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Spatial and temporal characterization of SCIAMACHY limb pointing errors during the first three years of the mission

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Limb scattering retrievals of atmospheric minor constituent profiles require highly accurate knowledge of the tangent heights during the measurements. The limb scattering measurements of the Scanning Imaging Absorption spectrometer for Atmospheric CartographY (SCIAMACHY) on Envisat are affected by tangent height errors of up to 2 km. This contribution provides a summary of the temporal and spatial variation of the SCIAMACHY limb pointing errors during the first three years of the SCIAMACHY mission. The tangent height errors are retrieved from the limb measurements in the UV-B spectral range. A seasonal modulation of the monthly mean tangent height offsets is identified with amplitudes of 800 m (220 m) before (after) the improvement of the Envisat orbit propagator model in December 2003. Even after the December 2003 orbit model improvement a constant offset component of about 1 km is present. Furthermore, pointing discontinuities are identified that coincide with the daily updates of the on-board orbit propagator model. In order to reduce the errors in ozone profile retrievals caused by pointing errors to less than 5%, the tangent heights have to be known to within 250 m.

1. Introduction

UV/visible limb scattering is a powerful technique to remotely sense the chemical composition of the terrestrial atmosphere. It combines global coverage – typical of nadir backscatter measurements (e.g., with TOMS (Total Ozone Mapping Spectrometer) (Heath et al., 1975) or GOME (Global Ozone Monitoring Experiment) (Burrows et al., 1999) – with a high vertical resolution on the order of 2–3 km – typical of solar occultation measurements (e.g., with SAGE (Stratospheric Aerosol and Gas Experiment) (McCormick et al., 1989) or POAM (Polar Ozone and Aerosol Measurement) (Lucke et al., 1999)). In the past few years a series of new atmospheric remote sensing instruments applying the limb scattering method was launched: SOLSE/LORE (Shut-

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the Ozone Limb Sounding Experiment/ Limb Ozone Retrieval Experiment) flying on NASA's space shuttle in 1997 and again in 2003 (McPeters et al., 2000; Flittner et al., 2000), OSIRIS (Optical Spectrograph and InfraRed Imager System) on Odin (Llewellyn et al., 2004), SAGE III (Rault, 2005) on a Meteor-3M spacecraft, and SCIAMACHY on the European environmental satellite Envisat (Bovensmann et al., 1999). Furthermore, the limb scattering technique will also be employed by the future OMPS (Ozone Mapping and Profiling Suite) mission on a NPOESS (National Polar-Orbiting Operational Environmental Satellite) satellite, scheduled for launch in 2008. Satellite-based limb scattering measurements were used already more than 2 decades ago for satellite observations of mesospheric ozone profiles (Rusch et al., 1984) and upper stratospheric NO₂ profiles (Mount et al., 1984) using the UV spectrometer on SME (Solar Mesosphere Explorer). Yet, the greatly enhanced computing power now makes profile retrievals possible for extended altitude ranges (and also other constituents), since spherical radiative transfer (RT) models can be run online in full multiple scattering mode.

One of the main issues for all existing limb scattering instruments is the accuracy with which the tangent heights (THs) can be reconstructed (von Savigny et al., 2004). The requirements on the knowledge of orientation and position of the spacecraft are particularly strict for limb viewing instruments, because of the large distance between the satellite and the sampled air volume (about 3000 km). For instance, an angular difference of only 1 min of arc translates to a TH difference of about 1 km. Furthermore, tangent errors of only a few hundred meters can lead to significant errors in the retrieved trace gas profiles: 500 m TH error leads to errors in the retrieved ozone concentrations of up to 10% in the stratosphere (von Savigny et al., 2005b¹) and up to 20% in the mesosphere (Rohen et al., 2005). The reason for the larger errors in the mesosphere is the larger vertical gradient, i.e. smaller scale height, of mesospheric ozone

¹von Savigny, C., McDade, I. C., Griffioen, E., Haley, C. S., Sioris, C. E., and Llewellyn, E. J.: Sensitivity Studies and First Validation of Stratospheric Ozone Profile Retrievals from Odin/OSIRIS Observations of Limb Scattered Solar Radiation, Can. J. Phys., revised, 2005b.

