Deriving Stratospheric Trace Gases From Balloon-borne Infrared/Microwave Limb Sounding Measurements

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Abstract. Infrared (IR)/microwave limb sounding is a well-established technique for remote sensing of the Earth’s atmosphere. The developments in IR/microwave limb sounding have triggered the demand for adequate and reliable analysis models and methods.

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INTRODUCTION

Infrared (IR)/microwave limb sounding is a promising technique for atmospheric remote sensing because numerous trace gases have spectral signatures in this spectral range. TELIS (TErahertz and submillimeter LImb Sounder) [1] is a new balloon-borne cryogenic heterodyne spectrometer used to investigate the vertical distributions of stratospheric trace gas species associated with ozone depletion and climate change. The instrument utilizes state-of-the-art superconducting heterodyne technology and allows limb sounding of the Earth’s atmosphere within the submillimeter and far IR spectral range. TELIS was developed by a consortium of major European institutes that include the German Aerospace Center (DLR), the Netherlands Institute for Space Research (SRON), and the Rutherford Appleton Laboratory (RAL). Each institute is responsible for one channel: a highly compact 500 GHz channel by RAL, a 480-650 GHz channel based on the Superconducting Integrated Receiver (SIR) technology by SRON, a tunable 1.8 THz channel with enhanced stability by DLR. Together with MIPAS-B, TELIS acts as a technology prelude to further spaceborne submillimeter/millimeter limb sounding missions.

This paper provides a brief description of the forward model and inversion methodology. Particular emphasis is placed on the feasibility study of the 1.8 THz channel. Besides, first ozone retrieval from one real terahertz measurement observed in 2010 flight is presented.

FORWARD MODEL AND INVERSION METHODOLOGY

In order to solve ill-posed nonlinear inverse problems arising in the atmospheric remote sensing, a new retrieval code, called PILS (Profile Inversion for Limb Sounding) which is dedicated to high resolution IR/microwave radiative transfer calculation and efficient inversion scheme, has been developed.

The forward model is built on GARLIC (a modern FORTRAN reimplementation of the line-by-line code MIRART [2]). GARLIC/MIRART (see also IRS2012-449 for GARLIC verification) is originally designed for IR applications with arbitrary geometries, instrumental field of view and line shape functions.

The inversion module employs the optimization solvers in the PORT Mathematical Subroutine Library for the nonlinear least squares fitting. Inverse problems are frequently ill-posed and multi-parameter Tikhonov regularization is used to stabilize the inversion process.

To obtain the derivatives of the measurements (radiance) with respect to the state vector comprising the discretized atmospheric profiles and all considered auxiliary parameters, automatic differentiation [3] is used. PILS utilizes TAPENADE [4] for returning the derivative code. It can offer both accurate derivatives and considerable computational speed-up as compared to the finite difference method.
1.8 THZ CHANNEL FEASIBILITY STUDY

The 1.8 THz channel measures the signal at local oscillator frequency between 1790 GHz and 1880 GHz. The spectrum is recorded in the intermediate frequency domain ranging from 4 GHz to 6 GHz (2 GHz bandwidth). The primary scientific goal of the 1.8 THz channel has been to measure the time-dependent chemistry of chlorine (Cl) and to achieve the closure of chemical families (NO\textsubscript{y}, Cl\textsubscript{y}, HO\textsubscript{x}) inside the polar vortex.

**Sensitivity Analysis of Expected Error Sources for OH Retrieval**

The hydroxyl radical OH is considered as one of the main chemical species controlling the oxidizing capability of the global atmosphere. TELIS has the ability to measure OH in the stratosphere using 1.8 THz channel.

In this study, we have carried out an error analysis for examining how imperfect instrumental knowledge affects the performance of the OH retrieval. We retrieve OH from a single limb scan that largely resembles typical TELIS observations by the 1.8 THz channel. The added noise is described by a Gaussian distribution. OH and O\textsubscript{3} are considered as the target molecules of multi-profile fitting in this section.

For TELIS a linear radiometric calibration approach is employed. However, the nonlinearity problem in the signal chain influences the radiometric accuracy. Therefore, the radiometric calibration of TELIS is simulated in order to investigate the nonlinearity effect on the retrieval. As the nonlinearity is caused by saturation effects in the amplifier chain, it leads to a compression of the measured output compared to the linear case. The compression in the hot load measurements is estimated to be 10-30%. The modeled calibrated spectrum with the compression of 30% is used for retrieval.

