RETRIEVAL OF WATER VAPOR FROM JASI MEASUREMENTS:

METHODOLOGY AND CASE STUDY APPLICATION

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1. INTRODUCTION

The Infrared Advanced Sounding Interferometer (IASI) satellite instrument will be the first operational weather interferometer to be launched in 2005 as the primary scientific instrument on board the METOP-1 polar orbiting satellite. This Michelson type fourier transform spectrometer samples the infrared contiguously from 645-2760 cm\(^{-1}\) with an unapodized spectral resolution of 0.25 cm\(^{-1}\). One of the instrument's primary objectives will be to improve upon the vertical resolution and accuracy of temperature and water vapor estimates from the current suite of operational sounders. The instrument is also designed for detection of additional trace gases and improved cloud characterization.

In this study, measurements from IASI are simulated to estimate profiles of both temperature and humidity. The forward model used to simulate the measurements and Jacobians is described in Section 2.1. Due to the abundance of channels spanning most of the thermal infrared spectrum, a more efficient algorithm is proposed which utilizes only about 1% (~85) of the original 8461 channels, retaining those channels whose sensitivity to temperature and humidity perturbations is a maximum as will be discussed in Section 2.2 below. We employ an optimal estimation cyclic retrieval algorithm which solves first for temperature, then water vapor. Section 2.3 summarizes the optimal estimation retrieval algorithm and describes the input covariance matrices used to retrieve the temperature and humidity state given the simulated measurements. The retrieval algorithm is applied to both a standard climatological profile and then to a longitude-height slice at 79° W on 15 September 1999 (i.e., through the core region of Hurricane Floyd in the Western North Atlantic Ocean). Section 3 presents some of the results of this case study application. A summary of the
work presented herein as well as suggested modifications for future work on the IASI retrieval problem are given in Section 4.

2. IASI DATA SIMULATION AND RETRIEVAL METHODOLOGY

2.1 Forward Modeling

For the successful retrieval of temperature or humidity within the framework of an optimal estimation approach as adopted here, the underlying physics of the measurement need to be properly modeled by a forward model solving the radiative transfer equation. At the same time, proper modeling of the derivative of the forward model with respect to the state (also termed "weighting matrix" or "Jacobian") is quite important, especially with regard to computational efficiency, since non-linearities in the problem of interest demand an iterative state estimation. The general forward model equation mapping the state (atmospheric profile) into measurement space (satellite-measured radiance or brightness temperature spectrum) takes the form (Rodgers 2000)

\[ y = F(x) + \varepsilon, \]  (1)

where \( y \) is the measurement vector, \( F(x) \) is the forward model operator for a given state \( x \), and \( \varepsilon \) is the measurement error. The measurement error characteristics should be known in terms of systematic biases and random instrument noise. The measurements \( y \) should in fact be corrected for biases before using them in the retrieval so that \( \varepsilon \) can be statistically well characterized by a measurement error covariance matrix. Inserting reasonable temperature and humidity test profiles for \( x \), Eq. (1) was used to confirm that the presence retrieval problem is moderately non-linear only so that we can apply Eq. (1) in linearized form, i.e., replace \( y = F(x) \) by \( y - y_0 = K_0(x - x_0) \), where \( K_0 = \frac{\partial F(x)}{\partial x} \) is the Jacobian (evaluated at state \( x_0 \)) and \( x_0 \) is a suitable reference state (Rodgers 2000).

For computing \( F(x) = T_B \) (\( T_B \) = brightness temperature) and \( K_0 \), the fast radiative transfer model RTIASI (Matricardi and Saunders 1999) was used, which uses temperature, humidity, and ozone profiles as input and then furnishes simulated IASI brightness temperature measurements and temperature and humidity Jacobians for any desired subset of IASI channels. The model calculates level-to-space transmittances on 43 pressure levels spanning from 0.1 hPa (~65 km height) to the surface. We use these same levels, the so-called "ATOV5 pressure level grid", also as our retrieval grid (all 43 levels for temperature, the lowest 28 levels for humidity).
2.2 Channel Reduction Procedure

For each individual IFOV pixel, full IASI spectra will contain 8461 channels from 645 - 2760 cm\(^{-1}\) with 0.25 cm\(^{-1}\) spectral resolution, which is an enormous amount of information. For the retrieval of temperature and humidity, it is not practical nor an advantage to use all these pieces of information, which are highly redundant for this purpose as instructively shown by Rodgers (1996). Thus a sensible strategy is required in order to eliminate those channels from the data processing, which will degrade rather than improve retrieved profiles since they will not add any appreciable new information while adversely affecting the conditioning of the inverse problem.