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number density. The retrieval errors associated with pointing errors strongly depend on the shape of the minor constituent profile and will differ to a certain extent from species to species.

It has been recognized early during the SCIAMACHY mission that the TH information provided in the data files is affected by errors of up to 3 km (von Savigny et al., 2003; Kaiser et al., 2004). To investigate the apparent pointing errors a pointing retrieval from the limb measurements themselves was implemented based on the well established “knee” technique (Sioris et al., 2003; Kaiser et al., 2004) in the UV spectral range.

The main purpose of this paper is to complement the special issue of Atmospheric Chemistry and Physics on SCIAMACHY calibration, validation and first results with a detailed description of the retrieved spatial and temporal characteristics of the SCIAMACHY limb pointing errors. High pointing accuracy is a crucial prerequisite not only for all scientific applications – e.g., studying polar chemical ozone loss in both hemispheres – but also for algorithm diagnostics/improvements and all validation activities. The paper is structured as follows: Sect. 2 provides a brief overview of the numerical method to retrieve pointing information from limb scattering observations in the UV-B spectral range. In Sect. 3 a detailed description of the temporal and spatial pointing variability is given. Section 4 illustrates with sample stratospheric O₃ profile retrievals how the retrieval accuracy can be improved by performing a pointing retrieval prior to the minor constituent profile retrieval. Conclusions are presented in Sect. 5.

2. Method and data set

The method used to perform limb pointing retrievals from SCIAMACHY limb scattering observations is based on the now well established knee-technique (Janz et al., 1996; Merkel et al., 2001; Sioris et al., 2003; Kaiser et al., 2004). Basically, the maximum (i.e., the “knee”) in the UV limb radiance profiles caused by absorption in the Huggins/Hartley bands of O₃ (Sioris et al., 2003; Kaiser et al., 2004) or Rayleigh extinction (Janz et al., 1996; Merkel et al., 2001) provides a suitable signature for point-

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ing retrievals. For the present analysis the TRUE (Tangent height Retrieval by UV-B Exploitation) (Kaiser et al., 2004) code (Version 1.4) is employed. It uses the SCIAMACHY UV limb scattering measurements in the 295 nm to 305 nm spectral range and THs ranging from about 35 km to 50 km. This TH range includes the knees of the wavelengths considered. The TH retrieval is based on SCIAMACHY Level 1 data. An optimal estimation scheme is used together with the radiative transfer code SCIRAYS (Kaiser and Burrows, 2003) to adjust a constant TH offset:

$$\text{TH offset} = \text{engineering TH} - \text{retrieved TH}$$

The engineering THs are the ones provided in the Level 1 data sets. For all TH retrievals shown here, the background atmosphere climatology in Nagatani and Rosenfield (1993) and the UGAMP (Universities Global Atmospheric Modeling Programme) (Li and Shine, 1995) O₃ profile climatology – based on 5 years of SME, SAGE II, and SBUV O₃ measurements – is used for the pointing retrievals. A more detailed description of the TRUE method itself is given in Kaiser et al. (2004) and will not be repeated here.

In the used spectral window (295 nm to 305 nm) the knee in the limb radiance profiles is solely due to absorption by O₃. Thus, the pointing retrieval is only possible if the atmospheric O₃ profile is known or can be estimated with high accuracy. Conversely, the most important source of error of the retrieved THs is an inaccurate O₃ profile. Particularly the altitude range between about 40 and 55 km is crucial for the spectral range considered here. Sensitivity studies showed (see Kaiser et al., 2004) that scaling the O₃ profile by factors of 0.8 and 1.2 leads to differences in the retrieved THs of up to 1 km. Scaling the O₃ profile by factors of 0.5 and 2.0 leads to differences of up to 3 km. Therefore, the accuracy of the retrieval technique is generally not better than about 1–2 km if mid-latitudes – with significant latitudinal and zonal variability in the O₃ field, particularly in the winter hemisphere with its enhanced planetary wave activity – are considered. But, if the stratospheric O₃ field is horizontally relatively homogeneous, then a retrieval precision of 300 m or better can be achieved. Since stratospheric and lower mesospheric O₃ is particularly variable at mid- and high latitudes, but generally

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less in the tropics, only SCIAMACHY limb measurements between 20° N and 20° S are used. For all orbits analyzed a mean TH offset for this latitude range was determined. Thus, for each orbit a single TH offset was derived and is shown in the following Figures. It must be noted that by looking at the TH offsets only at tropical latitudes a possible latitudinal dependence of the TH offset cannot be investigated. For further information on the error budget of the pointing retrievals see Kaiser et al. (2004).

