1 INTRODUCTION
SSM/I is a seven channel radiometer which operates at 19.35, 22.235, 37., 85.5 GHz in vertical (V) and horizontal (H) polarizations except at 22.235 GHz where only the V polarization is available. After the launch of the first SSM/I on board F-8 DMSP satellite, SSM/I total precipitable water vapour (TPW), wind speed (WS) and cloud liquid water path (CLW) were retrieved separately with regression algorithms. Several problems were found in the products derived from the algorithms reported in Hollinger (1991), and many 'improved' regression algorithms have flourished afterwards. However, there is one critical point common to any of these regression methods: their performances are limited by a simplified handling of non-linearities and/or by the poor quality of the a priori information. This problem is particularly critical when clouds are present in the field of view (FOV) as the retrieval problem becomes highly nonlinear.

Variational methods offer an alternative approach for the estimation of the geophysical parameters from SSM/I observations (Phalippou 1995). The geophysical parameters are estimated simultaneously following the theory of optimal estimation, and are therefore the best set of parameters that explain the observed radiances, while being consistent with the available a priori information. In addition, an estimation of the errors of the 'retrieved' products can be computed and the quality control is easier. This paper presents the theory, the implementation and the results of a 1-dimensional variational method (1DVAR) for the estimation of the humidity profile, the wind speed and the cloud liquid water path over oceans, using SSM/I observations and ECMWF forecast fields with their error covariances.

2 THEORY
The principles of nonlinear optimal estimation in the context of satellite data assimilation has been discussed by Eyre (1989). Let us define $x$ as the state vector (hereafter called control variable) formed by the atmospheric and surface variables. We seek the best estimate of $x$ knowing the a priori or background vector $x^b$ given by the ECMWF first guess (FG) (see section 3) and the coincident SSM/I observation vector $y^o$. We denote by $y(x)$ the operator mapping the control variable $x$ into the observation (radiance) space $y$, i.e. $y(x)$ is the radiative transfer model which calculates the radiances.
corresponding to the control variable \( x \). When the errors in the observations and the errors in the a priori information have Gaussian distributions and are uncorrelated, then the likelihood function (also called cost function) is given by:

\[
J(x) = \frac{1}{2} (y(x) - y^*)^T (O + F)^{-1} (y(x) - y^*) + \frac{1}{2} (x - x^b)^T B^{-1} (x - x^b)
\]  

(1)

where \( O \) is the expected error covariance of the observations, \( F \) is the expected error covariance of the radiative transfer model (forward operator) and \( B \) is the expected error covariance of the background \( x^b \). By definition, the best estimate of \( x \) corresponds to the maximum of the probability density function and is found by minimizing the cost function. The two terms in (1) represent the observation and the background costs and are often noted \( J_o \) and \( J_b \) in the literature. In this study \( x \) is a 22-element vector which contains the Naperian logarithm of the specific humidity profile on 20 levels, the wind speed and the cloud liquid water path.

The Newton method has been used to find the minimum of the cost function. The only lower bounds specified were on the wind speed and on the cloud liquid water path, where the bounds were set to zero. The use of the logarithm of the specific humidity alleviates the lower bound problem, but the humidity supersaturation still needs to be controlled. This has been achieved by adding an ad hoc constraint term \( J_{sat}(x) \) to the cost function.

The complete cost function \( J(x) \) to minimize is then written as:

\[
J(x) = J_o(x) + J_b(x) + J_{sat}(x)
\]  

(2)

During the minimization the \( n \)th estimate of \( x \) is calculated as follows:

\[
x_{n+1} = x_n - [H(J(x_n))]^{-1} \nabla J(x_n)
\]  

(3)

where \( H \) is the Hessian operator and \( \nabla \) is the gradient operator with respect to \( x \).

It can be shown that the a posteriori error covariance matrix \( S(x_n) \) of the estimation \( x_n \) is equal to the inverse of the Hessian.

