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Spectral sensing of atmospheric temperature and humidity profiles: Sensitivity of the technique

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SPECTRAL SENSING OF ATMOSPHERIC TEMPERATURE AND HUMIDITY PROFILES: SENSITIVITY OF THE TECHNIQUE

by

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February / février 2001

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ABSTRACT

This memorandum present a theoretical analysis on a remote sensing technique for the retrieval of atmospheric temperature and humidity profiles based on a IR Fourier transform spectrometer (FTIR). The sensitivity of the method is studied using a set of simulations based on a physical model using real atmospheric profiles from meteorological radiosondes. This study shows that the method is mostly sensitive to temperature and relatively insensitive to humidity. In all cases, its sensitivity stays relatively weak and is mostly concentrated to the lower altitude. However, since the emission and the transmission of the atmosphere are closely related, it is likely that this last one can be evaluated with a fair precision. This theoretical study has increased our knowledge of the system, which should lead to a performance improvement.

RÉSUMÉ

Ce mémorandum présente l'analyse théorique d'une technique de télédétection des profils atmosphériques de température et d'humidité qui se base sur l'utilisation d'un spectromètre IR à transformée de Fourier (FTIR). Pour étudier la sensibilité de la méthode nous utilisons des simulations tirées d'un modèle physique de l'atmosphère et des données atmosphériques en provenance de mesures par radiosondes. Cette étude montre que la méthode est surtout sensible à la température et dépend très peu de l'humidité. Dans tous les cas, sa sensibilité demeure relativement faible, particulièrement à basse altitude. Toutefois, étant donné la relation physique étroite entre l'émission et la transmission atmosphérique, il est possible que cette dernière puisse quand même être évaluée avec un précision satisfaisante. De plus, l'analyse théorique a permis de mieux comprendre la mise en oeuvre de la technique, ce qui permettra d'en améliorer la sensibilité.

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EXECUTIVE SUMMARY

The Canadian Forces are using a variety of electro-optical systems for the remote sensing of target characteristics. In the past few years, the development of passive IR spectral sensors has grown to a point where it is now considered as a vital technology for the remote monitoring of battlefield environments, providing unique information on the ongoing manoeuvres. However, the performance of that equipment depends strongly on the atmospheric conditions. This is especially true in mid- and thermal IR where the atmospheric transmission and emission vary strongly with the temperature and water vapour content. For this reason, many of the remote sensing techniques working in these bands need a good knowledge of the atmospheric conditions to work correctly. To be useful, the atmospheric parameters need to be known precisely for each location at any time. However, the major source of meteorological information, i.e. the radiosondes, cannot provide the necessary information in the fast moving modern battlefield. Ideally, the atmospheric parameters should be known in *real time*.

In order to obtain this information the Defence Research Establishment Valcartier (DREV) is currently developing a passive FTIR technique for the passive remote monitoring of the atmospheric parameters. This technique is based on the inversion of the atmospheric emission spectrum in mid- and thermal IR. The sensitivity of the method is studied using a set of simulations based on a physical model using real atmospheric profiles from radiosondes as inputs. The analysis shows than the method is mostly sensitive to the temperature and relatively insensitive to the humidity. In all cases, its sensitivity stays weak and is mostly concentrated to lower altitudes. Even if this sensitivity is poor, it may be still valuable in the correction of the atmospheric absorption since the atmospheric absorption and extinction are strongly coupled. This point still needs to be verified. In addition, this analysis allows us to precisely assess the method which will help to design a much sensitive system in the future.

This technology has applications in the remote monitoring of the battlefield gaseous contents and for the atmospheric correction in the hyperspectral imaging. The results of this work may also have a significant impact on several other remote sensing applications involving atmospheric pollution monitoring from the ground or an airborne platform. In addition, this work contributes directly to Canadian inputs to TTCP CBD AG-46, TTCP SEN AG-4 and NATO TG-16 international technical groups.

1.0 INTRODUCTION

Modern Defence organisations are using a variety of Electro-Optical remote sensing techniques for target detection, reconnaissance and surveillance. A good knowledge of atmospheric parameters such as the humidity and temperature is essential for the efficient application of these techniques. Unfortunately, the atmosphere is a very dynamic medium and these parameters need to be frequently updated. To solve this problem, the Defence Research Establishment Valcartier (DREV) is currently developing a technique for the remote sensing of atmospheric temperature and humidity profiles using infrared emission spectra (Refs. 1-2).

This remote sensing technique is now in its final evaluation phase. As part of the validation process, a series of meteorological radiosondes that provided in-situ temperature and humidity profiles were lunched at DREV on July 6-7, 1998 and on March 20, 1999. Simultaneous measurements of the infrared sky spectrum were carried out. From this dataset, we have been able to directly compare the measured atmospheric profiles with those obtained by the inversion of the infrared spectra. To better assess the limitation of the inversion method, a series of end-to-end simulations based on the measured profiles of March 10, 1999 has been performed. Since, these simulated spectra are free of any observational error, we were able to play with the parameters and explore the method without experimental constraints. This technical memorandum presents the results of this simulation study.

This work was carried out at DREV from February 1998 to January 2000 under Thrust 2d, Work Unit 2da25: Gaseous Emission Monitoring for Surveillance. During this period the author worked as a Postdoctoral fellow of the Natural Sciences and Engineering Research Council of Canada (NSERC).