3. Results

3.1. General overview

Figure 1 shows the retrieved TH offsets for all orbits – between July 2002 and February 2005 – available at IUP/IFE Bremen and averaged over the tropical limb measurements as described in Sect. 2. The derived TH errors cover the range between about -0.5 km and 2.5 km, and there is (a) significant scatter in every month (about ± 0.5 km), and (b) an apparent seasonal variation in the TH offsets. Summer 2003 shows a gap in the coverage lasting from 26 May 2003 until 12 September 2003. Due to a software error, the Level 0 data taken during this period was not processed by the Level 0-1b processor, and therefore the SCIAMACHY Level 1 files did not contain any limb data. However, this gap will be closed after the next reprocessing of the Level 1b data set is completed.

The amplitude of the seasonal variation is suddenly reduced in December 2003. This is due to an improvement of the orbit propagator model onboard the Envisat spacecraft, that was implemented on 13 December 2003. Apart from the seasonal variation and the usual variability of the retrieved TH offsets there are also several additional pointing anomalies. On 21/22 June 2004 during the orbits 12071 to 12086 negative TH offsets between -1 and -2 km were retrieved. This anomaly was due to a star tracker failure. On 11–13 December tests were carried out to investigate the performance of the improved on-board orbit model. These tests also led to significant TH errors. More

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variability than usually was also observed in November 2003, May 2003, and several months in 2002. It is important to note in this context, that in 2003 and particularly 2002 the number of available orbits was significantly smaller than in 2004 and 2005. This can also be seen in Table 1, that presents an overview of the monthly mean TH offsets, their standard deviations and the number of orbits used in this study.

3.2. Seasonal variation between July 2002 – November 2003

The seasonal variation of the monthly mean TH offsets for the period before the December 2003 improvement of the Envisat orbit model is shown in Fig. 2, together with a model fit composed of a linear and a sinusoidal term. Note that the shown error bars correspond to the standard deviations of the retrieved TH offsets about the monthly mean value. The variability mainly originates from the longitudinal variation discussed in Sect. 3.4. All parameters (i.e., c_1 , c_2 , c_3 , c_4 , c_5) were fitted for. The derived constant offset (black dotted line), the linear increase (blue solid line) and the sinusoidal variation (red dashed line) are shown separately and superimposed (black solid line). The amplitude (c_3) of the sinusoidal variation is about 800 m, the fitted period ($2 \times c_5$) is 11.7 months – consistent with an annual variation within the error bars – and the phase (c_4) is about 7 months with respect to the beginning of year 2002. Amplitude, period and phase of the sinusoidal variation are in very good agreement with pointing retrievals from the two other atmospheric chemistry sensors on Envisat: GOMOS (Global Ozone Monitoring by Occultation of Stars) and MIPAS (Michelson Interferometer for Passive Atmospheric Sounding). The reported annual variation in pitch pointing errors derived from both instruments is between 3×10^{-2} and 4×10^{-2} degrees (Duesmann et al., 2004), corresponding to about 1.5–2 km, in excellent quantitative agreement with the amplitude of 800 m found in this study. The cause of the apparent annual variation in the TH offsets was identified as an inconsistency between different coordinate systems (Duesmann et al., 2004).

