The ECMWF implementation of three dimensional variational assimilation (3D-Var): Experimental results

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SUMMARY

In this paper we assess the performance of the three dimensional variational data assimilation scheme, in the light of the results from the extensive pre-operational programme of numerical experimentation. Its performance is compared with that of the previous operational scheme at ECMWF, which was based on Optimal Interpolation. The main features of the new scheme are illustrated, in particular the effects of non-separable structure functions and the improved data usage. TOVS cloud-cleared radiances are for example used directly without a separate retrieval step. Scatterometer data are assimilated in the form of ambiguous winds with the ambiguity removal taking place within the analysis itself. Problems encountered during the tests are discussed and the solutions implemented are explained.

The over-all impact on forecast accuracy in the troposphere of the Northern Hemisphere extra-tropics is neutral for geopotential and positive for wind and temperature. The impact is neutral in the tropics, and significantly positive in the Southern Hemisphere. The stratospheric analyses and forecasts have improved in all regions. Other positive results include a clear improvement in near-surface wind analyses over oceans, in particular in the vicinity of tropical storms. This is predominantly due to the assimilation of scatterometer wind data.

1. INTRODUCTION

A new analysis scheme, based on variational methods (Lorenc 1986; Talagrand and Courtier 1987; Courtier and Talagrand 1987), became operational at ECMWF (European Centre for Medium-Range Weather Forecasts) on the 30th of January, 1996. It replaced the Optimal Interpolation (OI) scheme (Lorenc 1981; Shaw et al. 1987; Undén, 1989), which had been operational since the beginning of operational forecasting at ECMWF in 1979. This paper is the third and final part of a detailed description of the new scheme and its characteristics. The companion papers by Courtier et al. (1997) (Part I) and Rabier et al. (1997) (Part II) discuss the formulation and the structure functions, respectively, while this paper (Part III) presents experimental results.

3D-Var produces upper-air analyses of temperature, vorticity, divergence, specific humidity and surface pressure for numerical weather prediction (NWP). The analysis is performed directly in terms of the forecast model's spectral representation, on model levels. Analyses are produced every six hours using data from a six-hour time window centred around the analysis time. Observation processing, quality control, background error computation and surface analysis remain from the OI system in the version of 3D-Var discussed here, although they have recently been replaced by new modules or algorithms.

The purpose of this paper is to document some of the most important results obtained from a very extensive programme of experiments comparing 3D-Var and OI. We will try to answer two questions: Have the anticipated improvements materialized? What were the main difficulties during the pre-operational tests? Some problems did emerge and their solutions will be presented here. The degree of balance in the tropical mass-wind analysis was one of the areas which received attention, as did the humidity analysis.

The results in terms of mid-latitude forecast impact varied very significantly between individual two-week test periods. In some periods 3D-Var performed clearly better than OI, in other periods the situation could be the reverse. These variations are very difficult to interpret, and for now have to be seen as random variations in the relative performance of the two schemes. We will show that samples greater than fifty cases were required for reliable estimation of mid-latitude forecast impact. At the time of operational implementation we had accumulated 120 cases of 3D-Var and OI at operational resolution - the average unequivocally showing a

Northern Hemisphere impact that was neutral in terms of geopotential and slightly positive in terms of temperature and wind - and a significantly positive impact in the Southern Hemisphere. Other positive results reported in this paper are a significant improvement in the stratospheric analyses and forecasts and an improvement in the analysis of the low-level wind fields over sea (predominantly due to the assimilation of scatterometer winds), especially in the definition of tropical cyclones.

Section 2 gives a general summary of the main features of the 3D-Var analysis scheme, some of which have been presented in greater detail in Parts I and II. The experimental programme is detailed in section 3, followed by a presentation of the over-all forecast impact in section 4. Section 5 presents results illustrating the main characteristics of the 3D-Var analysis, mainly with respect to the non-separable representation of background errors. The problems encountered during the pre-operational tests, and their solutions are described in section 6. Conclusions and current developments are given in section 7.

2. 3D-VAR FEATURES

Some remarks on 3D-Var's main features are given here in order to guide the interpretation of the results later in this paper. More detailed descriptions have been given in Parts I and II.

2.1 Observations

An important incentive to the development of 3D-Var was that variational schemes are more flexible than OI in their use of observations. 3D-Var allows the relationships between observed quantities and the analysis variables to be (weakly) non-linear. These relationships (defined as observation operators in Part I) can also depend on more than one of the analysis variables. Such observations will have an influence on the analysis of several variables simultaneously, i.e. the 3D-Var scheme is multi-variate, with respect to the observations. Later in this paper we will examine the influence of radiosonde geopotential data on the humidity analysis, as an example of multi-variate effects. The non-linear and multi-variate aspects of the scheme have been studied by *Cardinali et al.* (1995) with respect to two-metre temperature and ten-metre wind data from SYNOP and SHIP. The non-linear and multi-variate aspects have also been important considerations in determining the best strategy for the assimilation of satellite data, such as TOVS radiances and scatterometer winds.

The new scheme is more easily adapted to new types of data. In addition to the data previously used by OI, the first operational implementation of 3D-Var uses TOVS radiance data (*Andersson et al.* 1994) and ambiguous scatterometer wind data (*Gaffard et al.* 1997). Experiments using total column water vapour from the SSM/I instrument of the DMSP satellite, are under way (*Phalippou* 1996; *Phalippou and Gérard* 1996).

The TOVS data are used directly as radiances after cloud-clearing by NOAA/NESDIS (*McMillin and Dean* 1982; *Reale et al.* 1986), whereas in OI they are used in the form of layer thicknesses and precipitable water content data, retrieved by a one-dimensional variational analysis scheme (*Eyre et al.* 1993; *McNally and Vesperini* 1996) prior to the analysis. The use of thicknesses has been retained in 3D-Var in the extra-tropical stratosphere above 100 hPa and in the Arctic, as will be discussed in section 6c). The incorporation of the retrieval process with the analysis itself, as in 3D-Var, can produce a better combination of the information in the different types of data and in the background (*Andersson et al.* 1994). TOVS data have a dominant role for the assimilation in the Southern Hemisphere (*Andersson et al.* 1991), and later in this paper we present results showing a clear 3D-Var improvement of the forecast performance there.

