COMPARISON OF SCIENTIFIC SCIAMACHY PRODUCTS WITH GROUND-BASED MEASUREMENTS

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ABSTRACT

Measurements taken in the framework of the Ground-Based Measurements and Campaign Database Subgroup (GBMCD) of the Atmospheric Chemistry Validation Team (ACVT) are compared to selected preliminary results of scientific algorithms to determine atmospheric parameters from measurements of SCIAMACHY. Presented are comparisons with algorithms to determine NO_2 total column, CH_4 and CO total columns, ozone profiles from limb and detection of PMCs. NO_2 total columns are compared with three ground-based DOAS stations. Three algorithms to determine CH_4 and CO total columns are compared with FTIR measurements taken at Kiruna, Ny-Ålesund and Jungfraujoch. First limb ozone profiles are compared with ozone sondes from Ny-Ålesund, Hohenpeißenberg, and Neumayer station (Antarctica) and Lidar measurements from Lauder. A method for detecting polar mesospheric clouds from limb measurements is compared to the observation of noctilucent clouds with the UBonn Lidar at the Esrange near Kiruna. All results show the potential of SCIAMACHY to detect the anticipated and even further products.

1 INTRODUCTION

SCIAMACHY (Scanning Imaging Absorption Spectrometer for Atmospheric CHartographY) on-board Envisat is a spectrometer designed to measure sunlight, transmitted, reflected and scattered by the earth atmosphere or surface in the ultraviolet, visible and near infrared wavelength region. Observing geometries are nadir, limb, solar and lunar occultation.

SCIAMACHY measurements yield the amounts and distribution of O_3, BrO, OClO, ClO, SO_2, H_2CO, NO_2, CO, CO_2, CH_4, H_2O, N_2O, pressure, Temperature, aerosol, radiation, cloud cover and cloud top height. These are anticipated as operational products from nadir and/or limb measurements as total columns and profiles, respectively.[1].

At the time of the Envisat Validation Workshop, only a limited number of operational products from SCIAMACHY were available. First results of the validation of ozone and NO_2, calculated by the near-real-time- (NRT-)processor,are presented in [2], further products are not available or show unphysical results [3]. Limb products, e.g. profiles which will be made by the offline- (OL-)processor only, were not available at all to the validation teams.

Beyond the development of the operational processor, other groups in the scientific community also develop algorithms to determine atmospheric parameters from SCIAMACHY measurements. Such products are are not only of general scientific interest, the work on them is also useful for the development or improvement of the operational systems. Scientific products are used in the verification team by comparing the results of the operational and the scientific algorithms to draw conclusions for the quality of both. Scientific algorithms, which are too slow for operational usage but very accurate can be used to verify the simplifications used in the operational retrieval. Additionally, scientific products can prove the concept of improved or alternate algorithms, which in the future may be used for the operational system. Analyzing the sources of errors in scientific products can help in identifying calibration problems, one example is the probable altitude shift in the current limb products, see section 4.

To determine the quality of the scientific products, co-operation with the validation scientists for comparisons with independent measurements is necessary. Because these validation activities are not foreseen in the official schedule, only limited activities are possible on a best effort basis. Nevertheless, case studies or validation on limited datasets is very useful for the development of scientific products.

Here a short and for sure incomplete list of scientific developments is given. Beyond NO_2 total column from nadir measurements, which will be presented in section 2, the DOAS groups at the University of Bremen (Germany) and at the University of Heidelberg (Germany) also works on the other UV-vis minor trace gases (BrO, SO_2, HCHO, OClO) and ozone. For nadir IR-products, scientists at Heidelberg, Bremen and SRON (Space Research Organization Netherlands, de Bilt, The Netherlands) have first algorithms available. First goals are methane and CO, but also for water vapor and CO_2 work has been started. First Comparisons for methane and CO are given here in section 3. At KNMI (Royal Netherlands Meteorological Institute, de Bilt, The Netherlands) scientists work on cloud and aerosol information. Scientists also work on the exploitation of limb and occultation measurements from SCIAMACHY. At the University of Bremen, two different approaches for retrieving limb ozone profiles are used. One of these by Christian von Savigny will be compared to ozone sondes and Lidar measurements in section 4. Additionally, limb profiles of NO_2, BrO and OClO are successfully retrieved by SAO (Smithsonian Astrophysical Observatory, Cambridge, USA) and the Bremen group. Work on deriving IR limb profiles has been started at the University of Bremen. Additionally, the occultation group in Bremen works on solar (and also lunar) occultation to derive ozone, NO_2, and BrO profiles. Scientists also work on products, which are not foreseen as operational products. In section 5 the detection of noctilucent clouds (NLCs) with SCIAMACHY is shown. At least at SAO and Bremen, work already started to exploit the limb-nadir matching pattern of SCIAMACHY operations to derive tropospheric columns.

All these efforts to get most out of SCIAMACHY measurements suffer at the time of the Envisat Validation Workshop from following limitations:

- The quality of the radiances/irradiances of the operational products is limited. The polarization correction is wrong, problems are known for the pixel-to-pixel gain and etalon. The wavelength calibration can be improved.
- The amount of available level 1b products from SCIAMACHY. Usually, scientific algorithms are based on the radiance/irradiance products of SCIAMACHY (level 1b products). These are currently not available to a wider community. A limited set of institutions has received a set of products via a satellite link, which is primarily used to disseminate level 0 products to the institutions involved in calibration and instrument monitoring during the commissioning phase. A very small subset of products is available in the verification team, where scientists from many institutions participate.
- For all algorithms based on the near-infrared channels 7 and 8, the time-depended transmission of the ice-layer has to be taken into account.
- Scientific algorithms are not part of an operational system, e.g. usually the amount of data that can be processed is limited.

In the following sections, first comparisons for the products mentioned above with ground-based measurements will be given.

2 COMPARISON OF NO_2 COLUMNS

Vertical columns of NO_2 in the distributed SCIAMACHY products are currently of limited quality [2]. At the University of Bremen, Andreas Richter uses the DOAS approach also utilized in the operational processor to generate scientific NO_2 columns. Instead of using the solar irradiance an earthshine radiance is used as a reference spectrum. This approach avoids uncertainties in the absolute calibration of irradiance and radiance. For the reference spectrum, a pacific ground-scene was selected, which can be expected to be completely unpolluted. e.g. without enhanced tropospheric NO_2 values.

