Simultaneous Retrieval of Chlorine Monoxide and Ozone Profiles from High Resolution Millimeter Wave Spectra

Martin Kuntz, Hermann Berg, Gerd Hochschild, Gerhard Kopp, Richard Krupa
Forschungszentrum Karlsruhe GmbH, Institut für Meteorologie und Klimaforschung
Postfach 3640, D-76021 Karlsruhe, FRG

INTRODUCTION

Modern mathematical techniques suitable for analysis of high resolution spectra are the constrained linear inversion (CLI) [1] and the optimal estimation method (OEM) [2]. In millimeterwave radiometry both techniques are commonly applied to the retrieval of single profiles, which is appropriate as long as the signatures of the different atmospheric constituents to be retrieved are well separated in the measured spectra. If the spectral lines, however, significantly overlap, the inversion of the measured data requires the joint retrieval of several constituents simultaneously. This is especially true if the measured spectra are perturbed by standing waves of instrumental origin so that each spectrum should be retrieved as a whole in that one can also fit the spectral undulations. In this report we give a short description of the joint retrieval algorithms used for the inversion of the high resolution spectra measured from February to April 1996 in Kiruna (see Kopp et al. this issue) and during March 1997 in Svalbard (see Hochschild et al. this issue), using a ground-based millimeterwave radiometer.

STANDARD INVERSION TECHNIQUES

Linearization of the equation of radiative transfer, assuming an n-point quadrature rule for the integration, and taking into account the finite number of measurements m results in a system of linear equations

$$\mathbf{Af} = \mathbf{g}$$

or a least squares problem

$$\min |\mathbf{Af} - \mathbf{g}|,$$

where $\mathbf{A}$ is the Jacobian matrix, dimensioned $m \times n$, $\mathbf{g}$ is a m-vector of measured intensities, and $\mathbf{f}$ is the n-vector of unknowns representing the sought profile. Since $\mathbf{A}$ is always close to being singular, a priori information is introduced in form of an additional linear equation system

$$\mathbf{Bf} = \mathbf{r}$$

(CLI) or in form of an a priori profile $\hat{\mathbf{f}}$ and a priori covariances $\mathbf{S}_{\mathcal{E}}$ and $\mathbf{S}_{\mathbf{f}}$ (OEM) in order to stabilize the solutions. The regularized profiles are then given by

$$\mathbf{f}_\gamma = \left[\mathbf{A^T C A} + \gamma \mathbf{B^T B}\right]^{-1} \left[\mathbf{A^T C g} + \gamma \mathbf{B^T r}\right]$$

and

$$\mathbf{f}_\gamma = \left[\mathbf{A^T S}_{\mathcal{E}}^{-1}\mathbf{A} + \mathbf{S}_{\mathbf{f}}^{-1}\right]^{-1} \left[\mathbf{A^T S}_{\mathcal{E}}^{-1}\mathbf{g} + \mathbf{S}_{\mathbf{f}}^{-1}\hat{\mathbf{f}}\right]$$

for the CLI and OEM, respectively. The diagonal matrix $\mathbf{C}$ in the above equations was not originally provided by Twomey [1], but has been suggested by Menke [5], and permits weighting of the measurements for each frequency channel individually.

JOINT RETRIEVALS

When performing joint retrievals, however, the vector $\mathbf{f}$ is a concatenation of several individual profiles $\mathbf{f_i}$ and the matrix $\mathbf{A}$ is given by a succession of Jacobian matrices. A priori information therefore has to be provided for each profile to be retrieved individually. Assuming no correlation between the profiles among each other the solutions may be written as

$$\mathbf{f}_\gamma = \left[\mathbf{A^T C A} + \begin{pmatrix} \gamma_1 \mathbf{B_1^T B_1} & \mathbf{O} & \cdots \\ \mathbf{O} & \gamma_2 \mathbf{B_2^T B_2} & \\ \vdots & & \ddots \end{pmatrix} \right]^{-1} \left[\mathbf{A^T C g}_\mathcal{E} + \begin{pmatrix} \gamma_1 \mathbf{B_1^T r_1} \\ \gamma_2 \mathbf{B_2^T r_2} \\ \vdots \end{pmatrix} \right]$$