The scatterometer data are presented to 3D-Var as pairs of wind observations - the two winds in each pair having approximately opposite wind direction. The choice of the most likely direction (the so called ambiguity removal process) is made during the 3D-Var minimisation - a method suggested by *Stoffelen and Anderson* (1997), using the information in the background and surrounding observations. The use of ERS scatterometer data in 3D-Var has improved the analysis of the low-level wind fields over sea (*Gaffard et al.* 1997). A tropical cyclone case is presented in section 5e).

2.2 Background

The 3D-Var specifications of observation errors (detailed in Part I, appendix B) and background errors (Part II, section 3.3) are generally more realistic than the OI specifications. The non-separable representation of background errors (in 3D-Var) is more accurate, especially for temperature, than the separable one used by OI. It gives, for temperature, significantly sharper horizontal correlations and broader vertical correlations. This effect was first discussed by *Phillips* (1986) and has been discussed thoroughly in Part II. On the other hand, OI has different correlation structures in different geographical areas which 3D-Var (being global) has not. In other words: the 3D-Var correlation model is non-separable, isotropic and globally homogeneous, and the OI correlation model is separable, isotropic and only locally homogeneous within 'analysis boxes'. There are therefore visible and significant differences between analysis increments produced by 3D-Var compared to OI, as will be illustrated in section 5. Wind increments are smaller due to tuning of background errors and broader vertical correlations; temperature increments are smaller, particularly near the surface, and they have a larger vertical scale in the free atmosphere giving a very different response to AIREP temperature data, for example. The stratospheric increments are more large scale and much smoother in 3D-Var, for all variables, due to the increase in length-scale with decreasing pressure given by the non-separable background errors.

Another advantage of the new scheme is that the level of noise (gravity waves) is controlled within the analysis itself. 3D-Var thereby combines several tasks which traditionally have been performed in separate steps: 1) retrieval of TOVS data, 2) ambiguity removal for scatterometer wind data, 3) analysis and 4) initialisation. This should lead to a better combination of the information in the different types of data and in the background.

3. EXPERIMENTAL PROGRAMME

The variational analysis scheme has undergone a very comprehensive programme of testing and assessment of its impact, during a period of two years, first at T106 resolution and later at full operational T213 resolution. 3D-Var has been run in parallel with OI at T106 resolution for a total of 146 days in seven separate periods, in all four seasons, and at T213 for a total of 163 days in four separate periods (Table 1). Approximately half-way through the experimentation there was a major change in the forecast model. The prognostic cloud scheme of *Tiedtke* (1993) was introduced, along with a modified scheme for gravity wave drag (*Lott and Miller* 1997) and a grid point representation of specific humidity together with a revision of the semi-Lagrangian scheme (*Ritchie et al.* 1995). The initial conditions for the new prognostic cloud variables are provided by the unmodified first-guess values (*Jakob* 1994). This new model version is referred to as cy13r4 in Table 1.

All data assimilation experiments were run with a six-hour cycle, using all data from a six hour time window centred at the analysis time. 3D-Var assimilations were compared with equivalent OI assimilations at the same resolution, using the same model version. Ten-day forecasts were run from each day at 12 UTC. The forecasts were verified against their own analyses when available, i.e. forecasts from 3D-Var assimilations were verified against 3D-Var analyses (otherwise operational analyses were used), and similarly for OI forecasts. Anomaly correlation and root-mean-square (rms) of forecast error were studied. Forecasts were used to verify against radiosonde observations. Two sets of observations not used by either analysis scheme were used to verify aspects of the analyses, namely SSM/I TPW (total precipitable water) for the humidity analysis and ERS-1 altimeter winds for the low-level wind analysis over sea. Satellite cloud images were also used in some instances.

The first set of experiments (A1 to A6 in Table 1) produced acceptable results in the mid-latitudes, but a deficiency affecting the tropical mass-wind balance was identified. In the continued experimentation, and in fact up to and including the operational implementation, the mid-latitude formulation was kept virtually un-changed as work concentrated on the tropics: experiments B1 to B3 had a multi-variate (balanced) tropical analysis; B4 and B5 a uni-variate one (see Part I). There were some important changes to the humidity analysis in experiment B5, which will be discussed below. The TOVS data usage was slightly adjusted between each of the T213 experiments. A model change of the shallow convection parametrisation was incorporated in the 3D-Var experiment B5, to reduce a systematic over-estimation of trade wind inversion height. It had an impact on 850 hPa temperature forecast scores and is assumed not to significantly affect the results presented in this paper.

Apart from the assimilations listed in Table 1, a very large number of experiments were carried out testing the 3D-Var sensitivity to various types of data (TOVS, ERS-1 and AIREP temperatures), and to some parameters of the formulation.

4. FORECAST IMPACT

The quality of an analysis scheme for the purpose of NWP is primarily judged by its ability to produce good quality forecasts. In the case of ECMWF, the emphasis is on the three to seven day range.

The assessment of 3D-Var forecast impact turned out to be more difficult than expected. There were very large variations between different two-week test periods (A1 to A5 in Table 1), in terms of 500 hPa mid-latitude forecast scores. 3D-Var was sometimes superior to OI and sometimes the situation was the reverse. There could be periods of five or more consecutive days of very significant difference in forecast performance between the two schemes. Careful study of such periods led to the conviction that very large samples were required to make an accurate assessment. The differences in forecast performance in individual periods could not be ascribed to deficiencies in the 3D-Var formulation or data usage. It was concluded that in excess of fifty cases were required for reliable results. The results of T106-experiments A1 to A6 (not shown) can be summarized as ambiguous for the Northern Hemisphere, in terms of 500 hPa geopotential, with an indication of a positive result for the Southern Hemisphere.

4.1 Aggregate of large sample

Given the need for a large sample we will not attempt to make a distinction between seasons. Instead we present an aggregate comprising all experiments obtained after the change of forecast model version: experiments B3 to B5 (Table 1). This is the most homogeneous set of experiments available with respect to extra-tropical performance, with a total of 120 cases. The tropical analysis was, however, modified substantially in B4 which limits us to using B4 and B5 for assessment of the tropical performance.

The 500 hPa geopotential rms, averaged over the 120 cases, is shown in Fig. 1, for Europe, North America, the Northern and Southern Hemispheres, in Fig. 1a) to d) respectively. OI is shown as a full line and 3D-Var dashed. The panels on the left show the results in absolute terms and the panels on the right in terms of relative differences, expressed in percent. The vertical bars represent 95 percent confidence levels. We can see a slight advantage for 3D-Var in the European area for days six to eight (Fig. 1a). There is a neutral result for North America (Fig. 1b) as well as for the Northern Hemisphere (Fig. 1c) as a whole. The result for the Southern Hemisphere (Fig. 1d) is significantly in favour of 3D-Var, from day 2 to day 6.

