ASSIMILATION OF REMOTELY-SENSED OBSERVATIONS

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Summary: This paper considers some of the problems that arise concerning the assimilation of remotely-sensed observations into numerical weather prediction models, including the options and compromises that have to be faced in deciding whether and how to pre-process the observations prior to assimilation. These issues are discussed first in general and then in relation to some specific observation types: TOVS radiances, satellite winds and cloud imagery, SSM/I data, scatterometer data and radio occultation data. Results of recent work in these areas at ECMWF are summarized or referenced.

1. INTRODUCTION

Most papers on data assimilation start from the assumption that the observations have already arrived "at the door" of the data assimilation system. This paper focuses mainly on another problem: what are the options and compromises that we face in deciding how to present observations to the data assimilation system, particularly in relation to remotely-sensed data.

The techniques of variational data analysis provide a framework for effective and consistent assimilation of meteorological observations of widely differing types, and they allow us to overcome some limitations of earlier analysis methods. In particular, observations that are related in a nonlinear manner to the variables to be analyzed can be handled without the approximations inherent in linear analysis methods. Also, through the concepts of an "observation operator" and its adjoint, we obtain a means of projecting information from the space of the analyzed variables into that of the measured variables, and back, in a consistent manner. Both of these aspects are important for many types of remotely-sensed observation where the links between the measured and analyzed variables are both complicated and nonlinear (sometimes very nonlinear).

In principle, the variational approach allows us to consider assimilation of observations close to their "raw" form, reducing the need for various forms of "pre-processing" or "retrieval" operation. In this way, the error characteristics of the observations themselves are usually simpler and more easily described. However, this approach requires more complex observation operators, which are themselves sources of error. Thus, for each observation type, we are faced with a compromise between the complexity of the pre-processing (prior to assimilation) and the complexity of the observation operator within the assimilation scheme. This problem is discussed in section 2, following a description of the general features of variational assimilation of observations. In section 3, examples are presented for a range of satellite observations, and assimilation options and associated compromises are discussed. In section 4, the potential of four-dimensional variational data assimilation (4DVAR) to exploit more fully the information in remotely-sensed observations is considered.

This paper addresses principally the assimilation of observations of the atmosphere, with emphasis on the troposphere. However, many satellite instruments intended for tropospheric monitoring are also sensitive to changes in surface (land or sea) variables. Therefore it is not usually possible to pose the assimilation problem as one involving purely atmospheric variables; surface variables must be considered simultaneously.

This paper is intended as a review. It draws mainly on work performed at ECMWF in this field during the period 1990-95; more detailed accounts are to be found in the papers referenced. More importantly, it attempts to provide a synthesis of the general ideas that have developed in relation to this work, ideas that are guiding plans for future developments in the assimilation of remotely-sensed data.

2. GENERAL CONSIDERATIONS

2.1 The variational approach

The variational approach to the assimilation of data into a numerical weather prediction (NWP) system has been described by a number of authors (e.g. Lorenc 1986; Le Dimet and Talagrand 1986). It takes the following form: we try to minimize a penalty function J(x) with respect to a control variable x (containing our description of the atmospheric state to be analyzed), where J(x) measures the degree of fit to the observations, to background (a priori) information, and possibly also to other physical and dynamical constraints. If observations and background information have unbiased, Gaussian errors, then the maximum likelihood penalty function is given by:

$$J(x) = \tfrac{1}{2}(x-x_b)^T B^{-1} (x-x_b) + \tfrac{1}{2}(y-H(x))^T (O+F)^{-1} (y-H(x)) + J_c \qquad (1)$$

where y is the vector of observations, H(x) is the vector of equivalent values corresponding to the state x, O is the expected error covariance of the observations, F is the expected error covariance of the "observation operator" H, x_b is the background state (e.g. a short-range forecast), B is its expected error covariance, and J_c (optionally) represents other constraints. ^{T} and $^{-1}$ denote matrix transpose and inverse respectively.

