

Joint Temperature, Humidity, and Sea Surface Temperature Retrieval from IASI Sensor Data

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Abstract

We discuss a joint retrieval algorithm of temperature, humidity, ozone, and sea surface temperature (SST; more precisely, this is the surface skin temperature of the ocean) for the IASI (Infrared Atmospheric Sounding Interferometer) instrument. The algorithm is based on optimal estimation methodology and was carefully tested under realistic conditions (using high resolution ECMWF analysis fields). The algorithm contains in a first step an effective and fast channel selection method based on information content theory, which leads to a reduction of the total number of IASI channels (>8400) to about 3 % only (~ 250), which are subsequently used in the retrieval processing. We show that this reduction is possible without significant decrease in performance compared to using many more (order 2000) channels. The clearly improved performance of the joint algorithm compared to more specific retrieval setups is exemplified as well. Finally, the application of the algorithm to AIRS (Advanced Infrared Sounder) data, a next step planned, is addressed.

Introduction

The IASI (Infrared Atmospheric Sounding Interferometer) instrument will be part of the core payload of the METOP series of polar-orbiting operational meteorological satellites currently prepared for EU-METSAT (first satellite to be launched in 2005). IASI is a Michelson type fourier transform interferometer which samples a part of the infrared spectrum contiguously from 645 cm^{-1} to 2760 cm^{-1} ($\sim 3.6 \mu\text{m}$ - $15.5 \mu\text{m}$) with an unapodized spectral resolution of 0.25 cm^{-1} . Compared to existing operational satellite radiometers, this high spectral resolution instrument allows significantly improved accuracy and vertical resolution of retrieved temperature and humidity profiles, and also delivers ozone profiles and sea surface temperature (SST). The instrument is also designed for detection of additional trace gases and improved cloud characterization.

In this study, simulated IASI measurements are used to estimate temperature and humidity profiles and the surface skin temperature. We used the fast radiative transfer model RTIASI for forward modeling and simulating the IASI measurements (see subsection *Forward Modeling*). Due to performance and numerical reasons a fast channel selection method based on information content theory, which leads to a reduction of the total number of IASI channels (>8400) to about 3 % only (~ 250), is introduced in the subsection *Channel reduction procedure*. The retrieval of the atmospheric variables is prepared by following the Bayesian approach for an optimal combination of *a priori* data and new measurements using a fast converging iterative optimal estimation algorithm (Rogers, 2000) (see subsection *Retrieval Algorithm*). The retrieval algorithm is applied to a quasi realistic METOP/IASI orbit track for September 15, 1999. Results for this case study are presented in the section *Results*. A summary of the work presented here as well as suggested improvements and future steps on the IASI retrieval problem are given in the section *Summary and Outlook*.

Data Simulation and Retrieval Methodology

We briefly describe our retrieval scheme in this section, the forward modeling involved, main aspects of the retrieval algorithm itself, and the important procedure of information content based channel reduction. The description follows (Lerner et al., 2002), and (Weisz et al., 2003) and more details can be found there. Those earlier studies used the same methodology as applied here but were linked to the development of single parameter (temperature-only and humidity-only) retrieval schemes.

Forward Modeling

For a successful retrieval of atmospheric parameters within the framework of an optimal estimation approach as adopted here, the underlying physics of the measurement needs to be properly modeled by a forward model solving the radiative transfer equation. At the same time, a proper modeling of the "Jacobian matrix" (also termed "weighting function matrix", i.e., the derivative of the forward model with respect to the state vector) 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 atmospheric state into the measurement space (satellite-measured radiance spectrum) has the form (Rogers, 2000):

$$\mathbf{y} = \mathbf{F}(\mathbf{x}) + \epsilon, \quad (1)$$

where \mathbf{y} is the measurement vector, $\mathbf{F}(\mathbf{x})$ is the forward model operator for a given state \mathbf{x} , and ϵ is the measurement error. The measurement error characteristics should be known in terms of systematic biases and random instrument noise. The measurements \mathbf{y} should in fact be corrected for biases before using them in the retrieval to characterize ϵ statistically well by a measurement error covariance matrix. Inserting reasonable test profiles for temperature and humidity, equation (1) was used to confirm that the present retrieval problem is moderately non-linear only, i.e., we can apply equation (1) in a linearized form by replacing:

$$\mathbf{y} = \mathbf{F}(\mathbf{x}) \quad \implies \quad (\mathbf{y} - \mathbf{y}_0) = \mathbf{K}_0(\mathbf{x} - \mathbf{x}_0), \quad (2)$$

where $\mathbf{K}_0 = \partial\mathbf{F}(\mathbf{x})/\partial\mathbf{x}|_{\mathbf{x}=\mathbf{x}_0}$ is the Jacobian Matrix (evaluated at state \mathbf{x}_0) and \mathbf{x}_0 is a suitable reference state (Rogers, 2000).