There is a clear indication that the very short-range (day one and two) scores in the Northern Hemisphere are slightly worse with 3D-Var. Investigations have shown that this can be attributable to a relatively large-scale forecast error component, predominantly in the sub-tropical areas, which clearly does not project on the rapidly growing modes and does not impair the usefulness of the 3D-Var forecasts. The problem may be due to an imperfect treatment of tides, or alternatively an incorrect specification of structure functions for the largest scales.

Forecast verifications of geopotential at 1000 hPa show a very similar picture (not shown) to what has been presented for 500 hPa. Verification in terms of wind and temperature generally show a more positive impact of 3D-Var, than in terms of geopotential. Wind forecasts at 200 hPa, for example, have clearly improved compared to OI in both hemispheres (Fig. 2a and b). Fig. 2c and d show a similar positive result for temperature at 200 hPa.

4.2 The stratosphere

The stratospheric forecast performance of 3D-Var has been a subject of particular attention in view of the improved description of background errors there (Part II). The verification indeed shows a very substantial gain over OI in terms of temperature, wind and geopotential, from 100 hPa and above. In Fig. 3 we show, as an example, the rms of 50 hPa wind (a and b) and temperature (c and d) forecast error for the two hemispheres. There

is a clear improvement over the entire forecast range. The stratospheric analysis will be discussed in the next section, 5(d).

4.3 Case-to-case variability

The large variability is best illustrated by scatterplots of the type shown in Fig. 4. Here, 3D-Var forecast performance as measured by rms 500 hPa geopotential error (x-axis) is plotted against OI performance (y-axis), each marker representing one 5-day forecast. There are 120 markers in all: circles represent summer cases (May to October) and triangles winter (November to April). The cross represents the mean. The points near, or on, the diagonal represent cases with equal 3D-Var and OI forecast quality. Points above the diagonal indicate cases in which 3D-Var has out-performed OI, and vice versa for points below the diagonal. The figure shows the European area, i.e it corresponds to Fig. 1a. There is a large number of cases in which one scheme is better than the other, with an approximately equal incidence of poor (and good) forecasts with both schemes. The same is true for all Northern Hemisphere areas (not shown). In the Southern Hemisphere, for days 2 to 6, however, there is a significant shift in the cloud of points in favour of 3D-Var (also not shown).

Figure 4 gives the impression of a relatively random variation in forecast performance. However, there was a tendency for poor (good) forecasts to appear in batches over periods of five days or more. To illustrate this we have picked out the best and the worst 14-day periods from the 120-case sample. The two 14-day averages of rms forecast error at 500 hPa are shown in Fig. 5. The bad period (Fig. 5a) occurred at the end of experiment B3 (950501-950514) and the good period (Fig. 5b) is B5 (960116-960129). Any conclusions drawn from study of either of these two periods in isolation would be entirely inaccurate. We therefore reiterate the importance of large enough samples for the evaluation of data assimilation schemes.

4.4 The tropics

There were repeated changes to the tropical analysis during the experimentation. We therefore restrict the presentation to reflect results obtained with the final configuration only, i.e. experiment B5 and the first two weeks of B4 which were re-run with the final version of 3D-Var. The tropical sample thus comprises 28 cases, 14 in January and 14 in August/September. For the tropics we choose to present forecast verifications against observations rather than against own analyses. This is because in the tropics the latter verification method is quite sensitive to the choice of verifying analysis.

The forecast verification against observations are shown in Fig. 6 for wind at 850 hPa (a) and 200 hPa (b). We can see that 3D-Var and OI perform equally well at 850 hPa and that OI has an advantage at 200 hPa out to day six. Geopotential scores show an advantage for 3D-Var (not shown). Temperature scores show that 3D-Var is better in the lower troposphere whereas OI is better in the upper troposphere (also not shown).

4.5 Summary

The assimilation and forecast experiments show a neutral impact of 3D-Var with respect to OI, in terms of geopotential in the troposphere of the Northern Hemisphere extra-tropics. The scores for wind and temperature show a slight advantage for 3D-Var, while the very short-range forecast scores have deteriorated somewhat. The Southern Hemisphere has improved significantly, whereas there is a mixed result in the Tropics. The clearest improvement is in the stratosphere in both Hemispheres and in the Tropics.

5. ILLUSTRATION OF 3D-VAR CHARACTERISTICS

In order to facilitate the validation of the new scheme, it was initially the intention to use the same observation errors in 3D-Var as in OI and to use a globally averaged set of the OI background error statistics. It soon became apparent that this strategy was unhelpful because it compounded the restrictions of the two schemes, i.e. the separability of OI and the global homogeneity of 3D-Var. The direct use of TOVS radiances required a more accurate representation of the temperature background errors than could be achieved by the separable model (*Andersson et al.* 1993). It was thus decided to derive and implement non-separable background error statistics for

3D-Var, as presented in Part II, following *Parrish and Derber* (1992). Some observation errors had to be adjusted, too, (see tables in appendix B, Part I) since those had in some instances been set artificially high (or low) to compensate for deficiencies in the OI background error formulation.

Part II reports on some very significant improvements brought by the non-separable formulation: 1) The horizontal structures broaden with height in the stratosphere; 2) The geopotential vertical correlations are broader than those for wind; 3) The temperature correlations are broader in the vertical and sharper in the horizontal; 4) The temperature standard errors are smaller and 5) The wind standard errors in the stratosphere are smaller than used in OI. The filtering properties of the 3D-Var analysis are therefore different from OI. This can be seen from study of analysis fit to data (section a) and three examples illustrating the response to surface pressure data (section b), to AIREP temperature data (section c) and to stratospheric radiosonde data (section d). The near-surface wind and tropical cyclone analysis is discussed in (section e).