2.0 INVERSION METHOD

The remote sensing technique we used is based on the inversion of the thermal infrared spectrum of the atmosphere. At the core of the inverse problem a set of linear equations are used to describe a physical process. From this set of equations it is possible to recover the physical state of the system from an observable parameter, in our case a spectrum. A good introduction to the theory of inverse problems can be found in Twomey (Ref. 3)

Establishing this set of equation alone is a complex task which necessitates a very good knowledge of the physics of the problem. In the case of atmospheric emission the construction of the appropriate set of equations is beyond the scope of this work. In fact, this work is based on a modified version of the FASCODE program especially developed for this task. This code allows us to calculate the variation of the emission from different atmospheric layers in relation to the temperature and the vapour content.

2.1 Direct Approach

Mathematically, the physical system can be described by a set of equations in a matrix A which transforms a profile **f** into a spectrum **g**

$$\mathbf{g} = \mathbf{A}\mathbf{f}$$

Therefore the inverse problem can be formulated by

$$\mathbf{A}f = \mathbf{g} + \varepsilon \rightarrow f' = \mathbf{A}^{-1}\mathbf{g}$$

where ε is the noise contribution. The least-square form of this equation is generally preferred, since it is much stable, i.e.

$$f' = (\mathbf{A}^t\mathbf{A})^{-1}\mathbf{A}^t\mathbf{g}$$

Unless the physical model is well behaved, the solution will be extremely unstable and useless. Mathematical techniques allow one to somewhat stabilise this equation. However, even then, when used for atmospheric remote sensing the method is not very reliable since the physical model is highly non-linear. As a consequence, we prefer to use a differential approach in which we do not invert the profile but instead produce a first order correction to it.

2.2 Differential Approach

In this scheme, a reference spectrum is first taken simultaneously with the launch of a radiosonde. This allows the use of a linear approximation for the set of equations which is a much better approximation in this case. It also alleviates the problem caused by the calibration of the spectrometer. This calibration is quite difficult to evaluate in absolute terms but is much easier to handle in relative terms between successive measurements.

With the knowledge of the state of the atmosphere, and through atmospheric modelling, it is possible to construct the Jacobian matrix which will be used for the inversion. Following this modification, the variables are now: $\mathbf{A} \rightarrow \mathbf{J}$, $\mathbf{g} \rightarrow \delta$ and $\boldsymbol{f}' \rightarrow \phi$,

$$\phi' = (J^t J)^{-1} J^t \delta$$

Unfortunately, this set of equations is very badly conditionned since there is strong correlation between the signal produced by each level of the atmosphere. During the inversion process, the noise is strongly amplified by a factor of the order of 1/min (eigenvalue). In a system of equations which is strongly correlated like ours, the minimum eigenvalue is very low (<<0.001). Since the typical noise level in our observation is approximately 0.4 K (0.25 K on the measurement and the reference), this would translate in a typical error in the temperature measurement larger than 400 K! It is possible to select the optimum region of the spectrum to obtain the best signal. Even in the best situation, the set of equations is still strongly correlated.

However, it is possible to increase to stability of the set of equations by adding some *a priori* knowledge. First, the information on the noise behaviour was introduced in the system:

$$\phi' = (J^t \sigma J)^{-1} J^t \sigma^{-1} \delta$$

Measurement of the entropy of the eigenvalues distribution of this system of equations confirms that this increases the amount of information available by about 3.7% (see Fig 2.1). Unfortunately, this is still not enough to stabilise the system.

2.3 Stabilization of the solution

Fortunately, mathematical artifacts allow us to further reduce the amplification of the noise. Indeed, we can introduce a damping factor, which is simply added to the diagonal of the set of equations. This operation allows us to artificially increase the eigenvalues. This operation effectively reduces the noise amplification effects but at the price of a systematic error. We can also use a second parameter, called smoothing. This parameter favours a solution with a smoother behaviour. Unlike damping it does not reduce the amplification of the noise but in some way, averages it. This property has the advantage of not introducing any bias, but may however remove some physical « spikes » in the data. In both cases, this operation is equivalent

