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# Physical-statistical retrieval of water vapor profiles using SSM/T-2 sounder data

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**Abstract.** The feasibility of retrieving water vapor profiles from downlooking passive microwave sounder data is demonstrated by usage of a retrieval algorithm which extends Bayesian optimal estimation. Special Sensor Microwave T-2 (SSM/T-2) downlooking sounder data, consisting of brightness temperature measurements sensitive to water vapor, are used together with total water vapor content data for computing tropospheric water vapor profiles. The significant nonlinearity in the cost function, an implication of the corresponding (nonlinear) radiative transfer equation, necessitates several extensions of the well-known optimal estimation inversion scheme. We supplemented the scheme by simulated annealing and iterative a priori lightweighting and obtained a powerful physical-statistical hybrid algorithm. Retrievals based on SSM/T-2 data were compared to atmospheric analyses of the European Centre for Medium-Range Weather Forecasts (ECMWF). A statistical validation of the retrieved profiles is presented. The comparisons indicate an approximate accuracy of about 15 to 20 percent for relative humidity.

## 1. Introduction

Straight-forward retrieval techniques fail to give reasonable results in ill-posed nonlinear inverse problems like retrieving water vapor profiles from downlooking sounder data. Both difficulties, ill-posedness as well as nonlinearity, can be overcome by a sensible combination of physical and statistical retrieval methods.

After describing the sensor characteristics of the microwave sounder SSM/T-2 we introduce such a combination, finally resulting in a powerful hybrid inversion algorithm. Retrieved water vapor profiles are validated by comparison with ECMWF analyses. In contrary to standard inversion methods, an improved accuracy and stability is achieved, which is confirmed by the statistical results of the validation.

## 2. The Sensor SSM/T-2

The SSM/T-2 sensor is a five channel, total power microwave radiometer with three channels placed symmetrically about the 183.31 GHz water vapor resonance line and two "window channels" (near 90 and 150 GHz, respectively). Humidity sounding can be seen as the primary application of the sensor, taking advantage of the low sensitivity of the microwave region to clouds.

There are 28 observations (beam positions) per scan for each of the five channels, with each observation having a spatial resolution of approximately 48 km at coincident centers for all channels. After each scan period, four discrete calibration measurements of a hot-load target, and cosmic background radiation are monitored [*Littlejohn*, 1995]. Generally, the sensor is thought to work with a maximum unbiased measurement error of 1.0 K brightness temperature. We used this estimate for the variances forming the diagonal elements of the measurement error covariance matrix, $\mathbf{S}_\varepsilon$.

## 3. Water Vapor Profiling

As shown by various authors (e.g., *Wang et al.* [1983], *Ulaby et al.* [1986]) the radiative transfer equation to be used for describing the problem of constituents sounding (and thus, water vapor profiling), provides a nonlinear mapping from state space into measurement space. Using $\mathbf{y}$ as the vector of measurements, $\varepsilon$ as the vector of measurement noise, $\mathbf{x}$ as the state vector, and $\mathbf{f}$ as the forward model function, the physics of radiative transfer reads

$$\mathbf{y} = \mathbf{f}(\mathbf{x}) + \varepsilon\,. \tag{1}$$

The state vector has to comprise the profile, while the measurement vector assembles the brightness temperatures of the five different channels. Additionally, the total precipitable water content (TPW) has been included into $\mathbf{y}$ as a sixth measurement. The water vapor profiles $\mathbf{x}$ are described using relative humidities at eight different height layers, spaced 2 km vertically (range: 2 to 16 km). Thus, the forward operation $\mathbf{f}$ consists of the channel weighting functions and, for the TPW measurement, of a spatial integration over the state.

When turning to establish a forward model operator in matrix form, $\mathbf{K}$, this matrix is considerably dependent on the actual state $\mathbf{x}$. Nevertheless, linearization about a certain state is possible and Eq.(1) can be written as

$$\mathbf{y} = \mathbf{K}(\mathbf{x})\,\mathbf{x} + \varepsilon\,. \tag{2}$$

Since we have to cope with a nonlinear mapping when aiming at retrieving water vapor profiles from downlooking microwave sounder data, the weighting functions of the SSM/T-2 sensor at different states are not the same. When trying to find a solution iteratively, the forward operator $\mathbf{K}$ changes its features with each step of iteration, thus making it impossible to apply a fixed inverse operator on the measurement vector $\mathbf{y}$ to give a retrieval estimation of the state, $\mathbf{x}_{retr}$. Therefore, we developed an advanced optimal estimation algorithm for solving this nonlinear retrieval problem.