5.1 Fit to data

Statistics of observation departures from background and first guess are plotted in Fig 7. The figure shows rms of observation-minus-background as full line and rms of observation-minus-analysis dashed, for radiosonde height and u-component wind data, accumulated over a 14-day period. The fit to radiosonde height data is relatively similar in the two systems (dashed lines show observation minus analysis). Wind data, however, are fitted much more closely by OI than by 3D-Var. The quality of the background is nonetheless similar (full line, showing observation minus background). It appears that the 3D-Var scheme filters the wind data more heavily than OI. This can be explained by the fact that the vertical correlations for wind are broader in 3D-Var, especially over the data dense continental areas where OI uses very sharp vertical correlations. The OI structure functions were especially tuned in this manner in order to fit data closely in jet-stream situations (*Lönnberg* 1988). The effect is in fact most noticeable in data dense areas (e.g. North America and Europe) where OI fits the data very closely, whereas the 3D-Var filters the data and produces a smoother analysis. It should be remembered that the quality of the background (a six hour forecast) is similar in the two schemes. This is an indication that some of the closer fit to the observations of OI is in some sense compensated by the better 3D-Var balance, so that the short-range forecasts are of similar accuracy.

The stronger smoothing of wind data in data dense areas is not entirely satisfactory and could be a contributor to the development of errors in the medium-range forecasts. A set of three 14-day assimilations was run in order to test the sensitivity to the broadness of the 3D-Var structure functions. One experiment used artificially sharpened structure functions, one used broadened functions and one was the un-modified control. The modifications were obtained by multiplying the auto-correlation spectra by 0.8^{n} and 1.5^{n} respectively (and re-normalising to obtain correlation spectra, as in Part II, section 3b), giving sharper/broader structure functions in the vertical as well as in the horizontal. The sharp structure functions gave a closer fit to wind data while in terms of forecast performance (not shown) they gave an improvement in the European area, a neutral result for the Northern Hemisphere and a very poor result for the Southern Hemisphere. The broad structure functions degraded the Northern Hemisphere slightly and improved the Southern Hemisphere. The best over all was the control assimilation. We concluded that geographically varying structure functions are desirable; this would require a generalisation of our present 3D-Var formulation (as discussed in Part I, section 3a-vi). These issues are currently subject to further investigation, with the aim to introduce more geographical variation in 3D-Var in the near future.

5.2 Response to AIREP temperature data

The response to temperature data has changed considerably with the introduction of 3D-Var. The OI temperature structure functions are very sharp in the vertical, with negative lobes either side of the observation. The 3D-Var temperature structure functions are broader and change sign at about the tropopause level (see Fig. 8a, Part II). The temperature horizontal length scale, however, is shorter in 3D-Var (approximately 300 km) compared to OI (500 km). Fig. 8 shows temperature cross-sections of 3D-Var (a) and OI (b) analysis increments, orientated from North to South in the North Atlantic. These analyses have not used TOVS data and there are no radiosonde data affecting the area of interest. The diagrams show the response to AIREP temperature and wind data when used in conjunction with surface pressure data - a frequent condition in the North Atlantic and in the North Pacific. We can see that the AIREP data in OI give rise to increments which are localized between 300 and 100 hPa, and that

the surface pressure data produce temperature increments near 850 hPa (as expected from the OI ps-T cross correlations). There are generally small increments in the mid troposphere. In 3D-Var, on the other hand, these two data types produce temperature analysis increments which are more broadly distributed in the vertical and tend to have maxima in the mid-troposphere, away from the data. There appears to be an interaction between the AIREP data and the surface pressure data in 3D-Var, which is absent in the more localized OI analysis. This tendency for broader temperature analysis increments in 3D-Var is a feature imposed by the specified background error statistics. It has been explained in Part II that the temperature vertical correlations are unrealistically sharp in OI due to the separability assumption.

In view of the different response to AIREP temperature data, assimilation experiments were run excluding just these data in both 3D-Var and OI, for a period of fourteen days. The results indicated a neutral forecast impact in both schemes (not shown).

5.3 Barotropic component of surface pressure analysis

The non-separable analysis gives broader (sharper) vertical response to larger (smaller) horizontal scales (Fig. 9, Part II), i.e. it takes into account the fact that the large-scale components of forecast error tend to be more barotropic than the small scale components. This effect can be clearly demonstrated in an analysis of surface pressure data only. Fig. 9 shows the analysis increments in a 3D-Var analysis of surface pressure data from SYNOP, SHIP, BUOY and PAOB. The left-hand panel (a) shows 1000 hPa and the right-hand panel (b) shows 300 hPa, in the Antarctic region. Comparing the two plots, we see that the small-scale increment at 100 E has less vertical propagation than the larger-scale increments at 140 E and 160 W. The two increments have similar amplitude at 1000 hPa, but at 300 hPa they differ by a factor two - the large-scale increment having the bigger amplitude. That is to say, the small-scale surface pressure increment decays with height primarily within the troposphere, whereas the large-scale pattern penetrates into the lower stratosphere. The cross-correlation between surface pressure and temperature (Fig. 9b, Part II) confirms this behaviour, as the correlation for high wavenumbers (small scales) is confined to the lower troposphere, whereas for low wavenumbers there is one maximum in the troposphere and a secondary maximum in the lower stratosphere. This feature of 3D-Var arises from the improved specification of background error statistics. It appears to be especially important for the use of single-level data in data sparse areas such as the Southern Hemisphere oceans.

5.4 Stratospheric analysis

Mid-latitude wind forecast errors σ_U are related through geostrophy to geopotential forecast errors according to the formula $\sigma_U = \sigma_p / fl_i$, where f is the Coriolis parameter and l_i is the length-scale of the geopotential forecast error correlation spectum at level i. In a separable analysis scheme (like ECMWF OI) l_i is constant in the vertical $(l_i = 500 \text{ km})$ which forces σ_U and σ_P to have the same vertical variation. In 3D-Var on the other hand, l_i varies from approximately 500 km in the troposphere to 1000 km at the top of the model, causing σ_U to increase with height less rapidly in the stratosphere than σ_P . This plus the direct effect of having broader structure functions at higher levels has a large impact on the stratosphere, creating isolated 'bulls-eyes'. This shows most clearly in maps of analysed potential vorticity on isentropic surfaces. Figure 10 shows 3D-Var (top) and OI (bottom), at 475 K.

The indication is that the OI analysis produces dynamically inconsistent structures ("blobs" of potential vorticity) by drawing to the wind observations in an inappropriate way. The benefits of the better 3D-Var analyses are translated to lower medium-range forecast errors in the stratosphere, as we have seen from Fig. 3, section 3, in both hemispheres.