For simulating the measurement vector and calculating $\mathbf{F}(\mathbf{x}) = \mathbf{T}_B$ (\mathbf{T}_B : brightness temperature) and the Jacobians \mathbf{K}_0 , the fast radiative transfer model RTIASI (Matricardi and Saunders, 1999) was used, which uses temperature, humidity, and ozone profiles and some surface parameters (e.g., surface skin temperature, surface air temperature, etc.) as input and then furnishes simulated IASI brightness temperature measurements and Jacobians of the input atmospheric species for any desired subset of IASI channels. This model calculates level-to-space transmittances on 43 fixed pressure levels spanning from 0.1 hPa (~ 65 km height) to surface. We used these same levels, the so called "ATOVS pressure level grid", also as our retrieval grid (all 43 levels for temperature, the lowest 28 levels for humidity).

Retrieval Algorithm

We approach the inverse problem associated with equation (2), i.e. the retrieval of temperature and humidity profiles and of SST \mathbf{x} , from brightness temperature measurements, \mathbf{y} , by the concept of Bayesian optimal estimation described in detail by (Rogers, 2000). With the assumption of Gaussian probability distributions and a linearized forward model, we choose a fast converging iterative optimal estimation algorithm (Rogers, 2000):

$$\mathbf{x}_{i+1} = \mathbf{x}_{ap} + \mathbf{S}_i \mathbf{K}_i^T \mathbf{S}_\epsilon^{-1} [(\mathbf{y} - \mathbf{y}_i) + \mathbf{K}_i(\mathbf{x}_i - \mathbf{x}_{ap})], \quad (3)$$

where the subscript i is the iteration index. $\mathbf{x}_{i/i+1}$ and \mathbf{x}_{ap} are the iterated and *a priori* state vectors, respectively (\mathbf{T} , $\ln \mathbf{q}$, and SST combined in one state vector), and \mathbf{S}_i is the retrieval error covariance matrix, defined by:

$$\mathbf{S}_i = [\mathbf{S}_{ap}^{-1} + \mathbf{K}_i^T \mathbf{S}_\epsilon^{-1} \mathbf{K}_i]^{-1}. \quad (4)$$

Here \mathbf{S}_{ap} is the *a priori* error covariance matrix. The optimization scheme expressed by equation (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 (Rogers, 2000). In applying equation (3), the iteration was initialized with $\mathbf{x}_0 = \mathbf{x}_a$ and state estimate \mathbf{x}_i , measurement estimate $\mathbf{y}_i = \mathbf{F}(\mathbf{x}_i)$, weighting function matrix $\mathbf{K}_i = \partial\mathbf{F}(\mathbf{x})/\partial\mathbf{x}|_{\mathbf{x}=\mathbf{x}_i}$, and retrieval error covariance estimate \mathbf{S}_i , were updated at each iteration step i until the convergence criteria were reached.

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 (Rogers, 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. This method leaves equation (3) unchanged, just \mathbf{S}_ϵ is modified in its diagonal according to:

$$\mathbf{S}_\epsilon(n, n) = \max \left[\frac{(\mathbf{y}(n) - \mathbf{y}_i(n))^2}{\alpha}, \sigma_i^2(n) \right] \quad (5)$$

where i is the iteration index, $\mathbf{y}(n)$ is the measurement value of channel n , $\mathbf{y}_i(n) = F_n(\mathbf{x}_i)$ is the forward model measurement, α is a (free) control parameter set to 4 for this study, and $\sigma_i^2(n)$ is the variance of the measurement noise for channel n (the original $\mathbf{S}_\epsilon(n, n)$ 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.