The optimal solution is found by minimizing the penalty function J(x) with respect to x or by solving its gradient equation:

$$\nabla_x J(x) = B^{-1}(x - x_b) + \nabla_x H(x)^T (O+F)^{-1} (y - H(x)) + \nabla_x J_c = 0 . \tag{2}$$

The evaluation of this expression involves either the computation of a Jacobian matrix, $\nabla_x H(x)$, or else the application of the adjoint operator which effectively performs the multiplication by $\nabla_x H(x)^T$ without the need to evaluate the full Jacobian matrix.

The expression for J(x) is general regardless of the dimension of x; this analysis method can be applied to a one-dimensional, vertical problem at a single horizontal location (analogous to conventional "retrieval" of a vertical profile), to a 2-dimensional problem (e.g. analysis of a surface field), in 3 dimensions (e.g. to analysis of the state of a global or regional atmospheric model), or in 4 dimensions (i.e. to 3 space dimensions, but with the observations distributed over time). This leads to descriptions of the variational technique applied to such problems as "1DVAR", "2DVAR", "3DVAR" and "4DVAR" methods respectively.

In order to apply these methods we need, for each observation type, an appropriate observation operator, H. This will involve a set of operations for "interpolating" the state x to the observation "location". For conventional observations of variables contained in x, the concepts of "interpolating" and "location" can be interpreted literally. However, for remotely-sensed observations they have to be generalized to include a projection from the space of the control variable to that of the measurement. For example, part of the observation operator for satellite radiance measurements is a radiative transfer model. Other remotely-sensed observations involve equivalent models as described below.

Eq.(1) applies to Gaussian errors. This arises because the penalty function appropriate to the maximum likelihood solution can be associated with the logarithm of a probability density function (PDF); the log of a Gaussian PDF leads to a quadratic term in J(x) (see Lorenc 1986). However if the PDF defined by the error characteristics is known to have some other, non-Gaussian form, then a corresponding form for J(x) can be derived. Such approaches are appropriate both for objective quality control (e.g. see Ingleby and Lorenc 1993, and its references) and for the direct analysis of observations for which the errors are known to be non-Gaussian.

It should be noted that an accurate observation operator, H, is crucial for the effective exploitation of the information contained in the observation. The "observation increment", $(y-H(x_b))$, is usually small in a modern NWP system, for most observations most of the time. An inaccurate observation operator may even lead to an observation increment, and hence an analysis increment, of the wrong sign. It is possible to compensate for this by appropriately large values in the expected error covariance, F. However, if they become much larger than the corresponding values in O, then we shall fail to exploit the potential information contained in y. Similarly, if either O or F is mis-specified, then we shall also misinterpret the information in the observation. It is therefore a general requirement for progress in this area that we develop an accurate observation operator for each observation type, ideally more accurate than the observation itself, and that we perform studies to characterize the errors of the observations and their operators in order to specify adequately the corresponding error covariances.

2.2 Data assimilation and model validation

Figure 1 gives a schematic representation that offers an alternative perspective on a variational data assimilation system. At the bottom we represent the continuous cycle of forecast and assimilation found (in some form) in all assimilation systems. At the top we have the "raw" observations which undergo some pre-processing, of varying degrees of complexity, before presentation to the data assimilation system itself. The NWP fields are "interpolated" (as defined above) through the observation operator to give what we may call "forecast observations". These are now in the space of the pre-processed observations, with which they can be compared. The difference between the observation and the "forecast observation" — the observation increment — can now be "mapped" back into the space of the model variables, and the process iterated if necessary. The process of "mapping" involves both interpolation and weighting, and it is the main concern of data assimilation theory.

