APPLICATION OF 3D MC RTM “TRACY-II” ON SCIAMACHY LIMB MEASUREMENTS IN THE UV/VIS SPECTRAL RANGE

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ABSTRACT

Nitrogen and halogen compounds play a major role in atmospheric chemistry, e.g. as catalysts responsible for ozone loss. Limb measurements provided by the SCanning Imaging Absorption spectroMeter for Atmospheric CHartographY (SCIAMACHY) on the ENVISAT satellite allow to retrieve stratospheric profiles of various trace gases on a global scale, among them BrO for the first time.

In the limb observation mode the instrument is measuring scattered light with a non-trivial distribution of light paths. By means of spectroscopy and radiative transfer modeling the measurements can be inverted to retrieve the vertical distribution of stratospheric trace gases.

For that purpose, Differential Optical Absorption spectroscopy (DOAS) is applied on the spectra in the UV/VIS region, yielding slant column densities (SCDs) of the respective trace gases (O3, NO2, BrO and OClO) in the first step. Second, the trace gas SCDs are converted into vertical concentration profiles applying radiative transfer modeling.

The Monte Carlo method benefits from conceptual simplicity and allows realizing the concept of full spherical geometry of the atmosphere and also its 3D properties, which is important for a realistic description of the limb geometry and allows accounting for horizontal gradients of trace gases. Moreover the model is assuming every light path in terms of probability to take place, allowing to estimate the statistical error of the RTM calculations.

This presentation will discuss the application aspects of the full spherical 3D Monte Carlo radiative transfer model “Tracy-II” for the profile retrieval from measurements in the SCIAMACHY limb geometry. In particular, the effect of horizontal inhomogeneous distributions of trace gases on the retrieval of profiles will be investigated.

1. INTRODUCTION

In recent years besides nadir observational geometry(e.g. [1, 2, 3, 4, 5, 6, 7]), measurements in limb geometry are providing further opportunities, namely, to extract moderate resolution profile information by measuring backscattered light viewing air masses at different elevation angles. Satellite instruments such as the Optical Spectrograph and Infrared Imager System (OSIRIS) on the Odin satellite [8], SCIAMACHY on ENVISAT [9], also the Stratospheric Aerosol and Gas Experiment (SAGE III) on the Meteor 3 have limb observation possibilities [10].

The SCIAMACHY instrument on the ENVISAT satellite is flying in a near polar Sun synchronous orbit having an inclination from the equatorial plane of approximately 98.5° and is performing one orbit in 100 minutes with equator crossing time of 10:00 in descending mode. The satellite probes the atmosphere at the day side of Earth in alternating sequences of nadir and limb measurements. Limb scans are performed with approximately 3.3 km elevation with swap across flying direction of 960 km at tangent point (TP) consisting of 4 pixels. The field of view (FOV) is 0.045° in elevation and 1.8° in azimuth that corresponds to approximately 2.5 km and 110 km at TP respectively. SCIAMACHY is measuring in the UV-vis-NIR spectral range 240 – 2380 nm having spectral resolution of approximately 0.25 – 0.55 nm in UV-vis range. For more instrumental details please refer to [9].

The aim of this study is to demonstrate a possibility to correct for horizontal gradients that appears in the measurement sensitivity area of the instrument characterized by very slant and thus long lines of sight through the atmosphere crossing large areas.

The 3D radiative transfer modeling allows the introduction of a 2D air mass factor concept (discretized not only in altitude but also e.g. in latitude) allowing the simultaneous inversion of many limb scanning sequences.

2. RETRIEVAL ALGORITHM

A retrieval algorithm of NO2, BrO and OClO vertical profiles from the SCIAMACHY limb measurements was developed at the Institute of Environmental Physics at the University of Heidelberg (IUP Heidelberg) [3, 11]. It allows efficient acquisition of the trace gas profiles, and shows good agreement of the retrieved BrO and NO2 profiles with balloon measurements [12, 13, 14].

Trace gas retrieval from SCIAMACHY measured limb spectra is done in two steps as illustrated in Fig. 1. In the first step, slant column densities (SCDs) of the trace gases are derived from the SCIAMACHY limb spectra by Differential Optical Absorption Spectroscopy.
(DOAS). Second, the trace gas SCDs are converted into vertical concentration profiles applying radiative transfer modelling either by the optimal estimation method or a least squares approach. For the algorithm details please refer to the [11].

