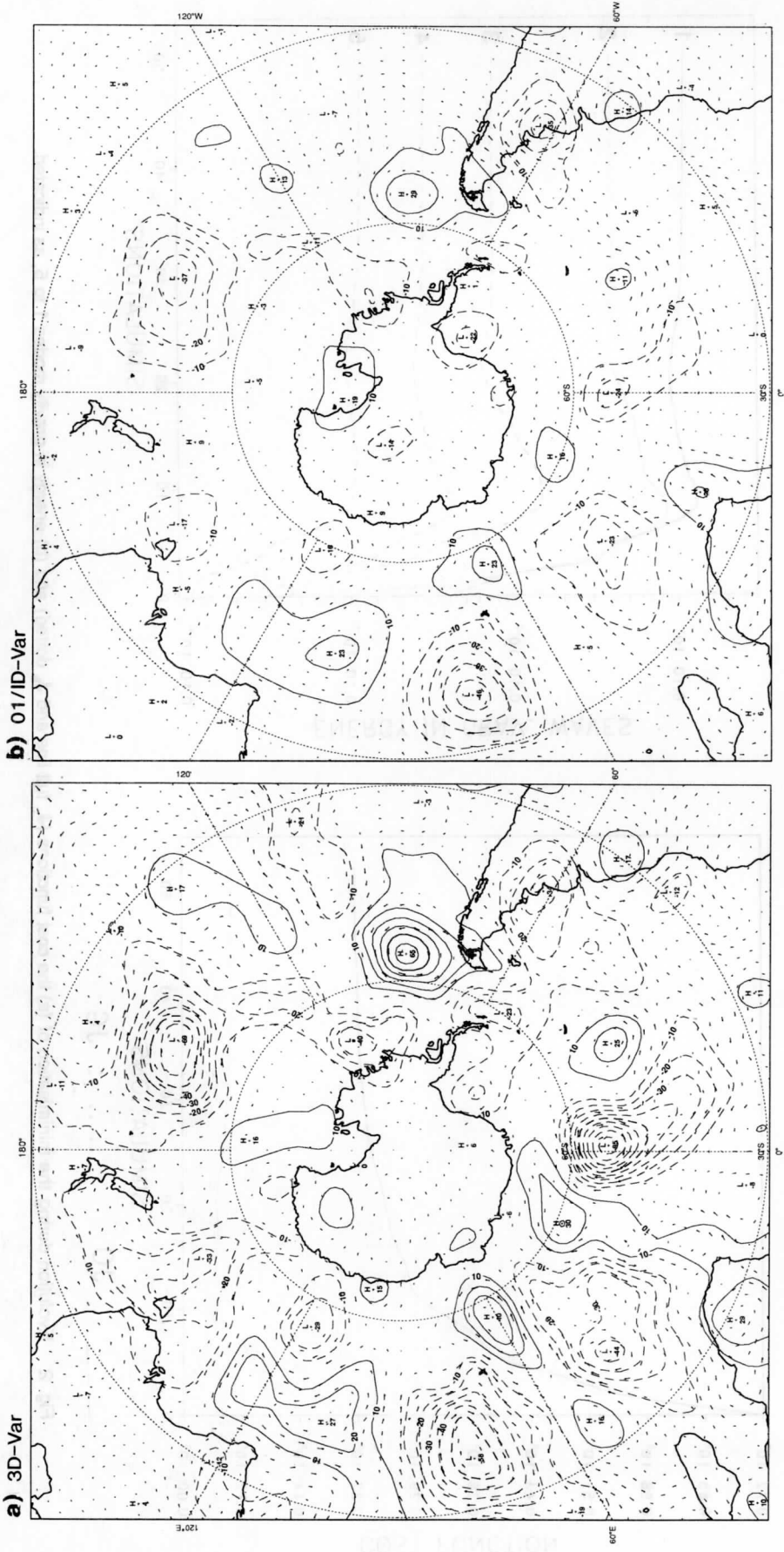


Fig. 3 Analysis increment of geopotential height and wind at 500 hPa, 890209-12UT, with a contour interval of 10 metres, negative dashed. a) is 3D-Var and b) is 01/ID-Var