When presented with a new type of observation, we need to learn how to assimilate it effectively. We can use the data assimilation system to help in the learning process in the following way: the new observation is passed through the system illustrated in Fig.1, up to the generation of the observation increment. During the learning period, the new observations are not allowed to affect the analysis (i.e. they are given zero weight). However, the observations increments are stored, and their spatial and statistical properties are studied. From these statistics we can learn not only about the error characteristics of the observation type and its operator, but also about the error characteristics of the

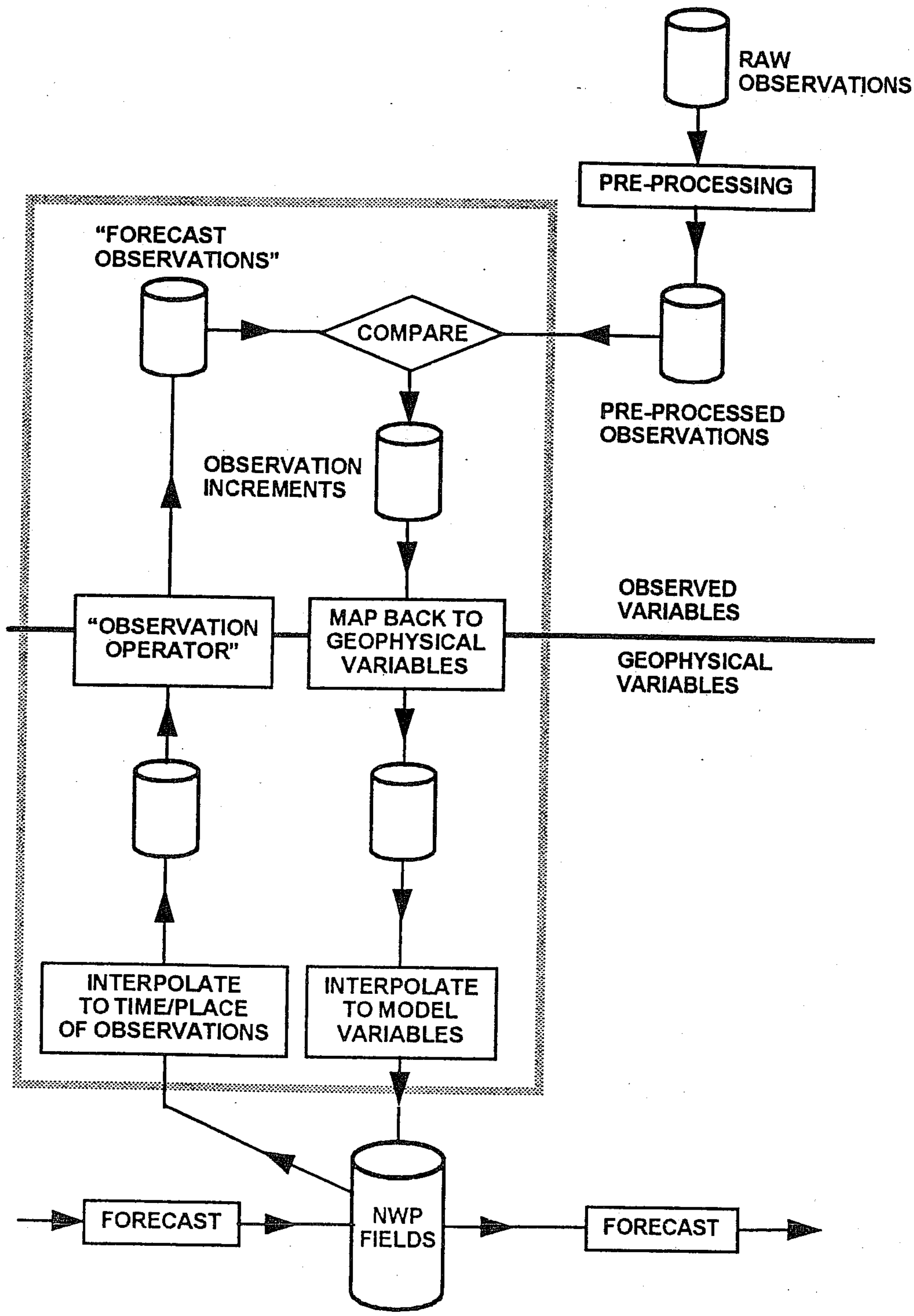

Fig.1 Illustrating schematically the variational assimilation of observations into a NWP model.

NWP fields. In this way, the process of learning how to use the new observations can provide valuable "validation" information on the NWP model itself, particularly concerning its systematic errors. Examples of such activities are cited below.