3 BACKGROUND FIELDS

For each SSM/I observation location, the background vector \( x^b \) has been computed by interpolating in time and space the three 6 hour ECMWF forecasts -called First Guess (FG)- which spanned the SSM/I observation time. The new prognostic cloud scheme (experimental at the time of this study, and now operational) was included in the ECMWF model.

3.1 Humidity profile

A simple and objective way to select which parameters should be included in the control variable \( x \), is to analyze the information content of the radiances with respect to those parameters. This can be
achieved, for instance, by comparing the diagonal elements of the error covariance matrix of the background, i.e. $B$, with the diagonal elements of the \textit{a posteriori} expected error covariance $S$. Using this method, we have found that SSM/I radiances improved mainly the error in the humidity profile retrieval between the surface and 300 hPa, which corresponds to ECMWF level 13.

3.2 Clouds

The vertical location of each cloudy layer (i.e. the top and base of each cloudy layer) and the phase of the water in the cloud (liquid/ice ratio) are the most important \textit{a priori} cloud parameters for retrieving the cloud liquid water path. The primary benefit of having a cloud background field derived from NWP is that the vertical location and the extent of the cloud are given in a manner consistent with the physics and the dynamics of the atmosphere. For instance, this will ensure that clouds are located at the maximum of the relative humidity profile.

In order to perform the radiative transfer simulation the liquid/ice profile of the cloud is required. Because of the lack of 'ground truth' it is quite difficult to validate the errors of ECMWF forecast cloud fields, and the error covariance matrices have not yet been estimated. Since the structure functions of the vertical cloud profile are not known, the structure of the cloud background was retained, and only the cloud liquid water path has been used as the cloud control variable. The standard deviation of the cloud liquid water path background has been set to 0.2 Kg$m^{-2}$ which represent a weak constraint.

3.3 Surface conditions

The ocean surface contribution to SSM/I radiances depends on the sea surface temperature (SST) and on the sea surface roughness which can be related to the surface wind speed. The ECMWF SST has been used as a parameter in the radiative transfer model, but was not included in the control variable. It is well known that the wind speed can be retrieved from SSM/I measurements (see for instance Goodberlet \textit{et al.} 1992). The wind speed has been included in the control variable. An error in background wind speed of 2 m$^{-1}$ has been assumed following the results of (Stoffelen and Anderson 1994).

4 RADIATIVE TRANSFER AND CALIBRATION

The radiative transfer model (forward operator) maps the control variable $x$ into the radiance space and thus it is the heart of a variational retrieval system. The radiative transfer model has to represent as accurately as possible the \textit{a priori} knowledge of the radiative properties of the atmosphere and of the
4.1 Atmospheric contribution

The atmosphere is described along the vertical by the pressure, temperature, specific humidity and cloud liquid water density on the 31 ECMWF model levels, i.e. between the surface and the top of the atmosphere which is about 10 hPa. Oxygen and water vapour are the two main atmospheric gases absorbing in the microwave spectrum. The absorption from O₂ and H₂O has been computed following (Liebe 1989).

For the clouds, liquid water absorption alone has been considered in this study, because of the uncertainties and complexity of radiative transfer modelling in scattering atmospheres. The FOVs affected by volume scattering due to rain or appreciable amount of ice-cloud have been detected at the pre-processing stage and after minimization (see section 5.3). The cloud absorption is calculated using the Rayleigh approximation which is valid for the liquid droplet spectrum of most non-precipitating clouds at SSM/I frequencies. The liquid water is assumed to be at the air temperature.

4.2 Sea surface contribution

The sea model used in this study is split in two parts: the foam-free sea model and the foam model itself.

(a) Foam-free Sea Model

The foam-free sea model is based on the geometrical optics (GO) approximation of scattering by a rough surface. The basic idea of the GO model is to represent the sea surface as a collection of flat facets, each one acting as a specular surface element. Each facet is described by its slope components along and across the wind direction. The Cox and Munk (1954) bidimensional slope distribution has been used in this study.