The improved quality of stratospheric analyses has also been noted in a report from the Danish Meteorological Institute (*Knudsen* 1996). ECMWF stratospheric analyses were compared with radiosondes in the Arctic and a marked reduction in bias of layer mean temperatures was found, after the introduction of 3D-Var.

5.5 Near-surface wind and tropical cyclone analysis

The near-surface analysed wind fields have been verified against an independent dataset, namely the ERS-1 altimeter winds. The ERS-1 altimeter produces wind speed observations every 7 km along the satellite track. In order to obtain comparable scales the average of 20 successive observations was compared with the analysed wind speeds. Results for the test period from the 8th of August 1995 until the 5th of October 1995 for the Southern Hemisphere show an improvement in the standard deviation of error of 0.22 ms⁻¹, from 1.99 ms⁻¹ in OI to 1.77 ms⁻¹ for 3D-Var. A lesser improvement was found in the Northern Hemisphere, and virtually no change in the tropics. The improvement in near surface wind has translated into a considerably better quality of first-guess and forecast ocean wave height. A comparison of first-guess wave height produced by the WAM model (*Komen et al.* 1994) with ERS-1 altimeter wave heights shows a reduction in standard deviation of wave height forecast in the Southern Hemisphere suggests an improvement of wave forecast skill (at the 60% level) of about half a day, while from day 3 onwards the standard deviation of wave height error is reduced by about 5% (not shown). The main part of the improvement is thought to derive from the use of ERS-1 scatterometer wind data in the 3D-VAR analysis.

Figure 11 shows an example of an analysis of a tropical cyclone - in this case tropical cyclone Karen, on 31 August 1995. Panel a) shows the observed scatterometer winds for an orbit which passes directly over the cyclone position (indicated by a large dot, at 20 North, 52 West). Panel b) shows the background (six-hour forecast) valid at the same time, and panel c) shows the 3D-Var analysis. The OI analysis is not shown, but is similar to the background field in this case. This is because few conventional data exist in this area, and ECMWF OI does not use scatterometer wind data. We see that the 3D-Var, when using the ERS-1 winds, has produced a good analysis of the cyclone. In every ERS-1 location 3D-Var has the choice between two equally probable winds with approximately opposite directions. This very rarely leads to any difficulties; the wind analyses are always horizontally consistent (*Gaffard et al.* 1997).

This is a striking example of favourable impact of the additional data used in 3D-Var. Statistically, over the whole experiment period we see a significant improvement of the definition of the analysed wind field in and around tropical cyclones. Table 2 shows the result of a subjective study of all reported tropical cyclones (hurricanes, typhoons and tropical storms) in the period between 19950828 and 19950918 comparing the position and intensity of the cyclones in the 3D-Var and OI analyses and forecasts. In a sample of 65 cyclone analyses 29 were improved, 30 were equal and 6 were worse. The improved analyses led to better forecasts in the short range (day 1 and day3), Table 2. *Tomassini et al.* (1997) studied all tropical cyclones in the North Atlantic in the period 19950824 to 19950908 and found that the mean positional error in analyses had been reduced from 173 km in OI analyses to 111 km in 3D-Var.

5.6 Discussion

Figure 12 shows root-mean-square of the difference between 3D-Var and operational analyses of 500 hPa geopotential, for the 120 days of B3 to B5. We see that the two analyses generally are very close over the Northern Hemisphere continents (less than 5.0 m rms difference), and that larger differences (7.5-10.0 m rms) occur over the Atlantic and Pacific oceans. The largest differences are, as expected, in the Southern Hemisphere midlatitudes (in excess of 15 m) and over the Antarctic, where the analysis is most uncertain, due to relatively sparse data-coverage.

The two most sensitive areas at initial time for medium-range forecasts for Europe are firstly eastern North Pacific and secondly eastern Canada with the Labrador Sea and adjoining parts of the North Atlantic (Rabier et al. 1996). The analyses in these areas are mostly influenced by TOVS and single level data, such as surface pressure data from ships, and wind and temperature data from aircraft reports. We have seen from the results presented in this section that there are significant differences between 3D-Var and OI in the analysis response to such data, in particular. This may explain some of the large case-to-case variability in relative forecast skill, reported in section 3.

6. Developments during pre-operational tests

During the pre-operational tests, the team of people scrutinizing the results included the developers of the scheme, together with experts in physical parametrisation, diagnostics and operational forecasting. This brought into focus aspects of the new scheme which could otherwise have been overlooked. The investigations revealed important shortcomings in (a) the tropical mass/wind balance, (b) the humidity analysis and model spin-up, and (c) the precise configuration for TOVS data usage. The resulting developments are presented in this section.

6.1 Tropical mass/wind balance

The tropical mass/wind balance is imposed by the J_b term of the 3D-Var objective function. The control variable is split into two parts, a balanced and an unbalanced one, defined by a projection onto the Hough modes of the model (see Part I, section 3d). The desired degree of balance is achieved by explicitly assigning different weights to the two parts.

The original formulation used in all experiments prior to B1 (Table 1) was incorrect in that it did not produce balanced multi-variate increments as intended. In fact most of the geopotential increments disappeared when initialised by NNMI (non-linear normal mode initialisation). The information from data was not retained and local temperature biases developed in the tropics in the 3D-Var assimilations. The tropical forecasts were also inferior to OI.

In experiments B1 to B3 a corrected multi-variate formulation was used. It produced balanced analysis increments which were retained by initialisation. The multi-variate formulation produced better tropical forecast scores than previous experiments, but some serious problems affecting the wind analysis emerged. Figure 13a shows the mean analysis increments of surface pressure for the South American region, averaged over 14 days (19950421 to 19950514), all at 18 UTC, approximately local noon. We see average positive increments over most of the Amazon basin, with a maximum of 2.0 hPa. The existence of these increments indicate a systematic model underestimation of the surface pressure at local noon. With the multi-variate formulation, 3D-Var produced strong wind increments on the same regional scale to balance the mass increments, Fig. 13b. The resulting wind analysis is not in agreement with near-surface wind observations (not shown) and therefore erroneous.

