DATA ASSIMILATION AND FORECAST EXPERIMENTS AT ECMWF USING THE '3I' RETRIEVAL SCHEME FOR SATELLITE SOUNDINGS
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ABSTRACT

We report on a retrieval, data assimilation and forecast experiment on satellite sounding data from the NOAA-9 and NOAA-10 polar orbiting satellites during a 15½ day period in January-February 1987, using the operational ECMWF system (as it was in late July 1988). Retrievals have been produced globally at a high resolution through the 3I (Improved Initialization Inversion) scheme developed at LMD, Paris, and implemented at ECMWF. The 3I retrieved temperature profiles have been compared with the operational NESDIS retrievals (SATEMs).

We show that the large air-mass dependent biases, characteristic of the NESDIS retrievals, also occur with 3I but with smaller amplitude. The cause of some large local 3I retrieval errors are explained and their impact on analysis and forecasts demonstrated. The implication of using a very large volume of satellite soundings (14000 soundings per 6 hours) in the ECMWF data assimilation system is also discussed. The experiment has led to further improvements of the 3I scheme.

1. INTRODUCTION
At ECMWF an extensive series of experiments has been carried out using satellite vertical sounding data from the NOAA polar orbiting satellites. The observing system experiment related to satellite soundings provided by NESDIS statistical retrieval scheme has been discussed in Andersson et al. (1989). Kelly et al. (1989) has studied the quality of NESDIS current physical retrievals and Zhang et al. (1989) has documented the humidity aspects of the experiments.

It was found that the statistical SATEM retrievals of TOVS (TIROS-N Operational Vertical Sounding) satellite data in the ECMWF analysis forecast system (as configured in late July 1988) had a negative impact on analyses and forecasts (Andersson et al., 1989) in the Northern Hemisphere. Synoptic and statistical investigation of the SATEM data for the

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study period (30 January to 14 February, 1987) showed serious defects in the statistical retrievals. The defects included important air-mass dependent biases in the data. These lead to geographically fixed biases of substantial magnitude.

This paper will discuss the work which has been done in cooperation with LMD (Laboratoire de Météorologie Dynamique) in Paris using the 3I retrieval scheme. The 3I method (Improved Initialization Inversion) has been developed at LMD by Chédin and Scott (1985). In the past, 3I retrievals have been produced for numerous but limited areas throughout the globe e.g. Flobert (1988b) and Claud (1989). They have been used in limited area data assimilation as for example the Norwegian 'LAM50' system (Claud et al., 1989), but have not previously been used as input to a global assimilation system.

At ECMWF the analysis system is based on a three dimensional multivariate Optimum Interpolation (OI) scheme for mass and wind, and on a three dimensional univariate OI scheme for relative humidity. All the scientific aspects of this analysis scheme are documented in Lorenc (1981), with the more recent development explained in Lönnberg et al. (1986), Lönnberg (1988) and Undén (1989). The aspects related to the interface between the OI analysis and the SATEMs are discussed in Kelly and Pailleux (1988).

The data assimilation is cycled once every six hours and uses conventional observations, satellite derived cloud track winds, and satellite derived profiles of temperature and humidity. These profiles are provided operationally by NESDIS (National Environmental Satellite, Data and Information Service).

The use of 3I in data assimilation involves the replacement of the NESDIS SATEMs with the corresponding 3I profiles. The NESDIS retrieval scheme of February 1987 was a statistical one (Reale et al., 1986), with a resolution at about 250 km. The 3I retrieval scheme, as implemented at ECMWF (Flobert, 1988a), has a resolution at about 100 km and produced a total of 30000 soundings per six hours. The increased horizontal resolution of the 3I profiles compared with the operationally received product has introduced the need for data screening as the current analysis has a practical limit of about 15000 soundings.

The following section outlines the details of the experiment and Section 3 gives a brief introduction to the 3I scheme. The quality of the 3I and NESDIS soundings is intercompared in Section 5. Sections 6 and 7 describe their impact on ECMWF analyses and forecasts. We demonstrate that the 3I soundings are of better quality than the statistical NESDIS soundings in some respects but there are several cases of local data problems with 3I. These local data problems are discussed in four case studies in Section 8. We conclude by presenting the improvements of the 3I scheme carried out to remedy the identified problems.
and we discuss the implications of using a very high density of satellite sounding data in the ECMWF analysis system.

2. THE DETAILS OF THE EXPERIMENT
The experiment comprises three data assimilations over the period 30 January 00 UTC to 14 February 12 UTC, 1987. This period was chosen because of the meteorological situation and the availability of the two satellites, NOAA-9 and NOAA-10, providing a global data coverage every six hours. The complete set of raw radiances, cloud-cleared radiances and soundings was provided by NESDIS. The three assimilations, labelled (1) OPS-Jul88, (2) NoSATEM and (3) 3I (HR) are specified as follows:

(1) OPS-Jul88 used the operational soundings produced by NESDIS with a density of about 5000 soundings globally per six hours. The retrieval scheme at the time was a statistical inversion scheme (Reale et al., 1986).

(2) NoSATEM used the same assimilation code but used no satellite sounding data, neither thicknesses nor precipitable water content.