(b) Sea Foam Model

Although the sea foam is an inhomogeneous medium, we have made the usual assumption that the foam contribution to the sea surface apparent radiance can be described by the fractional foam cover C₇ and by the foam emissivity. The fractional foam cover has been computed as an exponential function of the wind speed following Monahan and O’Muircheartaigh (1980).

(c) Sea surface model tuning
When the Stogryn (1972) foam emissivity model was used in the retrieval method presented in section 2, several problems were found for moderate and high wind speeds (above 10 m s\(^{-1}\)). The analysis of the results indicated a problem with the sea surface model. The sea foam modelling was first suspected, as its role is crucial at high wind speeds. A simple test was then done by setting the sea foam emissivity to unity regardless of frequency and polarization. The results immediately improved for all the aspects. It must be pointed out that although this empirical tuning against the radiances and the background is done through a correction on the sea foam emissivity alone, it represents an overall simple tuning of the complete sea modelling (roughness+foam).

4.3 Observation errors and forward operator errors

The F+O matrix has been assumed diagonal and the square root of its diagonal terms have been set to 2 K for the 19, 22 and 37 GHz channels and 3 K for the 85 GHz channels. Although these values are subjectively specified, we have verified that the \textit{a posteriori} variances are consistent with previous estimates of the accuracy of the retrieved parameters, as reported in the literature (see section 5).

Since the ECMWF fields are assumed to be globally unbiased, the mean differences over a large number of cases between observed and simulated radiances are expected to be zero at the end of the minimization for each channel. If this is not the case, then a bias exists in the radiances or in the forward model or in both. Ideally a bias correction scheme must process a large number of data to be statistically representative and the quality control must be efficient to ensure that the radiative process which are not represented by the forward model are screened out (scattering by cloud or rain for instance in this case). These conditions were not met in this study and a very simple iterative estimation of the biases has been done by processing several SSM/I scenes and using the estimated biases from the previous scene as an input for the current scene. Using this method, the estimated brightness temperature biases are equal to -2.35 K at 19 GHz, 0.25 at 22 GHz and 1.8 K at 85 GHz in V and H polarizations. No correction is necessary at 37 Ghz. These biases were added to the measurements before attempting the retrieval presented in the following section.

5 RESULTS AND DISCUSSION

The results presented in this section are for an ascending SSM/I (F-11 satellite) pass between 60° South and 60° North for the 4 January 1994. The ascending local crossing time is 17:04. The land areas represented in white in Fig. 1-3 are Africa, the coasts of Spain, Ireland and Iceland. This scene includes a large variation in the meteorological parameters of interest for this study. Figures 1.a, 2.a,
and 3.a show that the background (i.e. ECMWF fields) total precipitable water vapour varies between 5 and 60 Kg m⁻², the wind speed between 0 and 20 m s⁻¹ and the cloud liquid water path between 0 and more than 0.4 Kg m⁻². The highest wind speed and cloud liquid water path are associated with a frontal system in the Atlantic. The retrieved humidity fields, the wind field and cloud liquid water path are presented and analyzed in the sub sections 5.1 to 5.3.

5.1 Humidity fields
Although the 3 dimensional humidity fields are retrieved, the results are presented as total precipitable water vapour for convenience. Figures 1.a and 1.b show the background TPW and the TPW retrieved with the present method. The TPW retrieved with the method of Alishouse et al. (1990), hereafter referred as Alishouse TPW, is used as an independent ‘ground truth’ as the number of oceanic radiosoundings are too sparse to provide useful comparison for a single scene. The Alishouse algorithm is based on the regression between TPW derived from radiosonde observation and SSM/I measurements. The accuracy of Alishouse TPW is of the order of 2 to 4 Kg m⁻² depending on weather conditions. Alishouse TPW is shown in Fig. 1.c, where the black areas corresponds to precipitation detection. As this screening might also reject non-precipitating heavy cloud in which we are interested, a 1DVAR retrieval is however attempted when rain is detected by the Alishouse test.