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3.3. Seasonal variation between December 2003–January 2005

As mentioned before the amplitude of the seasonal variation of the TH offset after December 2003 is markedly smaller than before. The monthly mean TH offsets together with the model fit is shown in Fig. 3. The linear term (c_2) is about a factor of 3 smaller than before December 2003. The amplitude of the sinusoidal component was found to be about 220 m. The fitted period ($2 \times c_5$) of the sinusoidal variation is only about 9 months. However, within the error bars the derived variation of the mean TH offsets is also in agreement with an period of 12 months. At present, we cannot state with certainty that the 9 month period is real. Moreover, a constant component (c_1) of about 1 km is present. The comparison of SCIAMACHY limb O_3 profile measurements in 2004 with an extensive set of independent measurements (Brinksma et al., 2005²) also yielded an altitude offset of about 1–1.5 km. When comparing Figs. 2 and 3 a difference in the phase of the sinusoidal variation between the two periods can be identified: e.g., TH offset assumed a minimum in March 2003, but a maximum in March 2004. In summary, the pointing retrievals suggest that the December 2003 improvement of the orbit propagator model led to (a) a reduced seasonal variation, (b) a reduced linear change, and (c) an increased constant offset component of the TH offsets.

3.4. Longitudinal variation of the TH offsets

Kaiser et al. (2004) report sudden limb pointing discontinuities of up to 2.5 km that occur within a few limb measurements, i.e. within a few minutes. These discontinuities coincide in time with updates of the on-board orbit model that occur twice per

²Brinksma, E. J., Bracher, A., Lolkema, D. E., Segers, A. J., Boyd, I. S., Bramsted, K., Claude, H., Godin-Beekmann, S., Hansen, G. Kopp, G., Leblanc, T., McDermid, I. S., Meijer, Y. J., Nakane, H., Parish, A., von Savigny, C., Swart, D. P. J., Taha, G., and Piters, A. J. M.: Geophysical Validation of SCIAMACHY Limb Ozone Profiles, Atmos. Chem. Phys. Discuss., submitted, 2005.

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day, always approximately at the same geographical locations: (a) around 60° – 70° W between about 20° N and the equator – corresponding to the Caribbean and/or the northern part of South America – and (b) around 100° E and 45° S, i.e., south-west of Australia. For easier reference the updates are called “Caribbean” and “Australian” updates in the following sections. To check if pointing discontinuities occur systematically at these locations, the longitudinal variation of the 20° S to 20° N mean TH offset is shown in Fig. 4 for several months before and after the orbit model improvement in December 2003.

A closer inspection of Fig. 4 shows that for the months before December 2003 (left column) the Caribbean update (near 60° W) is in many cases associated with considerable pointing discontinuities, reaching values of about 2 km for example in May 2003. However, the magnitude of the discontinuities differs significantly from day to day. The impact of the Australian update on the TH offsets is not as obvious, but manifests itself in many cases in a bump around 100° E. Its magnitude is also highly variable but generally less than about 0.5 km. After the Australian update the retrieved TH errors increase almost linearly from orbit to orbit (the longitudes of the equator crossings move from east to west), until the Caribbean update takes place, and the THs are corrected again. Although this appears to be a repeating pattern a simple parametrization that would allow for an analytical TH correction is not possible due to the apparent random variability of the magnitude of the discontinuities.

Interestingly the months after December 2003 exhibit a distinctly different longitudinal variation of the mean tropical TH offsets. The large pointing discontinuities previously associated with the Caribbean updates are not present any more. However, the Australian update now shows a more pronounced TH jump with values of up to about 800 m, and even more in a few cases.

It is important to realize that some of the features present in the retrieved longitudinal variation of the TH offsets may in part be retrieval artifacts originating from differences between the actual middle atmospheric O_3 profile and the assumed climatological and zonally averaged UGAMP O_3 profile. Any zonal variation in the true atmospheric O_3

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field will introduce a zonal variation in the TH retrievals to a certain extent. However, there is no doubt that the retrieved pointing discontinuities, that coincide exactly with the daily updates of the on-board orbit propagator model are real and not spuriously introduced by differences between the O_3 climatology and the actual O_3 profile. Furthermore, the panels (a)–(e) of Fig. 4 show for many days a nearly linear increase of the TH offset between the Australian and the Caribbean update. This behavior is consistent with a slow pointing drift from orbit to orbit, until the pointing is corrected again, and indicates that the pointing retrieval is precise to within a few hundred meters.