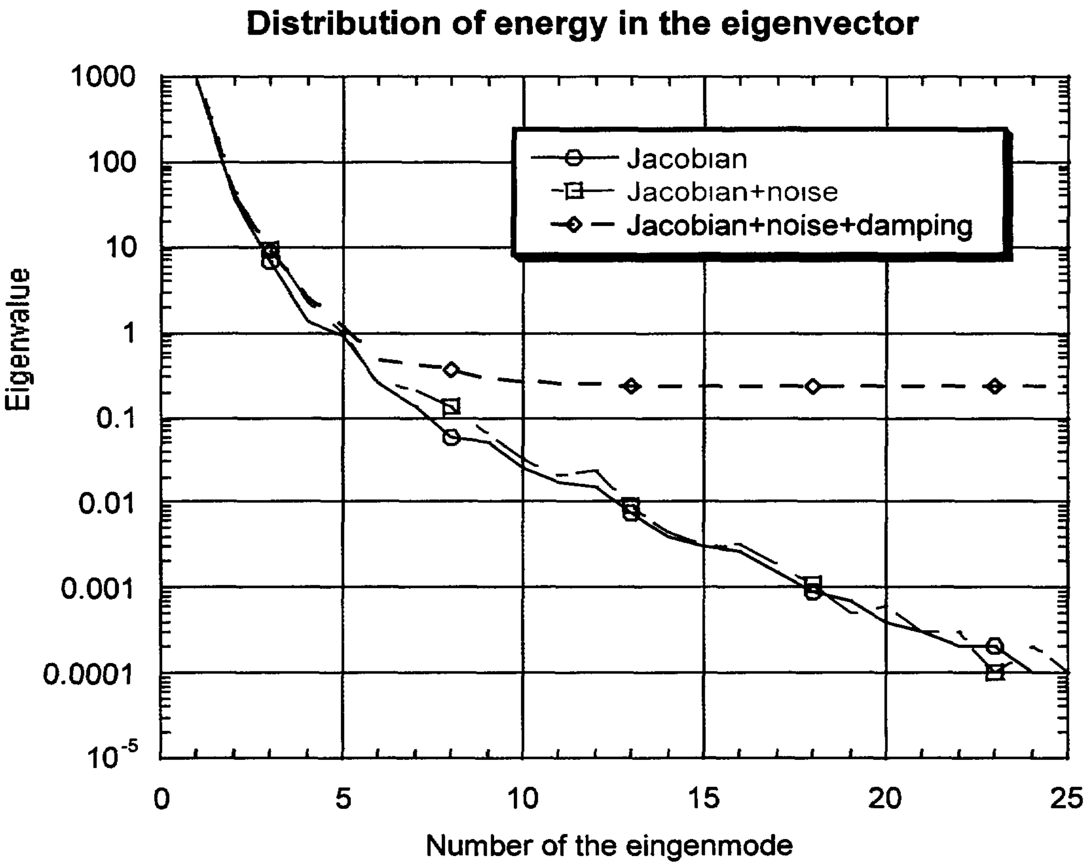

FIGURE 1 - Energy distribution in the eigenmode. The energy distribution for the original Jacobian, the Jacobian with the addition of the noise matrix and the final Jacobian are shown. By definition, the total energy is equal to 1000.

to adding some information to the system and from this point the difficulty is to find the right mixture between "physical" and added information.

The introduction of the damping factor modifies the equations in this way:

$$\phi'=(J^t\sigma J+\gamma I)^{-1}J^t\sigma^{-1}\delta$$

A smoothing factor can also be introduced in order to stabilise the equation further:

$$\phi'=(J^t\sigma J+\gamma I+\lambda H)^{-1}J^t\sigma^{-1}\delta, \text{ where } H=I^2.$$

In its original implementation this method introduced four free parameters to the inversion: two for the temperature and two for the water content. All these free parameters had to be adjusted as a function of the atmospheric conditions in order to optimise the inversion. Finding the right combination of parameters was therefore a serious burden and one of the main limitations of this procedure.

We can determine the correct value by comparing the simulated data with the real ones. In our case, we used simulated data in order to avoid any instrumental effect. The quality of the inversion was evaluated using the quadratic error between the inverted and the true profile. These simulations demonstrate than the effects of the smoothing and damping factors were strongly correlated. Therefore, we could use only the damping factor in the inversion procedure without reducing significantly the performance of the method. This greatly simplified the search for an optimal combination of factors which at that point can be obtained after half an hour of computation on a AMD-K6 (350 MHz) using Matlab compared to 4-5 hours with the previous procedure. The faster procedure also allows using a much finer grid for the search of the optimal solution.

At some point, it was not obvious if the inversion had to be optimised for the temperature or the humidity profile. This question was partially answered when numerous simulations showed than the two parameters where nearly independent of each other. Therefore, they could be optimised separately on their respective profiles; the combined solution being very close to the optimum.

2.4 Working in the Information Space

However, this situation was still not completely satisfactory since the temperature and humidity are not perfectly orthogonal (in the sense that a variation of one parameter influences the result of the second). The solution to this problem was not to add directly the damping parameters to the interaction matrix but to the matrix of the eigenvalues of the system. The equation used to solve the problem is now:

$$\phi'=[\mathbf{O}^t(\gamma \mathbf{I}+\mathbf{E})\mathbf{O}]\mathbf{J}^t\sigma^{-1}\delta$$

where **O** is the eigenvector matrix equivalent to $\mathbf{J}^t\sigma\mathbf{J}$, and **E** the eigenvalue matrix. This technique takes care of all the cross-correlations between the different levels and between the water and the temperature. In that sense, it is the *optimal inversion method.* As a bonus, it only needs one parameter to characterise the optimal damping factor. This simplifies largely the optimisation of the inversion.

This approach, however, has a price: we loose contact with the physical reality of the problem. In addition, in this space, the use of a smoothing parameter is not possible since it induces a correlation between the equations that we want to avoid in order not to reduce even further the eigenvalues of the system. In theory, the smoothing parameter can still be introduced before the orthogonalisation of the system of equations. However, it is not clear if this will help since it introduces some correlation between the different atmospheric layers. This is still an open question since we have not explored this scheme.

The addition of the damping factor in the information space slightly increases the total amount of information embedded in the system of equations. Overall, the final set of equations has 9.7% more information than the original one (see Fig. 2.1). Further progress in the formulation of the problem will be possible if additional constraints can be added. As an example, a statistical model of the atmospheric behaviour could be introduced to further constrain the model. At this moment the system of equations does not contain very much information. In fact, the total amount of information is 22 times less than an orthogonal system with 30 degrees of freedom. Overall, the system has slightly more than one degree of freedom.

3.0 STABILITY OF THE JACOBIAN

The huge variability of the meteorological conditions raises the question about the stability of the Jacobian used in the inversion from day to day or even within the course of a day. In addition, the impact of the fluctuation of trace atmospheric compounds (NO_X, O_3, CFC, etc) on the inversion is raised. The question must be solved if we want to determine the maximum time duration for which we can use a Jacobian without proceeding to the launch of a new radiosonde.