## 4. A Hybrid Optimal Estimation Algorithm

All five channels of SSM/T-2 have been used for the purpose of water vapor profiling over sea, and only the first three channels (around the 183.31 GHz water vapor absorption line) over land. The TPW has been included as



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complementary measurement; it can be measured well by other sensors (e.g., *Wang et al.* [1992], *Shibata* [1994]). For an initial validation of the profiling algorithm, the TPW has been estimated from ECMWF analyses. A random perturbation has been applied to the calculated TPW values (the standard deviation of the perturbation set to 20 percent of the values) in order to conservatively account for retrieval errors of genuine satellite-derived TPW values.

The ill-posedness of the profiling problem implies that the measurement vector **y** is not to be inverted directly into water vapor profiles $\mathbf{x}_{retr}$. We thus employ a Bayesian approach using some a priori knowledge on the state, $\mathbf{x}_{ap}$. A $\chi^2$ cost function of the form (cf. *Rodgers* [1976])

$$\chi^2 = (\mathbf{y} - \mathbf{f}(\mathbf{x}))^T \mathbf{S}_\varepsilon^{-1}(\mathbf{y} - \mathbf{f}(\mathbf{x})) + (\mathbf{x} - \mathbf{x}_{ap})^T \mathbf{S}_{ap}^{-1}(\mathbf{x} - \mathbf{x}_{ap}), \quad (3)$$

$\mathbf{S}_{ap}$ denoting the covariance matrix of the a priori profile, has to be minimized, finally yielding $\mathbf{x}_{retr}$. Rather high nonlinearities in the cost function, Eq.(3), and the intention to retrieve information on the state from the measurements rather than from the a priori, led us to combine advanced tools to cope with nonlinearity as well as to stress the information brought in by the measurement. In the following sections, the principal characteristics of the hybrid algorithm are described.

### 4.1 Choice of an A Priori Profile

A subset of the TIGR data set (see, e.g., *Chédin et al.* [1985], and references therein), the TIGR/IASI (Thermodynamic Initial Guess Retrieval / Infrared Atmospheric Sounding Interferometer) data set, has been used to obtain a proper a priori state for the retrieval problem. The data set contains 43 representative atmospheric states (comprising pressure, temperature, and humidity), which are assigned to some latitudinal and temporal conditions, so the climatological reasonableness is met while an independent piece of information is brought in.

A "library search" has been employed: That profile is taken from the catalogue of representative profiles which gives forward calculated brightness temperatures that are closest to the measured brightness temperatures. This search for a minimum-cost a priori assures that the a priori is statistically reasonable in terms of the cost function value, Eq.(3). It is a relevant prerequisite to be near a "reasonable" state, a state, which clearly is assumed to happen in the atmosphere and which is not too far from meeting the measurement. In practice we ran the full algorithm for five different a prioris to finally ensure a best physical estimate, $\mathbf{x}_{retr}$.

### 4.2 The Marquardt-Levenberg Iteration Algorithm

Starting with an a priori selected as outlined above, we employed a Marquardt-Levenberg iteration (*Marquardt* [1963]) to find the minimum of the Bayesian cost function, Eq.(3), in a mathematically rigorous and efficient way. In case of (strong) dependence of the retrieved state on the a priori due to the ill-posedness of the downlooking sounding problem, the a priori is, however, still well reflected in the retrieved state after applying a simple physical retrieval; most physical retrievals are thus confined to rather close regions around the a priori.

Another drawback of a gradient method like the Marquardt-Levenberg iteration is the necessity of calculating the weighting functions explicitly. As this usually is implemented as a numerical perturbation of the forward model, numerical residual errors may induce a severe deterioration of the retrieval accuracy near the minimum, where the cost function surface is very flat. Both statistical tools described below are not vulnerable to this particular problem.

### 4.3 Simulated Annealing

In order to further improve the treatment of the inherent nonlinearity of the problem, we used a simulated annealing technique (cf., e.g., *Laarhoven* [1996]). The method of simulated annealing is a random (Monte Carlo like) statistical search algorithm for a minimum with capability to escape from local minima. In our context, the cost function was not highly distorted, but we had to face the problem of a fairly flat cost function which possesses several local minima, all at about the same cost function value. The multiple annealing algorithm (e.g., *Liu et al.* [1995]) furnishes capability of examining large regions of state space without being restricted to accepting only clear cost value improvements.

Briefly outlined, the simulated annealing works as follows (see *Rieder* [1998] for details). Starting with the state provided by the Marquardt-Levenberg iteration, the annealing algorithm is run iteratively. At each step, we applied a random perturbation to the best state estimate of all previous steps. The best $\chi^2$ value after all annealing steps applied was taken to be the one associated with the best estimated state.