(3) 3I (HR) used 3I-soundings with a density of about 14000 soundings globally per six hours. The 3I algorithm is described by Chédin et al. (1985) and Chédin (1988) and was implemented at ECMWF by Flober (1988a).

Fifteen 10-day forecasts were run from each assimilation with the operational resolution (T106) and with the July 1988 version of the ECMWF model. The comparison between OPS-Jul88 and NoSATEM has been discussed in detail in Andersson et al. (1989).

3. THE 3I RETRIEVAL ALGORITHM
The inversion algorithm ‘3I’ (Improved Initialization Inversion) which was developed by the Atmospheric Radiation Analysis (ARA) group at Laboratoire de Météorologie Dynamique (LMD) during the last few years falls into the category of direct non-iterative physio-statistical methods, and gives results whose accuracy, as demonstrated at international conferences (International TOVS working group), is among the best.

The principle on which the 3I algorithm is based relies on a pattern recognition approach. The inversion of the radiative transfer equation is split into two steps, which both take satellite measurements as their data sources. The first step inverts these measurements according to the principle of best initial profile out of the large selection of atmospheric situations that were archived in advance and classified in groups according to latitude (tropical, mid-latitude, polar) and season. This library of
atmospheres, Tigr (TOVS Initial Guess Retrieval data set), consists presently of about 1200 situations carefully selected by statistical analysis methods out of about 10000 samples. Transmissions, radiances and weighting functions for all sounding channels have been calculated in advance for each particular situation. For each of them, calculations have been performed for 10 viewing angles between 0° (nadir) and 60° (the maximum value for angular scanning, see Fig.1), for 10 values of ground pressure (observations over elevated terrain), and for two types of surfaces (land and sea).

First, a similarity analysis is performed by comparing the measured radiances with the calculated radiances corresponding to each archived atmospheric situation and establishing a distance between two such situations. The most similar situation of those archived (or the mean of a few situations around the most similar) is taken as the initial solution.

From the initial profile obtained in this manner, the second step performs the inversion of the radiative transfer equation by means of a Bayesian type direct estimation method (maximum a posteriori probability), which aims at minimizing the deviation between the observations and the initial solution.

The perturbation, if not occultation, due to clouds would prevent retrieval of temperature profiles and other parameters in overcast areas, and also cause large gaps in the inversion fields, if it were not possible to find equivalent clear columns for such cases. Equivalent clear columns are the radiances the sounder would have measured if no cloud had perturbed the observations.

The manner in which the influence of clouds on observations is decoupled forms an essential aspect of the infra-red/microwave coupling performed by the 3I algorithm. In the case of cloudy spots, a first initial solution is obtained by comparison between observations and situations in the Tigr library for a restricted number of channels which are not sensitive to the effect of clouds (stratospheric channels and microwave channels). Using this initial set as a starting point, the cloud clearing algorithm based on the so called ψ-method is initiated. This method finds a clear equivalent from the difference between the observed and initial values of a microwave channel whose weighting function is close to that of the infra-red channel in question. For a cloud-insensitive (microwave) channel, integrating approximately the same atmospheric layers, this difference accounts for the major part of the discrepancy between the initial value and the real equivalent clear value of the infra-red channel. This procedure is iterated once. The ψ-method makes use of the potential offered by microwave measurements for obtaining information through clouds, and relies on the educated Tigr data base. The ψ-method is equally applicable to
Fig. 1  Horizontal resolution and scan patterns for HIRS (small ellipses) and MSU (large ellipses). The arrow is the sub-satellite track. The black square delimits an area of about 100 km x 100 km: a '3I-box'. The ten divisions, from nadir to limb, correspond to the ten viewing angles.

Fig. 2  Modified data assimilation cycle using 3I soundings in place of NESDIS soundings.
both partially cloudy and overcast areas, provided the microwave channels are not contaminated (for example by heavy rainfall) to any significant degree.

The 3I system is presently in use at numerous centres in the world, for both research and routine applications.

4. **THE RETRIEVAL SUITE AT ECMWF**

The output of the 3I retrieval package are temperatures at standard levels, relative humidity up to 300 hPa and cloud amount and height. The interface for the mass/wind analysis is via the seven thick layers (Kelly and Pailleux, 1988) which is the same as for NESDIS SATEMs. However it was now possible to use the relative humidity directly rather than converting it to the layer precipitable water content of NESDIS SATEMs. In addition use was made of the cloud information to provide a bogus saturated layer immediately below the cloud. The humidity aspects of this experiment are documented in Zhang et al. (1989).

In order to perform global 3I processing it was first necessary to modify the RTPP (International TOVS Processing Package) pre-processing programs (data handling, earth-location, radiance calibration, moisture and short-wave radiation corrections) provided by the University of Wisconsin to pre-process up to eight global TOVS (TIROS-N Operational Vertical Sounder) orbits in any six hour period, Fig.2. Use was made of the six hour forecast to compute radiances using the 3R (Rapid Radiance Recognition) fast forward model (Flobert et al., 1986), in order to perform quality control of the raw MSU radiances prior to mapping. Some work was also required to modify the MSU mapping for global processing (MSU mapping involves the interpolation of the MSU observations (large ellipses) to the positions of the HIRS spots (small ellipses), see Fig. 1). Next the 3I programs were interfaced to the ECMWF forecast fields. 3I allows for the use of some parameters such as surface temperature and pressure from the first-guess which are used to help guide the initial profile search in the TIGR data set.