1989 02 10-12 UTC, 500hPa height AN difference

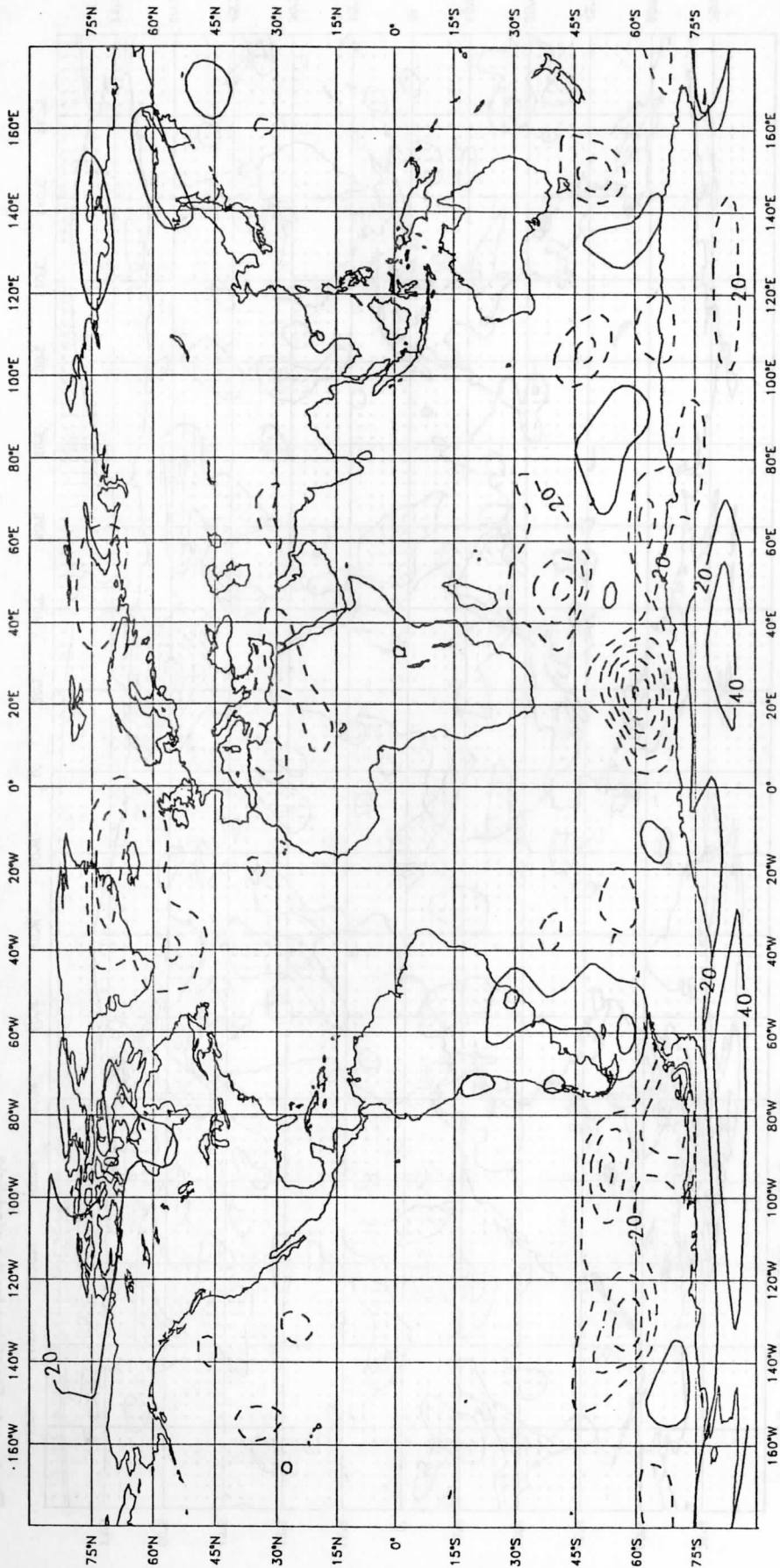


Fig. 4 Geopotential differences at 500 hPa at the end of the assimilation period (890210-12UT) between 4D-Var performed with conventional observations plus TOVS radiances and 4D-Var performed with conventional observations only. Negative differences are dashed, and the contour interval 30 metres.