A Priori error Covariance Matrix

For the elements of \mathbf{S}_{ap} we used an auto-regressive model variant and adopted \mathbf{S}_{ap} to be non-diagonal such that there exists inter-level correlation and the non-diagonal components fall off exponentially from the diagonal, i.e.:

$$\mathbf{S}_{ap}(i, j) = \sigma_i \sigma_j \exp \left[-\frac{|z_i - z_j|}{L} \right], \quad (6)$$

where σ_i and σ_j are the standard deviations at height (log pressure) levels z_i and z_j , respectively, and L is the correlation length. For temperature $L = 6$ km was set and the standard deviation settings were divided into 3 latitude regions -0° to 30° , 30° to 60° , and 60° to 90° – with the specifications given in table 1. For humidity we have $L = 3$ km and the standard deviation values grow from 20% at surface to 100 % at 500 hPa, then they are staying constant until 300 hPa and decrease to 50 % at 100 hPa (the shape of the curve was set in this way to approximately satisfy the ECMWF standard deviations for humidity).

| pressure [hPa] | temperature errors [K] | | |
|----------------|------------------------|-----------------------|-----------------------|
| | $0^\circ - 30^\circ$ | $30^\circ - 60^\circ$ | $60^\circ - 90^\circ$ |
| 1.00 | 6.0 | 8.0 | 9.0 |
| 50.00 | 1.5 | 2.0 | 2.5 |
| 1013.25 | 1.5 | 2.0 | 2.5 |

Table 1: Standard deviation values for the temperature *a priori* error covariance matrix.

Measurement Error Covariance Matrix

In order to create an appropriate (and consistent) measurement error covariance matrix \mathbf{S}_ϵ , we assumed the squared IASI 1c noise values (obtained from Peter Schluessel, EUMETSAT, personal communications, 2000) to be our diagonal elements. Since they are specified at a reference temperature $T_r = 280$ K the values are modified according to the actual brightness temperature, based on the Planck law. The temperature factor to be multiplied by the noise values is evaluated in form of (z_1/z_2) with:

$$z_1 = T_B^2 \exp \left[\frac{c_2\nu}{T_r} \right] \exp \left[\frac{2c_2\nu}{T_B} \right], \quad (7)$$

$$z_2 = T_r^2 \exp \left[\frac{2c_2\nu}{T_r} \right] \exp \left[\frac{c_2\nu}{T_B} \right], \quad (8)$$

where ν is the wavenumber and $c_2 = hc/k$ is the second radiation constant. Finally the temperature modified 1c noise values are superposed with an 0.2 K forward model error value to roughly account for errors in the forward model ((Collard, 1998), (J. Eyre, The Met. Office, personal communications 2000)). The impact of the RTIASI forward model error on the IASI retrieval accuracy is described in (Sherlock, 2000). Figure 1, bottom, shows the raw IASI 1c noise values and the modified values, according to a brightness temperature calculated for the U.S. standard mid-latitude summer profile.

For the off-diagonal elements we assume a correlation c_{ij} between the three nearest neighboring channels of 0.71, 0.25, and 0.04, according to $S_{ij} = c_{ij} \sqrt{S_{ii} S_{jj}}$, which we also have to account for in S_ϵ . This produces a covariance matrix with a rather steep descent from the main diagonal (Peter Schluessel, EUMETSAT, personal communications, 2000).

Simulation of the measurement vector

Since we do not have true measurements, we add a random noise factor $\Delta \mathbf{y}$ to the simulated measurements in order to generate quasi realistic data. For the noise modeling (receipt obtained from Peter Schluessel, personal communications, 2000) we first create normally distributed random numbers with standard deviation values according to the diagonal elements of the measurement error covariance matrix. Since RTIASI calculates apodized radiances and brightness temperatures, respectively, we apodize this noise with a Gaussian function of a full width at half maximum of 0.5 cm^{-1} ($\sigma = 0.212 \text{ cm}^{-1}$). The resulting values are shown in Figure 1,top.

