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NONLINEAR RETRIEVALS OF WATER VAPOUR FROM THE UARS MICROWAVE LIMB SOUNDER (MLS)

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ABSTRACT

The Microwave Limb Sounder (MLS) on the Upper Atmosphere Research Satellite (UARS) measures water vapour concentration in the stratosphere and mesosphere. The version 4 algorithm used at present to retrieve the concentration from the radiance measurements has a number of limitations. We describe work which attempts to circumvent some of these limitations.

The two main limitations of the current algorithm are that (1) The retrieval assumes linearity and (2) The concentration is retrieved onto a grid with a 5.3 km spacing. The theoretical vertical resolution of the instrument is better than this. To overcome limitation (1) we use a non-linear iterative retrieval; we overcome limitation (2) by using a vertical grid with a 2.6 km spacing. We show that both these measures result in a useful improvement. These improvements are planned to be incorporated in version 5 algorithms now under development for MLS. ©1998 COSPAR. Published by Elsevier Science Ltd.

INTRODUCTION

The Microwave Limb Sounder (MLS) is an instrument on the Upper Atmosphere Research Satellite (UARS). UARS was launched in September 1991 and is still operating at the time of writing, mid 1995, although water vapour measurements ceased in April 1993. MLS is designed to measure temperature and the concentration of several trace molecules in the stratosphere and mesosphere. It receives thermally emitted microwave radiation using a parabolic dish antenna whose field of view is scanned vertically across the earth's limb. The incoming radiation is fed via a superheterodyne receiver into several filter banks which are centred on the frequencies of rotational transitions, or spectral lines, of the target molecules. One filter bank (known as Band 1) is targeted at two oxygen lines; the mixing ratio of oxygen is known so this bank is used to determine temperature and pressure. The other five banks are used to measure trace species concentration. See Barath *et al.* (1993) for further details.

This paper concentrates on the filter bank (Band 5) which is centred on the 183.3 GHz transition of the water molecule. The data from these filters provide information on the water vapour content of the atmosphere between altitudes of 16 km and 90 km. The UARS project has already processed is data to give profiles of water vapour concentration and the results have proved very useful (Lahoz *et al.*, 1996). They do, however, have a number of problems; this paper describes some work which attempts to cure those problems.

RETRIEVAL THEORY

Basic Theory

For all retrievals, we make use of the optimal estimation equations. Suppose that we have a vector $\mathbf{y}$ which we can measure and which is related in a known way to another vector $\mathbf{x}$ which we want to know. In our case, $\mathbf{x}$ is a profile of water vapour concentration and $\mathbf{y}$ is a set of radiances from Band 5 of MLS. We write the relationship between $\mathbf{x}$ and $\mathbf{y}$ as:

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

where $\mathbf{b}$ is a vector of quantities which are required to calculate $\mathbf{y}$ but which we do not wish to retrieve. We linearise $\mathbf{F}(\mathbf{x}, \mathbf{b})$:

$$\mathbf{y} = \mathbf{F}(\mathbf{x}_L, \mathbf{b}_L) + \mathbf{K}(\mathbf{x} - \mathbf{x}_L) + \mathbf{K}_b(\mathbf{b} - \mathbf{b}_L). \quad (2)$$

The optimal estimation equation then gives $\hat{\mathbf{x}}$, the best estimate of $\mathbf{x}$ as:

$$\hat{\mathbf{x}} = \mathbf{x}_a + \mathbf{S}_a\mathbf{K}^T(\mathbf{K}\mathbf{S}_a\mathbf{K}^T + \mathbf{K}_b\mathbf{S}_b\mathbf{K}_b^T + \mathbf{S}_y)^{-1}(\mathbf{y} - \mathbf{F}(\mathbf{x}_L, \mathbf{b}_L) - \mathbf{K}(\mathbf{x}_a - \mathbf{x}_L)). \quad (3)$$

In this equation $\mathbf{S}_y$ is the covariance matrix of $\mathbf{y}$ *i.e.* its diagonals are the squares of the measurement errors in each element of $\mathbf{y}$, while its off-diagonal terms indicate known correlations between these errors. The vector $\mathbf{x}_a$ is an *a priori* profile and $\mathbf{S}_a$ is its covariance matrix. The equation combines the *a priori* profile and the radiances with weights depending on their errors, the retrieved profile relaxes to the *a priori* profile in regions of the atmosphere where the measurements provide no information. The error covariance of $\hat{\mathbf{x}}$, $\hat{\mathbf{S}}$, is given by

$$\hat{\mathbf{S}} = \mathbf{S}_a - \mathbf{S}_a\mathbf{K}^T(\mathbf{K}\mathbf{S}_a\mathbf{K}^T + \mathbf{K}_b\mathbf{S}_b\mathbf{K}_b^T + \mathbf{S}_y)^{-1}\mathbf{K}\mathbf{S}_a. \quad (4)$$