2.3 **Limitations and compromises**

For each observation type we need an observation operator, H. In calculating a value H(x), we must simulate accurately the characteristics of the observation at the point that it is presented to the assimilation system. This includes the simulation of any pre-processing that the observation has undergone. It is therefore very important that the observation operator and the pre-processing are correctly matched.

Observations create special problems if their simulation involves variables not represented in the control variable, x. This can be a particular problem for remotely-sensed data which tend to contain non-local information; although the measurements are sensitive mainly to changes in the atmospheric state in the domain to be analyzed, they may also be sensitive to changes outside this domain (e.g. to the atmosphere above the top of the NWP model, or to surface variables not represented in the model, at least not in the control variable). Also, the measurements may be sensitive to "difficult" variables such as cloud; such variables may be difficult to include in the control variable and, even if they are included, it may be impracticable to represent the spatial scales that significantly affect the measurement. Even though we may have no desire to analyze these scales, it is important to represent their effects on the measurement, if it is to be interpreted correctly.

Examples of these problems, and of the approaches we may take to address them, are given in the next section for some specific observation types.

There is a further problem, primarily of a logistic nature but nevertheless important: the development and maintenance of complex observation operators and matched pre-processing requires expertise specific to each observation type. We have yet to devise a strategy whereby all centres active in data assimilation for NWP or climate analysis can have effective access to this expertise. It will certainly not be feasible for all centres to duplicate expertise for every remotely-sensed data-type in this rapidly-growing field. New networks are required whereby "satellite centres", and other centres of observational expertise, develop and distribute appropriate observation operators, together with information on the error characteristics of the observations and their operators. In the meantime, it may be necessary to restrict the assimilation of remotely-sensed "raw" observations to those data types where most benefit is expected. This point is illustrated further in the examples considered below.

3. SOME EXAMPLES

3.1 **TOVS radiances**

The TIROS Operational Vertical Sounder (TOVS) instruments constitute the current implementation of operational satellite sounding radiometers on the NOAA satellite series — see Smith et al., 1979. Measurements from these instruments are sensitive to atmospheric temperature and humidity (and other variables — see below). Recent moves to assimilate TOVS radiances directly, rather than retrieved profiles of temperature and humidity, have resulted from difficulties experienced in obtaining consistent positive impact in NWP using the latter approach. There are many sources of practical problem with both approaches, but the fundamental problem in assimilating retrieved profiles is that their error characteristics are very complex, highly dependent on the atmospheric state, and not amenable to representation through simple covariance matrices. This problem originates from the fact that the retrieval problem is ill-posed; the retrieved profiles are "pseudo-observations"; they contain not only observed information but also components coming from the background or prior information used to constrain the retrieval (see Eyre et al. 1993). The problem of "prior-dependence" is common to many quantities retrieved from remotely-sensed data. However it is sufficiently acute for TOVS data to warrant significant investment in methods for assimilating radiance information more directly.

Such methods have now been implemented or are under development in several NWP centres. From 1992-96, ECMWF used operationally a 1DVAR scheme (Eyre et al. 1993) as the interface between TOVS cloud-cleared radiances and the "optimal interpolation" (OI) analysis scheme. The UK Meteorological Office implemented a similar 1DVAR scheme (described by Gadd et al., 1995) in April 1996. The prior-dependence problem still arises at the 1DVAR/analysis interface, but since both systems are under local control it is easier to address this problem and to limit its effects. In February 1996, ECMWF implemented a 3DVAR system for TOVS radiances and other observation types, in which the interface problem is removed (Andersson et al. 1994). However, in 3DVAR we have to address different problems in relation to TOVS; the control variable contains (at present) only the NWP model's prognostic atmospheric variables (wind, temperature and humidity). The radiances in many channels are partially sensitive either to the temperature above the model top (10 hPa) or to surface variables (see Fig.2). An interim solution to this problem is to use the 1DVAR as a "pre-processor" to supply information to the 3DVAR on these additional variables. (Within 1DVAR, it is technically simpler to extend the control variable to include all parameters required for accurate solution of the associated radiative transfer problem.) Within the same framework some experiments