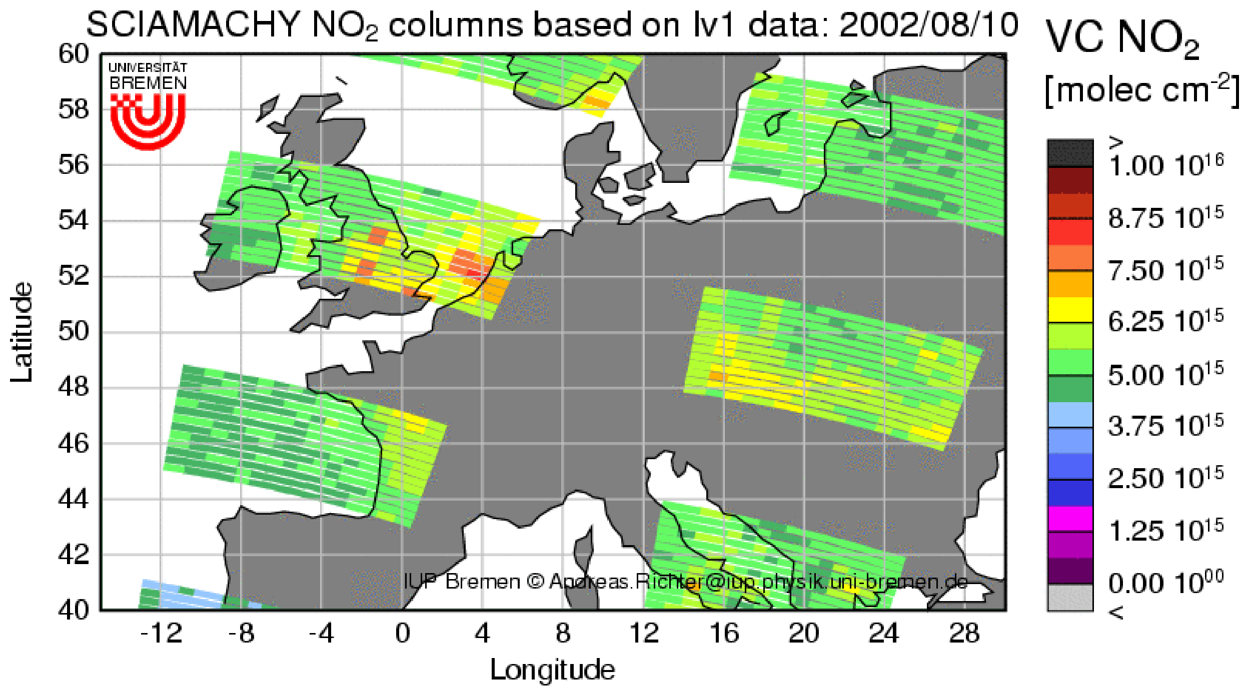

Figure 1: NO_2 columns over Europe on August 10th, 2003, calculated with the scientific DOAS algorithm at the University of Bremen from SCIAMACHY nadir measurements. The high spatial resolution allows the identification of individual sources of tropospheric pollution, for example the industrial centers in Great Britain or Roma in Italy.

A climatological value for the NO_2 column in this area is used. In principal, the assumed amount of total NO_2 in the reference spectrum is a free parameter of this retrieval.

Enhanced spatial resolution, compared to the predecessor instrument GOME, gives improved possibilities to identify sources of NO_2, for example urban pollution. Figure 1 shows the outcome of the above explained retrieval, enhanced values are observed for industrial areas in Great Britain and the Netherlands, Roma can also be identified. The relative behavior of the retrieved NO_2 values are reasonable and as expected.

The absolute values are examined by comparing these values with measurements of the ground-based DOAS network. Figure 2 shows comparisons with the stations located in Ny-Ålesund, Bremen and Nairobi, which are operated in the framework of AOID 331 [4]. Given are the DOAS measurements for morning (DOAS AM) and evening (DOAS PM) and the available retrievals from SCIAMACHY with a ground-pixel center within 300 km from the station. For Ny-Ålesund, all values agree within 5 – 10 % with the ground-based observation. For Bremen and Nairobi, the lowest retrieved values in most cases fits well with the morning DOAS observations. Higher values from SCIAMACHY are enhanced tropospheric NO_2 contributions caused by urban pollutions of the cities Bremen and Nairobi. Ground based DOAS instruments primarily detect the stratospheric NO_2 column only, actually they are corrected for tropospheric pollution. Therefore, enhanced values from the satellite are expected and the retrieved columns fits well with the ground-based observations.

3 Comparison of CH_4 and CO

Vertical column densities of important atmospheric trace gases (CH_4 , CO, CO_2, H_2O, and N_2O) can be derived from the SCIAMACHY near infrared (NIR) nadir measurements. Operational data products are derived with the BIAS (Basic Infrared Absorption Spectroscopy) retrieval algorithm. At time of the Envisat validation workshop, these operational products contain no physical meaningful results [3].

Here, three approaches for deriving CH_4 are compared to ground-based Fourier Transform InfraRed (FTIR) measurements. In the following paragraphs, these approaches are briefly described.

WFM DOAS (Weighting Function Modified Differential Optical Absorption Spectroscopy) is a modified DOAS algorithm mainly being developed for the retrieval of trace gas vertical column densities from SCIAMACHY and GOME/ERS-