1989 02 10-12UTC 500hPa wind AN difference

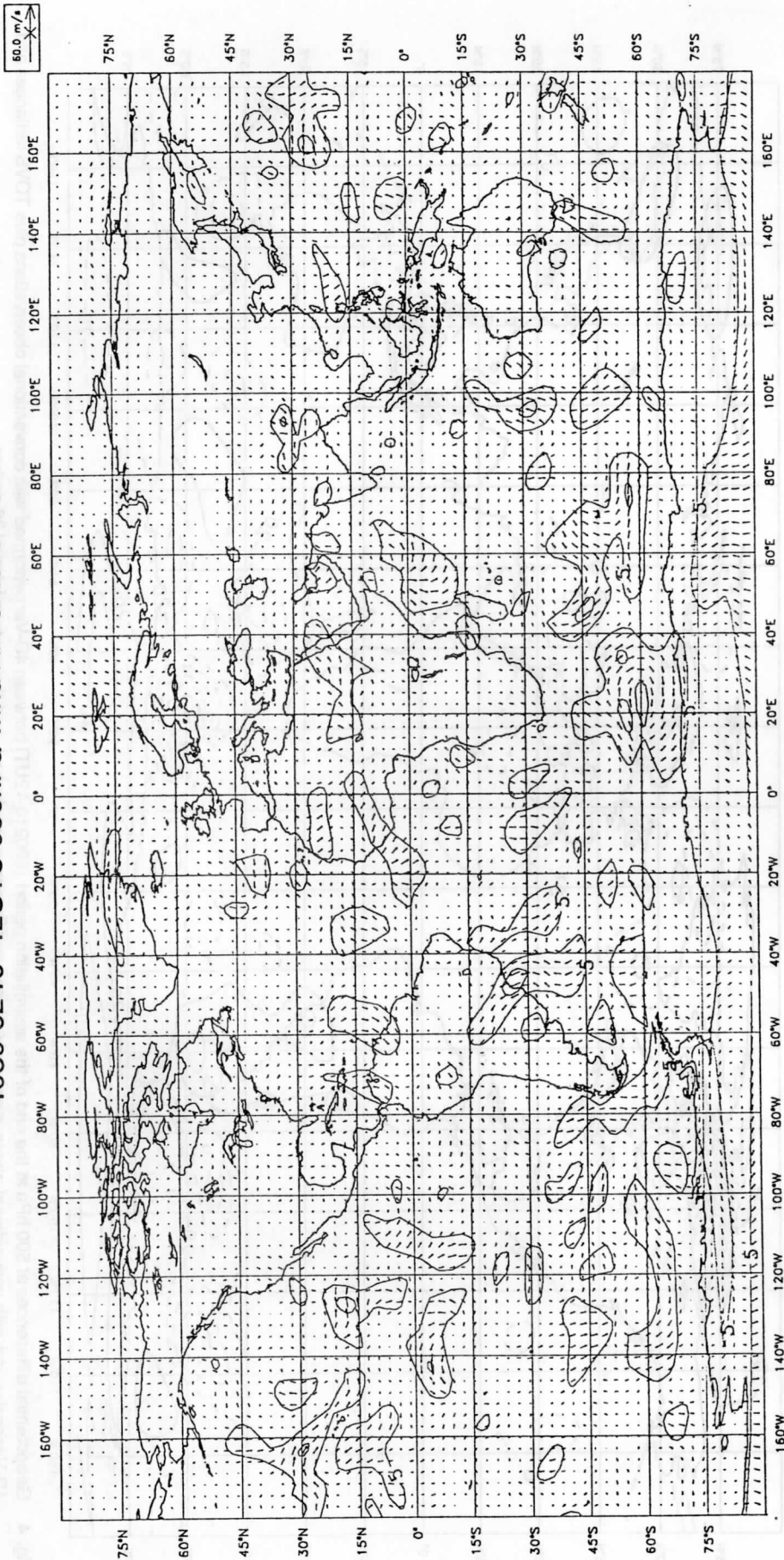


Fig. 5 As Fig.15 but for the wind field.