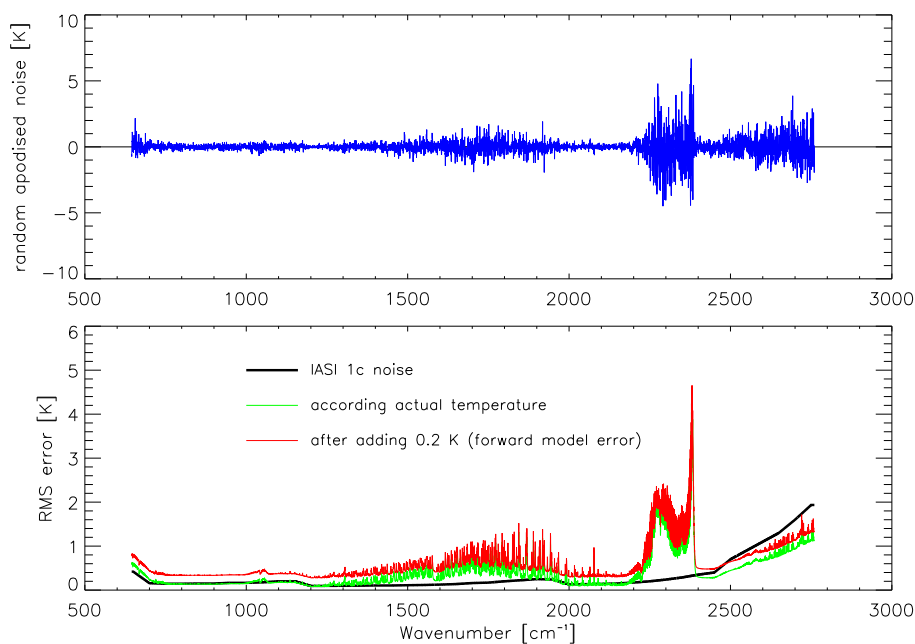


Figure 1: Top: Random apodized noise values versus wavenumber. Bottom: Square roots of the diagonal elements of the measurement error covariance matrix S_ϵ .

Channel Reduction Procedure

Since the full IASI spectra contain 8461 channels it is essential to reduce this number and somehow remove redundant information for computational and performance reasons. Hence, our task is to find a subset of channels which is sufficiently sensitive to the retrieved variables. Therefore we remove the channels above 2500 cm^{-1} (spectral range $< 4 \mu\text{m}$ – here residual solar contribution becomes important) and those channels whose "foreign" gas emissions contribute significantly to the measured brightness temperature (i.e., $975.0 \text{ cm}^{-1} - 1100 \text{ cm}^{-1}$, $1220 \text{ cm}^{-1} - 1370 \text{ cm}^{-1}$, and $2085 \text{ cm}^{-1} - 2200 \text{ cm}^{-1}$). At this point we have still about 5700 channels, which is still too much for our purpose.

Therefore we perform a further reduction of the number of channels by utilizing two different methods: the information content theory and the maximum sensitivity approach.

In information content theory one seeks to know how much information is contained in a possible outcome by knowing it. If we select the channels sequentially by retaining the channels with highest information content (H) and removing them from subsequent calculations, we may write:

$$H_i = \frac{1}{2} \log_2 |\mathbf{S}_{i-1} \mathbf{S}_i^{-1}|, \quad (9)$$

where $\mathbf{S}_{i/i-1}$ is the retrieval error covariance matrix. For \mathbf{S}_0 the *a priori* error covariance matrix \mathbf{S}_{ap} was used.

As a simplified and faster alternative of using information content theory we can also use an approach, which is solely based on the weighting function matrix scaled by the measurement errors. It is desirable to selectively choose those channels whose instrument noise is small or the measurement sensitivity to temperature and humidity perturbation is high. This is achieved by using the following channel selection criterion which maximizes the sensitivity-to-error ratio, a matrix denoted by \mathbf{H} :

$$\mathbf{H} = \mathbf{S}_\epsilon^{-\frac{1}{2}} \mathbf{K}, \quad (10)$$

where \mathbf{S}_ϵ is again the measurement error covariance matrix (with dropping the non-diagonal elements for this purpose) and \mathbf{K} is the Jacobian Matrix.

Results

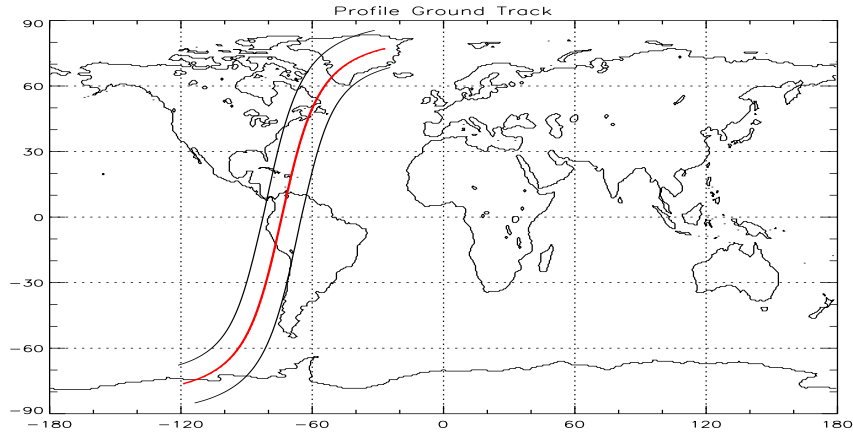


Figure 2: Simulated quasi-realistic swath of the IASI instrument. The red line delineates the suborbital track for which retrieval performance examples are shown.