A recent paper by *Daley* (1996) demonstrated that formulations based on the application of the linear balance equation or a Rossby-Hough expansion imply a tropical coupling between the mass and rotational wind forecast errors which does not seem to exist in reality. Daley constructed a filtered form of the linear balance equation which was essentially un-coupled in the tropics, and closer to reality. This explains our difficulties with the balanced formulation. As described in Part I (section 3d) a uni-variate formulation was developed. Like ECMWF OI, it produces virtually zero wind increments in response to mass data (and vice versa) on (or very close to) the equator, gradually becoming more geostrophic further away from the equator. The scheme is fully multi-variate poleward of 30°N and 30°S.

The behaviour of the uni-variate formulation of 3D-Var in the tropics is very similar to OI, as expected. A large part of the mass increments is rejected by initialisation and the appearance of some noise in the vertical profiles of temperature is inevitable, in the upper troposphere.

6.2 Humidity analysis

The analysis variable of the 3D-Var humidity analysis is specific humidity. The main data for the humidity analysis are radiosonde specific humidity, SYNOP two metre relative humidity and TOVS radiances in channels HIRS-10, 11 and 12. Several other TOVS channels also have a weak dependency on humidity, which is taken into account. There can also be a weak influence on the humidity analysis from surface pressure data and radiosonde geopotential data through the virtual temperature effects of the hydrostatic equation (Appendix A, Part I).

6.2.1 Humidity affected by geopotential data

One problem of the humidity analysis was the appearance of large positive analysis increments at the lowest model levels, over some sub-tropical land areas (Saudi Arabia, North Africa, Mexico and Southern United States), at local mid-day. These areas are characterised by high temperatures and dry conditions. The moistening could be as high as 5 g/kg and was at variance with most available humidity data. Investigations showed that these humidity increments occurred at radiosonde locations and were caused by geopotential observations rather than humidity data. Figure 14 shows the resulting mean two metre specific humidity over the Arabian Peninsula and the mean error at selected SYNOP stations. The plotted numbers represent mean differences between the 3D-Var analyses and observations of two metre specific humidity, in the period 950824 to 950829, 12 UTC. The analysis error is between 4 and 10 g/kg (too moist) at several SYNOP stations in northern and central Saudi Arabia.

We have seen that geopotential data can be fitted by changing both temperature and humidity. In the absence of any other data, the relative changes of humidity and temperature when fitting geopotential data are governed by the background error standard deviations (of temperature and humidity). The conclusion was therefore that there was a problem with the specification of humidity background errors σ_q in hot and dry conditions. 3D-Var at the time used a background specification of $\sigma_q = 0.15q_s(T, p)$ i.e. 15% of saturation specific humidity. At relatively high temperatures, e.g. 305 K, this gives a background error of almost 5 g/kg. The findings led to the modified specification, as given in Part II section 4. An easier but less correct solution would have been to disable the dependency on humidity of the geopotential observation operator. This would, however, produce inconsistencies between the humidity analysis and the geopotential data.

6.2.2 Spin down

A second problem of the 3D-Var humidity analysis was a marked spin-down of the tropical convection during the first six hours of forecasts starting from 3D-Var analyses. There was an increase in the six-hour precipitation, relative to OI. One suspicion was that the analysis increments over tropical and sub-tropical oceans were too large and that a too vigorous redistribution of the tropical humidity by the analysis contributed to the excessive precipitation. Study of radiosonde minus model humidities gave an indication that the humidity background errors should be reduced in the tropical oceanic boundary layer. This resulted in the formulation given in Part II, section 4, but did not solve the spin-down problem. Later, it was discovered that some relatively small volumes of supersaturation were present in the 3D-Var analyses. In the incremental 3D-Var (Part I, section 5a) the final analysis is created by adding the low-resolution analysis increments to the high-resolution background. This was done without checking for supersaturation (or negative humidity). When this was rectified, the spin-down problem was reduced. Figure 15 shows an example of the time evolution of precipitation in forecasts from OI (a), un-corrected 3D-Var (b) and (c) 3D-Var after modification of the humidity analysis. The spin-down problem is clearly visible in the un-corrected 3D-Var. The corrected 3D-Var is more similar to OI.

6.2.3 Stratospheric humidity

A third problem with the 3D-Var humidity analysis occurred in the stratosphere. There are no in-situ or satellite humidity data used in the stratosphere. Monitoring of the stratospheric humidity revealed a slow but systematic linear increase with time. The globally averaged humidity above 100 hPa increased from 2.5 10^{-6} to 3.5 10^{-6} kg/kg during a period of 45 days. The forecast model has not been seen to show this systematic behaviour in long runs. Investigations showed that the analysis introduced small, but generally positive, humidity analysis increments in the stratosphere at each analysis. The mechanism behind the problem turned out to be small, but non-zero, vertical correlations between troposphere and stratosphere, which allowed the systematic component of the tropospheric increments to spread into the stratosphere. The solution implemented was to set the vertical correlations between the levels above 100 hPa and all other levels to exactly zero and to set the background error above 150 hPa to a very small value (1.25 10^{-8} kg/kg).

6.3 TOVS data usage

The precise configuration of TOVS data usage is a product of many years of experimentation - first with NESDIS retrieved data, later using 1D-Var retrieved data in OI and finally using a combination of radiances and retrieved

data in 3D-Var. The original intention was to simply use radiances everywhere on the globe instead of retrieved thicknesses, restricting the set of radiances to surface insensitive channels over land and to cloud insensitive channels where clouds were detected. This strategy was modified due to the results obtained by *Kelly* (1993) pointing out difficulties in using radiances in the stratosphere. The top of the ECMWF model is currently at 10 hPa, whereas many TOVS channels have a significant contribution from radiation above this level. Kelly found that extrapolation errors caused analysis errors in the upper stratosphere. Assimilations using NESDIS retrieved thicknesses above 100 hPa did not have this problem. The set of radiances for use in 3D-Var was thereby reduced to those that can be described as being predominantly 'tropospheric', and NESDIS retrieved thicknesses were introduced in the extra-tropics between 100 hPa and 10 hPa. This closely mimics the TOVS data usage of ECMWF OI from December 1995 onwards (*McNally and Vesperini* 1996). There are plans to extend the model higher into the stratosphere and at that point the TOVS data usage will need to be readdressed.