As a first filter only based on the general quality of the measurements, the IASI noise model described by Barnett and Susskind (1999) is used to eliminate those channels whose brightness temperature noise estimate exceeds 1 K (corresponding to the error which should not be exceeded in retrieved temperature profiles). This leads to all channels > 2420 cm\(^{-1}\) (wavelengths shorter than \(\sim 4.1 \, \mu m\)) being dropped, reducing the number of channels from 8461 to about 7100. More recent (unpublished) noise estimates place those channels with wavenumbers greater than 2600 cm\(^{-1}\) above the 1 K threshold (P. Schluessel, EUMETSAT, private communicate, 2000).

Including channels in which emissions from trace gas species other than the ones best aiding temperature and humidity retrieval (i.e., CO\(_2\), H\(_2\)O) significantly contribute to increasing the retrieval error. Thus, with the luxury of *kilo* channel availability, we remove those bands of channels which contain significant contributions from such "foreign" trace gases, i.e., O\(_3\) (700-720 cm\(^{-1}\), 1000-1080 cm\(^{-1}\)), N\(_2\)O and CH\(_4\) (1267-1312 cm\(^{-1}\)), and N\(_2\)O, CO, and O\(_3\) (2092-2355 cm\(^{-1}\)).

After the removal of these bands we apply a channel selection criterion which maximizes the sensitivity-to-error ratio (termed the "H sensitivity ratio") by exploiting information about the sensitivity of the individual channel (as a function of wavenumber and pressure level) and the associated instrument noise characteristics (a function of wavenumber), i.e. we employ the matrix measure,

\[
H = S_e^{-1/2} K_0
\]  

where \(S_e\) is the measurement error covariance matrix. Thus, given an atmospheric profile, the temperature and humidity Jacobians (dimension *number of channels* × *number of levels*) are obtained and those channels with large noise or contaminated by "foreign" gases are removed. Next, starting from the top pressure level downwards, the top two (three) channels with maximum H values for temperature (humidity) at a specific level are selected and subsequently removed from further searches at lower pressure levels. We are left with a total of 86 channels (43 levels × 2 channels/level) in temperature and 84 channels (28 levels × 3
channels/level) for water vapor. Figure 1 displays the channels selected using the above procedure. For temperature (panel a), more channels are selected that flank the CO₂ absorption band near 15 μm. It can easily be seen that for water vapor (panel b), most channels in the broad 1500 cm⁻¹ water vapor absorption band are selected for the retrieval in addition to channels near 14 μm. Alternatively one could apply this technique from the surface upwards, but it was found only to slightly improve temperature and humidity retrievals below 750 hPa while worsening retrievals above 750 hPa. The allowance for more channels per level did not improve retrieval performance and actually increased the number of iterations required to reach our convergence criteria (discussed below). Other (less efficient) channel selection methods were explored (e.g., Rodgers 1996) but showed no distinct advantage in using them for the present retrieval application (see Rabier 2000 in these proceedings for a better description of channel selection methods).

Figure 1: Channel selection via "H-sensitivity ratio." a) Selected temperature channels (86 total) and b) Selected water vapor channels (84 total) indicated by dark diamonds overlaid on the RIASI generated Tₜ spectrum for a standard tropical profile.
2.3 Optimal Estimation Retrieval Algorithm

We approach the inverse problem associated with Eq. (1), the retrieval of temperature and humidity profiles \( x \) from brightness temperature measurements \( y \), by the concept of Bayesian optimal estimation described in detail by Rodgers (2000). Since the problem of interest is moderately nonlinear, we chose an iterative optimal estimation of the form

\[
x_{i+1} = x_a + S_i K_i^T S_e^{-1} \left[ (y - y_i) + K_i (x_i - x_a) \right]
\]

where subscript \( i \) is the iteration index, \( x_a \) is an a priori profile (for temperature or humidity), and \( S_i \) is the retrieval error covariance matrix defined by

\[
S_i = [S_e^{-1} + K_i^T S_e^{-1} K_i]^{-1}.
\]