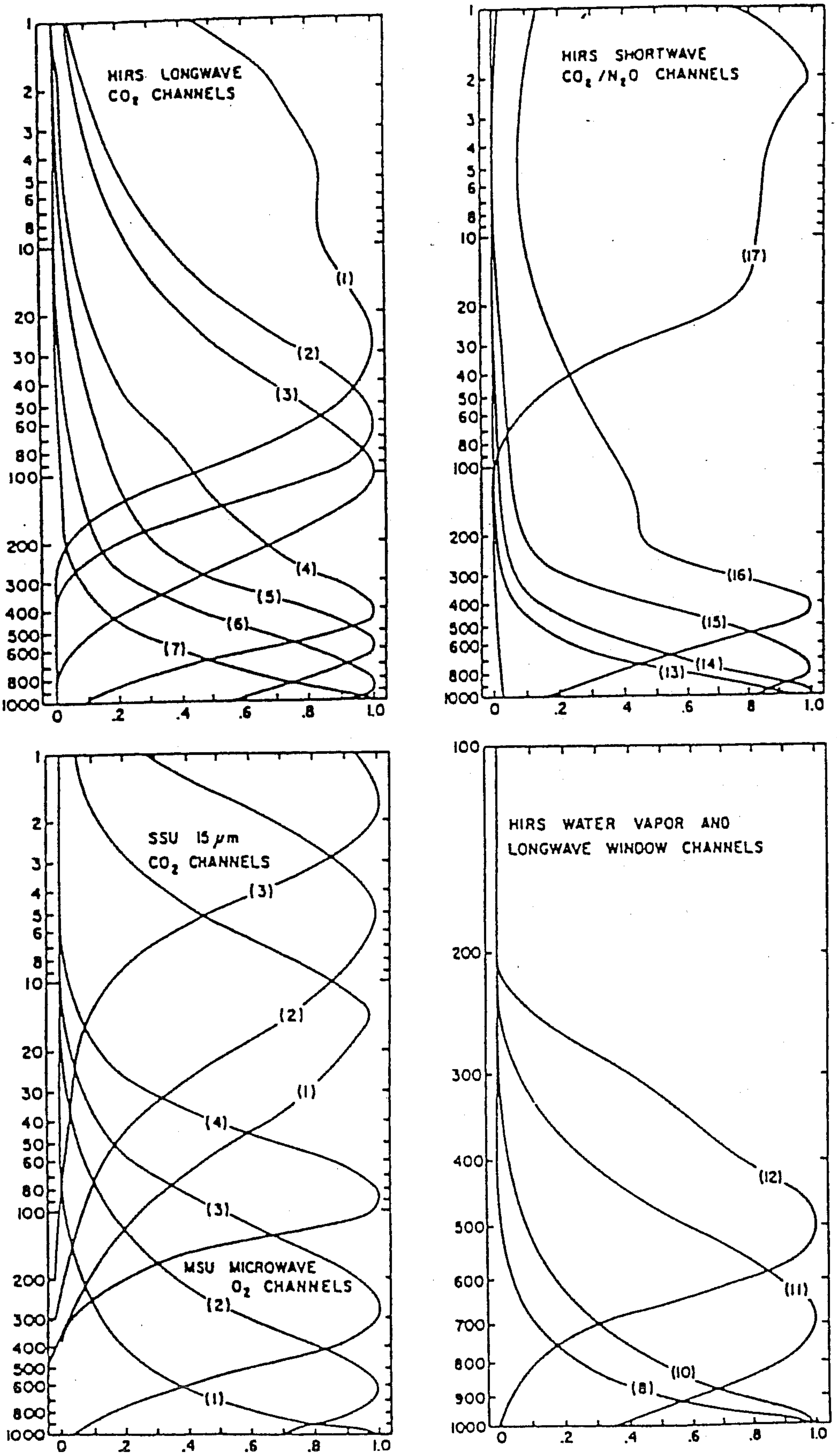

Fig.2 Weighting functions for TOVS channels (from Smith et al., 1979).

have also been conducted on the impact of TOVS radiances within a 4DVAR system (see section 4).