Atmospheric variation can strongly affect the useful « diagnostic bandwidth ». In fact, an enlargement of the 10 microns windows is expected in dry air. Since the most sensitive wavelengths are those at which the transmission is near 50%, we expect to observe a shift of the peak of sensitivity to the humidity level. In a way, the Jacobian matrix may become blind to the humidity profile. Therefore, a fine-tuning of the bandwidth used for the inversion should be based on the expected atmospheric profile. On the other hand, this effect is not expected to be very strong for the inversion of temperature since it is mostly derived from the CO_2 absorption, which is not expected to change very much.

An analysis of the elements of the Jacobian matrix itself supports this naïve interpretation. Here, we compare the elements of the Jacobian produced with the real atmospheric profiles measured with a radiosonde launched at DREV in April and July 1998. The element of the matrix in the CO_2 band does not change much if we compare a Jacobian generated from a summer profile and one generated from a winter profile (see Fig. 2). The humidity signal however is much more variable as the relative variation of concentration of water in the atmosphere (2-3x) is larger than the relative variation of the temperature (10%) (see Fig. 3).

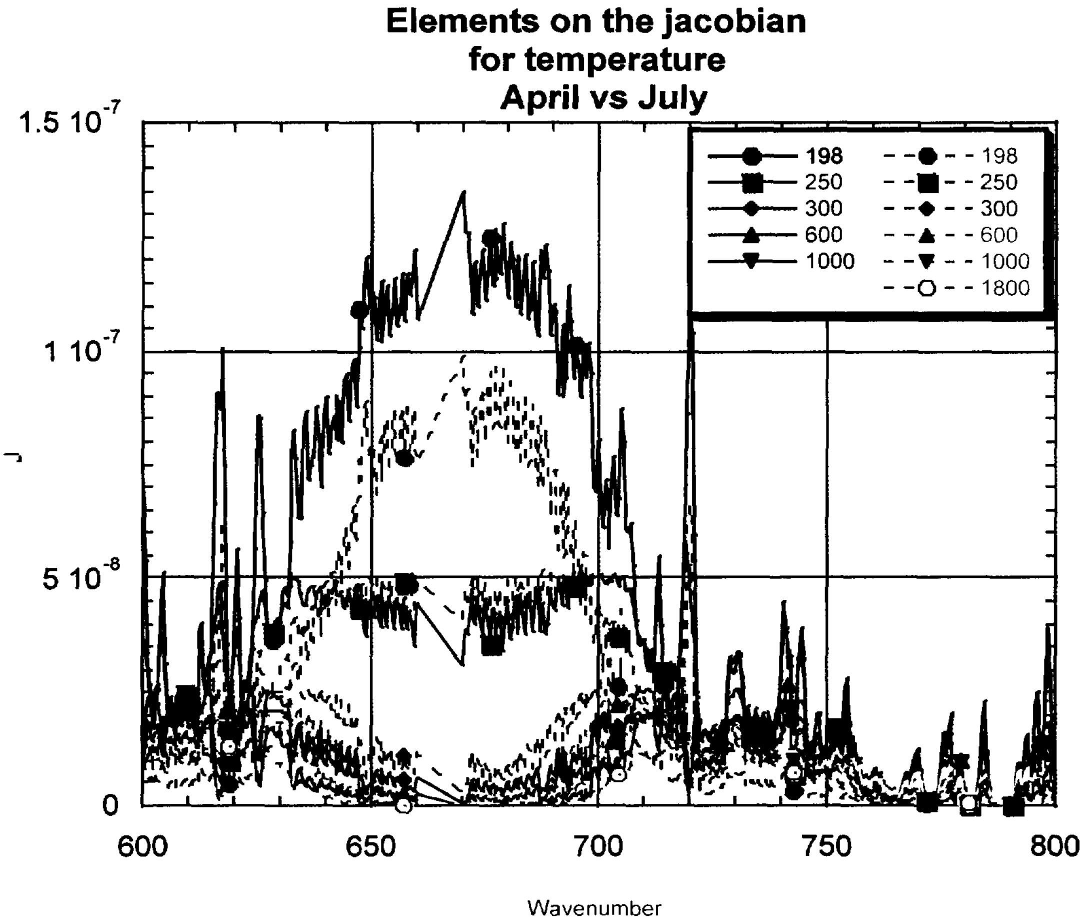

FIGURE 2 - Variability of the Jacobian: Elements of the Jacobian for the temperature. Comparison between a summer (full line) and a winter (broken line) atmospheric profile. Each curve refers to the contribution of a different altitude.