In Eq. (4), \( S_e \) is the a priori error covariance matrix, and the other quantities are as defined earlier. The optimization scheme expressed by Eq. (3) is usually termed the Gauss-Newton method and provides a reliable maximum a posteriori estimate for "small residual" inverse problems as the one dealt with here (Rodgers 2000). In applying Eq. (3), the iteration was initialized with \( x_0 = x_a \) and state estimate, \( x_i \), measurement estimate, \( y_i = F(x_i) \), weighting matrix, \( K_i = \partial F(x)/\partial x \mid_{x=x_i} \), and the retrieval covariance estimate, \( S_i \), were updated at each iteration step \( i \) until convergence was reached. Convergence was determined based on the scalar "cost function" measure

\[
\chi^2 = [y - F(x_i)]^T S_e^{-1} [y - F(x_i)] + (x_i - x_a)^T S_e^{-1} (x_i - x_a).
\]

If \( \chi^2 \) is less than the number of degrees of freedom (approx. the number of channels, \( N_{\text{chan}} \)), then convergence is obtained when the iteration step \( (\chi^2_{i+1} - \chi^2_i) < 0.1 N_{\text{chan}} \) is met and the profile with the minimum \( \chi^2 \) value (either \( x_i \) or \( x_{i+1} \)) is retained. In the event a maximum of 12 iterations is reached without convergence as defined, the profile \( x_i \) with the minimum \( \chi^2 \) value is retained and properly flagged. Convergence is usually obtained with 2 to 3 iterations for temperature and 3 to 4 iterations for humidity retrievals. The computationally demanding part in the estimation scheme is the calculation of the forward model Jacobian \((K_i)\), which must be performed at each iteration step (by the RTIASI model).

Dependent on the quality of the a priori profile, the first or the first two steps may need special aid with convergence due to linearization errors, which is often dealt with in extending the Gauss-Newton scheme to the Levenberg-Marquardt scheme (e.g., Rodgers 2000; Rieder and Kirchengast 1999). We utilized the more simple but for the present purpose equivalently effective extension introduced by Liu et al. (2000), termed the "D-rad" method. Leaving Eq. (3) unchanged, just \( S_e \) is modified in its diagonal according to

\[
S_e(m_m) = \max \left[ \frac{(y(m) - y_i(m))^2}{\alpha}, \sigma_\alpha(m)^2 \right]
\]
where \( i \) is the iteration index, \( y(m) \) is the measurement value of channel \( m \), \( y_i(m) = F_m(x_i) \) is the forward-modeled measurement, \( \alpha \) is a (free) control parameter set to 10 for this study, and \( \sigma(m)^2 \) is the variance of measurement noise for channel \( m \) (the original \( S(m,m) \) values). Liu et al. (2000) found the "D-rad" extended Gauss-Newton algorithm to perform equally well or better than the Levenberg-Marquardt algorithm in aiding convergence when a poor initial guess profile was given.

The a priori error covariance matrix \( S_a \) reflects the uncertainty in our knowledge of how close the a priori profile \( x_a \) is to the "true" profile \( x \) we desire to estimate. In order to reflect the typical smooth character of a priori profiles, we use an auto-regressive model variant and adopt \( S_a \) to be non-diagonal such that there exists inter-level correlation and the non-diagonal components fall off exponentially from the diagonal; i.e.,

\[
S_a(i,j) = \sigma_i \sigma_j \exp\left(-\frac{|z_i - z_j|}{L}\right)
\]  

(7)

where \( \sigma_i \) and \( \sigma_j \) are the standard deviations at height (log-pressure) levels \( z_i \) and \( z_j \), respectively, and \( L \) is the correlation length. For temperature, \( L = 3 \) km was set and the standard deviations were assumed to grow linearly in \( z \) (log-pressure) from 2 K at the surface to 15 K at 70 km (~14 K at the top level 0.1 hPa). For humidity, \( L = 1 \) km and the standard deviations were assumed to increase linearly from 0.25 at the surface to 0.4 at 700 hPa (in \( \ln(q) \) units, corresponding to fractional uncertainty, used for specifying humidity profiles in the retrieval scheme). Above 700 hPa a constant value of 0.4 was maintained. These specifications of \( S_a \) roughly reflect uncertainties with which good climatological profiles reflect actual states in the atmosphere.