In the systems implemented so far at ECMWF for the assimilation of TOVS radiances, cloud-cleared data have been used. These have undergone substantial pre-processing, and it is worthwhile to ask whether there would be advantage in assimilating the "raw", potentially-cloudy radiances. Indeed such schemes have been developed and tested with 1DVAR (e.g. Eyre 1989). However there is a significant obstacle to extending this approach to 3D- and 4DVAR. The problem is that the cloud fields within the NWP model not only have significant deficiencies at the scales they represent but also do not attempt to represent the horizontal scales observed by the TOVS instruments. HIRS (the High-resolution Infrared Radiation Sounder — a component of TOVS) has a field-of-view (fov) of about 20 km and a small change in the fractional cloud cover within the fov can have a significant effect on the observed radiance. Cloud must be simulated on these scales if raw TOVS radiances are to be interpreted correctly. A possible solution to this problem is to include in the control variable a representation of cloud cover at the specific TOVS observation locations but, for the time being, the compromise adopted for TOVS is to treat clouds as a pre-processing issue and to present cloud-free or cloud-cleared radiances to the assimilation scheme.

In the development of the 1DVAR and 3DVAR systems for TOVS cloud-cleared radiances, the following problems have demanded considerable attention:

(a) The radiative transfer model used in the observation operator is subject to substantial bias errors (i.e. of the order of the true observation increment). Also, in some channels, the local biases exhibit considerable spatial variation, particularly when moving from polar to tropical air masses. These biases must be monitored and controlled if the radiance data are to be used effectively. As discussed in section 2.2, the assimilation system itself can provide statistics of observation increments (i.e. measured minus forecast radiances), allowing these bias problems to be studied and a bias correction scheme developed. Such a scheme is in routine operation at ECMWF (Eyre 1992), and similar schemes have been implemented by other centres using radiances directly.

(b) The effect of TOVS radiances on the analysis is very sensitive to the assumptions made within the assimilation/retrieval scheme concerning the vertical correlation of forecast error. This is because the TOVS weighting functions are broad (see Fig.2); they measure radiation from a layer of depth comparable to the structure functions defining the vertical correlation of forecast error. Therefore interpretations of the radiance signals are sensitive to the specification of these functions. It has been important to find a specification for the vertical correlation of temperature error that is consistent with observational studies and that provides consistent and acceptable structure functions for all model variables. Studies in this area have been performed and are reported by Rabier and McNally (1993).

The TOVS 1DVAR scheme was implemented operationally at ECMWF in June 1992 in the Northern Hemisphere extra-tropics. It provided consistent positive impact on forecast scores, with the greatest impact over North America (see Eyre et al. 1993). This is consistent with the fact that the largest analysis increments are made over the Pacific. These results confirm that, in modern global NWP systems, the impact of TOVS data is not primarily on the sub-synoptic scales (as once anticipated from the high spatial sampling density of TOVS) but on the longer waves. A plausible explanation for this is that, because of its intrinsically low vertical resolution, TOVS is "blind" to temperature features that are small-scale in the vertical, which are usually associated with features of small-scale horizontal structure. If features are sufficiently large-scale in the vertical to be observable, they tend to correspond to large-scale horizontal features.

In December 1994, the TOVS 1DVAR scheme was implemented globally within the ECMWF system. The associated experimentation provided an opportunity to study the impact of TOVS data on the humidity analyses in the tropics and sub-tropics. These impacts were found to be large. Validation studies using total-column water vapour retrieved from SSM/I (Special Sensor Microwave / Imager) data showed the impacts of TOVS to be generally positive, and particularly so in the region of the inter-tropical convergence zone, where the TOVS data tend to correct for large systematic model errors. These results are reported by McNally and Vesperini (1996). Not only do they provide a demonstration of the impact of TOVS radiances on humidity analyses, but they also illustrate the use of SSM/I data for model validation.