The algorithm was tested for a quasi-realistic orbit arc of metop with a full swath of the IASI instrument (more than 10000 profiles) with an ECMWF analysis field of September 15, 1999, 12 UTC, as "true" field (see left plots of Figure 3 for temperature, Figure 5 for humidity, and Figure 7 for SST), and the 24h forecast of this analysis as first guess (see right plots of Figure 3 for temperature, Figure 5 for humidity, and Figure 7 for SST – these are the *a priori*-minus-true plots). The simulation region (Figure 2) covers the western Atlantic Ocean and is also situated over the Humboldt stream. Parts of Greenland and of the Americas are covered as well. The red line shows the ground track of the quasi-nadir profiles which are shown as exemplary results of our simulation study.

The simulation study was done under clear air conditions. We emphasize on showing the significantly improved performance of the joint retrieval algorithm compared to the more specific temperature, humidity, and SST only retrievals (see Figure 4, Figure 6, Figure 8).

Another aspect highlighted is that there is no significant loss in the retrieval performance if one chooses fairly few channels (about 250) compared to many channels (about 2000).

Temperature Results

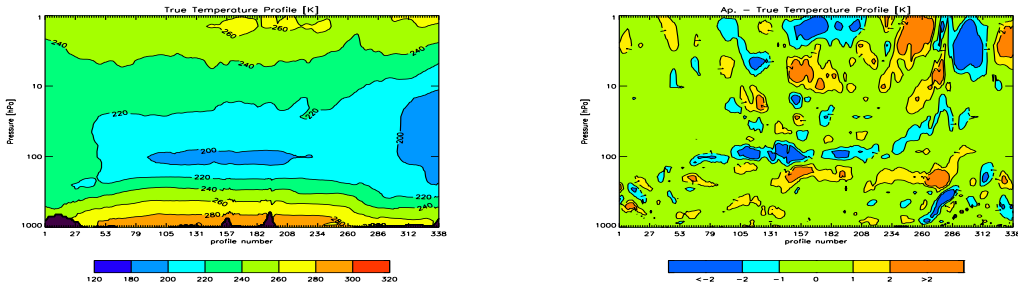


Figure 3: Left: "True" temperature profiles. Right: *A priori*-minus-true temperature profiles.

Figure 4, top left, shows the estimated temperature where IC (information content theory approach) with about 250 channels was used for channel selection. Comparing it with Figure 4, top right, where MS (maximum sensitivity approach) with few channels (also about 250 channels) was used, we can see that there is almost no difference between them. The MS approach is simpler and slightly faster than the IC approach but there is essentially no difference in performance, so if concerned about efficiency one might choose the simpler MS approach.