The measurement error figures were adopted from the IASI mission performance sensitivity study described in Barnett and Susskind (1999). The "reasonable" estimate case was chosen and the corresponding variances assembled into the diagonal of \( S_a \). Off-diagonal elements in \( S_a \) were set to zero, i.e., no cross-correlation between channels was assumed. Typical RMS error values range from 0.1 to 0.5 K in brightness temperature, with a relatively sharp increase at wavenumbers above 2200 cm\(^{-1}\). As noted earlier (section 2.3.1) we thus limited the wavenumber range utilized to < 2420 cm\(^{-1}\), above which expected noise exceeds 1 K for a background scene emitting at 280 K.

3. RESULTS

Before discussing results of applying the retrieval algorithm to a case study, it is instructive to understand where there might exist weaknesses or strengths of the algorithm by performing sensitivity tests to a well behaved profile like a standard climatological profile. This is done and displayed in Figure 2 whereby a standard U.S. midlatitude summer profile served as our background guess and a standard tropical
atmosphere was used as our "true" profile to simulate the actual measurements. This plot conveys how the algorithm performs with successive iterations until convergence is reached (in this case at iteration 3). Between about 250-900 hPa, the final retrieved humidity profile is within 10% of the actual "true" profile (Figure 2b). The difficulty in retrieving humidity at the lowest levels is reflected in the RMS error (Figure 2c) which is greatest near the surface and 200 hPa. Also, in plotting the Jacobians themselves (not shown), greatest sensitivity is observed in the mid-upper troposphere above 800 hPa. The light solid line in Figure 2c is the square root of the diagonal of the a priori error covariance matrix.

We also conducted a set of experiments whereby we perturb our initial background profile by a fixed and random amount for both temperature and humidity (Figure 3). In the case where we perturb our background humidity by ± 30%, we see temperature retrieval errors on the order of 3 K in the troposphere with slightly improved performance in the stratosphere. Random perturbations generate similar results with an exception near the surface where large retrieval error and initial perturbation gradients are present. For the retrieval of humidity, the sensitivity to background temperature differences is much more pronounced. For example, with temperature perturbations as small as 2 K at all levels, humidity retrieval errors at some levels can be as large as 150% and thus the algorithm is unable to reach convergence.

Figure 2: Specific humidity retrieval using standard tropical atmosphere as "true" and mid-latitude summer as a priori. "Final" retrieval corresponds to third iteration. Light solid line on panel c is root of the diagonal of error covariance matrix.
In Figure 4, a latitude versus height cross section of water vapor (g/kg) across Hurricane Floyd is displayed. Although infrared sounders are incapable of accurate retrievals below cloud layers, the simulated radiances are calculated without explicit knowledge of clouds. However, saturated profiles will produce very sharply peaked weighting functions and thus offer little information below these peaks. Therefore retrievals below model-calculated moist (or cloudy) layers are suspect. Figure 4a displays the actual ECMWF analysis while Figure 4b reveals the retrieved humidity and Figure 4c shows the difference between the two. The retrieved slice fails to show much structure and thus mimics the a priori profile. In this example a standard tropical atmosphere is assumed to 40° N with a standard midlatitude summer poleward of 40° N. Absolute differences are on the order of 30% or greater at most levels above 800 hPa. North of 40° N this trend is reversed. What Figures 4a-c show is the need for a better first guess and a priori error covariance matrix. This is clearly displayed in Figures 4d and 4e where the cyclic retrieval algorithm was initiated with the actual background humidity field. Resulting errors are reduced to less than 10% except near 200 hPa and in the vicinity of Floyd due to disregarding clouds as noted above. Part of the remaining error can also be attributed to the somewhat simplistic specification of the a priori error covariance matrix (which was assumed static for every profile in the slice).
Figure 4: Latitude versus height cross section of specific humidity (g/kg) from (a) ECMWF specific humidity (g/kg) analysis on 15 September 1999 at 1200 UTC. (b) Retrieved humidity (g/kg) using optimal estimation cyclic algorithm. (c) Difference (%) of retrieved and “true” humidity field. (d) Retrieved humidity (g/kg) using “actual” background humidity to initiate cyclic retrievals. (e) Difference (%) of retrieved and “true” humidity field.

