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A.S. ZACHOR
R.D. SHARMA

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DR. ALVA T. STAIR, Jr.
Chief Scientist

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TESTS OF AN INVERSION ALGORITHM FOR SPECTRALLY RESOLVED LIMB RADIANCE PROFILES

A. N. Zachor
R. B. Shettle

Air Force Geophysics Laboratory (OPL)
Hanscom AFB
Massachusetts 01731

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Preface

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Tests of an Inversion Algorithm for Spectrally Resolved Limb Radiance Profiles

1. INTRODUCTION AND SUMMARY

Spectrally resolved infrared radiance profiles of the Earth's limb can be inverted to obtain vertical distributions of temperature and species concentration. The atmosphere below approximately 70 km, where LTE prevails and the undisassociated CO$_2$ distribution is known, can be probed using broadband limb measurements, as demonstrated by House and Ohring, Gille et al., Russell et al., and others. The added dimension of spectral resolution offers the potential of obtaining unambiguous information in the non-LTE altitude regime.

The limb spectral radiance profile cannot in general be expressed as a linear function of the vertical temperature and concentration profiles. Consequently, the inversion must generally be performed by some sort of recursive algorithm. Zachariet al. used a recursive direct nonlinear technique to recover vertical profiles of excited nitric oxide concentration and kinetic temperature above a 100-km altitude from spectral data measured by the balloon-borne SPIRE-CVF spectrometer. These inversions used SPIRE data for the NO fundamental band near 5.3 µm. Comparable results could have been obtained by an approximate linear method because ground state NO is optically thin for tangent paths above ~100 km.
for the fundamental band. That is, the measured radiance profile and the excited state density profile have a relationship that is approximately linear for this special case. A nonlinear method can be adapted more easily to the general, non-optically-thin case, which is why we chose to use the nonlinear method in our earlier study, referred hereafter to as ZSNS.

The direct nonlinear method starts with an initial guess for the solution profile, for example, the excited NO vertical density distribution. The corresponding limb radiance profile is computed and then the guess is relaxed according to some measure of the disagreement between the computed and measured limb radiance profiles. The relaxation equation used in the earlier study, Eq. (8) of ZSNS, revises the guess according to ratios of measured and computed radiance values. The process is iterated until the solution profile has converged.

The purpose of this study is to examine further the inversion capabilities of the relaxation method used in ZSNS, and to determine its sensitivity to noise. We were interested particularly in answering the following questions:

(a) How accurately can the method recover sharply-peaked distributions? In the limb viewing geometry, a layer far below the peak is observed through much denser layers above it.

(b) How accurately can the temperature profile be recovered when there is noise in the data? The temperature profile recovered in ZSNS had large, noise-like excursions.

These questions were answered by generating synthetic spectral limb radiance profiles and then inverting them, both before and after the addition of normally distributed pseudo-random numbers representing noise. We used the NO fundamental ($\Delta v = 1$) band and assumed that ground state NO is optically thin for the complete range of tangent paths involved in the simulations, which corresponded to tangent heights between 85 and 130 km. Thus, the equations used for the direct computation of radiance, spectral radiance and the relaxed guess are those given in ZSNS. The inversion method modified to handle the non-optically-thin case (and to recover ground state as well as excited state density) would be expected to have a slightly higher sensitivity to noise than will be indicated by the present results.

In the noise-free simulations, the excited NO vertical density profile was represented by a Gaussian function and also by a double-peaked distribution which is the sum of two Gaussians. The simulations with noise used only the double-peaked distribution. The added white spectral noise had two different rms levels, corresponding to maximum SN's of 500 and 100; these are the signal-to-noise values at the combination of wavelength and tangent height that produces the maximum limb spectral radiance. The spectral resolution was the same as the SPM2E instrument, approximately 0.05 pm, which resolves the NO band into 14 spectral elements.
The excited NO density profile NO* (H) was retrieved by inverting the synthetic limb profile of band radiance (integrated spectral radiance), whereas the temperature inversion used 13 profiles of spectral radiance. As in the ZSNS study, the NO* (H) solution and the set of solutions obtained by inverting each spectral radiance profile are combined to obtain the profile R(H, λ), the normalized spectral emission per unit volume as a function of altitude. The normalized spectral emission R(T, λ) was also computed for various temperatures T. A systematic comparison of the retrieved R(H, λ) and computed R(T, λ) yields the temperature profile T(H). The initial guess in each of the inversions consisted of a constant (altitude-independent) value.