A problem encountered with the 3I processing was the existence of large biases in particular air masses. An anomalous stratospheric vortex remained almost stationary over Europe with very cold temperatures near the surface and soundings differed from radiosondes by up to 10°C at some levels. In order to solve these bias problems, 3I was slightly revised to allow for a better balance between lower and upper parts of the atmosphere. Previously limited by matrix truncation to 10 hPa, retrievals were now computed up to the top of the atmosphere (0.05 hPa) although the retrievals were used, as before, up to 10 hPa. In addition, a small study was made with a series of satellite and radiosonde matches and a set of radiance bias corrections were computed which are
air-mass dependent (Kelly and Flobert, 1988). These tuned radiances were used in theesults presented here.

5. EVALUATION OF SOUNDINGS
5.1 Collocations with radiosondes
Collocations with radiosondes were made in order to assess the quality of the 3I soundings
and to validate the radiance tuning. These collocations were presented in Flobert (1988a)
together with the corresponding collocation statistics from the routine monitoring of NESDIS
soundings. Flobert (1988a) showed that 3I is consistently better than NESDIS in the lowest
layer, 1000/850 hPa. 3I is also less biased in northern latitudes, but overall there is a
striking similarity between the two retrieval schemes, both in bias and standard deviation.

During the first part of the study there was a strong anomalous circulation in the
stratosphere over most of Siberia and Europe. The stratospheric cold vortex was shifted
from its climatological position over the pole to Central Europe, causing a strong
cross-meridional temperature gradient over Russia. The operational soundings showed a
large negative bias relative to radiosondes over Siberia and China, mainly in the 50/30 hPa
layer, Fig.3a. It was suggested that the problems originated from improper tuning of the
regression coefficients of the statistical retrieval scheme; the tuning was performed within
latitude bands and the unusual circulation is likely to have made the tuning data set quite
different from the data set to which it was applied.

Similar, or slightly larger, bias appeared with the physical 3I scheme, Fig.3b. Calculations
with the 3R forward model (Flobert et al., 1986) has shown that this can be a case in which
there are several valid solutions to the radiative transfer equation and both retrieval
algorithms consistently went for a wrong solution rather than retrieving the abnormally
warm stratosphere. It is however to be noted that SSU data (Stratospheric Sounding Unit)
were not introduced in the 3I processing.

5.2 Comparison between 3I and NESDIS soundings
Direct comparisons with NESDIS soundings show that whole batches of 3I soundings often
disagree with NESDIS soundings by several degrees. In Fig.3 the subtropical air along 25°
North is 2 to 3°C warmer in 3I. Just north of the cold front, at (35°N,155°W), 3I is 3°C
colder. The tongue of warm air, near (43°N,130°W) is 3°C warmer in 3I. There are few
other upper-air observations in the area and it is difficult to know which retrieval scheme
is better.

The 3I soundings exhibit very little random noise; they appear coherent and smooth in the
horizontal. In such circumstances coherent air-mass bias is usually accepted by the
Fig. 3  Statistics of soundings collocated with radiosondes. Maximum distance difference is 150 km. Solid line: RMS (Root Mean Square Error), dotted line: standard deviation, dashed line: bias. a) Area over China for NESDIS and b) similar for 3I (20°-50°N, 90°-145°E).
analysis scheme in the absence of other data and has a direct impact on the analyzed fields. The very noisy NESDIS soundings near \(47^\circ\text{N},145^\circ\text{W}\), Fig. 4b, are on the contrary effectively smoothed and almost ignored by the analysis.

5.3 Comparison with first-guess fields

The stability index, \(T(1000/700) - T(500/300)\), was studied in Andersson et al. (1989) as a means of detecting deficiencies with the soundings. Global statistics of the stability departure from first-guess (FG) were presented for the operational NESDIS soundings, in the form of bias and standard deviation for the 15-day February 1987 period. The corresponding maps for 3I have been produced and they are presented here.

The patterns of a positive bias (retrieval less stable than FG) in the western North Pacific and western North Atlantic, and a negative bias (more stable than FG) in the eastern parts of these oceans occur with both retrieval schemes but are much less pronounced with 3I. However, 3I has very large biases over Europe and northeast Canada. The bias and standard deviation for clear and cloudy soundings are shown for NOAA-10 in Fig. 5a to 5d. Maps for NOAA-9 are shown in the Appendix. There is no significant quality difference between NOAA-9 and NOAA-10. The quality of the clear soundings is better than the quality of the other soundings, as expected. See for example the positive bias on the stability index of the cloudy soundings in the Southern Hemisphere, especially around 30° South.

In comparison with NESDIS (see Andersson et al., 1989 for maps), 3I appears to be better in most parts of the Atlantic, especially in the north. The NESDIS MSU (cloudy) soundings from NOAA-10 were much too stable in the mean over eastern North Pacific; the 3I soundings are unbiased there. The standard deviation of the stability deviation from the first-guess indicates that 3I overall is much better than NESDIS in the Northern Hemisphere in this respect.