and

$$\mathbf{f}_\gamma = \left[\mathbf{A^T S}_\mathcal{E}^{-1} \mathbf{A} + \begin{pmatrix} \mathbf{S_{f_1}^{-1}} & \mathbf{O} & \cdots \\ \mathbf{O} & \mathbf{S_{f_1}^{-1}} & \\ \vdots & & \ddots \end{pmatrix} \right]^{-1} \left[\mathbf{A^T S}_\mathcal{E}^{-1} \mathbf{g}_\mathcal{E} + \begin{pmatrix} \mathbf{S_{f_1}^{-1} \hat{f}_1} \\ \mathbf{S_{f_2}^{-1} \hat{f}_2} \\ \vdots \end{pmatrix} \right]$$

for the CLI and OEM, respectively. Note that the above variants on the CLI and OEM may be easily combined with the extension for retrieving mixing ratio profiles from spectra perturbed by spectral undulations of instrumental origin, as outlined by Kuntz [3]. In this case $\mathbf{f}$ also includes the amplitudes and phases of the standing waves which should be fitted in the inversion algorithm itself.

RESULTS AND CONCLUSION

As an example we consider the simultaneous retrieval of chlorine monoxide (ClO) and ozone (O_3) volume mixing ratio profiles from daytime and nighttime spectra measured on 17 March 1997 in Svalbard well inside the polar vortex applying the OEM (see Figures 1 and 2). The spectra have been inverted by fitting the standing waves in the inversion process itself rather than calculating daytime-nighttime difference spectra in order to eliminate the spectral undulations. This in turn allows to retrieve complete ClO and O_3 profiles over the entire altitude range rather than only daytime-nighttime difference profiles of ClO in the upper tropo- and lower stratosphere. The retrieved ClO profiles show a strong diurnal variation around $\sim$ 19 km with a maximum of $\sim$ 1.2 ppbv during daytime, while a second maximum in the altitude range between 30 and 40 km varies only slightly. A more complete discussion of the results is, however, beyond the scope of this paper.

We have demonstrated that the simultaneous retrieval of constituent profiles from ground based measurements in the millimeterwave range really works in practice and that it provides a useful means for determining mixing ratios of minor constituents in the altitude range between 18 and 50 km.

REFERENCES

[1] Twomey S., Introduction to the Mathematics of Inversion in Remote Sensing and Indirect Measurements, Elsevier Scientific Publishing, 1977.
[2] Rodgers C. D., Rev. Geophys., 14, 609-624, 1976.
[3] Kuntz M., Rep. 5719, Forschungszentrum Karlsruhe GmbH, Germany, 1966
[4] Kuntz M., G. Hochschild, R. Krupa, J. Geophys. Res., 102(D18), 21,965-21,975, 1997.
[5] Menke W., Geophysical Data Analysis: Discrete Inverse Theory, Academic, San Diego, Calif., 1989.