The results of the simulations are displayed in graphs in the following section. Examination of the results leads to the following conclusions:

1. In the dense-tree simulations the retrieved NO* (H) and T(H) were nearly identical to the models used to generate the synthetic limb radiance profiles, except at the very lowest altitudes, where the excited density was two orders of magnitude lower than the peak values. The errors at the low altitudes are very likely due to the fact that the synthetic emissions were inadvertently rounded to four significant figures. See Figures 3 and 4 in Section 2.

2. For S_A N_A_A = 300, the excited NO density can be retrieved with moderate accuracy down to density levels 50 times smaller than the peak. Below this density level, the accuracy degrades rapidly. It appears that the inversion technique we have used is less accurate at altitudes below the lower NO* peak than it is above the higher NO* peak, although the errors tend to be more systematic in the lower altitude range (see Figure 6).

3. For S_A N_A_A = 100, the errors in retrieved NO* density profiles have the same behavior as for the higher S_A case, except that the retrieved profile is accurate to levels 20 times lower than the peak (see Figure 7).

4. The accuracy in retrieved translational temperature degrades rapidly above some lower altitude limit and below some lower limit. However, for S_A N_A_A = 300 the peak error in T(H) is below approximately 10% over most of the range of altitudes. For S_A N_A_A = 100, the peak error is about 10-20% near the NO* peaks; the error decreases linearly to 0.5 K very slowly. The total NO density decreases with height one tenth the NO density decrease (see Figures 8 and 9).
(e) Examination of the results indicates that the random peak excursions in the retrieved temperature profile at the altitudes of the NO* peaks are approximately ±5°C for maximum spectral S/N = 500 and approximately ±25°C for (S\_A/N\_A)\_max = 100. The temperature profile that we retrieved from the SPIRE NO data (see ZSNS) has excursions of ±15°C near the altitude of maximum NO*, approximately 130 km. This would be consistent with the present simulation results if the spectral signal-to-noise of the SPIRE data for tangent height H\_T = 130 km was approximately 30 (after the data is averaged over 0.05 \( \mu \)m intervals, as done by ZSNS). Examination of the SPIRE data for this tangent height shows that the enhanced S\_A/N\_A is somewhat greater than 30, but probably not more than 60. Hence, the present results support the conclusions by ZSNS that detector noise was the major cause of the noise-like excursions in the temperature profile retrieved from the SPIRE NO data.

(f) The results emphasize the importance of achieving high signal-to-noise in limb spectral radiance measurements, and also of considering the tradeoffs between spectral resolution and signal-to-noise. This study did not consider the effects of smoothness constraints on the inversion solutions, which might reduce considerably the S/N requirement.

2. RESULTS OF SIMULATION

The single-peaked Gaussian distribution used to represent the excited density profile NO* (H) in the simulations is given by

\[
NO^*(H) = 5 \times 10^4 \exp \left( \frac{(H-115)}{5} \right)^2, \tag{1}
\]

where NO* has the units cm\(^{-3}\) and the altitude H is in kilometers. The density profile peaks at 115 km and is \( e^{-1} \) times the peak value at 110 and 120 km altitude. The double-peaked distribution, given by

\[
NO^*(H) = 5 \times 10^4 \left\{ \exp \left( \frac{|(H-115)/4, 3437|^2}{|H-100/4, 3437|^2} \right) \right\}, \tag{2}
\]

has a relative minimum at 107.5 km, where NO* is approximately one-tenth the maximum value \( \approx 5 \times 10^3 \) cm\(^{-3}\) which occurs at 100 km and 115 km.
The translational temperature profile used in the computation of synthetic radiances is the profile given by the Jacchia model for an exospheric temperature of 1050K (based on the U.S. Standard Atmosphere 1976). The profile is displayed in graphs that compare the model T(H) to the inversion results, which are described below. Figures 1 and 2 show the two different NO* (H) models and the corresponding computed limb profiles of band radiance. The computed limb spectral radiance profiles are not shown.

Figure 3 compares the single-peaked "actual" or model NO* distribution and the corresponding retrieved profile when no noise has been added to the synthetic band radiance profile. However, the synthetic band radiances were rounded to four significant figures before they were inverted. Note that the error is significant only at the lowest altitudes, where NO* (H) is less than 0.01 times the peak NO*. Figure 4 shows that the error has essentially the same behavior for the double-peaked case.