In Andersson et al. (1989) it was concluded that the NESDIS soundings have very little skill in measuring the tropospheric stability in the mid-latitudes, especially in the North Atlantic and in the Japan area. In the Subtropics, however, their quality seems comparable to the quality of the first-guess. The performance of 3I in these three areas is presented here in Fig. 6a to 6c along with the corresponding maps for NESDIS. These scatter plots should be compared with the corresponding ones for selected radiosondes presented in Andersson et al. (1989). Again, the 3I soundings appear to be better in the North Atlantic. The very large errors noted in the NESDIS soundings which gave too stable soundings in the cold-air out breaks to the south of Japan do not occur as much with 3I. In
Fig. 4 Observed 1000/700 hPa layer mean temperature, 870204-12 UTC in °C. Contour lines are a Cressman analysis of the observed values. a) is 3I, b) is NESDIS. The marked areas are areas with large differences between the two retrieval schemes.
Fig. 5 15-day statistics of observed deviations from first-guess stability, T(1000/700)-T(500/300) for 3I soundings, accumulated in 5x5° boxes. a) bias for NOAA-10 clear soundings and b) standard deviation. c) bias for NOAA-10 cloudy soundings and d) standard deviation.
Fig. 5 Continued.
Fig. 6 Observed tropospheric stability, $T(1000/700) - T(500/300)$, retrieved from NOAA-10, versus first-guess stability in °C, for three different areas, February 1987. 31 to the left and NESDIS to the right. a) North Atlantic (50°N-68°N, 40°W-5°E), b) South of Japan (25°N-35°N, 130°E-140°E) and c) Midway & Hawaii (19°N-29°N, 180°W-155°W).
the central Pacific (Hawaii and Midway Island) the 3I quality is comparable to that of NESDIS.

6. EVALUATION OF ANALYSES

3I analyses are different from OPS-Jul88 and NoSATEM analyses at all levels and for all variables. The humidity aspects are discussed in Zhang et al. (1989). Differences in analysed layer-mean temperature fields are either regional, local or related to synoptic situation (air-masses). Fig.7a illustrates them all. The 3I analysis is colder than OPS-Jul88 (NESDIS) in most of the Southern Hemisphere which suggests a problem with radiance tuning in the 3I experiment. Large local differences like those near (30°N,140°W), (35°N,60°W) and (50°N,10°W) are all, as will be discussed below, caused by differences in the pre-processing and quality control of contaminated or otherwise corrupt raw radiances. Biases tied to air-masses like those in the North Pacific and in the Labrador Sea are attributable to differences between the two retrieval schemes themselves, (one of which can be a different choice of initial profile for the retrieval) and to the fact that the large number of soundings in the 3I analysis gives larger weight to satellite soundings (in relation to the weight given to other data types and to the first-guess).

Much of the air-mass dependent biases (in layer-mean temperature) are artefacts introduced as a consequence of the inadequate vertical resolution of the soundings. This assumption is supported by the observation that the differences between the analyses in terms of calculated radiances (MSU2, 3 and 4) are very small in these areas.

Differences in the upper troposphere often compensate those in the lowest layers. Around 100 hPa the differences are small. In the top layer (30/10 hPa), Fig. 7b, the differences are very large (exceeding 5°C) and affect most of the Northern Hemisphere. 3I is noisier but the large differences can only be explained by the fact that 3I does not make use of the SSU channels (Stratospheric Sounding Unit). The impact of these stratospheric analysis differences on forecasts has not yet been studied in any detail.

7. EVALUATION OF FORECASTS

The study on the February 1987 dataset comprises fifteen 3I forecasts (3I HR), fifteen forecasts from a data assimilation with operational NESDIS soundings (OPS-Jul88) and a set of fifteen forecasts without satellite sounding data (NoSATEM).

All forecasts were run with the July 1988 version of the ECMWF forecast and analysis system which enables a clean comparison between the three data assimilations and between forecasts. The NoSATEM versus OPS-Jul88 comparison has been discussed in Andersson et
Fig. 7  Layer mean temperature difference between 3L analysis and OPS-Jul88 (NESDIS) analysis, 870201-12 UTC. a) is 1000/700 hPa and b) is 30/10 hPa. Negative differences are dashed.
al. (1989). Here the focus will be on the OPS-Jul88 versus 3I comparison, with NoSATEM retained as a reference.

Both anomaly correlation and RMS (Root Mean Square error) scores have been produced. The two methods of verification gave the same result and only anomaly correlation will be presented here. An anomaly correlation of 100% represents a perfect forecast. As a rule of thumb forecasts with an anomaly correlation below 60% can be considered synoptically useless. The verifying analysis was the operational analysis as produced at the time. It used the operational NESDIS soundings.

7.1 Northern Hemisphere

The 15 day mean scores for the Northern Hemisphere, Fig.8a, show that OPS-Jul88 has a slight advantage over 3I up to a forecast range of 5 days, but 3I is better at day 6. However NoSATEM is slightly superior to both satellite experiments up to day 7.

The day 3 and day 5 scores for the individual forecasts are presented in the form of scatter diagrams, Figs. 9a and 9b. At day 3 there are thirteen losses, one draw and only one win for 3I compared with OPS-Jul88. The largest losses occurred on 4, 8 and 9 February and the win on 2 February. The 4 February case will be discussed below together with some other cases with local 3I data problems. The scatter is relatively large and shows that the ECMWF system is sensitive to differences between satellite retrievals.