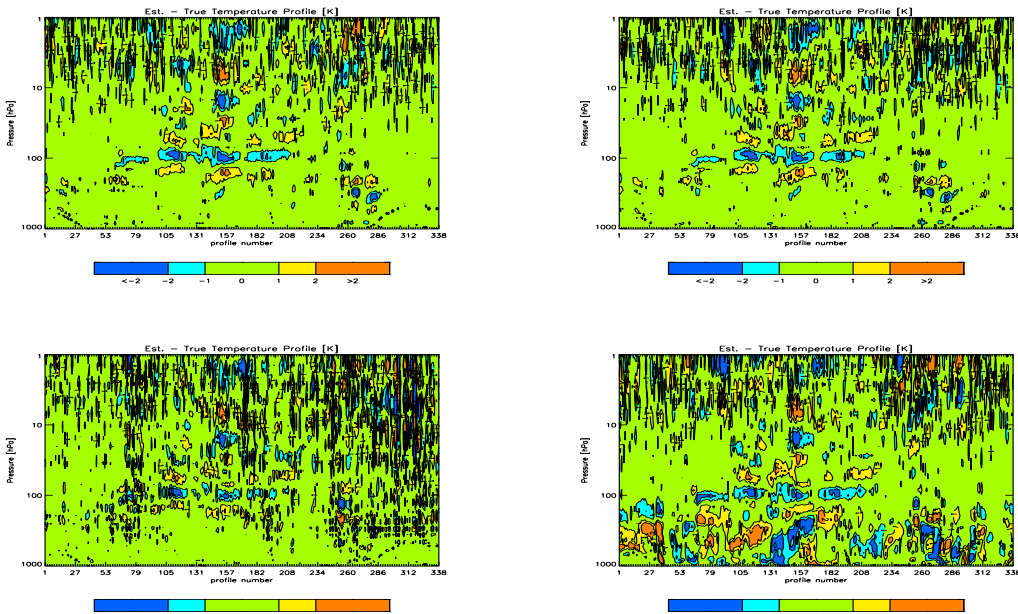


Figure 4: Estimated-minus-true temperature profiles. Top left: IC with few channels, top right: MS with few channels, bottom left: IC with many channels, bottom right: temperature-only retrieval.

Figure 4, bottom left, shows the estimated temperature for IC with many channels (~2000). One can see that using few channels in the retrieval results in no significant loss of information. Figure 4,

bottom right, shows the results for a temperature only retrieval. Here we recognize that the absence of the humidity retrieval produces a highly negative impact in the retrieval performance.

Humidity Results

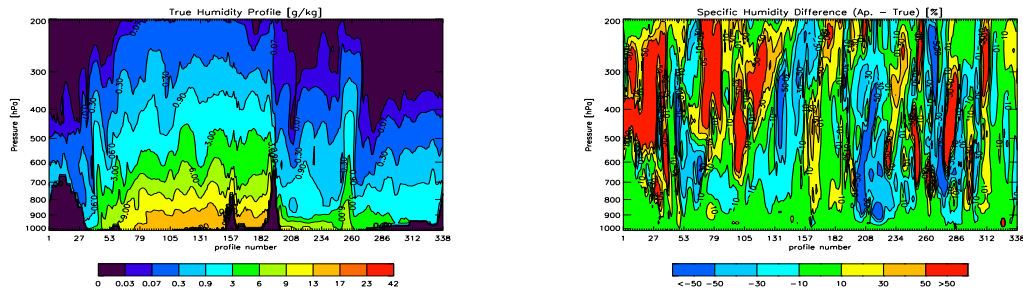


Figure 5: Left: "True" humidity profiles. Right: *A priori*-minus-true humidity profiles.

For the results of the different humidity retrievals nearly the same things as for the temperature retrievals can be said (see Figure 6). The not-so-bad result for the humidity-only retrieval is caused by a good choice in the temperature *a priori* profiles.

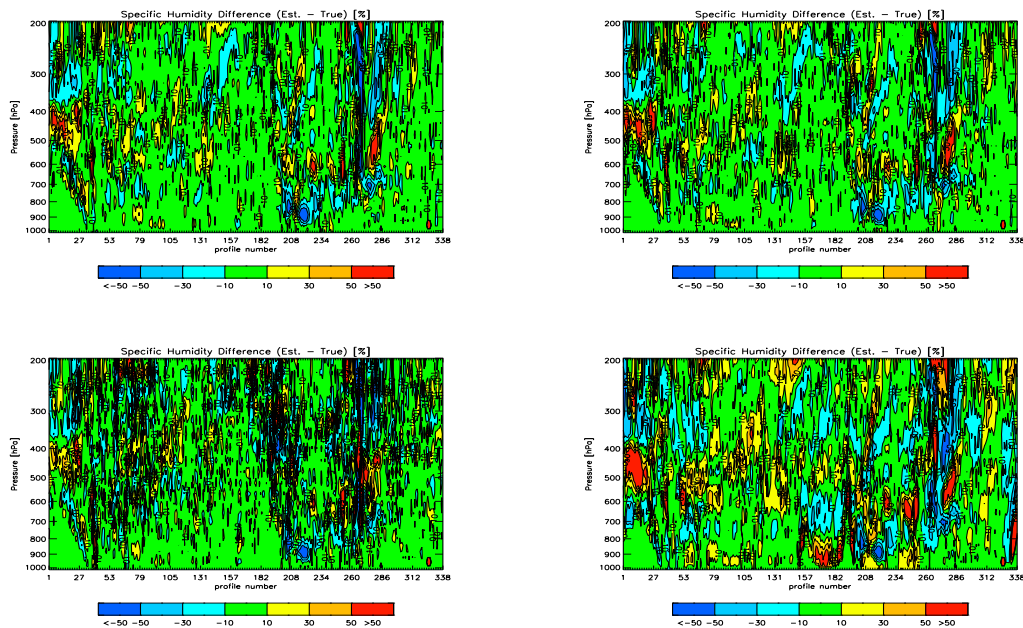


Figure 6: Estimated-minus-true humidity profiles. Top left: IC with few channels, top right: MS with few channels, bottom left: IC with many channels, bottom right: humidity-only retrieval.