In one of the test-periods, a ten degree temperature difference (between 3D-Var and OI) appeared in the lower stratosphere in the Arctic region. It was not obvious from diagnosis of the two analyses which of them was more correct. Experiments were run excluding some Arctic radiosonde stations to be used for verification. The results were inconclusive. However, forecasts from the 3D-Var analyses rapidly adjusted the Arctic temperatures to produce values close to those of the OI analyses. Further experimentation followed, replacing the radiances in the Arctic region, north of 70°North, with 1D-Var retrieved thicknesses. As a result the difference between the 3D-Var and OI analyses became sufficiently small that this became the solution for implementation. A better description of the Arctic background error, in particular a temperature vertical correlation matrix reflecting the low tropopause, may be necessary for the re-introduction of radiances to this area.

7. Conclusions and future directions

A three-dimensional variational analysis scheme (3D-Var) was implemented at ECMWF on 30 January 1996, replacing OI (Optimal Interpolation). In this three part paper we have presented the formulation of the new scheme (Part I), the specification of structure functions (Part II) and the results from pre-operational experimentation (Part III).

7.1 Summary

3D-Var uses a wide variety of meteorological data to produce global analyses of temperature, vorticity, divergence, specific humidity and surface pressure, directly on model levels using the model's spectral representation. The global analysis problem is solved simultaneously for all analysis variables by iteratively minimising the variational objective function. The objective function consists of three terms controlling the distance to the background (a six-hour forecast), the distance to the observations and the amount of gravity waves, respectively.

The background term includes a coupling between mass and wind. The coupling is achieved by separating the balanced part of the analysis increments from the un-balanced, through a projection on the model's Hough modes. The objective function for the un-balanced part is given a higher weight (corresponding to a lower variance) than the balanced part, which results in predominantly balanced analysis increments. The tropical analysis is univariate.

The observation term includes all observations used by the OI scheme plus the addition of scatterometer wind data. The scheme uses TOVS cloud cleared radiances instead of retrieved data in the troposphere, whereas retrieved layer mean temperatures are retained in the extra-tropical stratosphere above 100 hPa and in the Arctic. The data are related to the analysis variables through so-called observation operators, which can be multi-variate and weakly non-linear. This makes the scheme very flexible in terms of data usage, and facilitates the introduction of new data types. This has been explored in the use of TOVS radiances and in the use of directionally ambiguous scatterometer winds. Several projects are underway, aiming at including additional observational data in 3D-Var, e.g. SSM/I products, TOVS raw (as opposed to cloud-cleared) radiances, water-vapour winds and radiances from geostationary satellites. Additional scatterometer winds will also become available in the near future. These data are likely to improve primarily the analysis of the tropical wind field and the analysis of humidity.

A non-separable formulation of structure functions is used. This allows the horizontal length scale to vary in the vertical. It also results in shorter length scales for temperature than for geopotential and in vertically sharper correlation structures for wind than for mass. We have demonstrated that the structure function specification has a profound impact on the analysis increments, particularly with respect to single level data such as aircraft data and surface pressure observations. The current formulation is globally homogeneous. This is believed to be the cause of some 3D-Var analysis deficiencies in the tropics and in the polar regions.

The pre-operational tests at full operational resolution (T213) comprises a very large number of cases - in total 163 days, in five separate periods. This amount of experimentation was necessary because of a very large variability in forecast performance between the two schemes. We averaged the 120 cases run after an important model change (the prognostic cloud-scheme). On average over those 120 cases we found a neutral impact in the Northern Hemisphere extra-tropics in terms of geopotential, whereas wind and temperature scores were positive. In the Southern Hemisphere there was a significantly positive impact in terms of geopotential, wind and temperature. The tropical results were mixed. The main areas of difficulty during the pre-operational tests have been discussed in section 6 of this paper. They include the tropical mass-wind balance, several aspects of the humidity analysis and the precise usage of TOVS and SATEM data.

The stratospheric analyses are significantly better in 3D-Var, as seen from analysed potential vorticity for example. The 3D-Var structure functions are a better description of the true background errors in the stratosphere, displaying the characteristic increase in horizontal length scale with height which is not present in OI. The benefits of the better 3D-Var analyses are translated to lower medium-range forecast scores in the stratosphere, in both hemispheres. There is, nevertheless, undoubtedly scope for further improvement of the stratospheric analyses and forecasts.

The analysis of tropical cyclones has improved by the addition of scatterometer wind data. It has been shown that the mean positional error in analyses of North Atlantic tropical cyclones has been reduced from 173 km in OI to 111 km in 3D-Var (*Tomassini et al.* 1997). The improved analyses also led to better forecasts in the short range.

7.2 Current directions of work

The implementation of 3D-Var reported on in this paper relied on the OI scheme for quality control of the data and to calculate standard deviations of background error. The dependence on the OI scheme has, however, recently been removed. The quality control has been embedded within the variational analysis itself using the method described by *Lorenc and Hammond* (1988) and *Ingleby and Lorenc* (1993), and applied to a simulated LIDAR dataset in a two-dimensional variational analysis by *Dharssi et al.* (1992). We are now applying their technique to the global set of real observations. Results have shown that variational quality control is an adequate and efficient replacement for the traditional OI quality control. The checks against the background fields (the so called first-guess check) has also been replaced by a new module which does not rely on the OI codes.

The replacement for the OI calculation of standard deviations of background error is a two-part procedure which first estimates standard deviations of analysis error and then applies a simple error growth model (*Savijärvi* 1995) to estimate standard deviations of background error for the next analysis cycle. The standard deviations of analysis error are estimated using a low-rank approximation based on the leading eigenvectors of the Hessian matrix of the cost functional (*Fisher and Courtier* 1995).

The mass/wind balance is currently defined through a Hough-mode separation. Two deficiencies of this formulation have been discussed in this paper. Firstly, the mass-wind balance is not part of the change of variable transformation. This severely deteriorates the conditioning of the problem unless the same background error statistics are used for both the balanced and the un-balanced parts of the control variable. In practice we are forced to use the same correlations for vorticity as for divergence, although the results in Part II have indicated that this is a poor approximation. Secondly, the need to uncouple the mass and wind analyses in the tropics leads to the introduction of a transition zone in the sub-tropics which is fairly arbitrarily defined, at present. It was felt that these known deficiencies to the formulation were not severe, and could be left until after the first operational implementation. Work addressing these problems is now well under way. It involves a re-formulation of the

background term (J Derber, pers. comm.), based on a statistically modified linear balance equation. Results so far are promising, and there is scope for further improvements of the scheme in the future.