At day 5, Fig. 9b, there are two large wins for 3I. They occurred on the last two days of the experiment (13 and 14 February). However, both show very little impact up to day 3½ (not shown) and cannot easily be traced back to analysis differences. On average, the day 5 score in the Northern Hemisphere is a draw with NESDIS.

7.2 Southern Hemisphere

In the Southern Hemisphere the OPS-Jul88 forecasts are ahead of 3I throughout the first five days, Fig. 8b. One has to bear in mind that 3I has the initial handicap of its forecasts being verified against analyses that have been produced from the NESDIS soundings. This effect should be negligible, however, in the medium range.

The results at day 3 are curious because all forecasts are draws or almost draws except for two which are 'disasters' for 3I, Fig.9c. The two very bad 3I forecasts occurred on the adjacent days of 7 and 8 February. On the 7'th 3I suffered badly from 'jumps' in MSU2 and produced a batch of very unrealistic soundings as will be discussed below. The scatter in Fig.9d for day 5 is not in favour of either of the two experiments.
Fig. 8. 15-day average of 500 hPa height anomaly correlation for three sets of forecasts. Full line: OPS-Jul88 (NESDIS), dashed line: NoSATEM and dotted line: 3I. a) Northern Hemisphere, b) Southern Hemisphere, c) North America and d) North Pacific.
Fig. 9 Scatter diagram of 500 hPa height anomaly correlation for the 15 forecasts, comparison between OPS-Jul88 (NESDIS) and 3I. The cross indicates an average. 
a) Northern Hemisphere day 3, b) Northern Hemisphere day 5, c) Southern Hemisphere day 3 and d) Southern Hemisphere day 5.
7.3 Impact of sounding density

The scores for 3I relative to NESDIS reflect the difference in volume of data used in the two data assimilations (14000 for 3I compared to 5000 for NESDIS) as well as the methodological differences between the retrieval schemes. There is a negative impact of NESDIS statistical retrievals in the Northern Hemisphere in this period and therefore it is not so surprising that a larger negative impact is found when more satellite data is used, as in the 3I experiment. As shown in Andersson et al. (1989), most of the negative impact in the medium range occurred over North America, down-stream of the Pacific Ocean where the analysis relies heavily on satellite sounding data in the absence of conventional upper-air observations. The problem is magnified in the high density 3I experiment as can be seen from Fig.8c.

The importance of satellite data volume was confirmed in a lower density re-run of the first four cases. The 3I soundings were thinned to a resolution broadly equivalent to that of the operational NESDIS soundings. With the lower resolution 3I (3I LR) the scores improved in the Northern Hemisphere, Fig. 10a, particularly in the North American region, Fig. 10c. In the Southern Hemisphere there was no significant change, Fig. 10b.

There seems to be a potential to improve the results with a more intelligent screening of the satellite data, aimed at removing local biases and systematic deficiencies, before the data are presented to the analysis.

8. CASE STUDIES

Several forecasts with negative impact from 3I data were studied in more detail. In some cases it was possible to trace forecast errors back in time to the initial date and comparisons between the three data assimilations gave indications of possible explanations. Temperature soundings were compared between the two retrieval schemes, with radiosondes and with first-guess fields. Radiances were computed with the 3R forward model (Floquet et al., 1986) from first-guess and analysis fields and compared with observed radiances.

8.1 Shallow cold air out-breaks over warm ocean

During the first two days of the assimilation period there was a large discrepancy between the satellite soundings (both 3I and NESDIS) and the NoSATEM analysis over Davis Strait and the Labrador Sea between Greenland and northeast Canada. The satellite soundings were much too warm in the lowest layer, (1000/700 hPa). On 31 January 1987, 12 UTC there was an 8°C difference at one point, near (50°N,48°W), in the 850 hPa temperature field between 3I and NoSATEM analyses, Fig.11. The 3I temperature field looks unrealistic in this situation of strong cold-air advection as indicated by the pressure field.
Fig. 10 4-day average of 500 hPa height anomaly correlation for four sets of forecasts. Full line: OPS-Jul88 (NESDIS), dashed line: NoSAME, dotted line: 3I HR and dash-dotted line: 3I LR. a) Northern Hemisphere, b) Southern Hemisphere, c) North America and d) North Pacific.
Fig. 11 Analysis of mean sea level pressure in hPa, full lines, and 850 hPa temperature, dashed and shaded in intervals of 4°C, for western North Atlantic, 870131-12 UTC. a) is 3I and b) is NoSATTEM.
Fig. 12 shows cross-sections of the analysed temperature and wind along the line indicated in Fig. 11. The cross-sections in Fig. 12 show that there are large differences in analysed low level temperatures, lower tropospheric stability and jet speed. The peak value of the polar jet (at 57° North) is 45 m/s in the NoSATEM analysis but only 32 m/s in the 3I analysis. Also the subtropical jet (at 37° North) has been reduced by the use of satellite data, from 67 to 62 m/s. Also the boundary layer on the cold side of the front is different in the two analyses. The NoSATEM analysis has a marked unstable layer close to the surface (between 50° and 57° North) which is not present in the 3I analysis. The peak windspeed in the boundary layer is higher in the NoSATEM (36 m/s) than in the 3I (32 m/s) analysis.