We tested also a joint temperature-humidity profile retrieval between 200 hPa and 500 hPa, a region of special interest to us, in order to check whether the estimated humidity becomes better and significantly faster because of a more limited to channel selection for this region. It turned out, however, that this upper-troposphere-focused approach was only very moderately faster and, in particular, the retrieval performance degraded.

Sea Surface Temperature Results

To get a reasonably "bad" first guess for the SST (sea surface temperature) we perturbed the true SST with 3 K to demonstrate the performance of our retrieval algorithm for SST since generally the 24 hour forecast is clearly very close to the analyzed SST.

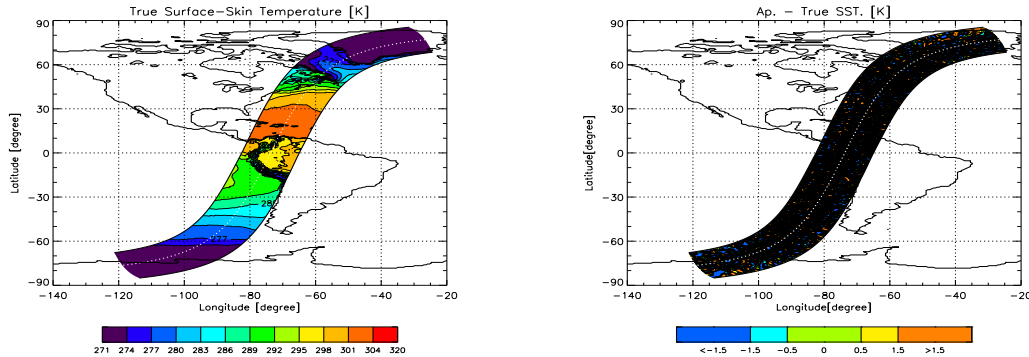


Figure 7: Left: "True" sea surface temperature. Right: *A priori*-minus-true sea surface temperature.

Figure 8, left, illustrates the quite improved performance of the joint algorithm compared to an SST-only retrieval (Figure 8, right). A further confirmation of this can be seen in the comparison of the average error bar plots for the joint and SST only retrieval (Figure 9, top left and right). The error bars of the SST-only retrieval show quite big rms errors and have also marked biases, which do not occur in the case of the joint retrieval. The comparison of the error bars between IC with few channels (Figure 9, top left) and IC with many channels (Figure 9, bottom) reflects that there is only very moderately accuracy gain in the use of many channels in the joint retrieval to get a good result for the SST retrieval given the very significant increase in computational cost for ~ 2000 channels relative to ~ 250 channels.

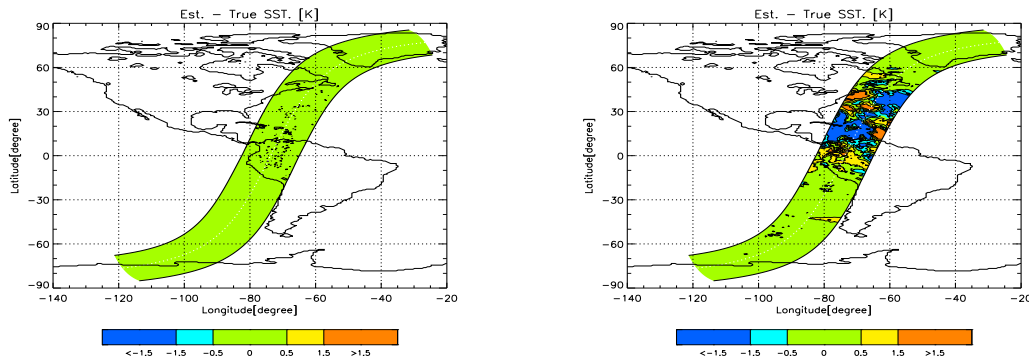


Figure 8: Estimated-minus-true sea surface temperature. Left: Joint \mathbf{T} , \mathbf{q} , and SST retrieval. Right: SST-only retrieval.