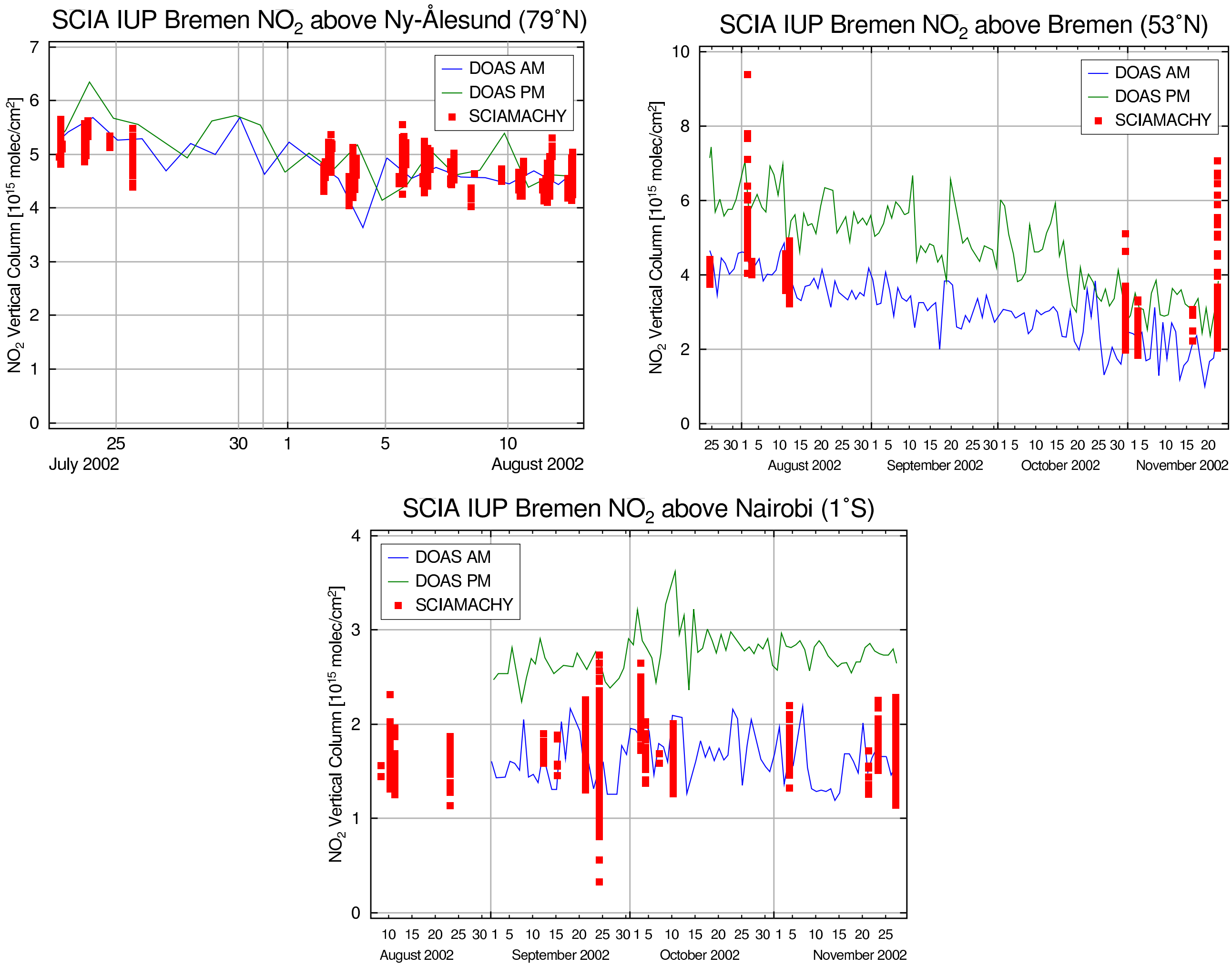

Figure 2: Comparison of Scientific NO_2 columns calculated with the scientific DOAS algorithm at the University of Bremen from SCIAMACHY nadir measurements with ground-based DOAS measurements at Ny-Ålesund, Bremen and Nairobi.

2 nadir radiance and solar irradiance spectra by Michael Buchwitz at the University of Bremen. WFM DOAS is based on linear least squares fitting (the logarithm of) a linearized radiative transfer model plus a low order polynomial to the logarithm of the ratio of a measured nadir radiance and solar irradiance spectrum [5]. The main difference with respect to standard DOAS is that the WFM DOAS reference spectra are derivatives of the radiance rather than trace gas absorption cross sections. The fit parameters are the desired vertical columns directly, i.e., there is no explicit airmass factor conversion. For this work, an additional correction function is used to improve the fit despite of the calibration problems in the level 1 product [6].

At the Space Research Organization Netherlands (SRON), Hans Schrijver develops an algorithm using an iterative maximum likelihood method for determining the atmospheric tracer concentrations from the radiance measurements. A modeled spectrum is then fitted to the measured spectrum in an iterative way. The calculation of the modeled spectrum starts with the calculation of optical depths deduced from a priori atmospheric profiles of the absorbing gases H2O, CH4, CO, and N2O, temperature and pressure. From these optical depths the earth radiance is calculated in a forward model, which is then transformed by a simplified instrument model to represent the radiation detected by the instrument detectors. Limits of the sensitivity of the retrieved CO and CH4 concentrations due to detector noise was described by [7]). This paper showed that retrieved concentration of CH4 has a precision of 1%, and that the lower limit for the precision of CO is down to 10% in most cases. This precision does not include model errors due to imperfect knowledge of the molecular spectrum, clouds, etc., and it furthermore depends strongly on the surface albedo, latitude, and the total column amount of the trace gasses.

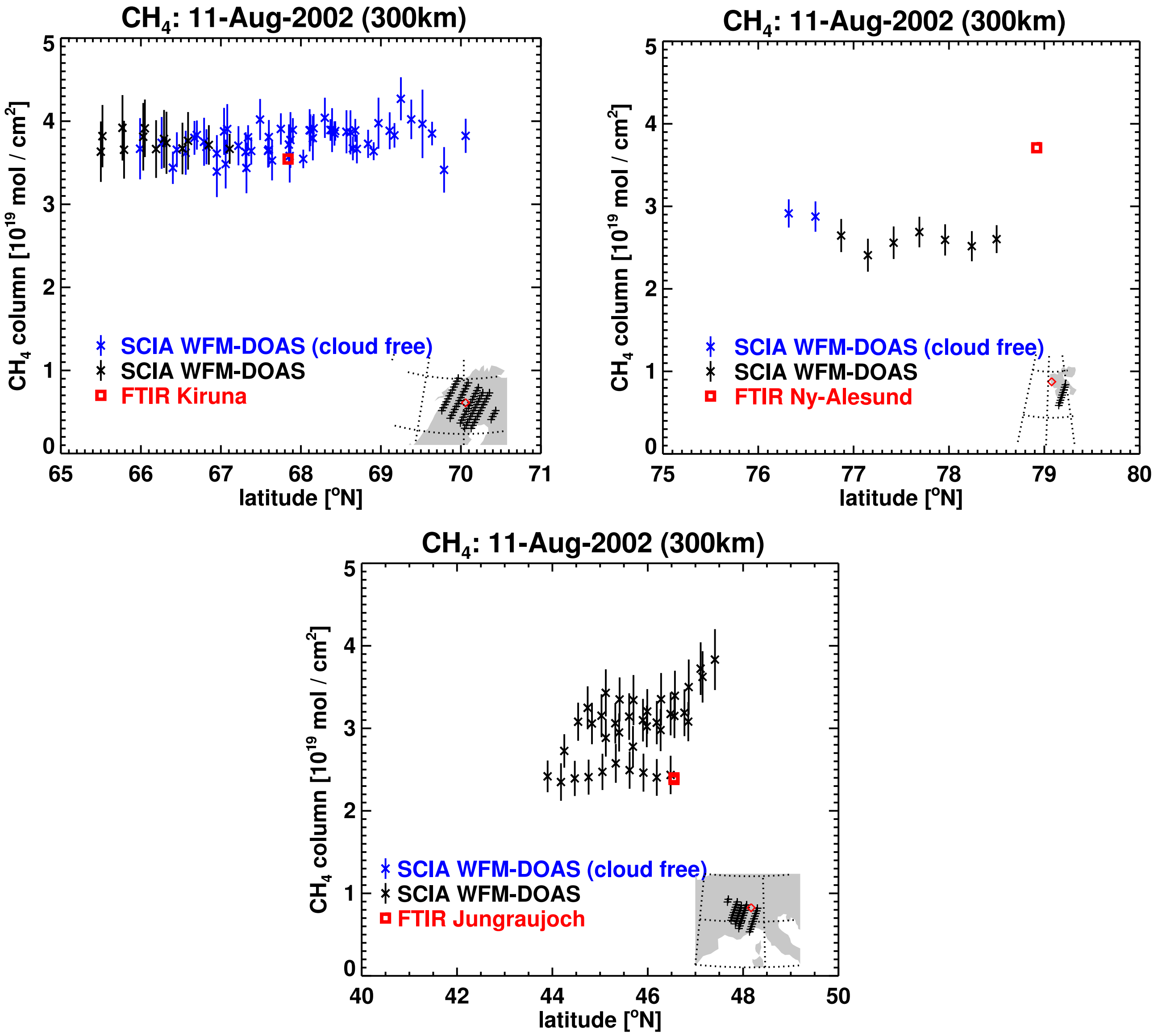

Figure 3: Methane vertical column densities calculated with WFM-DOAS (University of Bremen) from SCIAMACHY nadir IR measurements, compared with ground-based FTIR measurements from the stations Kiruna, Ny-Ålesund and Jungfraujoch. The retrieval results of the SCIAMACHY pixels within a radius of 300 km around each stations are shown, divided in cloud-free and cloud-contaminated pixels. The small maps in the lower left corner of the plots indicates the locations of the stations and the used SCIAMACHY ground pixels.