Fig. 13 shows cross-sections of the divergence fields corresponding to Fig. 11. In Fig. 13 it appears that the organised frontal structure present in the NoSATEM experiment has been much weakened by the use of satellite data.

A large forecast error developed from this region in the 3I forecast. At day 3 it can be found northeast of Iceland as a 303 m forecast error in the 500 hPa chart, Fig. 14. The scores for the Atlantic area are shown in Fig. 15. There is a dramatic drop in the 3I forecast score at day 2.

No obvious problems have been found with the radiances when compared with radiances calculated from the first-guess. The ice boundary was well to the northwest of the largest sounding errors. Both 3I and NESDIS retrieval schemes were erroneous. The most likely explanation is that the 1.5 to 3 km deep layer of cold arctic air over the relatively warm open sea surface gave a very weak signature in the radiances and so was not detected by either retrieval scheme. The necessary information was not there in the radiances alone.

8.2 Damped frontal activity
The NoSATEM forecast from 4 February 1987, in good agreement with actuality, produced a cut-off low as the last member of a family of cyclones in the eastern North Pacific. On the contrary, both satellite forecasts, 3I as well as OPS-Jul88, failed to develop this low. Large forecast errors travelled down-stream and had clearly a negative effect on the medium range forecasts for North America, North Atlantic and Europe, see Fig. 15b for North American scores. The NoSATEM and 3I analyses and 2-day forecasts are shown in Fig. 16a together with the verifying analysis. It is curious that all three waves along the frontal zone appear deeper and the temperature fields more amplified in the NoSATEM analysis than in the 3I analysis (which is similar to the OPS-Jul88 analysis in this respect, not shown). The wave near (30°N, 160°W) in the NoSATEM analysis (Fig. 16b) is the crucial one for the forecast.
Fig. 12  Analysis cross-section from northwest to southeast between Greenland and Canada (line marked in Fig. 11), 870131-12 UTC, showing winds in the plane of the cross-section, arrows, and perpendicular to it, full lines in m/s, as well as potential temperature, thin lines in Kelvin. a) is 3I and b) is NoSATEM.
Fig. 13  As Fig. 11 but for divergence in units of $10^{-5}$ s$^{-1}$. a) is 3I and b) is NoSATEM.
Fig. 14 500 hPa 3-day Northern Hemisphere forecast errors of forecast from 870131-12 UTC. Contours are -60, -20 (dashed), +20, +60 (full lines) in metres. Verifying analysis is the operational analysis from February 1987. a) 31 and b) NoSATEM.
Fig. 15 500 hPa height anomaly correlation for limited areas for the four following case studies. Full line: OPS-Jul88 (NESDIS), dashed line: NoSATEM, dotted line: 3i(HR). a) Forecast from 870131-12 UTC North Atlantic, b) 870204-12 UTC North America, c) 870201-12 UTC North America and d) 870207-12 UTC Southern Hemisphere.
Fig. 16  Mean sea level pressure in hPa, full lines, and 850 hPa temperature, dashed and shaded in 4°C intervals, for eastern North Pacific. a) 3I analysis of 870204-12 UTC and b) NoSATEM analysis. c) 3I 2-day forecast from 870204-12 UTC and d) NoSATEM corresponding forecast. e) verifying operational analysis of 870206-12 UTC.
The reduced temperature gradients in the mid-latitude frontal zones is an effect of the very systematic and organised air-mass biases of the satellite soundings. They in turn are caused by the limited vertical resolution of the observations, particularly in cloudy areas.

8.3 Rain contamination

The forecast from 1 February 1987 is a case of positive impact of the operational satellite data but the 3I forecast was not good over North America, see Fig.15c for the scores. 3I soundings were very inconsistent with NESDIS soundings and with the first-guess, along the frontal zone over eastern North Pacific. Fig.17a shows the 3I observed 1000/500 hPa temperature deviations from the first-guess. The soundings were up to 5°C too cold in a narrow band along the front, on average in the five kilometre thick layer. The measured MSU2 radiances were too cold compared to those calculated from the first-guess fields. Most of the soundings in the area had been rejected by the NESDIS processing.

The bad 3I soundings turned out to be caused by heavy rain. The simple rain test proposed by Phillips (1980), states that the MSU channels are likely to be contaminated if the MSU2-MSU1 brightness temperature difference is less than 12°C. Fig. 17b shows the observed values of the MSU2-MSU1 difference in the North East Pacific. Due to a programming oversight this test had not been included in 3I processing. Applied to our data, the test nicely identified the area along the front as affected by rain, Fig.17b, and the MSU data ought to have been rejected by the 3I system.

Similar bad data also appeared six and twelve hours earlier in the assimilation. In data assimilation their effect on the mid-tropospheric wind field was large. Fig. 18 shows a cross-section from northwest to southeast along the line indicated in Fig. 17b. The cross-section, Fig.18, shows a spurious feature in the isotachs in the 3I analysis just above and south of the front at 33° North. The associated vertical winds are excessive.