The comparison of Fig. 1.b and 1.c show that the spatial horizontal structure of 1DVAR-TPW agrees remarkably well with Alishouse TPW field. The background TPW is very close to the 1DVAR-TPW in the Northern Hemisphere. More differences between 1DVAR-TPW and the background appear in the Southern Hemisphere even at large scale. It is noticeable for instance that the humidity of the background is too large in the 10° to 30° South latitude band as confirmed by the 1DVAR and Alishouse retrieval.

The standard deviation of the difference between 1DVAR-TPW and Alishouse TPW is 1.4 Kg m⁻². Overestimation and underestimation of Alishouse TPW at respectively low and high water vapour content have been observed in the scatter plot (not shown). Such local biases have already been reported in Alishouse et al. (1990). They are due to the intrinsic nonlinearity of the retrieval problem which is difficult to handle when a regression type method is used.

The theoretical 1DVAR accuracy varies between 1 to 2 Kg m⁻² confirming once again the quality of SSM/I for oceanic humidity measurements.

5.2 Wind speed fields
Because of the lack of independent coincident wind speed measurements over ocean, the wind speed
derived from SSM/I using Goodberlet et al. (1992) algorithm is used for qualitative comparison purposes only. The background, the 1DVAR and the Goodberlet wind speed fields are shown in Fig. 2.a, 2.b and 2.c. The Goodberlet wind speed is not plotted (black areas in Fig. 2.c) when its accuracy is less than 2 ms\(^{-1}\) according to the accuracy flag system used by Goodberlet et al. (1992). This screening eliminates most of the frontal areas in the Atlantic where the higher wind speeds occurred. The comparison between the three wind fields show a good overall agreement. The fact that the 1DVAR retrieved wind field is smoother than the Goodberlet wind field is due to the background constraint. It is in particular noticeable that the 1DVAR wind speed differs only slightly from the background. One might expect such a result because of the strong (but objective) constraint imposed by the background term. As no particular unreasonable feature appears in the 1DVAR retrieved wind field, it could be assumed that the sea model is satisfactory for inverting SSM/I radiances. However, it is particularly difficult to demonstrate that the accuracy of the retrieved wind field is better than the accuracy of the background, i.e., that there is an improvement on the wind speed \emph{a priori} knowledge. This would need a comparison with collocated independent and accurate wind speed measurements.

This validation work is beyond the scope of this study, and we have simply calculated the theoretical 1DVAR wind speed accuracy (see section 2). This accuracy depends mainly on wind speed and to a smaller extent on the other parameters as suggested by the nonlinearity of the radiance sensitivities with respect to wind speed. The typical value of the 1DVAR retrieved wind speed accuracy is around 1.5 ms\(^{-1}\) for wind speeds lower than 12 ms\(^{-1}\).

Finally, we must emphasize the advantage of having a good quality wind speed background for the inversion in particular for the retrieval of wind and cloud liquid water path. For certain conditions the wind speed and the cloud have similar effects on the radiances (depolarization effect, increasing of radiances in H polarization). In these conditions the inversion problem is particularly ill-conditioned if no \emph{a priori} information is available, and a cloud signature can easily be interpreted as a wind speed effect and vice-versa. This problem affects most of the SSM/I regression algorithms which are used for retrieving separately wind speed and cloud liquid water path. This effect is visible for instance in Fig. 2.c where the speckle is believed to be due to cloud contamination. In the present method, when a cloud-wind ambiguity arises, the minimization will prefer to modify the cloud water path as the constraint on that parameter is weak compared to the wind speed constraint. This will give a chance to the algorithm to move away from the initial ambiguous solution. However, the drawback is that in case of gross error in the background wind speed, due for instance to the mis-location of a frontal system, the wind constraint can be too strong and not appropriate.
5.3 Cloud liquid water path

The background and the 1DVAR-retrieved CLW are shown in Fig. 3.a and 3.b. Because of the complete lack of ground truth for the cloud liquid water path and the large uncertainties existing in the available regression algorithms, the 85 GHz H polarized brightness temperature is used as cloud imagery. This SSM/I channel is sensitive enough to the cloud for identifying the moderate to heavy cloud patterns as shown in Fig. 3.c.