### 4.4 Iterative A Priori Lightweighting

In order to effectively mitigate the problem of arriving at states that resemble the a priori state too much, we used a further improvement by employing a Monte Carlo search algorithm (random search through state space) that subsequently reduces the influence of the a priori profile. This is achieved by iteratively giving less stress (termed lightweighting) to the a priori term in Eq.(3), through increasing the a priori covariance matrix $\mathbf{S}_{ap}$ to approach 3 times its values at the end of the iteration.

The new states are computed by a random perturbation of the best state so far, the perturbation being applied within a neighborhood region of n-dimensional (n being the number of state elements that form the state vector) Gaussian-weighted shape, centered around the actual state. The new state is accepted if the cost function value of the modified cost function is less than the one of its predecessor.

## 5. Validation With ECMWF Data

We used an ECMWF (European Centre for Medium-Range Weather Forecasts) data set for the purpose of having a global reference state ("ground truth") of the atmospheric parameters temperature (used as auxiliary input) and humidity. The ECMWF "atmospheric analyses" (joint estimates based on both measurements and weather forecast model results, obtained by an assimilation system) contain the relevant atmospheric parameters as quantities on a dense spatial and temporal grid. The analyses used here are organized on a grid of 31 height levels (at "model resolution"), a latitudinal and longitudinal grid of 1 x 1 deg, and are established every 6 hours (cf., e.g., *Technical Attachment of ECMWF* [1994]).

The suitability of using ECMWF data for the purpose of a validation of SSM/T-2 retrievals has been checked by computing the ECMWF-derived brightness temperatures in the forward direction and comparing these brightness tempera-

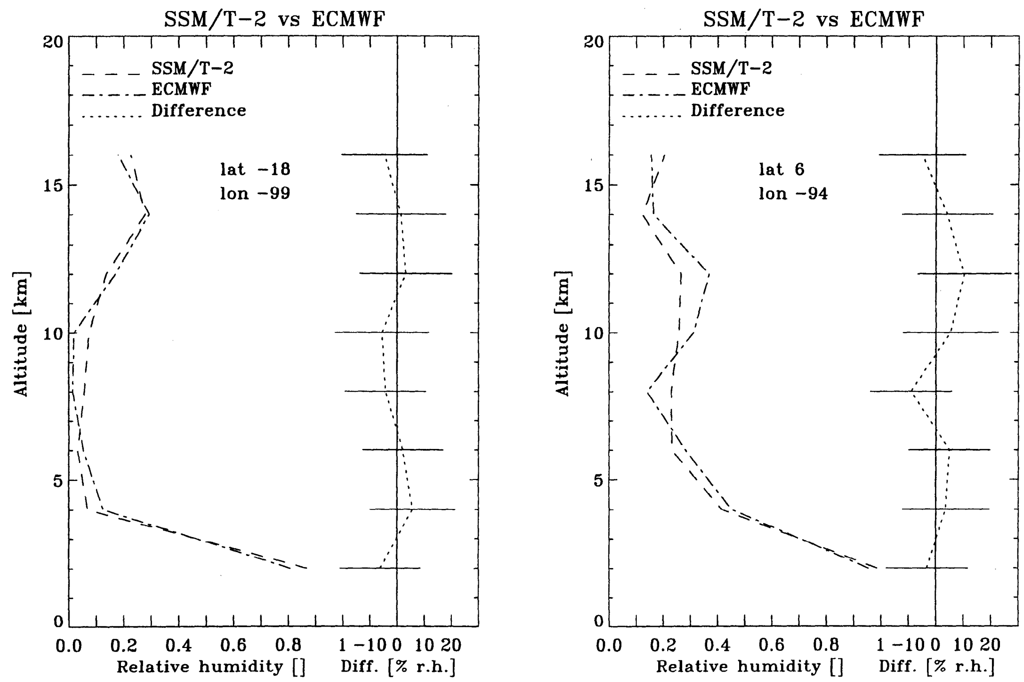


**Figure 1.** Retrievals over sea; dry atmospheric conditions (left), and moist atmospheric conditions (right), respectively. At altitudes above 12 km the profile derives mostly from the a priori profile.

tures to the measured SSM/T-2 quantities. From this we concluded that a routine global retrieval needed further input above ice and above land due to the unknown parameters of the surface radiation; thus, the window channels were excluded in those regions. Under clear sky conditions, the calculated brightness temperatures met the SSM/T-2 measurements accurately (to ~ 1–2 K). A proper knowledge of cloud and precipitation parameters were advantageous and could be provided by other sensors, but for the purpose of demonstrating some examples we estimated the necessary surface and cloud/precipitation parameters by empirical formulae [*Muller et al.*, 1994]. Since SSM/T-2 data are not included in the assimilation algorithm of ECMWF, the analyses are independent of the measurements and useful for validation.