A pseudo-correction scheme is implemented, that superimposes the nonlinearity onto the model spectra in iteration. Moreover, 5% uncertainty is assumed. The relative retrieval errors with respect to the true profile (Fig. 1) imply that the nonlinearity effect is more severe on O\textsubscript{3}, which causes a largest error at 15 km. It can be seen that the OH retrieval is not affected below 21 km because there is no strong OH line at lower altitudes. The errors with correction of 25% and 35% seem to be symmetric with respect to the case of 30% (above 25 km for OH).

![Relative error of OH and O\textsubscript{3} with respect to the true profile.](image)

**FIGURE 1.** Relative errors of OH and O\textsubscript{3} with respect to the true profile. The retrievals are done for the calibrated spectra with the compression of 30% in the hot load measurements. \(x_i\) and \(x_t\) represent the retrieved and true profiles, respectively. The dotted maroon horizontal line refers to the observing altitude of TELIS.

Uncertainties in the parameters used by the instrument module of the forward model may cause systematic biases in the retrieved vertical profiles. Excluding the nonlinearity error, sideband ratio and pointing error are studied by propagated error using the linear mapping which via the contribution matrix relates changes in the retrieved state vector to changes to the measured signal.

For an ideal double sideband receiver the sideband ratio is equal to one. However, in practice this ratio is estimated to lie in the range of 0.95 to 1.05 for the 1.8 THz channel. In the left panel of Fig. 2 the propagated errors introduced by a relative bias are shown. The large sideband ratio bias can result in significant error in the retrieval quality of OH. The sideband ratio measurements have been consolidated in latest laboratory campaign.
A pointing error can be characterized by systematic bias and random offset. TELIS receives its pointing information from a highly stable attitude and heading reference system equipped on MIPAS-B. As can be inferred from the right panel of Fig. 2, the uncertainty in systematic pointing bias can be another major error source for the OH retrieval.

![Fig. 2](image1)

**FIGURE 2.** Left: propagated error of sideband ratio onto the OH retrieval with the sideband ratio bias ranging from -0.1 to 0.1. Right: propagated error of pointing with the error on the systematic pointing bias.

### Multi-window Simultaneous Processing for HCl Retrieval

TELIS can measure two of three channels simultaneously. The retrieval capability of HCl by using multi-window is studied. We focus on two windows located in the 1.8 THz and 480-650 GHz SIR channels. In the retrieval, the state vector is constructed from the VMR profiles of the main target HCl and one auxiliary molecule O$_3$.

The averaging kernels (Fig. 4, left panel) for the multi-window case indicate a higher sensitivity below 20.5 km. An improvement in terms of the degree of freedom for signal is also obtained. The corresponding smoothing error in the right panel of Fig. 4 declares that the regularization results in less information loss at lower altitudes, and the measurement error below 20 km is decreased by about 10%. Therefore, the retrieval precision is better over the altitude range of 10-20.5 km compared to that using the 1.8 THz channel only.

![Fig. 3](image2)

**FIGURE 3.** Left: averaging kernels for HCl retrieval using the single-window measurement in the 1.8 THz channel, and the multi-window measurement in the 1.8 THz and 480-650 GHz SIR channels. Right: retrieval precision, smoothing and measurement errors for the single- and multi-window fitting.
FIRST RESULT OF O₃ RETRIEVAL

We retrieve O₃ from a limb scan in the 1.8 THz channel observed on 24 January, 2010. The retrieval grid is discretized in 1.5 km between 16 and 32.5 km which is equivalent to the tangent spacing. While dealing with the real measurements in the IR/microwave spectral range, the offsets at the lower tangent altitudes caused by broad continuum contributions shall be concurrently fitted at each retrieval altitude.

The retrieval result and corresponding averaging kernel are shown. Two SMILES products, the MLS and MIPAS-B retrievals are taken for comparison. Large discrepancies occur above 34 km due to the limited information above the observing altitude obtained by the TELIS instrument. Apart from that, a rather good agreement is found between 16 and 31 km.

![Comparison of O₃ retrieval between TELIS and SMILES, MLS and MIPAS-B products on 24 January, 2010.](image1)


CONCLUSIONS

A short overview of the forward model and inversion method dedicated to IR/microwave limb sounding has been given. Both synthetic and real TELIS measurements have been involved in the data analysis. The next step is to investigate ways to increase retrieval reliability and to consolidate the ozone products in 2010 and 2011 flights.

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