1989 0210-12UTC 500hPa wind AN difference

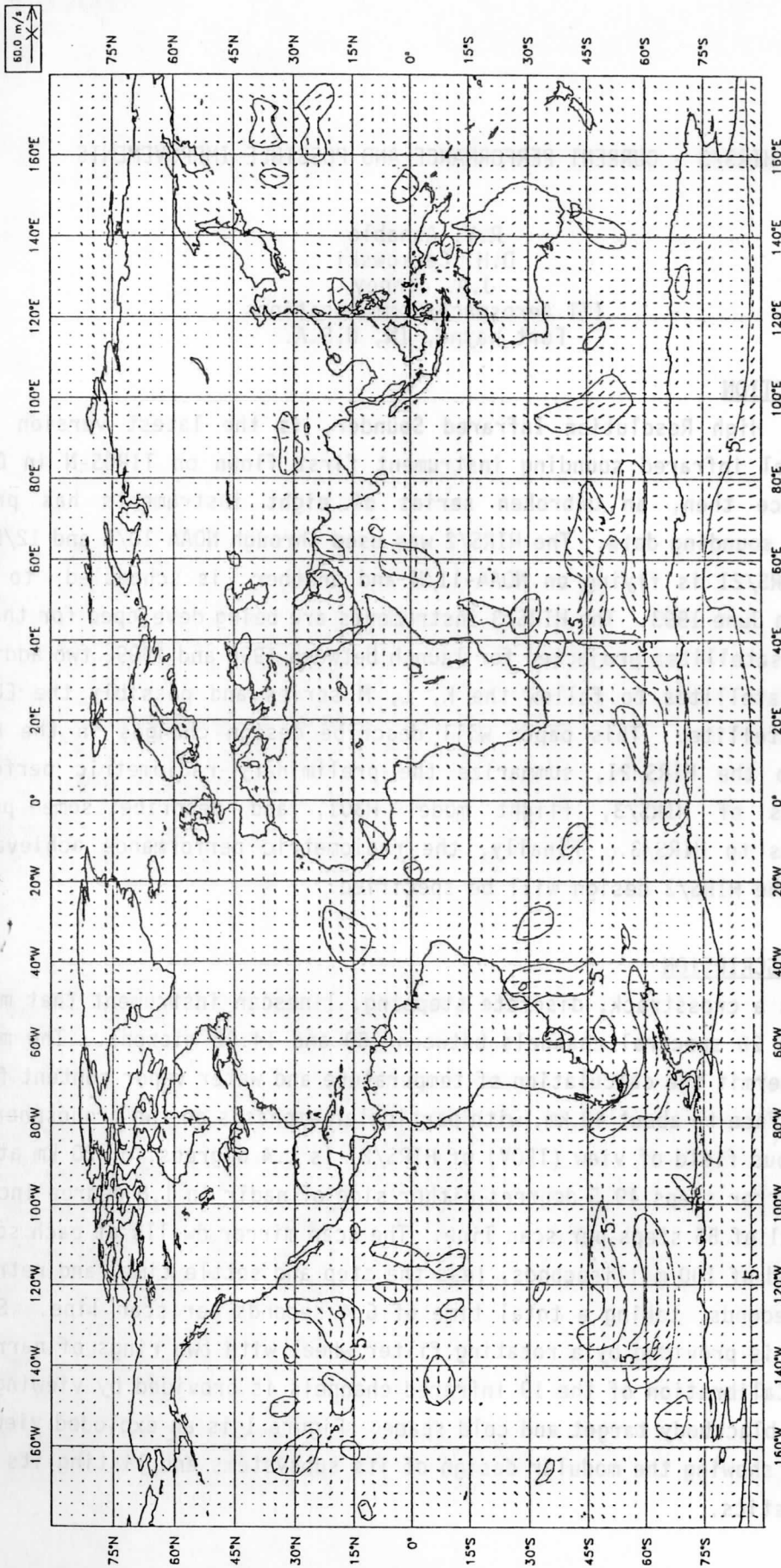


Fig. 6 As Fig. 16 but humidity TOVS channels HIRS-11 and 12 have been excluded from the assimilation using TOVS radiances.

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