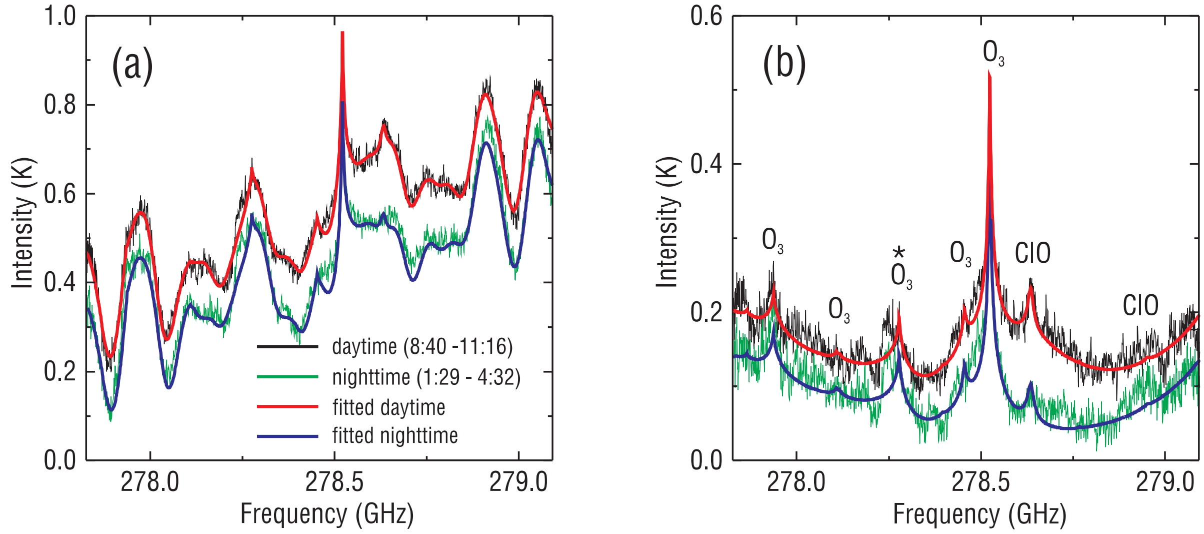

Figure 1: (a) Daytime and nighttime raw spectra of O_3 and ClO measured on 17 March 1997 in Svalbard with integration times indicated. Data are shown together with spectra that have been obtained by fitting O_3, ClO and a couple of standing waves simultaneously. Intensity, as equivalent black body radiation temperature in degrees Kelvin, is plotted versus frequency in GHz. (b) The same as (a) except that the spectra have been corrected for standing waves. The weak O_3-signature marked by an asteric originates from the lower sideband.

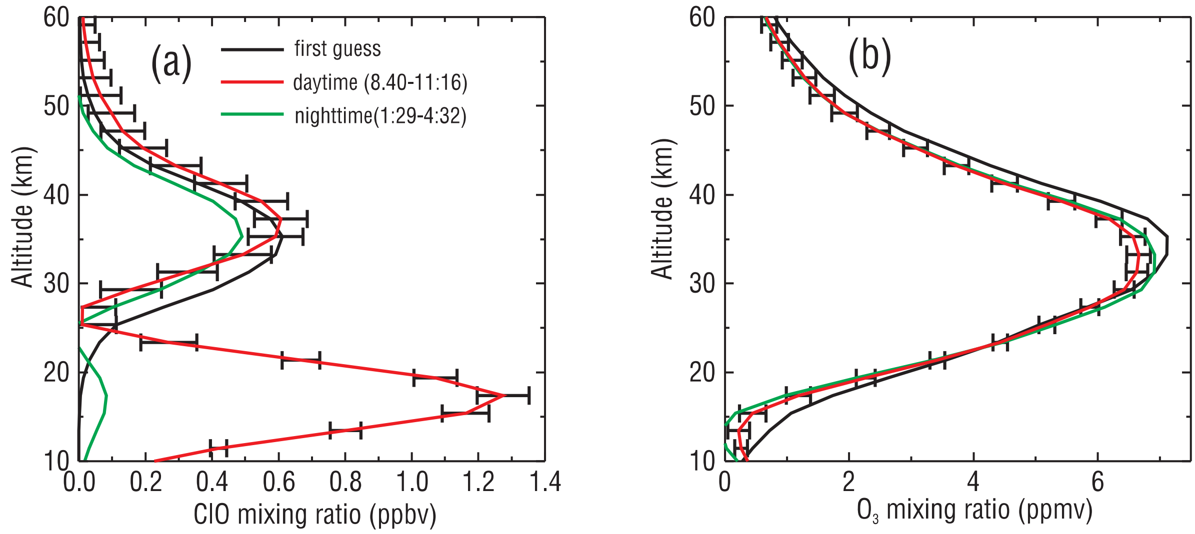

Figure 2: Retrieved daytime and nighttime mixing ratio profiles of (a) ClO and (b) O_3 from the measured spectra shown in Figure 1. Retrieved profiles are shown together with a first guess taken from the U. S. Standard Atmosphere (1976) for high latitudes. Error bars refer only to errors caused by noise. Systematical errors and errors due to the limited vertical resolution are not included.