The cross-section also shows important analysis differences with the NoSATEM analysis within the frontal zone at 37° North and differences in the analysis of the tropopause and the mid tropospheric stability in the deep polar air-mass at 55° North. The decreased frontal temperature gradient, the spreading of the jet in the horizontal, the smoothing of the tropopause and the redistribution of the static stability in the cold air-mass have all been found to be typical of both satellite data assimilations. They can, possibly, be attributable to the limited vertical resolution of the satellite soundings and the way the analysis draws for vertical features of the FG-OBS increments (Lönnberg, 1989).
Fig. 17 Eastern North Pacific, 870201-12 UTC. a) is observed 1000/500 hPa layer mean temperature deviations from first-guess, in °C. b) is observed MSU2-MSU1 brightness temperature difference in °C. The 12°C contour line is drawn.
Fig. 18 Analysis cross-section from northwest to southeast in eastern North Pacific, along the line marked in Fig. 17a, 870201-12 UTC, showing winds in the plane of the cross-section, arrows, and perpendicular to it, full lines in m/s, as well as potential temperature, thin lines in K. a) is 3I and b) is NoSATEM.
8.4 Corrupt radiances
The 3I forecast from 7 and 8 February 1987 are the only two clear defeats of 3I in the Southern Hemisphere, see Fig.15d for the scores on the 7th. The NESDIS and 3I analyses of the 7’th at 12 UTC have been studied in detail. Large data problems were found in the area between New Zealand and Antarctica. The analyses were different by 6°C in the 500/300 hPa layer, Fig.19. A large forecast error developed from there in the 3I forecast and had at day 4 reached (60°S,130°W). Fig.21 shows the forecast errors for day 1 and day 4 for both 3I and OPS-Jul88 forecasts.

The 3I soundings in the area look peculiar, with a temperature lapse rate totally different from that of NESDIS' soundings, Fig.20. The problem coincides with a jump in the MSU2 data of one orbit, as can be seen in deviations of the observed radiances from synthetic radiances calculated from the first-guess. The jump occurs between two lines (at 52° South) of one NOAA-10 orbit between 120° and 140° East, Fig.22. Normal values of the deviation should be close to +1.5°C because of the tuning of the forward model. The jump appears to be in the order of 1° Kelvin in brightness temperature. The figure incidently shows a considerable mismatch between NOAA-9 and NOAA-10 MSU2 in the area of (60°S,170°E). The 3I algorithm appears to be more sensitive than NESDIS to MSU2 variations resulting, in this case, in a negative effect. This problem should be overcome by rejecting MSU observations for which the difference with MSU calculated from the first-guess is too large.

9. FURTHER IMPROVEMENTS OF THE 3I SCHEME
In response to the problems highlighted by the present 3I experiments at ECMWF modifications have been made to the 3I algorithm. They are described in detail in Chédin et al. (1989). A summary of these refinements is presented below.

Rain detection test:
In the studied fifteen day period numerous areas, sometimes quite large, were affected by strong rain, contaminating the MSU observations. A test derived from Phillips work (1980) has been introduced aiming at rejecting such situations.

Cloud clearing:
The ψ-method for decontaminating infra-red cloudy radiances from the effects of the clouds has been refined. Instead of predicting the difference between the clear radiance and the corresponding initial guess by the difference between the observed and initial guess value of a microwave channel peaking at about the same pressure level, it is now predicted by a linear combination of such differences for several microwave channels. This solution overcomes the problem of different peak levels between infra-red and microwave channels.
Fig. 19 500/300 analysis difference between 3I and OPS-Jul88 (NESDIS) analysis at 870207-12 UTC, in °C, for an area between New Zealand and Antarctica. Full lines are positive and dashed are negative.

Fig. 20 All soundings in a box within 55 - 65 South and 130 - 140 West. a) is 3I and b) is NESDIS.
Fig. 21 500 hPa Southern Hemisphere forecast errors of forecast from 870207-12 UTC. Contours are -60, -20 (dashed), +20, +60 (full lines) in metres. Verifying analysis is the operational analysis from February 1987. a) 3I day 1, b) OPS-Jul88 (NESDIS) day 1, c) 3I day 4, d) OPS-Jul88 day 4.
Fig.22  Observed MSU2 brightness temperature deviation from radiances calculated from 3I analysis first-guess 870207-12 UTC, in °C, for an area between New Zealand and Antarctica. Values over land should be disregarded.
Estimation of the final solution from the initial guess:

Computation of the variance/covariance matrix of the vectors of the difference between the final solution and the initial guess has been made more sophisticated and is now in exact conformity with the on-line 3I retrieval algorithm. In particular the matrix calculations now take into consideration the initialization from near analogs approach (the so called distance circle), (Chédin and Scott, 1985), the cloud clearing algorithm (the θ-method) and the dependence on the viewing angle. A set of 120 more sophisticated covariance matrices are now used instead of 12 previously.

Minor refinements:

Other changes have been successfully tested. A new test for detecting low clouds, the inclusion of operational sea surface temperature maps in the water vapour retrieval, new MSU mapping, etc.

As shown in Chédin et al. (1989) these modifications resulted in significant improvements of the sounding quality.