4. Improvement of O_3 profile retrievals by pointing correction

In this section the improvement of the stratospheric O_3 profile retrievals applying the derived TH offsets is investigated with a sample coincident measurement with the LIDAR (McDermid et al., 1995; Leblanc and McDermid, 2000) at Table mountain (California, U.S.A.). The SCIAMACHY stratospheric O_3 profiles are retrieved exploiting the Chapuis absorption bands of O_3 using the technique (Version 1.61) described in von Savigny et al. (2005a). With this method stratospheric O_3 profiles can be retrieved in the 15–40 km altitude range with a vertical resolution of about 4 km and a theoretical accuracy of about 5–10% (von Savigny et al., 2005b¹). We use a limb measurement on 20 September 2004 (Orbit 13379) with a mean tangent point location of 35.8° N/–122.2° E made at 18:10:55 UTC. The location of the LIDAR instrument is 34.4° N/–117.7° E, and the measurement was made at 06:14:00 UTC. The time difference between the measurements is therefore 12:05 h. The TRUE pointing retrieval for orbit 13379 yielded a TH offset of 1.31 km. The comparison between the LIDAR profile and the SCIAMACHY retrievals is shown in Fig. 5. Since the LIDAR profile has a significantly higher vertical resolution, it was convolved with the SCIAMACHY averaging kernels. Apparently, the SCIAMACHY O_3 profile with corrected THs is in much better agreement than the uncorrected profile. In Fig. 6 the relative differences between SCIAMACHY and the LIDAR profiles as well as the relative difference between the pointing corrected and

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uncorrected SCIAMACHY profiles are shown. For this comparison the SCIAMACHY retrievals as well as the convolved LIDAR profiles were interpolated onto a regular 2 km altitude grid. The pointing corrected SCIAMACHY profile agrees to within about 10% with the collocated LIDAR measurement, whereas the uncorrected retrieval differs by up to 33%, and it shows a systematic high bias above the O₃ concentration peak and a systematic low bias below the peak. This is indicative of a vertical displacement of the retrieved profile. The retrieved TH offset of 1.13 km leads to relative differences between the corrected and the uncorrected O₃ profiles of up to 25% above the O₃ concentration peak and up to 20% below the peak. In order to reduce the retrieval error due to pointing errors to less than 5%, the TH accuracy has to be better than about 250 m. Note, that sensitivity tests showed that if the TH offset is less than about 3 km, then the O₃ profile retrieved without prior TH correction may just be shifted vertically. The difference in O₃ concentrations between prior TH correction and TH correction after the O₃ profile retrieval is only a few percent within the 15–40 km altitude range.

Although only an individual validation example is presented here it is typical of the improvement that can be achieved with a pointing correction (Segers et al., 2005; Brinksma et al., 2005²), and demonstrates the importance of high pointing accuracy for limb scattering retrievals.

5. Conclusions

Pointing errors are the main source of error for trace gas retrievals from limb scattering observations. Without accurate TH (tangent height) information the retrieved profiles cannot be fully validated, and not be used for most scientific applications. An overview of the spatial and temporal behavior of the pointing errors of SCIAMACHY limb scattering observations during the first 3 years of the mission has been presented. The TRUE method was applied to derive a mean TH offset – averaged over the tropical limb measurements – for each orbit. The main conclusions are:

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- 1) The retrieved TH offsets exhibit a seasonal variation, both before and after the December 2003 improvement of the orbit propagator model. Before December 2003 the amplitude of the seasonal variation was about 800 m, and it is significantly reduced to about 220 m after December 2003.
- 2) The constant offset component increased from about 0.5 km before December 2003 to about 1 km after December 2003. The presence of a tangent offset of about 1 km after the December 2003 orbit model improvement is in good agreement with comprehensive validation results for the year 2004 (Brinksma et al., 2005²).
- 3) The retrieved TH offsets show discontinuities of up to 2 km that coincide in time with updates of the on-board orbit propagator model. These updates occur two times per day. Before December 2003 the Caribbean update was associated with more pronounced discontinuities, whereas the Australian update manifested itself in bumps of generally less than 0.5 km. After December 2003 the longitudinal variation of the TH offsets differs from the period before. The pointing discontinuity associated with the Australian update is now more pronounced, and the Caribbean discontinuity has almost vanished.
- 4) A pointing correction performed prior to the trace gas profile retrievals significantly improves the accuracy of the profile retrievals. A TH error of only 500 m leads to errors in the derived O₃ concentration of 10% and more at certain altitudes. In order to reduce the profile retrieval errors due to TH errors to less than 5%, the TH accuracy has to be better than about 250 m.