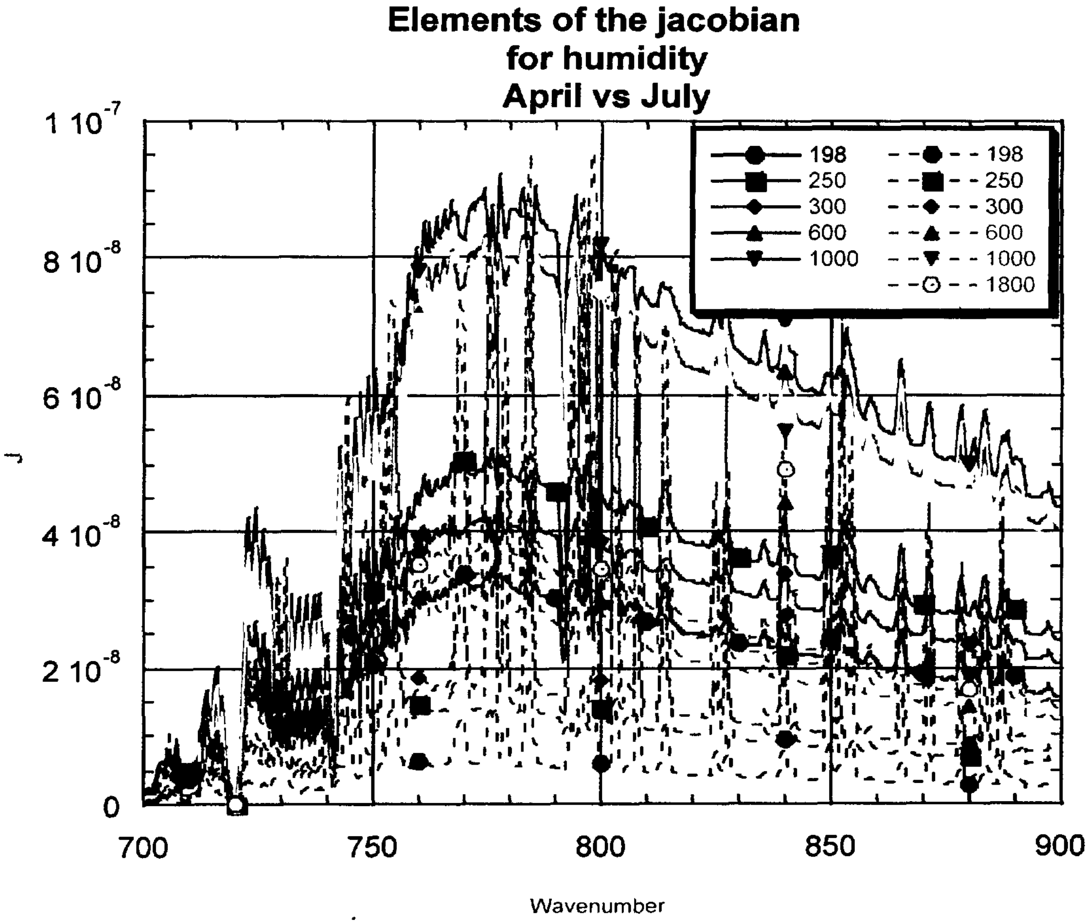

FIGURE 3 - Variability of the Jacobian: Elements of the Jacobian for the humidity. Comparison between a summer and a winter atmospheric profile. Each curve refers to the contribution of a different altitude.

4.0 PERFORMANCE OF THE METHOD

We tested the performance of the inversion technique in simulated cases. First, we simulated the performance of the algorithm in a situation where the atmospheric profile varied only slightly between measurements (e.g. a half-hour between measurements). This simulates a possible mode of operation of the system where the operator launches a radiosonde in order to calibrate the instrument at the beginning of its mission and then continuously updates the atmospheric profiles based on the result of the previous atmospheric inversion.

The first use of the simulation was to determine how the performance of the method varied with the level of radiometric noise. The quality of the inversion has been estimated using the standard deviation between the inverted profile and the real profile between the ground level and 5 km for the temperature and up to 3 km for the water content. Each of these simulated observations used an optimised-damping factor. Therefore, they simulate the best possible situation, where the instrument and the noise are perfectly controlled.

The result of the simulations shows that the performance of the system is only slightly degraded by the noise, since it is compensated by an increase of the damping factor. Unfortunately, even *without noise the simulation performs poorly*. We interpret this behaviour as a consequence of the lack of information in the system of equation. In fact, the inversion appears to be sensitive only to the temperature profile in the first two kilometres of the atmosphere and appears to be near nearly insensitive to the humidity at any altitude! The normalised sensitivity appears in Fig. 4. This result has been reproduced many times under various circumstances.

A closer examination of the Jacobian matrix provides us with an answer to this behaviour. If we examine the matrix we will notice that it is separated in four sub-matrices: temperature, humidity and cross-term between these two factors. If we examine the sub-matrix of temperature we observe a smooth decrease in the value of the elements with the altitude and with a large fraction of the power concentrated near the diagonal, which is an indication of a good mathematical behaviour (see Fig. 5). An examination of the humidity sub-matrix revealed a completely different behaviour. The value of the element *increases* with altitude and the power is spread all over the matrix. This is a clear indication of a very ill conditioned behaviour of the system of equations (see Fig. 6). When we isolate the sub-matrix and othogonalise it, the