The optimal estimation equation only works if Eq. 1 is linear or nearly so, and hence the linearisation of Eq. 2 is a good approximation. If Eq. 1 is only moderately nonlinear, we can use the optimal estimation equation iteratively. We do this by applying it once, and then using $\hat{\mathbf{x}}$ as a new linearisation point, recalculating $\mathbf{K}$ and $\mathbf{y}_L$ and applying the equation again. The process is repeated until $\hat{\mathbf{x}}$ does not change significantly from one step to the next. For more details, see Rogers (1976).

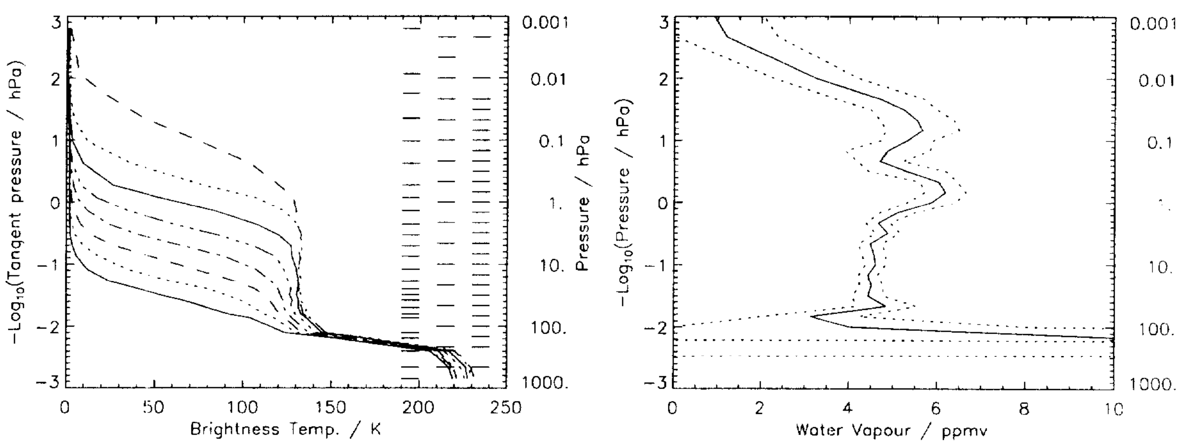

Fig. 1. The left panel shows typical measurements made during one scan in the MLS water vapour band. Each line shows the radiance in one channel, the dashed line at the top of the figure is channel 8 which is centred on the transition frequency. The solid line at the bottom is channel 1, centred 191 GHz from the line centre. Channels 9-15 are similar to channels 1-7 and are omitted for clarity. The three columns of horizontal lines indicate, from left to right, the tangent pressures for this particular scan, the retrieval grid used for MLS data versions 1 - 4 and the grid used in this paper. The right panel shows a profile of water vapour retrieved from these radiances; the dotted lines show its uncertainty.

Retrievals from MLS

Figure 1 shows an example of $\hat{\mathbf{x}}$ and $\mathbf{y}$ for a single MLS scan. The filter bank contains 15 filters; filter 8 is centred on the transition frequency while filters 1 and 15 are furthest away from it. Measurements are taken at 26 tangent levels; the tangent pressures vary from one scan to the next and are determined from the Band 1 measurements.

The production MLS retrievals (versions 1–4) have all represented the constituent profiles on a grid with 3 levels per decade of pressure, so that there are levels at 100 hPa, 46 hPa, 21.5 hPa, 10 hPa etc., these levels are spaced approximately every 5.3 km in height. This grid has a much coarser resolution than the scan pattern, especially in the lower stratosphere. It's spacing is also wider than the MLS field of view at 183 GHz. The retrievals described in this paper use the standard UARS pressure grid, which is twice as fine, with 6 levels per decade (approximately every 2.6 km). In order to make the retrieval stable on the fine grid it is necessary for the *a priori* covariance matrix $\mathbf{S}_a$ to have non-zero off-diagonal elements. These elements are assumed to form a gaussian about the diagonal with a correlation height of about 4 km in the stratosphere, increasing to 8 km in the mesosophere.