The position of the clouds and the cloud liquid water path of the ECMWF background agree reasonably well with the 1DVAR-retrieved cloud fields for the frontal system in the North Atlantic. More discrepancies can be observed in the Southern Hemisphere, in particular in the tropical and subtropical areas. The large differences between the background and the retrieved CLW occurring between 20° and 30° South are associated with a background TPW overestimation. The visual comparison between Fig. 3.b and 3.c show that the retrieved CLW is correlated with the 85 GHz H polarized brightness temperature, as one might expect as this channel is used in the retrieval process. Note that the problem of negative value of the retrieved cloud liquid path which appear in regression-based retrievals, is avoided here thanks to the positivity constraint used during the minimization (see section 2).

The retrieved CLW varies between 0 and 0.4 Kgm⁻². This last value is believed to be around the maximum CLW which can be retrieved with the present method. Indeed, above that value ice particles or/and rain are likely to occur in large amount producing a significant scattering of the radiation. The field of view affected by scattering have been detected at the pre-processing stage following (Ferraro et al., 1994) and at the 1DVAR post-processing stage by using a threshold on the value of the admissible observation cost function (see (2)). These two methods of rain detection give similar patterns, showing that the quality control of the 1DVAR retrieval can be done as a post-processing based on the value of the cost function for instance.

The CLW theoretical accuracy derived from (7) is typically equal to 0.02 Kgm⁻² for low to moderate cloud liquid water path, i.e. between 0.01 and 0.4 Kgm⁻². However, for high wind speed, i.e. above 15 ms⁻¹ the error increases dramatically and can reach 0.1 Kgm⁻² for a 20 ms⁻¹ wind speed.

6 SUMMARY AND CONCLUSION

A variational method has been described in this paper for the simultaneous retrieval of the atmospheric humidity profile, wind speed and cloud liquid water path from SSM/I observations. The method is based on the minimization of an objective cost function. The a priori information comes from the ECMWF first guess fields, the forward operator i.e. the radiative transfer model, their associated
covariance error matrices and the observation errors. The main purpose of this study was to
demonstrate the feasibility of the method with the present knowledge of the radiative transfer
modelling and to show its potential for NWP. The first results are very encouraging. However, several
problems have been identified which should receive further attention for using the full benefits of this
method for NWP, such as the tuning of the radiative transfer model, a better estimation of the biases,
an assessment of the off-diagonal elements. In order to do so, it is believed that SSM/I data have
to be inverted for a large number of orbits in order to have statistically robust results. For that reason,
we are currently developing a fast radiative transfer model and its adjoint to avoid excessive
computation time.

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Figure 1: Total precipitable water vapour, from left to right, a/ background, b/ IDVAR. c/ Alishouse algorithm.
Figure 2: Marine wind speed at 10 m. From left to right, a/ background, b/ lDVAR, c/ Goodberlet algorithm.
Figure 3: Cloud liquid water content, from left to right, a/ background, b/ IDVAR. c/ 85 GHz SSM/I

brightness temperature
TECHNICAL PROCEEDINGS OF

THE EIGHTH INTERNATIONAL TOVS STUDY CONFERENCE

Queenstown, New Zealand

5-11 April 1995

Edited by

J R Eyre

Meteorological Office, Bracknell, U.K.

Published by

European Centre for Medium-range Weather Forecasts
Shinfield Park, Reading, RG2 9AX, U.K.

July 1995