Humidity retrieval differences (Figures 4c and 4e) are mainly a result of initial temperature uncertainties as displayed in Figure 5. Problems of obtaining an accurate humidity retrieval in the troposphere are linked to temperature retrieval uncertainties on the order of 3-5 K (Figure 5a). When the cyclic algorithm is initiated with the actual humidity, temperature retrieval errors are < 2 K below 1 hPa with the exception near the tropical tropopause region near 5-20° N as is reflected in the upper troposphere in Figure 4e.
4. SUMMARY AND DISCUSSION

In this paper we have presented an algorithm to retrieve temperature and humidity from measurements made by the Infrared Atmospheric Sounding Interferometer (IASI), scheduled for launch aboard the METOP-1 satellite in 2005. Main features are a sensible channel reduction procedure followed by an iterative optimal estimation retrieval. A three-step procedure was introduced for down-selecting channels, which includes: exclusion based on a measurement noise threshold, “foreign” gas elimination, and a sensitivity-to-noise ratio ("H sensitivity ratio") maximization retaining 2 to 3 channels per retrieval level. This procedure results in reducing the number of channels to about 1% of the total number of IASI channels (~85 out of 8461).

An iterative linearized optimal estimation retrieval algorithm based on the “D-rad” (Liu et al. 2000) extended Gauss-Newton optimization scheme has been applied to simulated measurements. Standard climatological profiles were used to supply background thermodynamic information to demonstrate the sensitivity of the retrieval to initial background perturbations.

The retrieval of temperature performs quite well (less than 1 K difference from “true”) throughout most of the troposphere if the prescribed water vapor profile is well known (within 10%). Humidity retrievals are within 10% of the “true” humidity profile throughout most of the troposphere up to 200 hPa if the prescribed temperature profile is well known (within 2 K). Convergence is typically reached within 2-3 iterations for temperature and 3-4 iterations for humidity.

Temperature retrievals appear to be quite robust against uncertainties in prescribed humidity up to about 30 to 50%. Humidity retrievals are much more sensitive and prescribed temperature uncertainties should stay within 2 K. Humidity retrievals require a better a priori profile specification; initial profiles should be typically at least as close to the “true” ones as the U.S. standard mid-latitude summer profile to the standard tropical profile. Based on this observation a cyclic retrieval algorithm was implemented and applied in a
case study day. Results from this application further stressed the importance on the first-guess profile and corresponding error covariance matrix. Even with an idealized background humidity guess, problems with retrieving temperature (and subsequently humidity) were observed in clear air (subsidence) regions near the tropical tropopause, which arose mainly due to a somewhat simplistic a priori covariance specification.

The results of this study provide clear guidance for further advancements. Our current and future work plan includes: 1) More robust a priori guess profile selection involving either the use of an independent model analysis or a climatological look-up table. 2) Improvement of the channel reduction procedure to ensure reliable accuracy below 800 hPa and to generate a universal set of channels for most air masses. 3) Perform joint retrievals (i.e., stacking both temperature and humidity profiles into one state vector). 4) A thorough analysis of the retrieval process based on a Bayesian error analysis and characterization formalism. 5) Algorithm application to realistic IASI sounding geometry and high resolution weather analysis to test retrieval performance on mesoscale variability, with focus on the mid to upper troposphere. 6) Investigation of retrieving other parameters from IASI (e.g., sea surface temperature, integrated (mid to upper troposphere) water vapor, and cloud top height and temperature).

The results obtained so far strongly indicate that the high spectral resolution measurements from IASI indeed have potential to significantly outperform current operational sensors in temperature and humidity profiling and that they may become a future key database for the much needed monitoring of climatic changes in the thermal structure and especially the moisture distribution of the middle and upper troposphere. Lingering issues are still recognized in the retrieval of temperature and humidity below 800 hPa and near the tropopause.

5. REFERENCES


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