3.2 Satellite winds and cloud imagery

At present NWP centres assimilate "winds" (motion vectors) derived by tracking features in cloud imagery from geostationary satellites. Variational methods allow us to consider more sophisticated ways of using this information. Firstly, they permit alternative treatments of observational errors; rather than specifying observation error in terms of u and v (i.e. zonal and meridional wind components), we can specify them in terms of speed and direction, or as "rotated u and v" (i.e. along and across the direction of the wind). Also, it is possible to represent non-Gaussian error distributions through an appropriate non-quadratic penalty function. These possibilities may have advantages given the particular error characteristics of satellite winds.

Secondly, 4DVAR techniques can, in principle, extract wind information directly from sequences of images, without the need for an intermediate derived wind vector. Should we attempt to replace present satellite winds with such an approach? The answer at present, at least for global NWP systems, is clearly no: such models do not have the horizontal resolution to represent the cloud features that are tracked. Thus no appropriate forward operator can be constructed, and the pre-processing of the imagery to "winds" remains essential. Models of much higher resolution would be required before it would be possible to simulate the features that are tracked. Mesoscale models are now approaching the resolution where it might become feasible, given also a good representation of the cloud fields by the model.

There are other features of much larger scale apparent in satellite images, both for conventional window channels and for water vapour channels. 4DVAR techniques may well be able to extract wind information from sequences of such images, but full exploitation of cloud information in 4DVAR will require adjoints of the models' moist processes. In future "ozone channels" may also contain similar information on winds around the tropopause and in the lower stratosphere.

3.3 **SSM/I data**

Following the discussion above on TOVS data and on satellite imagery, it is pertinent to ask: how should we attempt to assimilate information in microwave imagery data from SSM/I — as radiances or as retrieved geophysical parameters? Theoretically, the answer is that the assimilation of radiances is likely to be closer to optimal, for the same reasons as for TOVS. However in practice there are logistical reasons for assimilating retrieved quantities if the difference in skill is negligible. It is therefore necessary to consider the information on each geophysical variable independently:

(a) Ice/snow cover. Here a static analysis of the retrieved quantities is adequate for NWP applications.

(b) Water vapour (total column). Assimilation of retrieved quantities is probably close to optimal. This is because the retrieval problem is only weakly nonlinear and not strongly prior-dependent (much less so than for this retrieval problem than for TOVS temperature profile retrieval). Preliminary experiments undertaken at ECMWF with 4DVAR to assimilate total column water vapour (TCWV) retrieved from SSM/I data are discussed in section 4.

(c) Sea-surface wind speed and cloud liquid water (total column). Here the retrieval problem is substantially more nonlinear and prior-dependent. For example, the amount of cloud liquid water retrieved is dependent on where it is assumed to be in the vertical. For this reason, ECMWF has developed a 1DVAR approach to the simultaneous retrieval of several variables to which the 7 channels of SSM/I are sensitive (see Phalippou 1996). The scheme is similar to that described by Prigent et al. (1994).

3.4 Scatterometer data

The assimilation of scatterometer data from the first European Remote Sensing satellite (ERS-1) has received considerable recent attention. Work has focused on two main problems: how to represent the observation operator, i.e. the transfer function through which the backscatter coefficients (σ^0s) are related to the wind vector near the sea-surface; and how to resolve the ambiguity between the two wind vectors, separated by roughly 180 degrees, that fit the measurements. We have identified three options for the assimilation of these data into a 3D/4DVAR system:

(a) to assimilate the σ^0s directly (as for TOVS radiances),

(b) to assimilate "ambiguous" retrieved winds, allowing other constraints within the variational analysis to resolve the ambiguities in an optimal way, or

(c) to assimilate winds for which the ambiguity has been removed through a pre-processing step.