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the retrievals were performed at the HLRN (High Performance Computing Center North). The HLRN service and support is gratefully acknowledged.

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Table 1. Monthly tangent height offset statistics.

Month	Year	mean TH offset/km	Std. dev. /km	Number of orbits	Month	Year	mean TH offset/km	Std. dev. /km	Number of orbits
July	2002	0.57	0.45	17	Nov.	2003	1.57	0.33	163
Aug.	2002	0.89	0.40	71	Dec.	2003	0.90	0.50	166
Sep.	2002	1.40	0.30	26	Jan.	2004	1.04	0.24	294
Oct.	2002	1.38	0.21	34	Feb.	2004	1.04	0.23	261
Nov.	2002	1.43	0.21	34	Mar.	2004	1.20	0.24	375
Dec.	2002	0.84	0.37	31	Apr.	2004	1.22	0.22	391
Jan.	2003	0.44	0.40	132	May	2004	1.12	0.17	405
Feb.	2003	0.25	0.37	136	June	2004	0.92	0.43	361
Mar.	2003	0.03	0.19	158	July	2004	0.73	0.24	307
Apr.	2003	0.06	0.26	166	Aug.	2004	0.68	0.24	334
May	2003	0.21	0.52	94	Sep.	2004	0.83	0.27	399
June	2003	—	—	0	Oct.	2004	0.83	0.23	199
July	2003	—	—	0	Nov.	2004	1.03	0.20	302
Aug.	2003	—	—	0	Dec.	2004	1.06	0.21	247
Sep.	2003	1.67	0.25	91	Jan.	2005	1.12	0.24	326
Oct.	2003	1.68	0.23	184					

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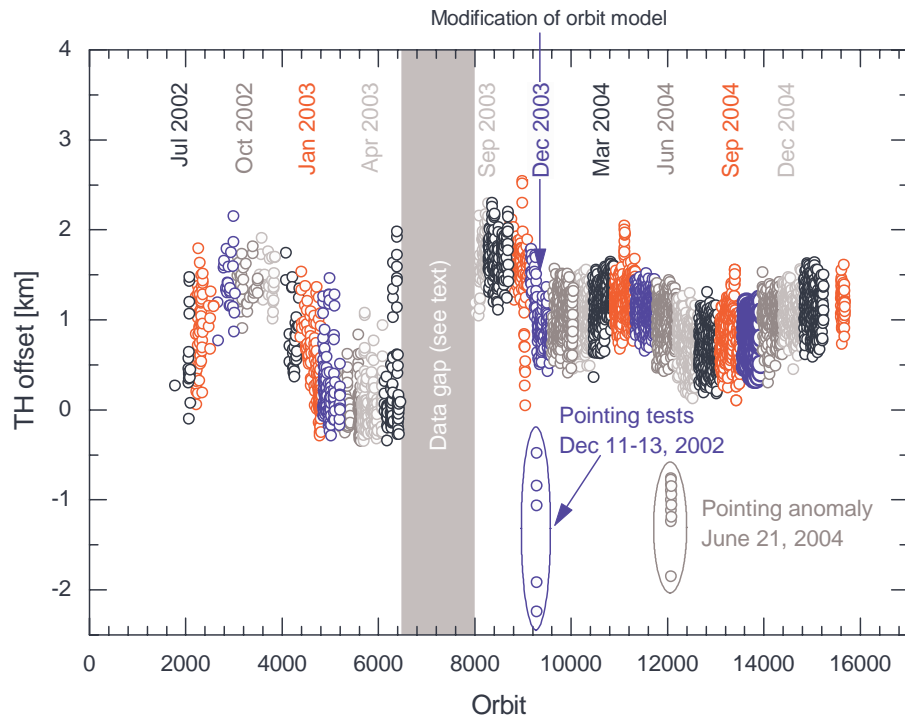


Fig. 1. Tangent height (TH) offset retrievals for all available orbits averaged over the tropical limb measurements between 20° S and 20° N between July 2002 and February 2005. In December 2003 an improvement of the Envisat orbit model took place. Before December 2003 a strong seasonal variation with an amplitude of about 800 m is present. After the update the amplitude is reduced to less than 250 m, but an offset of about 1 km remains.