### 5.1 Comparison of Individual Humidity Profiles

Two cases of individual retrievals are presented, demonstrating the feasibility of retrievals and revealing some properties of the hybrid algorithm used (Fig. 1). Case one is a retrieval under rather dry atmospheric conditions, case two is a retrieval under moist conditions. The particular locations are denoted in the middle of the panels, "lat" denoting the latitude and "lon" the longitude. All retrievals have been performed with samples of an (arbitrarily) selected SSM/T-2 orbit arc segment of Oct 20, 1995.

The panels display the SSM/T-2 retrieved profile, the corresponding ECMWF profile, and the difference of both. Furthermore, error bars indicate the standard deviations of the retrieval at the height levels used. The standard deviations of the retrieval have been calculated by taking the square root of the diagonal elements of the retrieval error covariance matrix, $\mathbf{S}_{retr} = (\mathbf{K}^T \mathbf{S}_\varepsilon^{-1} \mathbf{K} + \mathbf{S}_{ap}^{-1})^{-1}$.

### 5.2 Statistical Validation With ECMWF Data

When comparing retrievals with an ECMWF analysis, both retrieved profile and ECMWF profile errors are relevant. The error of the ECMWF humidity profiles can be assumed to be about 15 % relative humidity. We estimated the statistical error of the difference profiles, $\mathbf{x}_{retr} - \mathbf{x}_{ECMWF}$, by the standard deviation of the sample of difference profiles used.

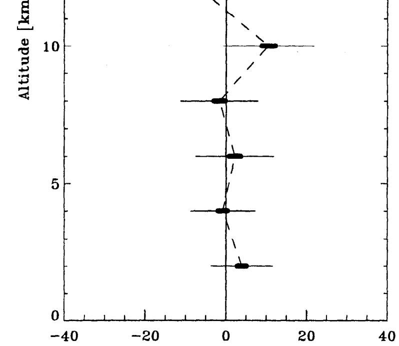


**Figure 2.** Statistical mean (dashed profile), standard deviation of mean (heavy short bars), and standard deviation (light longer bars) for retrievals-minus-analysis over sea (i.e., for SSM/T-2–retrieved minus ECMWF humidity profiles).

When performing retrievals over sea routinely, we used all five channels of SSM/T-2, whereby we weighted the two window channels to be less informative than the three atmospheric channels (the corresponding standard deviations in the measurement covariance matrix $\mathbf{S}_\varepsilon$ were set to 1.5 K, the standard deviations of the atmospheric channels being 1.0 K).

Figure 2 shows, as an exemplary validation result, a statistical error estimate for retrievals over sea. For this estimate we used a sample of 63 retrievals available along a sea track of the selected Oct 20 orbit arc (range: 11 to –64 deg latitude).

According to Fig. 2, the retrievals are fairly accurate at altitudes up to about 8 km. Besides the favorable contribution functions at lower altitudes [cf. *Rieder*, 1998], the TPW input stabilizes retrievals most at the moist lower height layers. This is also the reason why the error bars at lower altitudes are smaller, indicating more accuracy. The results show significant biases at some higher altitudes, though, perhaps due to weak estimates of cloud and precipitation parameters. Furthermore, at higher altitudes the measurements are not capable of supplying much information to the retrieval, causing larger standard deviations at these levels.

## 6. Summary and Conclusions

Spaceborne downlooking passive microwave radiometers are capable of providing not only column-integrated but also reliable height-resolved information on the atmosphere. The 183.31 GHz water vapor absorption line has been shown to furnish capability of providing information on the height distribution of relative humidity. A comparison to ECMWF humidity data revealed an accuracy of $\approx$ 15% for retrievals over sea.

To establish such retrievals, advanced techniques to cope with the inherent nonlinearities of the profiling problem have to be applied and a hybrid algorithm was developed to this end. Initialized with an a priori state obtained by a library search, a physical retrieval part with the efficient Marquardt-Levenberg algorithm combined with a statistical retrieval part with elaborated Monte Carlo methods, simulated annealing and a priori lightweighting, provided stable solutions.

Nevertheless, the task of routinely performing water vapor profile retrievals all over the globe based on spaceborne downlooking passive microwave measurements has to be tackled by a multi-sensor approach. This is needed in order to estimate parameters, which influence the radiative transfer but which cannot be probed around the 183.31 GHz line appropriately (and only partially by additional lines near 90 and 150 GHz). Most notably this includes ice/land surface effects and cloud/precipitation effects.

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