Option (a) is theoretically attractive (Thépaut et al. 1993). However it has been found that the highly nonlinear nature of the transfer function leads to error characteristics that are very difficult to represent satisfactorily in the σ^0-space. Also the retrieval of ambiguous winds from σ^0s is rather direct (not significantly prior-dependent). ECMWF's current preference is therefore for option (b); it is theoretically very close to (a), and recent experiments suggest that in some critical cases (e.g. where phase errors are present in the forecast wind field) it can avoid ambiguity removal problems encountered with (c). These problems may be considered as a source of non-Gaussian observational error, which are not adequately treated by the quadratic penalty function of eq.(1). Work at ECMWF in this area is reported by Stoffelen (1994) and Stoffelen and Anderson (1994, 1996).

3.5 **Radio occultation data and other limb sounding data**

Measurements of the refraction of radio waves passing from one satellite to another through the limb of the Earth's atmosphere contain information on the gradients of refractivity, and hence on the gradients of temperature and humidity along the path. With the advent of the Global Position Satellite (GPS) system, such measurements for the Earth's atmosphere are now possible (see Hardy et al. 1992) and recent results from the GPS/Met experiment are very encouraging (Kursinski et al 1996). Measurements of refracted angle can be pre-processed, using certain assumptions, to retrieve vertical profiles of refractivity and further to retrieve the temperature profile (if humidity effects are negligible or known) or the humidity profile (if the temperature profile is known). An analysis of the assimilation problem (Eyre 1994) has shown that there may be advantages in assimilating measured refracted angles directly, rather than via intermediate retrieved profiles, particular when strong horizontal gradients are present. Similar arguments can be applied to other measurements which make use of a limb-sounding geometry.

4. THE POTENTIAL OF 4DVAR

Compared with assimilation studies using 3DVAR, observing system experiments using 4DVAR have, to date, been rather simplified in a number of respects, including their spatial resolution and limited model physics. However these experiments have already suggested that 4DVAR has the potential to extract information from observations in new ways.

Assimilation of TOVS radiances over a 24-hour period gave rise to significant (and unexpected) impact on the tropical wind field. Investigation revealed that most of the impact came from the TOVS water vapour channels. Although the precise interpretation of the results is difficult, the effects noted are consistent with the assimilation system extracting dynamical information from the time-changes in the radiance fields for channels in water vapour absorption bands (Andersson et al. 1994). Similar impacts on the wind field were found when total column water vapour derived from SSM/I data were assimilated (Filiberti 1993). Thus 4DVAR offers hope that we might be able to use humidity-sensitive measurements to improve wind analyses, and also that we might achieve humidity analyses dynamically consistent with their associated mass and wind analyses.

The other promising development with 4DVAR has been in the assimilation of scatterometer data (Thépaut et al. 1993). Typically, in 3D assimilation experiments, the impact of scatterometer data on the analysis of low-level wind is clearly positive but the impact is not retained for long into the forecast. The main weakness appears to be in the inability of the 3D assimilation to project information from the boundary layer to higher levels in a dynamically consistent manner, which the NWP can then retain. Preliminary experiments with 4DVAR have shown the ability of surface wind data to affect the analysis up to the jet stream level through the flow-dependent structure functions implicit in the 4D system. This is a hopeful sign, particularly for more effective exploitation of scatterometer data, but also for other surface observations and single-level data.

5. CONCLUSIONS

Remotely-sensed observations, particularly from satellites, constitute a rapidly expanding source of new information with potential for application in NWP. The effective use of these observations is hampered by the complicated relationships that exist between the observed quantities and the variables of the NWP models. Variational data assimilation offers a framework within which these problems can be addressed in a coherent manner. However, careful attention is required to the most appropriate interface between the remotely-sensed data and the assimilation systems; the degree to which the observations are pre-processed prior to assimilation must be considered, and the "observation operator" within the assimilation system must be carefully matched to the pre-processing. The error characteristics of both the observations and their associated operators also need far more attention than they have received so far. The successful implementation of the strategies outlined in this paper will require a close collaboration between the "satellite centres", who provide the data and often carry the greatest expertise on their interpretation, and the "data assimilation centres". Such collaboration is required in order to specify the best NWP interface and hence the appropriate pre-processing of the observations, to share the expertise required to build accurate observation operators, and to specify adequately the associated error characteristics.

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