10. CONCLUSIONS

From the NOAA-9 and NOAA-10 raw radiances provided by NESDIS (Washington), the 3I scheme (cloud clearing and inversion algorithm) has been run in an experimental suite at ECMWF to produce global data sets of retrieved soundings. More than 30000 soundings on average have been produced for each 6 hour period from 30 January 00 UTC to 14 February 12 UTC in 1987. The quality of these soundings has been examined and compared to the quality of the operational NESDIS soundings. Around 15000 3I soundings were used in the main data assimilation and forecast experiment. In a shorter experiment only 5000 to 6000 3I soundings were used. Two similar data assimilation and forecasts experiments run on the same period, one without any SATEMs the other with operational NESDIS soundings, have been used for comparisons.

The results of this TOVS experimentation can be summarized in the following way:

a) The quality problems of the 3I soundings are very similar to the problems of the NESDIS soundings (produced through a pure statistical technique). This tends to show that the difficulties in the retrieval algorithms are related mainly to specific air-masses or specific weather systems; the difficulties seem to be of the same type regardless of the inversion algorithm.

b) However, the quality of the 3I soundings is on the average slightly better than the quality of the NESDIS soundings. In particular 3I is consistently better in the lowest
layer (1000/850 hPa) and the soundings exhibit very little random noise. This is more significant in the Northern Hemisphere, and has been found using various evaluation tools. One of the most useful tools is the one involving a vertical stability index (see Andersson et al., 1989). As an example, in several areas of the North Atlantic and the North Pacific bad vertical gradients were clearly identified in both NESDIS and 3I soundings, but to a larger extent in NESDIS.

c) Some specific 3I problems appeared. Many of them have been found to be related to rain-contamination and MSU ‘jumps’.

d) The impact of the 3I soundings on the analysis is large in terms of difference maps 3I analysis minus operational analysis, or 3I analysis minus NoSATEM. This is true at all levels and for all variables, including for humidity (Zhang et al., 1989). In terms of calculated radiances, however, the differences between the 3I analysis and the operational analysis are very small except in areas with contaminated or otherwise corrupt radiances. This suggests that the observed radiances are well assimilated in spite of the artificial temperature retrieval interface between the radiances and the analysis. In these circumstances large local temperature differences between the analyses are often artefacts, introduced because of the low vertical resolution of the radiance measurements via the choice of initial profile for the retrieval.

e) When using the 3I soundings at the same resolution as the NESDIS soundings in the analysis (5000 to 6000 soundings per analysis), the 3I forecast is neither better nor worse on average than the NESDIS forecast. This comparison has been made on four cases only: 31 January to 3 February 1987. The main 3I assimilation experiment has been run using three times more soundings (more than 15000 soundings per analysis). Then the 3I forecasts have been found on average worse than the operational forecasts. We have to remember that the experiments have been run with an analysis system where the quality control was not severe enough and where most of the poor quality soundings were actually accepted by the analysis, leading on average to a negative impact of SATEM data on the forecast scores (Andersson et al., 1989). It is likely that the data volume is the critical problem in the main 3I experiment. The OI data selection is not able to cope properly with a number of SATEMs three times larger than the operational one, especially in a context where the SATEM quality control is too loose. The global weight given to SATEMs is then probably too high compared for example to the global weight given to about 600 radiosondes (or much less at 06 and 18 UTC). This is the likely explanation of some bad forecast scores of the 3I experiment.
The data volume problem in OI points out the need of defining a more optimum interface between the TOVS information and the assimilation. So do different quality problems discussed in Kelly et al. (1989). The fact that the slight improvement of the 3I soundings (compared to the NESDIS ones) was not reflected in the forecast scores might seem surprising. However, it probably tells that there are still a lot of potential improvements in the way the TOVS data are utilized by the analysis scheme (which is also indicated by the overall small negative impact of the TOVS on the Northern Hemisphere forecast scores). In the 3I data assimilation the same observation error statistics were used as is operationally used for the NESDIS soundings (Kelly and Pailleux, 1988). The available observation error statistics are very crude with for example no regional variations and it ought to be enhanced by taking into consideration its dependence on retrieval scheme and region or air-mass.

For the near future (within the context of the present OI scheme) we can expect progress in the use of TOVS data from the development of a more integrated system where the retrieval and the analysis schemes are at least made consistent regarding quality control and data selection.

The first global assimilation of 3I TOVS retrievals has served as a validation of the 3I scheme. It has resulted in improvements of some particular aspects of 3I. These recent improvements are described in Section 8 and the results are encouraging.

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References


APPENDIX

In the main text maps were presented with bias and standard deviation of the difference between NOAA-10 SATEMs (retrieved by 3I) and the first-guess in terms of tropospheric stability, T(1000/700)-T(500/300), averaged in 5° by 5° boxes over the 15-day period (31 January to 14 February, 1987). The corresponding maps for NOAA-9 are presented here for reference, Fig. A1a to d.

In general the two satellites perform similarly. The only significant difference is the smaller bias for NOAA-9 cloudy retrievals along 30° South.
Fig. A1 15-day statistics of observed deviations from first guess stability, T(1000/700)-T(500/300) for 3I soundings, accumulated in 5° by 5° boxes. a) bias for NOAA-9 clear soundings and b) standard deviation. c) bias for NOAA-9 cloudy (MSU) soundings and d) standard deviation.
Fig. A1  Continued.