At the University of Heidelberg, Christian Frankenberg develops a near-infrared retrieval of vertical column densities, which is an iterative DOAS approach. The absorptions are calculated using an atmospheric model consisting of 50 height layers. For each layer the absorption cross sections of the respective trace gases are determined according to the prevailing temperature and pressure conditions (assuming a Voigt line-shape). Spectral line parameters were taken from the HITRAN database [8]. The derived total optical density is fitted to the sun-normalized measurement spectra by using an iterative DOAS technique.

In the figures 3, 4, and 5 the out-coming of the described algorithms for methane are compared to FTIR measurement in Kiruna [9], Ny-Ålesund [10] and Jungfraujoch [11]. Figure 6 shows the results for CO of WFM-DOAS. Whereas Kiruna and Ny-Ålesund values are taken at the same day as the SCIAMACHY measurements (August 11th, 2002), at Jungfraujoch station there is no measurement available for this day. Instead, the two measurements from August 8th and August 14th, 2002 are chosen for comparison. CO and CH_4 are mostly distributed in the lowest parts of the troposphere.

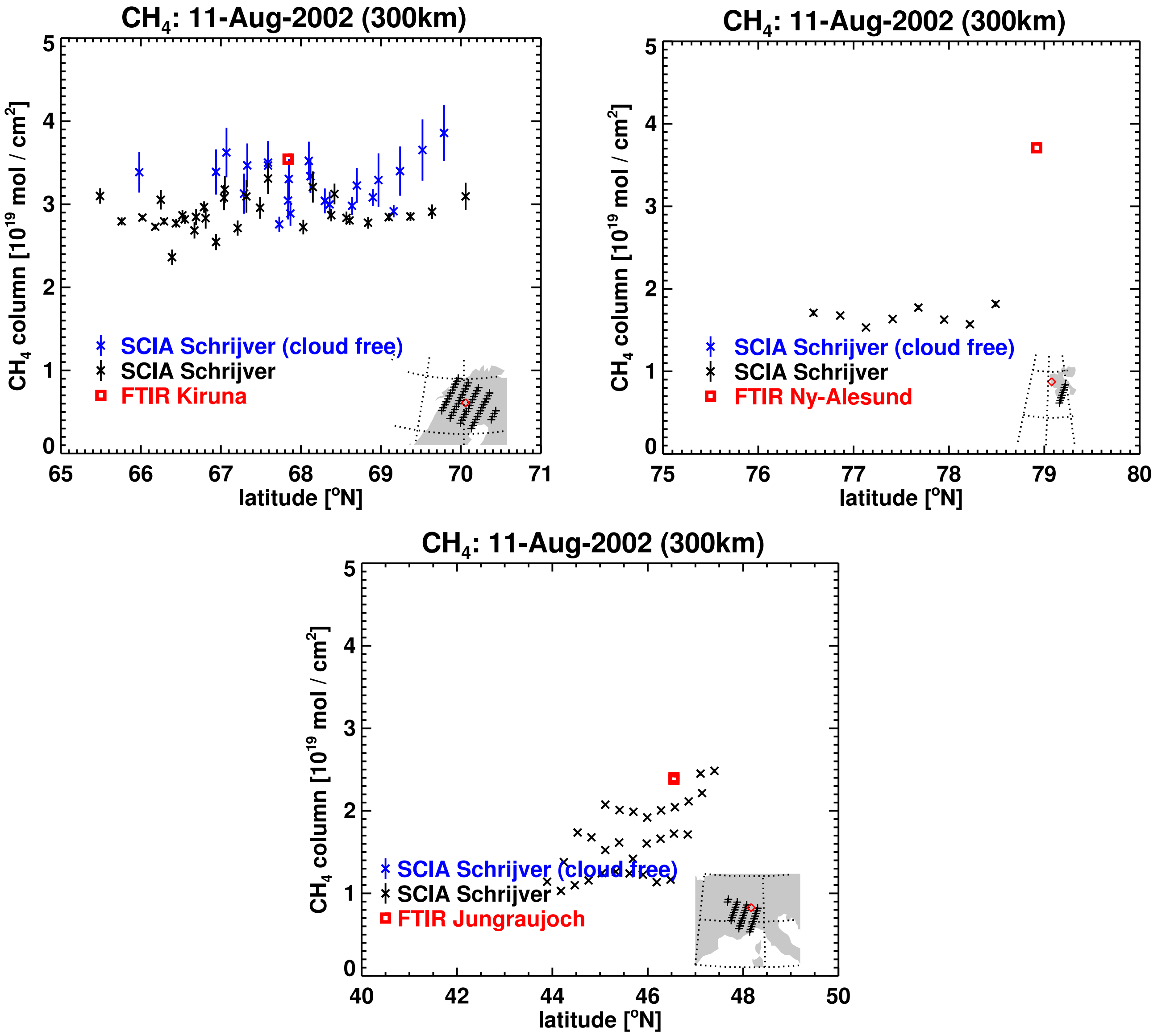

Figure 4: Methane vertical column densities calculated with the method by Hans Schrijver (SRON) from SCIAMACHY nadir IR measurements, compared with ground-based FTIR measurements from the stations Kiruna, Ny-Ålesund and Jungfraujoch. The retrieval results of the SCIAMACHY pixels within a radius of 300 km around each stations are shown, divided in cloud-free and cloud-contaminated pixels. The small maps in the lower left corner of the plots indicates the locations of the stations and the used SCIAMACHY ground pixels.

Therefore, only for cloud-free ground-pixels good agreement between satellite and ground-based measurement can be expected. A detailed analysis has to take into account properly the altitude levels of the stations and the ground-pixel scenes and the cloud coverage of the observed ground-pixel. This is beyond the scope of this paper, only first comparisons are presented here.