The current 3D-Var specification of background errors assumes non-separability and global homogeneity while OI assumes separability and has regional variation of the vertical correlations. In this paper we have stressed the advantages of non-separability and we have demonstrated the disadvantages of not having regional variation. Work is now progressing on introducing such regional variation in 3D-Var. There is ample evidence that there are geographical variations in the vertical correlations of background errors: The temperature and wind error structures are sharper in the tropics and subtropics than in the global average (Part II, Fig. 12); The variation of tropopause height with latitude makes the global average correlations less appropriate at high latitudes (*Kelly* 1993); There are also important differences between data rich and data sparse areas (*Lönnberg* 1988). In a gridpoint analysis it is straightforward to define the vertical background error correlations in gridpoint space with the required geographical variability - as was done in OI. In spectral 3D-Var, however, it is more difficult, but it has been shown that, with some restrictions, it is possible to modify the 3D-Var correlation model locally in gridpoint space (Part I, section 3b). This is done by distorting the vertical geometry of the model in an ad hoc way. The method has been implemented for testing in 3D-Var, with encouraging preliminary results. It is believed that it will improve the realism of the vertical structure functions in 3D-Var. The possibility of having variable horizontal length scales, along the ideas presented in section 3a-vi in Part I, will also be explored.

We have started studying the effects of increased vertical resolution of the stratosphere, and an extension of the model to 0.5 hPa. The vertical extension of the model is important for the assimilation of some relatively high-peaking TOVS channels. We shall also be looking at the benefits that can be derived from including ozone as a variable in the data assimilation system.

7.3 Future developments

A 4D-Var system relying on this 3D-Var formulation is now being tested. 4D-Var (four-dimensional variational assimilation) includes the time-dimension in the analysis step of the assimilation. It minimises an objective function measuring the misfit between a model trajectory and the available information (observations and background). Assuming the model is linear, this temporal generalisation of 3D-Var produces the same result at the end of the assimilation period as the Kalman filter, provided the model is perfect. As a consequence, it uses flow-dependent structure functions within the assimilation period, as illustrated by *Thépaut* et al. (1996). Recent results have shown good mid-latitude performance of a 4D-Var system on a 6-hour assimilation window (*Rabier et al.* 1996). It is hoped that such a system can be implemented operationally in the near future.

Although the 4D-Var system generates flow-dependent structure functions within the assimilation period, the structure functions assumed for the background are the same as in 3D-Var. A simplified Kalman Filter, currently under development, extends the 4D-Var system to include flow-dependence in the specification of the background term of the cost function. The basic formulation was described by *Courtier* (1993).

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TABLES

Name	Dates from/to	Resolution	Model version	No of days
A1	940101/940115	T106	cy11r7	15
A2	940303/940317	T106	cy11r7	14
A3	940401/940415	T106	cy11r7	15
A4a	930801/930815	T106	cy12r1	15
A4b	930816/930830	T106	cy12r1	15
A5	931001/931015	T106	cy12r1	15
A6	941206/950117	T213	cy12r1	43
B1	940613/940711	T106	cy13r4	29
B2	941206/950102	T106	cy13r4	28
B3a	950405/950421	T213	cy13r4	17
ВЗЬ	950422/950514	T213	cy13r4	23
B4	950824/951028	T213	cy13r4	66
B5	960116/960129	T213	cy14r2	14
Total				146+ 163

Table 1: List of data assimilation experiments in which 3D-Var has been run in parallel with OI. Cy13r4 marks an important model change including the introduction of the prognostic cloud scheme. Ten-day forecasts have been run from each day at 12 UT. Experiments at operational resolution T213 are highlighted in **bold**.

	An	Day 1	Day 3	Day 5	Day 7
3D-Var Improved	29	23	25	16	12
Neutral	30	32	26	32	18
Worse	6	10	14	12	6

Table 2: Subjective study of tropical cyclone position and intensity in analyses and forecasts, comparing 3D-Var with OI. The sample includes all hurricanes, typhoons and tropical storms in the period from 19950828 to 19950918.

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Fig. 4 Scatter diagram of r.m.s. of 500 hPa geopotential forecast error (metres), showing 3D-Var along the x-axis and OI along the y-axis. The same 120 cases as in Fig 1 are plotted. Winter cases are marked with a triangle and summer cases are shown with a circle. The cross indicates the mean.





Fig. 5 Average r.m.s. of 500 hPa geopotential forecast error for the periods 950501 to 950514 (a) and 960116 to 960129 (b). These were the two 14-day periods with the worst and the best 3D-Var performance, respectively. The full line is OI and 3D-Var is dashed.







Fig. 7 R.m.s. difference in u-component and geopotential height, of observation minus-analysis (dashed) and observation-minus-background (full lines), for all used radiosonde wind data in the Northern Hemisphere (north of 20 N, left), in the tropics (within 20N and 20 S, middle) and the Southern Hemisphere (south of 20 S, right hand panels), for the 14-day period from 19950824-12 to 19950906-12 UTC. The diagrams represent 3D-Var (a) and OI (b)







Fig. 8 North-south cross-section along 40 W, of analysis increments of temperature (K) 19930816-00 UTC for analyses without TOVS or SATEM data. a) is 3D-Var, b) is OI. Contour interval is 0.2 K.

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Fig. 9 Analysis increments of geopotential height at 1000 hPa (a) and 300 hPa (b) for an analysis using surface pressure data only (SYNOP, SHIP, DRIBU and PAOB). The contour interval is 10 metres, with negative contours dashed.







Fig 11 Tropical cyclone Karen, 19950831. Panel (a) shows the observed scatterometer wind for an orbit which passes directly over the cyclone position (indicated by a large dot, at 20 N, 52 W), (b) shows the background (six-hour forecast) valid at the same time, and (c) shows the 3D-Var analysis, interpolated to observation locations.





Fig. 13 Mean 3D-Var analysis increments (19950421 to 19950504, 18 UTC). a) shows surface pressure. Contour interval is 0.4 hPa, negative dashed. b) is mean vector wind increments. The legend indicates a 5 ms-1 wind arrow.



Fig. 14 Mean 3D-Var analysis of two metre specific humidity (19950824 to 19950829, 12 UTC. Contour interval is 2 g/kg. Plotted numbers indicate mean difference between observed and analysed humidity, at selected SYNOP stations.



Fig. 15 Global hydrological budget at model sea points showing total precipitation (full line) and evaporation (dashed). a) is OI, b) is 3D-Var and c) shows the modified 3D-Var which later became operational.