![Diagram of the algorithm applied for profile retrieval.](figure1.png)

**3. RADIATIVE TRANSFER MODELLING – SPATIAL SENSITIVITY**

We use the 3D full spherical Monte Carlo radiative transfer model “Tracy-II” [15, 16] to calculate box AMFs which are necessary to retrieve number density profiles of trace gases from measured SCDs. The model “Tracy-II” is an up-to-date version of the RTM “Tracy” [17]. The largest advantage of Monte Carlo models in the limb geometry is that they assume not only 3D shaping of Earth both for single and multiple scattering but also provide the possibility to simulate to a high degree an inhomogeneous atmosphere. They deal with microscopic processes in the atmosphere in a probabilistic way.

The detector sees either photons directly scattered from the incoming solar radiation into the line of sight (LOS) of the instrument, or photons already scattered by the atmosphere or the ground below. The limb geometry is characterized by relatively long paths of photons along the LOS after the last scattering event in comparison to the paths before the last scattering.

The instrument has different sensitivities for different places in the atmosphere even along the line of sight. For limb measurements this distribution varies a lot with elevation being impacted by extinction provided by scattering on air molecules. Also absorbers (especially ozone) and scattering by aerosols, clouds and reflection at the ground modify the measured light intensity.

In general the instrument has higher sensitivity to air masses closer to instrument since the light contributing to the measurement integrates along the line of sight. (See schematic view in Fig. 2)

![Schematic view of spatial sensitivity distribution. An example of contributing light paths is displayed. More crossing paths means higher sensitivity for particular region.](figure2.png)

A limiting factor for the retrieval at low altitudes is the high Rayleigh scattering probability i.e. the atmosphere is optically thick. For high altitudes, where the atmosphere is optically transparent a nearly symmetrical distribution across the tangent point (TP) of photons being scattered into the LOS can be observed. But at low elevations having optically dense atmosphere most of the photons visible by the instrument are contributing to the LOS at sites far from the TP in the direction of the instrument. For an illustration of scattering events in limb geometry as modelled by the 3D Monte Carlo RTM Tracy II, see Fig. 3. Besides the shifted sensitivity towards areas closer to the instrument this also means that the measured spectra practically do not contain information about the lower part of atmosphere.

Fig. 4 shows an example of box AMFs calculated for limb geometry. The low sensitivity for altitudes below 12-15 km can be realized. In fact, as will be seen later this fact allows to retrieve trace gases starting from above this altitude. On the other side, the maximum retrieval altitude is not determined by the sensitivity (as expressed by the AMFs) but low intensities that can be measured at high elevations giving lower signal to noise ratio.

**4. HORIZONTAL GRADIENTS**

Photochemically active species like ozone, BrO, NO2 and OClO can vary significantly in space and time due to their dependence on solar illumination, atmospheric chemistry and transport. The large sensitivity area of satellite limb geometry characterized with possibly large horizontal extension requires the consideration of the gradients of trace gas distributions inside this area.
Since the instrument is more sensitive to the air masses closer to the instrument this side will have a larger effect on measurement results.

If horizontal gradients exist, algorithms which do not account for horizontal variation of trace gases will introduce errors in the retrieval: If the concentration gradient in the instrument direction is positive this will lead to a higher concentration as in reality and the peak values will tend to appear at lower altitudes. In the case of a negative gradient lower values will appear.

Algorithms assuming homogeneous horizontal distributions do not take into account that the LOS is crossing areas with higher concentration than those that appears around tangent point.

5. TWO-DIMENSIONAL RETRIEVAL – THE IDEA

In order to account for these gradients we suggest a two dimensional retrieval where we combine consecutive limb scanning sequences and discretize the measurement not only in altitude but also in latitude. In
this approach we invert these consecutive measurements at once including in the retrieval the information about the horizontal sensitivity of the measurements simulated by the radiative transfer model. Thus, the 2D approach is distinguishing between air volumes at different areas along line of sight. Precondition for an improvement in respect to the conventional one dimensional algorithm is that the change of the atmospheric trace gas concentrations (particularly because of SZA change) in time is negligible. Also the distance between following scanning sequences should be as small as possible so that they in some extent overlap (see Fig. 5) and at least less than the sensitivity area of one limb measurement. Both criteria are fulfilled for the northern part of SCIAMACHY orbits, where 3 or 4 limb scanning sequences are made without nadir states between.