Figure 3 shows the comparisons of the WFM-DOAS approach. For Kiruna, the results fit quite well. Ny-Ålesund values are about 30% too low. At Jungfraujoch, some values fit quit well, but a large subset gives to high values. This can be explained by the high altitude of the station in the Alpes, so that many of the SCIAMACHY ground-pixels see methane further down.

The same comparison for the SRON approach is given in 4. In general, the results are the same, but the values are lower than for the previous comparison. For Kiruna, the values for cloud-free scenes are in general higher than for cloud contaminated scenes, which is the expected behavior.

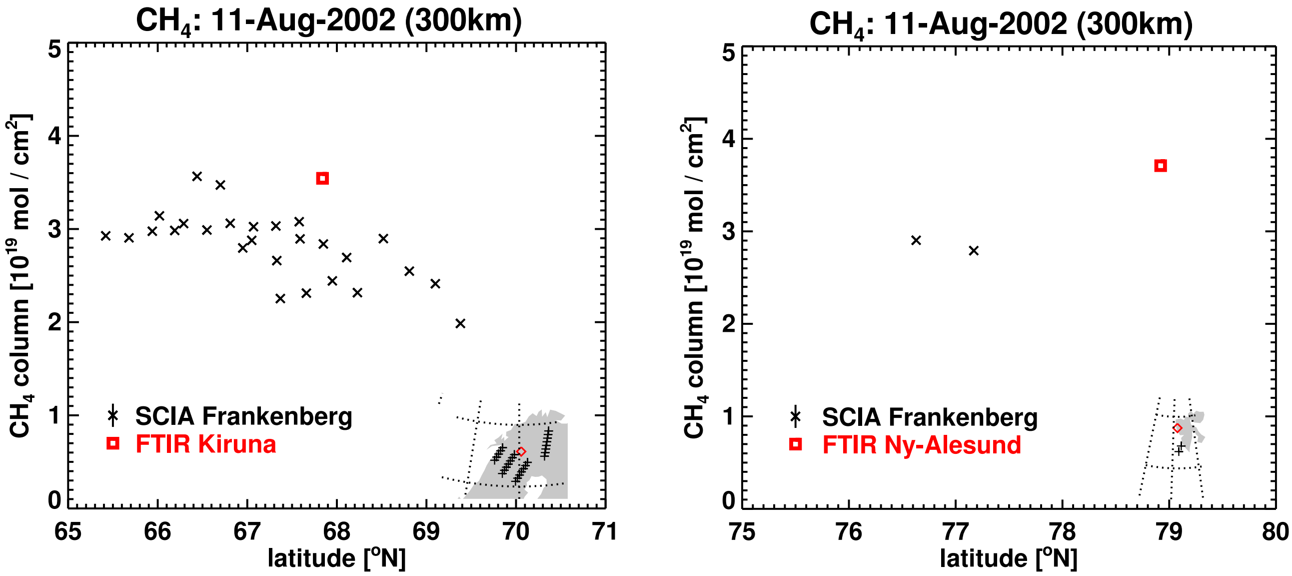

Figure 5: Methane vertical column densities calculated with the method by Christian Frankenberg (University of Heidelberg) from SCIAMACHY nadir IR measurements, compared with ground-based FTIR measurements from the stations Kiruna and Ny-Ålesund. The retrieval results of the SCIAMACHY pixels within a radius of 300 km around each stations are shown, cloud-free and cloud-contaminated pixels are currently not distinguished. The small maps in the lower left corner of the plots indicates the locations of the stations and the used SCIAMACHY ground pixels.

The comparison of the Heidelberg approach is shown in 5. Cloud-free and cloud-contaminated pixels are currently not distinguished. Here, results are only available for Kiruna and Ny-Ålesund. The Kiruna values are usually a bit too low. For Ny-Ålesund, the values are also a bit too low, but they fit better than the results of the other two approaches.

For the WFM-DOAS approach, a first comparison of CO retrieval results is given in figure 6. The retrieved values show high scattering with large error bars. For Kiruna and Ny-Ålesund, the values are about 30 - 50 % lower than the ground-based observation. For Jungfraujoch, the SCIAMACHY values fit quite well to the retrieved values within the error bars.

The first results of the scientific algorithms to detect methane and CO from SCIAMACHY nadir IR measurements give promising results, also there is still a lot of work to achieve high quality results.

4 Comparison of ozone profiles from limb measurements

At the University of Bremen, Christian von Savigny applied the method originally developed for the OSIRIS instrument to SCIAMACHY limb measurements to derive stratospheric ozone density profiles between 15 and 40 km altitude.

The method, which closely follows that of Flittner et al. [12] and McPeters et al. [13], is based on the analysis of normalized and paired limb radiance profiles in the center and the wings of the Chappuis-Wulf absorption bands of ozone. It employs a non-linear Newtonian iteration version of Optimal Estimation (OE) [14] coupled with the pseudo-spherical multiple scattering radiative transfer model SCIARAYS [15].

Here, first comparisons with ozone sondes launched from Ny-Ålesund [10], Hohenpeißenberg[16] and the Neumayer station (Antarctica) [10] and with Lidar measurement in Lauder are presented.

In Figure 7, the comparison with the ozone sondes are given. For the high northern latitudes (Ny-Ålesund), two matches with sondes launches are found within the available set of Level 1 products. On July 24th, the ozone-sonde shows a secondary maximum in the profile around 11 km. The SCIAMACHY ozone profile gives the same structure, but the maxima are moved up about 4 km. On August 7th, the sonde profile is matched quite well by the SCIAMACHY profile. Only the thin layers around the tropopause cannot be detected by this algorithm.

The two ozone sondes measurements at the Neumayer station (Antarctica) on October 10th and November 3rd both show reduced ozone content in the lower stratosphere. In both cases Neumayer is near the edge of the vortex, although at November 3rd the vortex is displaced towards Fireland and disappearing the following days. Again, the SCIAMACHY profiles fits the overall structure, but overestimates the altitude of the profile. Additionally, at the edge of the vortex for a quantitative validation the observed air-masses have to be very carefully checked because of the long light pass along the line of sight of the limb geometry.