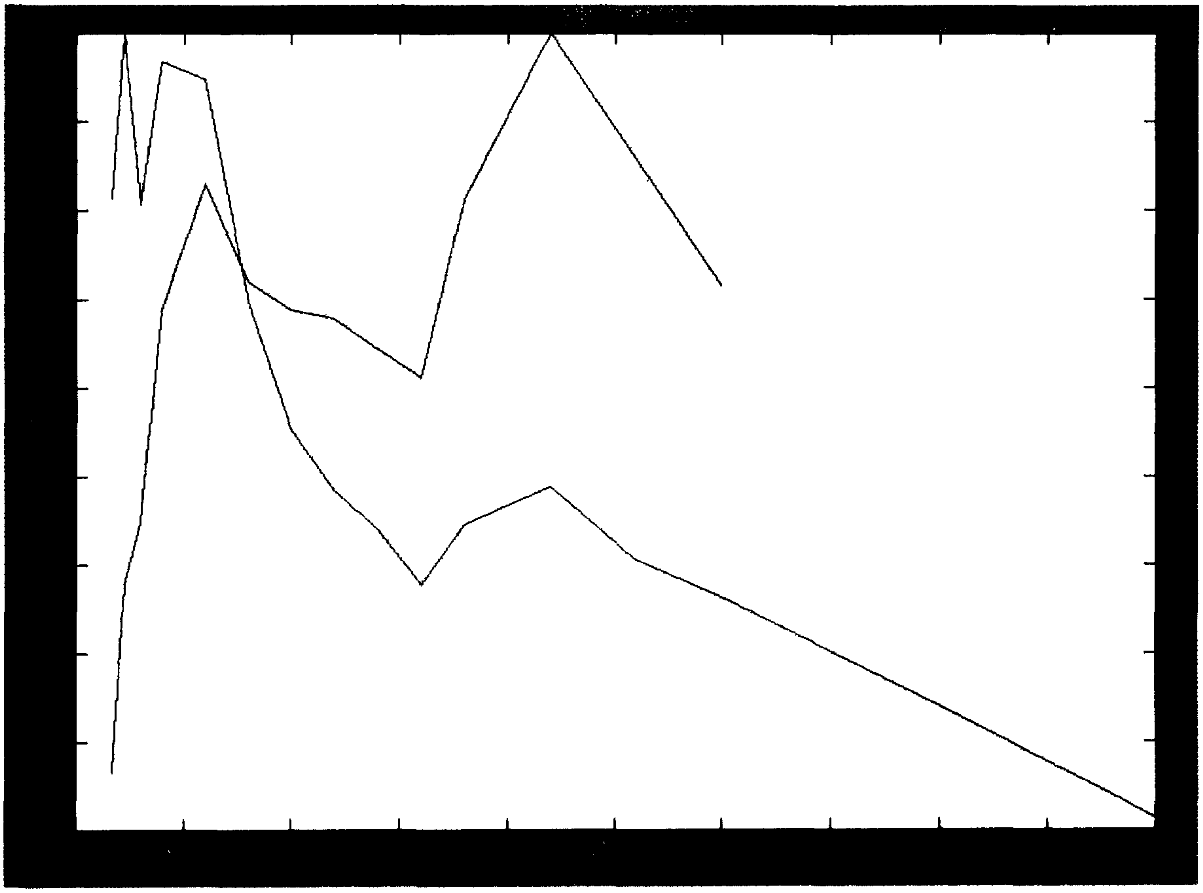

FIGURE 4 - Sensitivity with altitude: The blue curve is for humidity, the red one for temperature.