The MLS forward function $\mathbf{F}(\mathbf{x}, \mathbf{b})$ is moderately nonlinear in water vapour, especially where the radiances are large. The production MLS retrievals assume a linear forward function and therefore only apply Eq. 3 once. In order for this to be valid, larger values of $\mathbf{y}$ are not used. The retrievals described in this paper use the iterative approach described above and reject far fewer radiances.

RETRIEVAL TESTS

Method

In order to show that the retrieval procedure described above works properly, we test it on a case where we know the correct answer. To do this, we take a reasonably representative set of water vapour profiles and use the known function $\mathbf{F}(\mathbf{x}, \mathbf{b})$ to generate a set of radiances. We then apply Eq. 3 in an attempt to recover the original profiles. A set of 76 profiles is used. The profiles are located at times and places where MLS actually made measurements and the temperature, tangent pressures etc. are taken from MLS version 4 production data. Both the 'true' water vapour profiles and the *a priori* / initial guess are taken from a monthly zonal-mean average of SAGE II and HALOE data. Sufficient vertical structure is added to the 'true' profiles to ensure that the retrieval is given a stringent test.

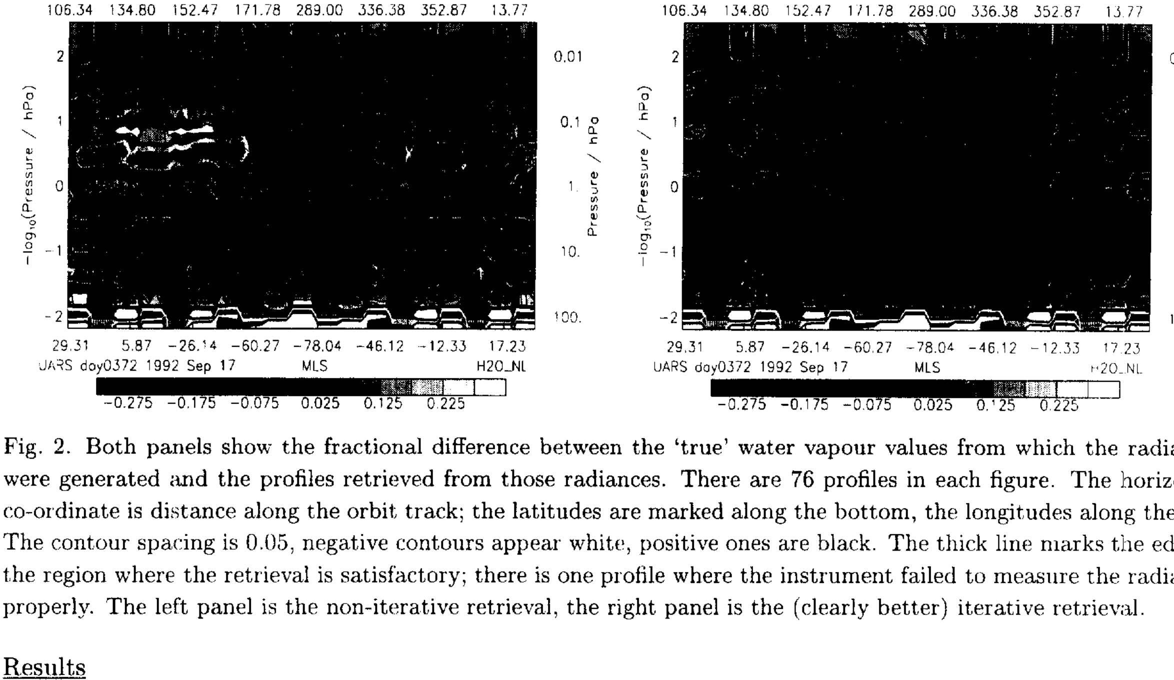

Fig. 2. Both panels show the fractional difference between the 'true' water vapour values from which the radiances were generated and the profiles retrieved from those radiances. There are 76 profiles in each figure. The horizontal co-ordinate is distance along the orbit track; the latitudes are marked along the bottom, the longitudes along the top. The contour spacing is 0.05, negative contours appear white, positive ones are black. The thick line marks the edge of the region where the retrieval is satisfactory; there is one profile where the instrument failed to measure the radiances properly. The left panel is the non-iterative retrieval, the right panel is the (clearly better) iterative retrieval.