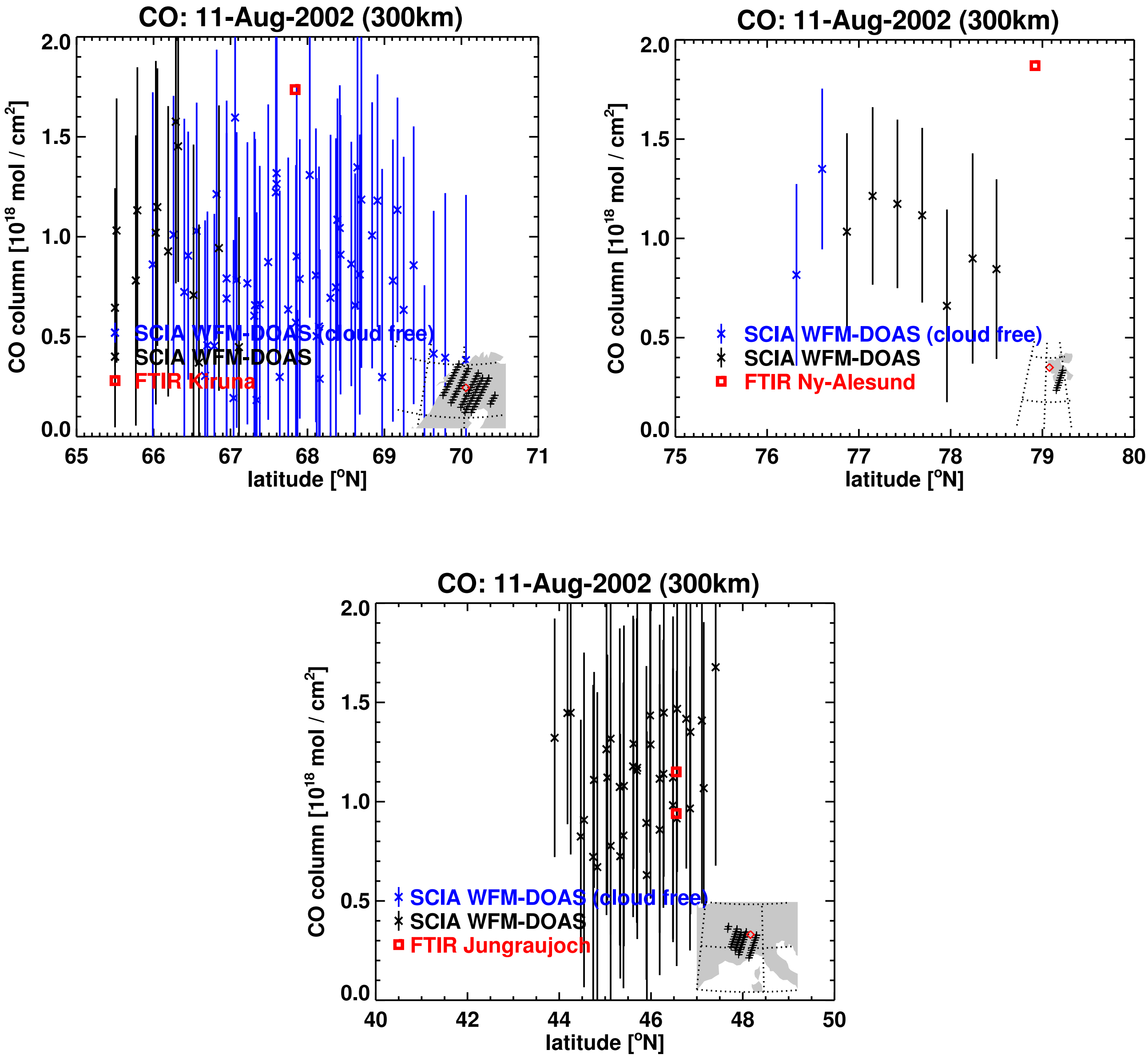

Figure 6: CO vertical column densities calculated with WFM-DOAS (University of Bremen) from SCIAMACHY nadir IR measurements, compared with ground-based FTIR measurements from the stations Kiruna, Ny-Ålesund and Jungfraujoch. The retrieval results of the SCIAMACHY pixels within a radius of 300 km around each stations are shown, divided in cloud-free and cloud-contaminated pixels. The small maps in the lower left corner of the plots indicates the locations of the stations and the used SCIAMACHY ground pixels.

In the mid-latitudes at Hohenpeißenberg, the observed profiles agree well at November 05th with the exception of again a small altitude offset. On November 22nd, the SCIAMACHY profile underestimates the amount of ozone around the maximum, but this might be also a physical difference, because the tangent point is a few hundred kilometers north of Hohenpeißenberg.

Six matches between the available level 1 products and Lidar measurements at Lauder are found, all in July and August 2002. The comparison is given in Fig. 8. Because the Lidar is measuring at nighttime, the measurement before and after the SCIAMACHY overpass is given. In general, we find the same behavior as before. The overall structures agrees well, whereas an altitude shift upwards can be observed, leading to an overestimation of the amount of ozone above the ozone maximum and an underestimation below.

Altitude shifts were also observed for other profile retrievals from limb and occultation [17]. Nevertheless, the overall