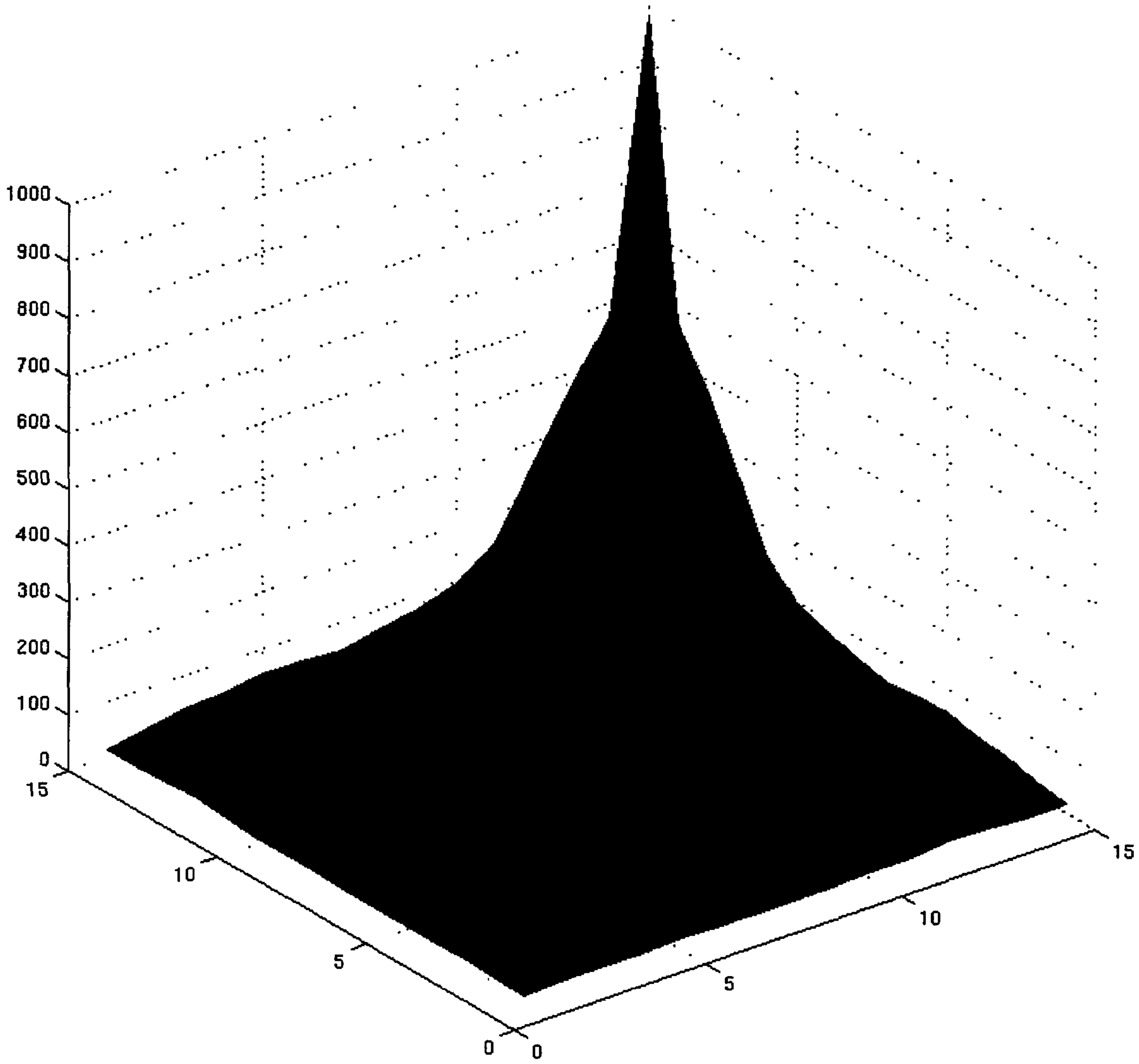

FIGURE 5: Elements of the Jacobian for the temperature-temperature sub-matrix

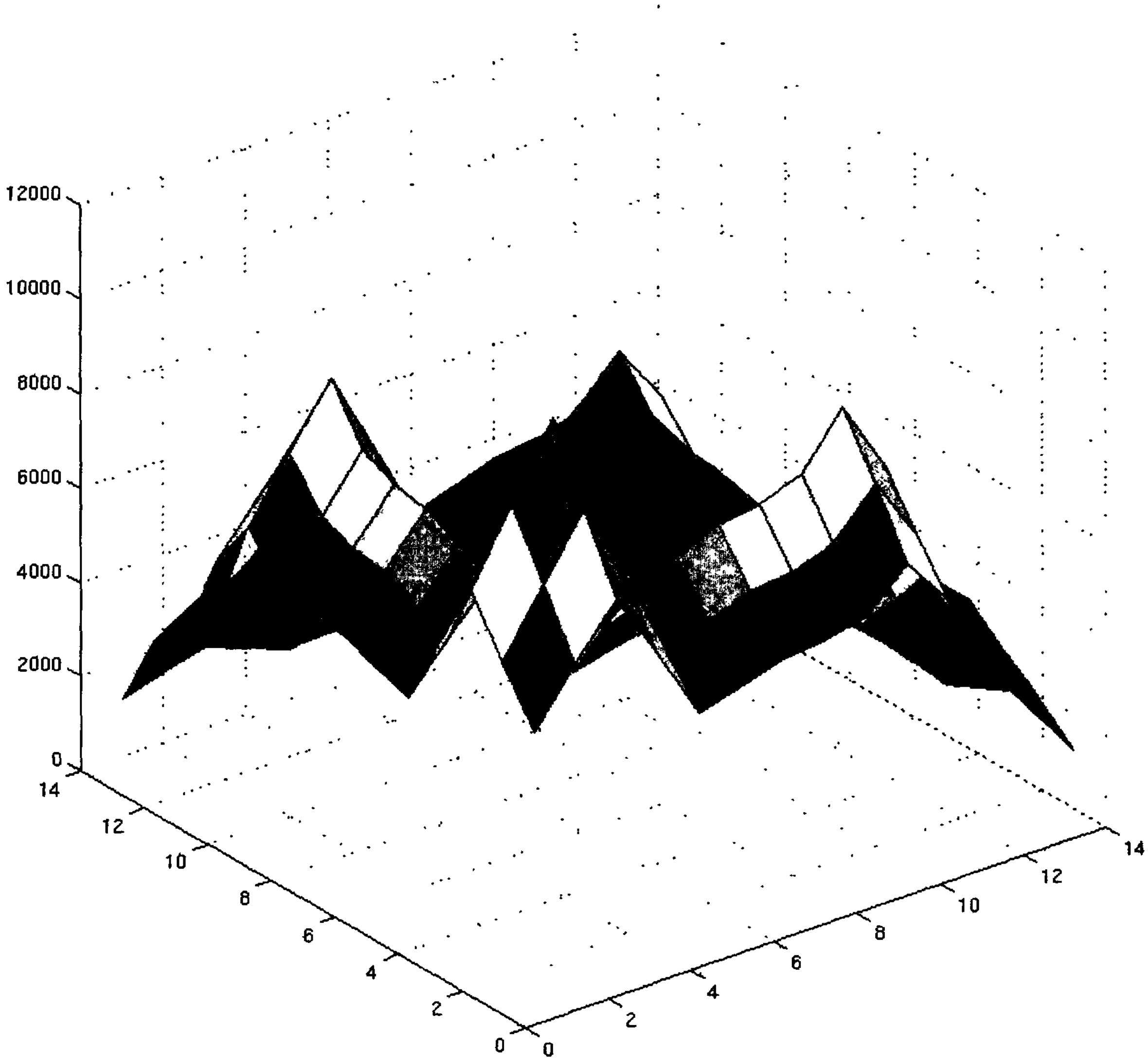

FIGURE 6: Elements of the Jacobian for the humidity-humidity sub-matrix

difference in behaviour is even more apparent. The temperature matrix demonstrates a drop in the value of the eingenvalue with the order of the eigenmode, which is relatively slow compared with the extreme drop of the humidity matrix for which nearly all the power is concentrated in one mode. This result tells us one thing: there is hope to measure the temperature profile but the situation appears rather disappointing for the humidity.