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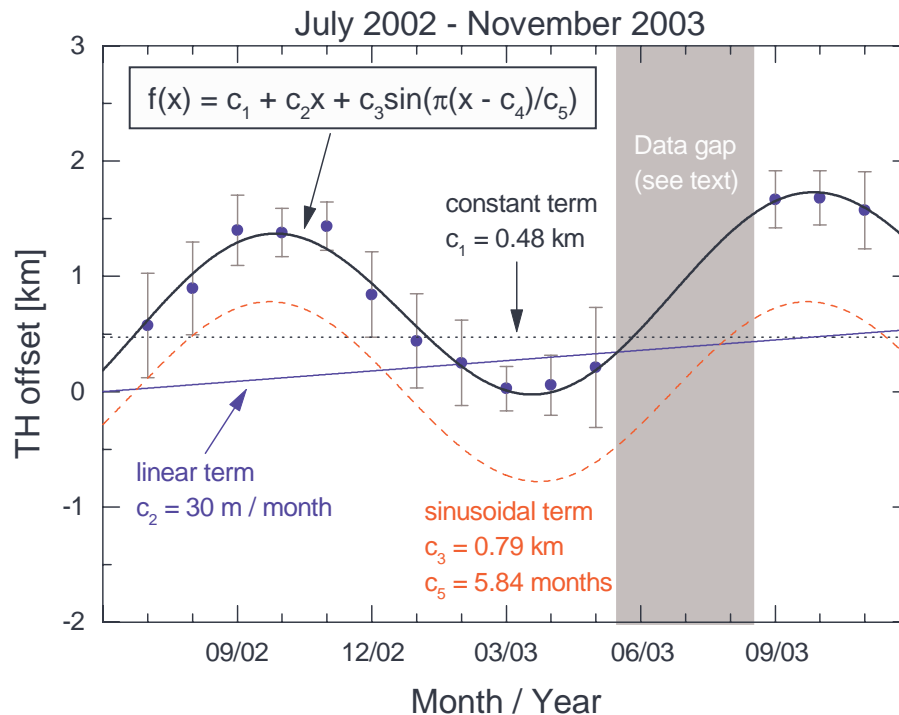


Fig. 2. The blue solid circles show the monthly mean TH offsets for the July 2002–November 2003 period. The error bars indicate the standard deviations about the monthly mean values. The TH offset variation was modeled with a superposition of a linear and a sinusoidal function. The amplitude of the sinusoidal function is $c_3 \approx 800$ m, and its period is $T = 2 \times c_5 \approx 12$ months.