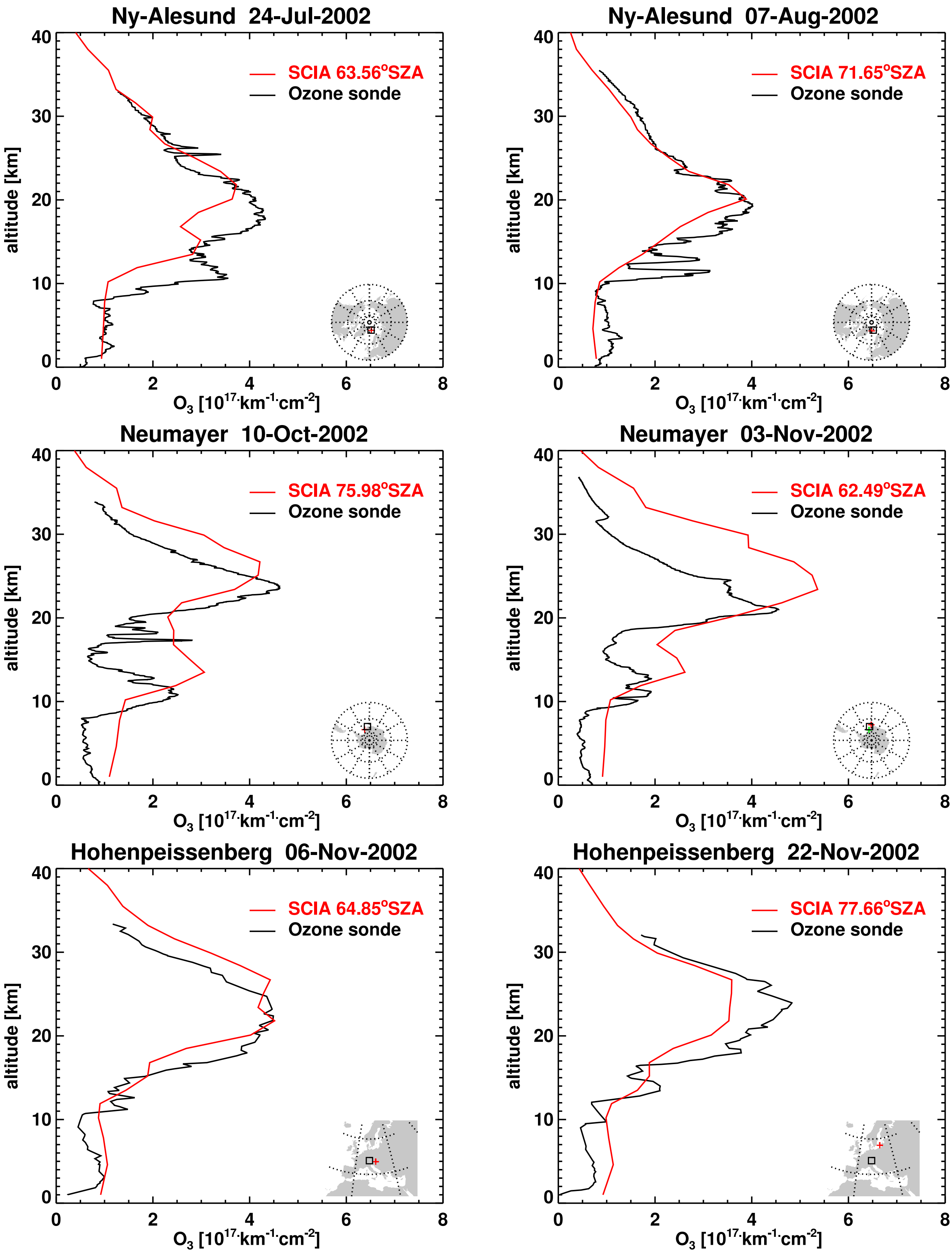

Figure 7: Comparisons of SCIAMACHY limb ozone profiles with ozone-sondes from Ny-Ålesund, Hohenpeißenberg and the Neumayer station (Antarctica). The small maps in the lower right corners indicates the location of the station the limb tangent point.

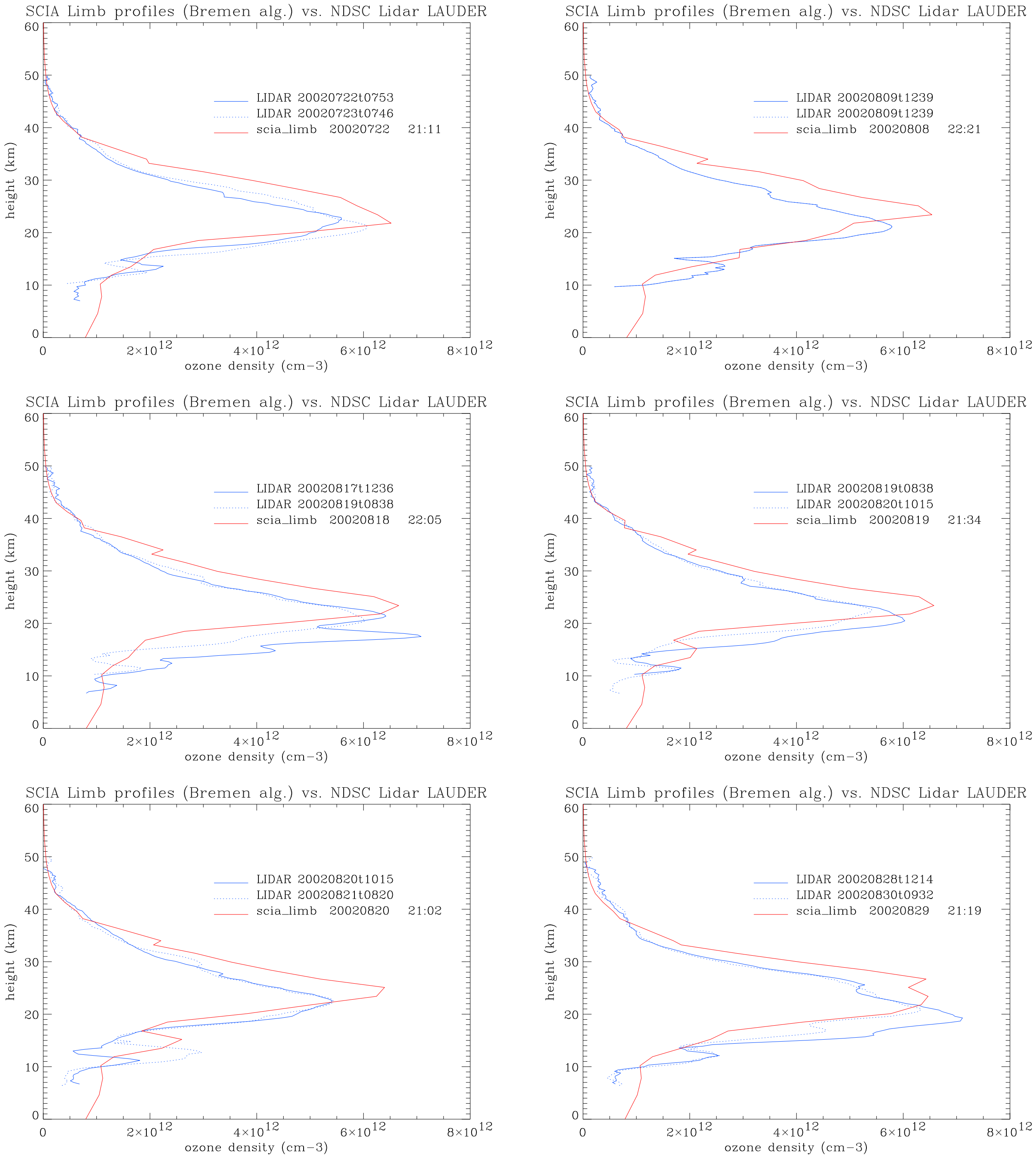

Figure 8: Comparisons of SCIAMACHY limb ozone profiles with Lidar profiles from Lauder. The lidar measurements from the night before and after the SCIAMACHY overpass is given. Figures are provided by Robert Koelemeijer,RIVM.