Figure 5. Spatial correlation of two successive limb scanning sequences. If the distance is small enough for the measurement areas to partially overlap, the measurement of air masses is made in different instrument positions.

6. 2 DIMENSIONAL BOX AIR MASS FACTORS

In order to retrieve profiles of the trace gas number density the inversion of directly measured slant column densities should be made. Box air mass factors are the connection.

The box AMFs depicted in Fig. 4 demonstrate only the sensitivity to vertically resolved atmospheric layers. For an instrument elevation $z$ they are defined as ratio of slant column density ($SCD_i$) of the particular atmospheric layer $i$ and the vertical column density ($VCD_i$) of this layer:

$$AMF_{iz} = \frac{SCD_{iz}}{VCD_i}$$

(1)

For the 2D inversion the air mass factors are discretized not only in altitude but also in latitude $j$:

$$AMF_{ijz} = \frac{SCD_{ijz}}{VCD_{ij}}$$

(2)

Figure 6. Comparison between 1D and 2D box air mass factors. The latitudinal distribution of the air mass factor along the line of sight of the instrument can be realized for 2D box AMFs. Introducing 2D AMFs in the retrieval is subordinating air masses measured not only in altitude but also in latitude.

The 2D box AMFs describe the spatial character of the sensitivity of limb measurements in a more appropriate way, see Fig. 6. The areas crossed by the lines of sight can be nicely seen. The higher sensitivity for the instrument side also can be realized from Fig. 6.

7. RESULTS

A retrieval of OCIO and NO$_2$ number densities as function of latitude and altitude, both for 1D and 2D approach, is plotted in Fig. 7. Lower values for OCIO appear for the latitude region where the second scanning sequence is localized. In the 2D retrieval approach, the model uses knowledge from the previous state assigning part of the measured slant column densities with high concentrations more to the North.
For the region with strong horizontal gradients, introduced by atmospheric photochemistry, large differences between both approaches can be seen. Since the 1D approach assumes a homogeneous horizontal distribution it is not taking into account that the LOS is crossing areas with higher concentration than those that appears around the tangent point. But the 2D approach at the same time is distinguishing between air volumes at different areas along the line of sight.

In the comparison shown in Fig. 7 lower concentrations for 2D retrieval of OCIO can be seen for latitudes below 65°. Also the peak is not so pronounced for the layer at 15-18 km altitude - the relation between the number density at 15-18 km with that at 18-21 km is decreasing. In the second case study we applied the 2D approach on the retrieval of NO₂ profiles (see right panel of Fig. 7). For the NO₂ retrieval where a negative gradient in the direction of instrument occurs the increase of the values in the 2D approach is visible for 21-30 km and latitudes of 55-65° where a substantial overlap of consecutive limb scanning sequences appears. However the difference between the 1D and the 2D approaches is smaller as for OCIO case because the gradient is smaller for NO₂.

8. CONCLUSIONS

SCIAMACHY provides scattered light measurements in limb geometry from which atmospheric trace gas profiles can be successfully retrieved. The two step approach (DOAS, RTM combined by optimal estimation) allows to investigate the effects of spectroscopy and radiative transfer on profiles separately. Assuming horizontal homogeneous trace gas distributions can lead to errors in retrieved profiles. The combination of SCIAMACHY limb scanning sequences in one inversion constraint allows taking into account the spatial correlation between them. The application of a simultaneous inversion of consecutive limb scanning sequences for SCIAMACHY UV/vis measurements is demonstrated for the first time. It allows the correction for cases with large horizontal gradients: peak concentrations and altitude is corrected in the right direction for both type of gradients (positive and negative). A small distance between limb scanning sequences improves the horizontal resolution of measurements; therefore an instrument using only UV/vis limb measurements would be an advantage.

9. REFERENCES