Summary and Outlook

We presented a retrieval algorithm for determining temperature, humidity and SST from radiance measurements made by the IASI instrument, scheduled for launch onboard of the METOP weather satellite series (first satellite to be launched in 2005). Main features are a sensible channel reduction procedure followed by an iterative optimal estimation retrieval. The channel reduction algorithm based on the information content theory makes the retrieval efficient – the procedure results in a reduction of the number of channels from more than 8400 to about 3% only (~ 250 channels). The retrieval performance does

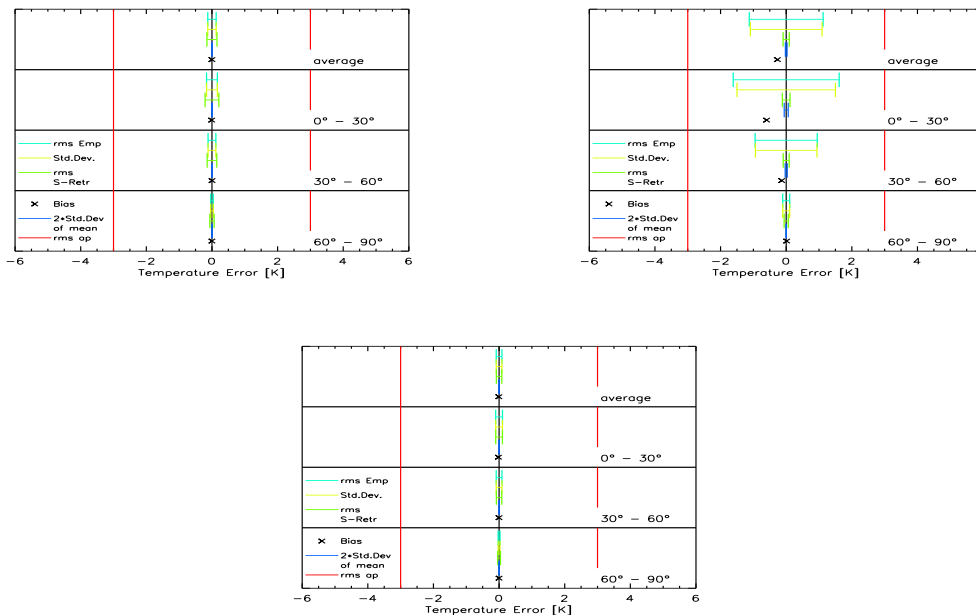


Figure 9: Top Left: SST error analysis for joint retrieval – IC, few channels. Top Right: Error analysis for SST-only Retrieval. Bottom: SST error analysis for joint retrieval – IC, many channels.

not significantly degrade due to this reduction. We also showed that the joint algorithm leads to a clearly improved performance compared to more specific retrieval setups, such as temperature-only or SST-only retrievals.

We obtain a retrieval accuracy of about 1 K in temperature and 15% in humidity with a vertical resolution of 1 km to 3 km in the troposphere. For the stratosphere we found that *a priori* data exhibit important influence. Some challenging areas arose in the mid-latitude regions and at heights with weak sensitivity of the weighting functions (e.g., the tropopause).

The results of this study provide guidance for further advancements. Our current and future work plan includes improvements of the *a priori* covariance matrices for temperature and humidity (e.g., usage of the relevant ECMWF *a priori* covariance matrices) and cross-testing the algorithm with another ground track region and analysis. Furthermore we work to complete the joint algorithm by including as well the retrieval of ozone profiles.

As a future step towards real data, the completed temperature, humidity, ozone, and SST algorithm will then be applied to AIRS (Advanced Infrared Radiation Sounder) data, where our domain of particular interest is the upper troposphere and its climatic variability in humidity and temperature.

Acknowledgments

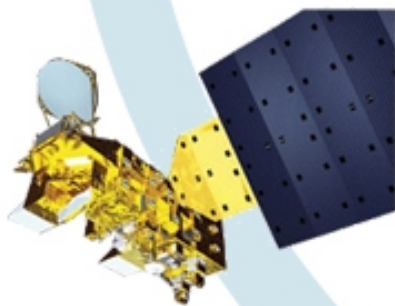
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