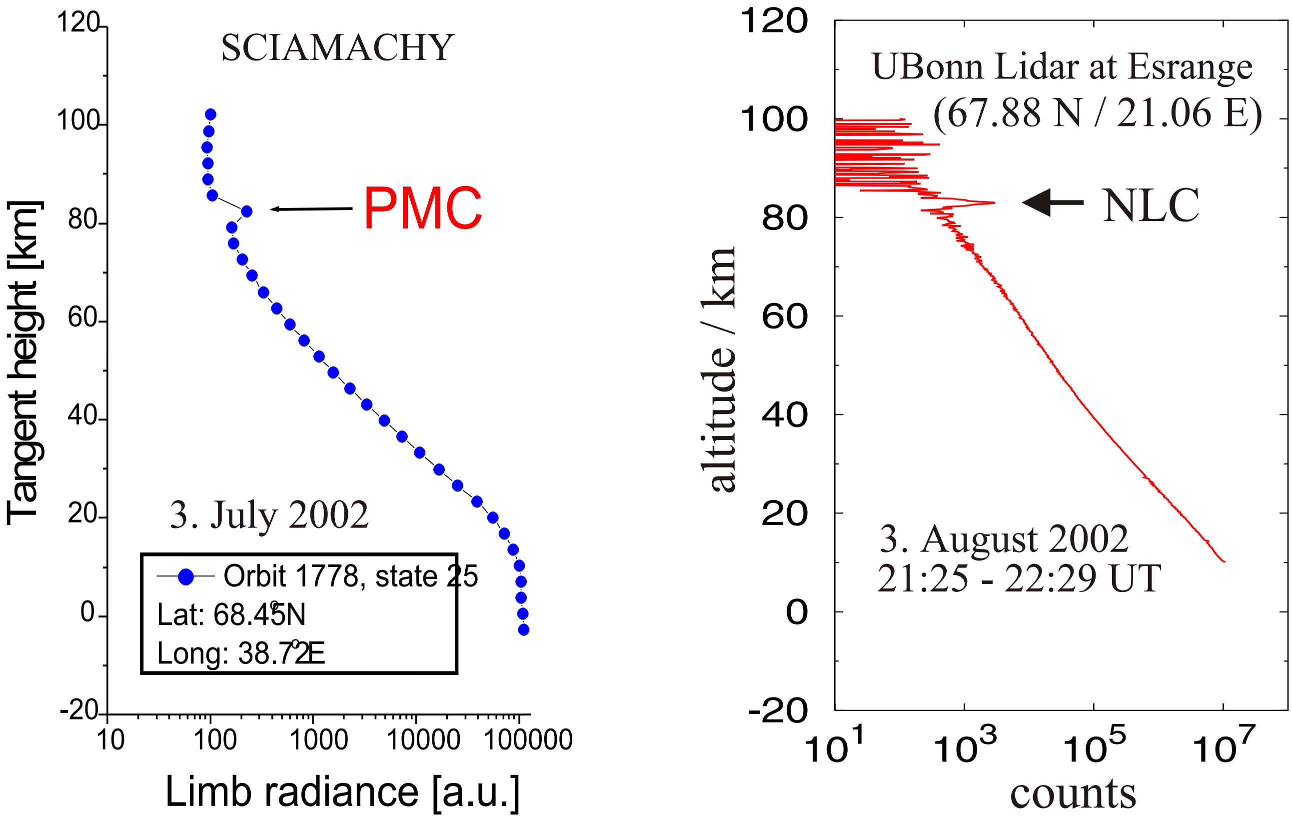

Figure 9: Example of possible PMC/NLC comparison. Shown are SCIAMACHY data of July 3rd (left panel) and Lidar data of August 3rd, 2002 (right panel). Although there is no spatial and temporal coincidence, the observed cloud altitude is quite similar.

agreement between ozone profiles retrieved by the used method from SCIAMACHY limb measurements and the ground-based observations is already very good.

5 Detection of PMCs

Polar Mesospheric Clouds (PMC) and Noctilucent Clouds (NLC) are two different names for the same phenomenon, namely clouds of ice particles which form at 82–83 km altitude, slightly below the cold summer mesopause. At this altitude temperatures fall frequently below 140 K and ice particles can form. This occurs during an approximately 12 week period cantered about two weeks after solstice, which comprises mid November to late February on the southern hemisphere and mid May to late August on the northern hemisphere. Satellite instruments as well as Lidars are able to observe these clouds.

NLCs are easily detectable with SCIAMACHY observations of limb scattered radiation, since the NLC backscatter appears as an anomalous enhancement of the limb radiance at the altitude of the NLCs, i.e. about 83 km. This is illustrated in Fig. 1. The detection algorithm checks for an increase in limb radiance that is greater than an exponential increase. Without the presence of a NLC in the instrument FOV the limb radiance would approximately increase exponentially with decreasing tangent height in the optically thin regime. This is because the atmosphere's background density increases roughly exponentially with decreasing altitude.

SCIAMACHY is not only capable of detecting and mapping NLCs, but information on the NLC particle sizes can be extracted as well. This is done by determining the spectral signature of the NLC backscatter in the UV spectral region, where multiple scattering and albedo effects are negligible [18].

The University of Bonn Lidar is located at the Esrange (68N, 21E) near Kiruna in northern Sweden [19]. During a validation campaign lasting from July 16th to August 31th, 2002, 36 measurement runs were performed. Relative density profiles and absolute temperature profiles as well as tropospheric and mesospheric aerosol layers could be measured and

Table 1: Observation dates of NLCs by the UBonn Lidar at the Esrange in July/August 2002

Date	18.07.	21.07.	22.07.	27.07.	29.07.	03.08.	04.08.	11.08.	16.08.
begin / UT	18:30	11:00	19:00	05:30	02:00	21:25	20:30	20:30	21:30
end / UT	21:00	16:00	23:10	06:30	04:00	22:30	21:30	22:30	23:00

products of the ENVISAT atmospheric instruments GOMOS, MIPAS and SCIAMACHY validated [20]. The Lidar is capable to perform nighttime as well as daytime measurements and thus able to observe NLCs independently of the solar zenith angle. During the measurement campaign NLCs could be observed on nine measurement runs. In Tab. 1 the NLC observation-dates of the UBonn Lidar at Esrange are listed.

Up to now there are no data available with coincident NLC-observations of SCIAMACHY and the UBonn Lidar, but the principles of validation can be seen from Fig. 9. Shown is a SCIAMACHY observation of a polar mesospheric cloud on July 3rd, 2002 at 68.45N and 38.72E. The Lidar observation (right panel) is on August 3rd, 2002 at 67.88N and 21.06E. Even though there is no spatial and temporal coincidence on these observations, the clouds are observed at the expected altitude in both measurements. For further analysis it is necessary to compare observations in close spatial and temporal coincidence.

These comparisons are also usable for validation of SCIAMACHY altitude registration.

6 CONCLUSIONS

First examples from various types of SCIAMACHY measurements were compared to independent ground-based measurements. From nadir UV-vis measurements, NO_2 columns by the University of Bremen algorithm show very good agreements with three stations of the ground-based DOAS network. For nadir-IR measurements, three algorithms from the Universities of Bremen and Heidelberg and from SRON show promising results for methane and CO (Bremen only), when compared to ground-based FTIR instruments in Kiruna, Ny-Ålesund and Jungfraujoch. This is very remarkable, because the calibration problems of the processor and the ice layer effects cumulate in the IR channels 7 and 8. First ozone limb profiles show good agreement to coincident ozone-sonde and Lidar measurements except the observed altitude shift up to 3 km of the profile. Because other limb and even occultation retrievals show similar offsets, this is a hint of an altitude problem in the level 1 product. As an example of a product not foreseen as an operational one from SCIAMACHY, the possibility of detecting noctilucent clouds was shown by similar observations of the UBonn Lidar. Such comparisons will be usable for validating the SCIAMACHY altitude registration.

The presented results clearly show the potential of the SCIAMACHY instrument to be used for determinating the anticipated and even further products. The unavailability of the majority of foreseen operational products at the time of the Envisat Validation Workshop is not a principle failure of the instrument. Scientific algorithms are already able to successful retrieve much more from SCIAMACHY measurement than the operational system. It's in there!

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