![Graph](image)

Figure 1. Single-peaked Gaussian Model for NO* (H) and the Limb Profile of Band Radiance, Determined by NO* (H) and the Model Temperature Profile T(H)

Figure 2. Same as Figure 1, Except the Model for NO5(II) is the Sum of Two Displaced Gaussian Functions.

Figure 3. Actual and Retrieved Excited Density Profiles NO5(II) for the Noise-free Case. However, the synthetic limb radiances profile was rounded to four significant figures.
Figure 4. Same as Figure 3 Except that the Actual NO$^+(H)$ is Represented by the Double-peaked Model

Figure 5 compares the actual or model T(H) to the temperature profiles retrieved for the single- and double-peaked cases, when only rounding noise is present. The errors in retrieved T(H) are significant at the same altitudes for which the retrieved NO$^+(H)$ has significant errors, that is, when NO$^+(H)$ is less than 0.01 times the peak NO$^+$. Figure 6 shows the retrieved double-peaked NO$^+$ vertical profile when the maximum spectral S/N is 500. The retrieved profile is in good agreement with the actual profile when NO$^+(H)$ is greater than ~0.01 to 0.02 times the peak NO$^+$. For a maximum spectral S/N of 100 the actual and retrieved profiles are in good agreement when NO$^+(H)$ is greater than approximately 0.02 times the peak NO$^+$; see Figure 7. However, at 107.5 km where NO (H) has a relative minimum, the relative error is approximately 40 percent.
Figure 5. Actual and Retrieved Temperature Profiles. The retrieved profiles are shown for both single-peaked NO$^+$ and Double-peaked NO$^+$. 

Figure 3 shows that accurate temperature profiles can be retrieved over the range of altitudes corresponding to NO (II)$ \geq 0,$ 10 NO$^+_\text{peak}$ when $S/N_{\lambda_{\text{max}}} \approx 500$. For the double-peaked model used in the simulations this altitude range is approximately 95-120 km; the error in this altitude regime is less than $\pm 20^\circ \text{C}$. 

Figure 3 shows that the retrieved profile has unacceptable large errors when $S/N_{\lambda_{\text{max}}} \approx 100$. The rms error in temperature is less than $\pm 10$-20 $^\circ \text{C}$ only near the peaks of the NO$^+$ distribution.
Figure 6. Actual and Retrieved Density Profiles NO*(H) for 
\(S/N_{\lambda_{\lambda_{\lambda}}} \quad \text{max} = 500\), 
Double-peaked Case

Figure 7. Same as Figure 6, Except 
\(S/N_{\lambda_{\lambda_{\lambda}}} \quad \text{max} = 100\)
Figure 8. Retrieved Temperature Profile for $S_{\lambda}/N_{\lambda} \text{max} = 500$, Double-peaked Case

Figure 9. Same as Figure 8, Except $(S_{\lambda}/N_{\lambda}) \text{max} = 100$
3. DISCUSSION

It appears that the nonlinear inversion technique investigated in this study is no less accurate below the peaks in concentration distribution than it is above the peaks, although the errors tend to be more systematic at the lower altitudes below a single or double peak.

Based on the results of this study, it is not surprising that the temperature profile retrieved from the SPIRE NO spectral data by ZSNS show noise-like excursions of ±75°C. The maximum $S/N_{\lambda}$ was between 30 and 60 for the SPIRE data. The present study implies that maximum spectral $S/N$s of the order of 500 are required to ensure acceptable temperature solutions.

Translational temperature profiles in the thermosphere have a characteristic smoothness exemplified by the model T010 used in the simulations. Based on the a priori knowledge (or assumption) of "smoothness", the retrieved temperature profile shown in Figure 9 would be judged "unacceptable". So-called smoothness constraints can be incorporated into the inversion algorithm to significantly reduce the $S/N$ requirement. For the double-peaked NO cases modelled in this study, it is estimated that the $S/N$ requirement can be reduced by a factor as large as two or three.

The study results indicate, nonetheless, the importance of considering the available tradeoffs between spectral resolution and signal-to-noise. High spectral resolution might be required, for example, when two or more species have overlapping spectral bands, or when the available data interpretation algorithm requires resolution of optically-thin portions of a strongly emitting band. When these constraints do not apply, one should opt for the minimum spectral resolution that gives the best contour (translational temperature). The tradeoffs obviously become more complex when the instrument must recover simultaneously the distributions of several species.
References


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D. Kurt

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