Why do these two components of the atmospheric spectrum differ so widely in behaviour? A good orthogonality between elements of the Jacobian means that we separate well the different layers of the atmosphere. It means that a different spectral signal exists for each layer of the atmosphere. Since the same kind of molecules are used for the inversion of each layer, the difference in spectrum can only be produced by one phenomenon: pressure broadening. The water vapour produces unresolved narrow lines and a wide continuum in the spectral region used in the inversion, which does not appear sensitive to pressure broadening (see Fig. 3). In contrast, the temperature measurement came from a strongly saturated CO_2 band. Pressure broadening can be observed for the CO_2 since it affects the wings of the band, which is resolved by our instrumental setup. As opposed to it, pressure broadening cannot be observed on the water vapour line since the resolution of the spectrometer is too low (1 cm^{-1} vs 0.1 cm^{-1}).

In addition, an increase of resolution of the bandwidth can also help. There is a saturated band of water vapour below 650 cm^{-1}, on the low frequency side of the CO_2 band (see Fig. 7). At this moment, this band is not used by the FTIR spectrometer since the response of the current detector is very poor at that wavenumber. However, for a system optimised for the remote sensing of the atmospheric parameters this would allow the use of a much reduced range of wavelengths, which will facilitate the optimisation of the detector.

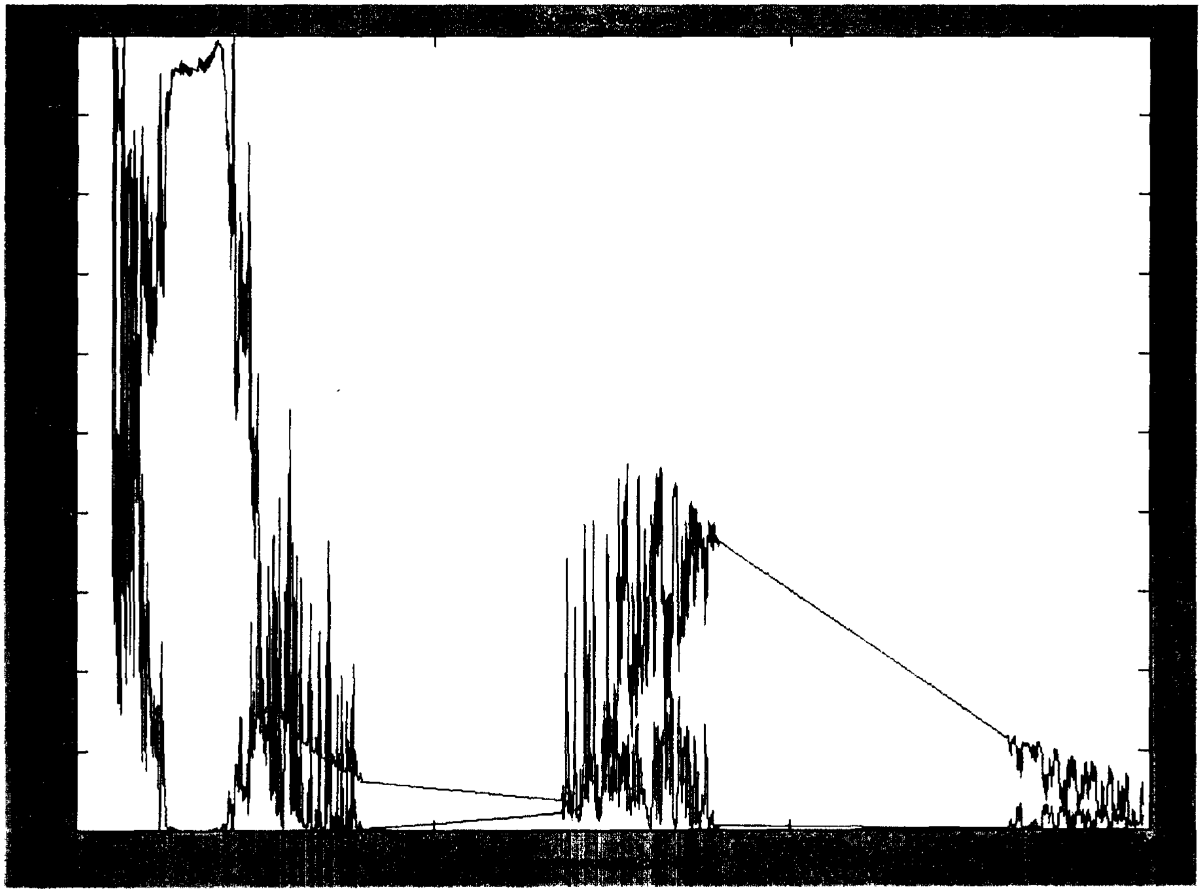

FIGURE 7 - Spectral distribution of the sensitivity. The red curve is for the temperature the blue curve is for the humidity.

5.0 CONCLUSION

Based on numerical simulations for the remote sensing of atmospheric temperature and humidity parameters by FTIR spectroscopy, we conclude that in the present analysis the system of equations used for the inversion of the atmospheric emission spectrum *does not* contain enough information to derive accurate atmospheric profiles. Only an increase in the total amount of information could improve the performance of the system. This could be done by increasing the spectral resolution until the atmospheric emission lines can be resolved or by extending the wavelength ranges. In addition, further constraints could be added to the inversion based on the statistical behaviour of the atmosphere. Multiple measurements of the atmospheric emission at different angles can also help.

Meanwhile, since the atmospheric emission and transmission are physically linked, it is possible that the weak accuracy of the atmospheric profiles derived by remote sensing would not affect much the quality of the estimation of the atmospheric transmission. Obviously, future simulations need to be done to confirm this.

6.0 ACKNOWLEDGMENTS

The author would like to thank Dr. Jean-Marc Thériault for many helpful suggestions related to this work. The expert technical assistance of Claude Bradette throughout this work is also gratefully acknowledged.

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