Results

Figure 2 shows the differences between the retrieved profiles and the true ones for both a single-step retrieval and an iterative retrieval. The improvement gained by using the iterative retrieval is clear, indicating that the problem is moderately nonlinear. In the above test, the retrieval algorithm is given vectors $\mathbf{y}$ and $\mathbf{b}$ which are exactly those used and generated by the forward function. Errors in the retrieved profiles are therefore due to smoothing and nonlinearity; this is why the iterative retrieval gives a nearly perfect, but somewhat smoothed result. In the real world, $\mathbf{y}$ and $\mathbf{b}$ will have errors; in this case we cannot expect the

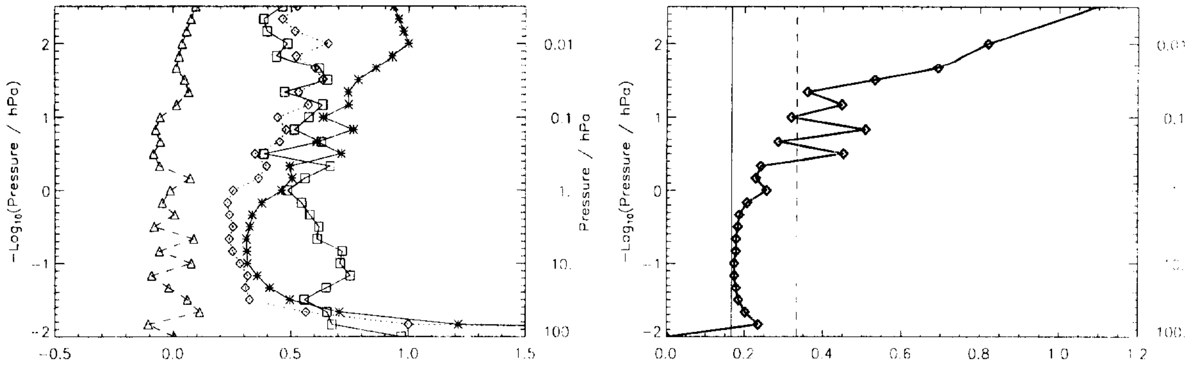

Fig. 3. The left panel shows the mean difference between true and retrieved (triangles), the root mean square (rms) difference (diamonds) and the average error bars (stars) for 75 profiles. The error bars are the square roots of the diagonal elements of $\hat{\mathbf{S}}$. In addition, the squares show the mean ratio of the rms difference to the error bars. This ratio should be approximately unity. The units on the horizontal axis are parts per million by volume (ppmv) except for the squares. The right panel shows the full width at half height of the averaging kernels. The units of half-width on the horizontal axis are -Log_{10}(Pressure / hPa). The vertical lines are the width of the 2.6 km grid used in this study (solid) and the standard MLS 5.3 km grid (dashed).

retrieval to return the true values of $\mathbf{x}$ exactly, but it should return them within the retrieved error bars, *i.e.* the square roots of the diagonal elements of $\hat{\mathbf{S}}$. To test this, we corrupt $\mathbf{y}$ and $\mathbf{b}$ with gaussian random noise with amplitudes given by $\mathbf{S}_y$ and $\mathbf{S}_b$ and re-run the retrieval. Note that in these tests $\mathbf{b}$ consists of the temperature profile and the 26 tangent pressures; the forwared model and its spectroscopic parameters etc. are assumed to be exactly known. The results displayed in Figure 3 show that the retrieved errors $\hat{\mathbf{S}}$ do indeed give a useful estimate of how far the retrieved profile deviates from the true one.

Vertical Resolution

The averaging kernel matrix $\mathbf{A} = \text{d}\hat{\mathbf{x}}/\text{d}\mathbf{x}$ have been calculated (Rodgers, 1990). The rows of this matrix are functions whose width is a useful indication of the vertical resolution of the measurement; these widths are plotted in Fig. 3. Note that they approach the 2.6 km grid spacing in the mid-stratosphere but are much larger in the mesosphere.

CONCLUSIONS

We have shown that the MLS forward function is sufficiently nonlinear that an iterative retrieval gives a superior result to a non-iterative one. We have also shown that it is practical to retrieve on the UARS grid with 6 levels per pressure decade, instead of the 3 levels per decade which MLS has used until now. The vertical resolution is about 3 km in the mid stratosphere, increasing to 6 or 7 km in the mesosphere. It is planned that the improvements described in this paper will be incorporated into MLS data version 5.

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