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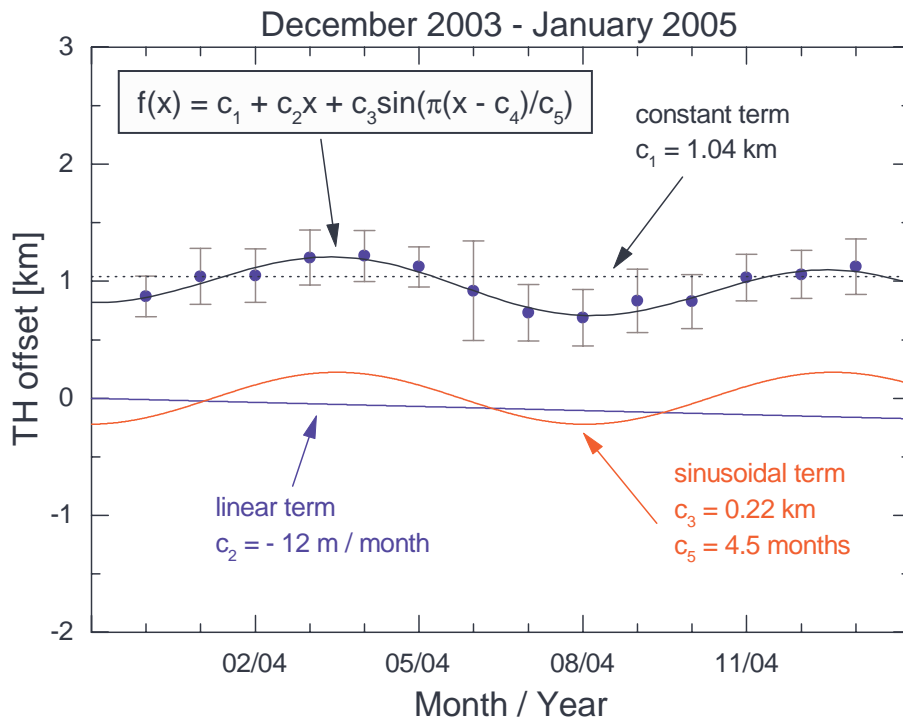


Fig. 3. Retrieved and modeled monthly mean TH offsets for the December 2003–January 2005 period. The amplitude of the sinusoidal modulations is reduced to about 1/4 of the value during the July 2002–November 2003 period (Fig. 2). However, a nearly constant offset of approximately 1 km remains.

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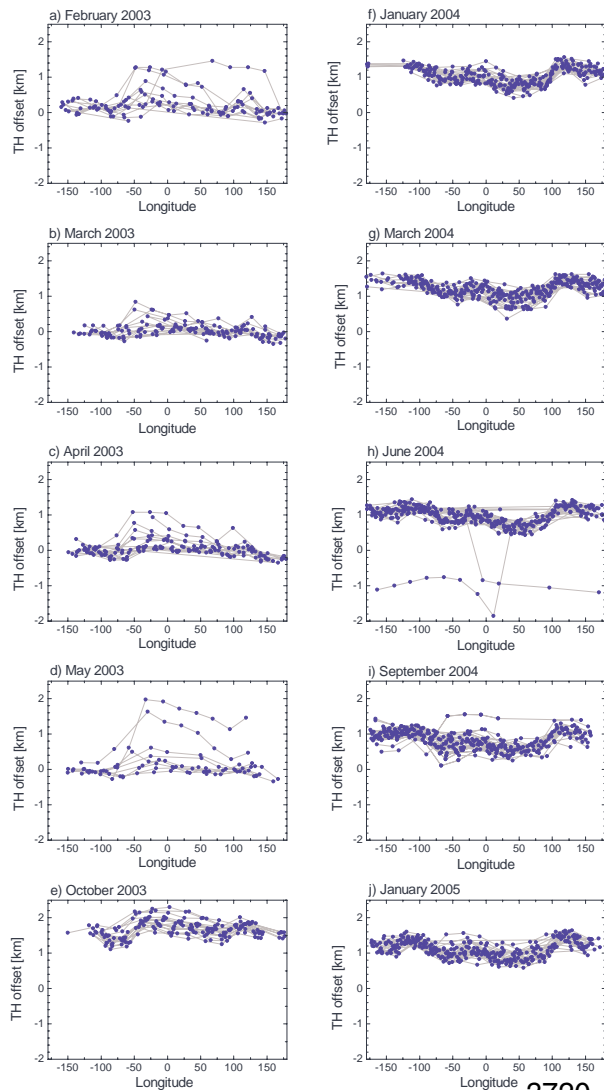


Fig. 4. Longitudinal variation of the retrieved mean tropical TH offsets for several months before (left column) and after (right column) the orbit model update in December 2003. For the months before December 2003 the repeating discontinuity at about 60° W – where the updates of the on-board orbit model take place – is clearly visible. After December 2003, the longitudinal variation of the pointing offsets is different. Although the Caribbean discontinuity is gone, the signature at around 100° E is more pronounced. The outliers in June 2004 are due to the previously mentioned pointing anomaly on 21/22 June.

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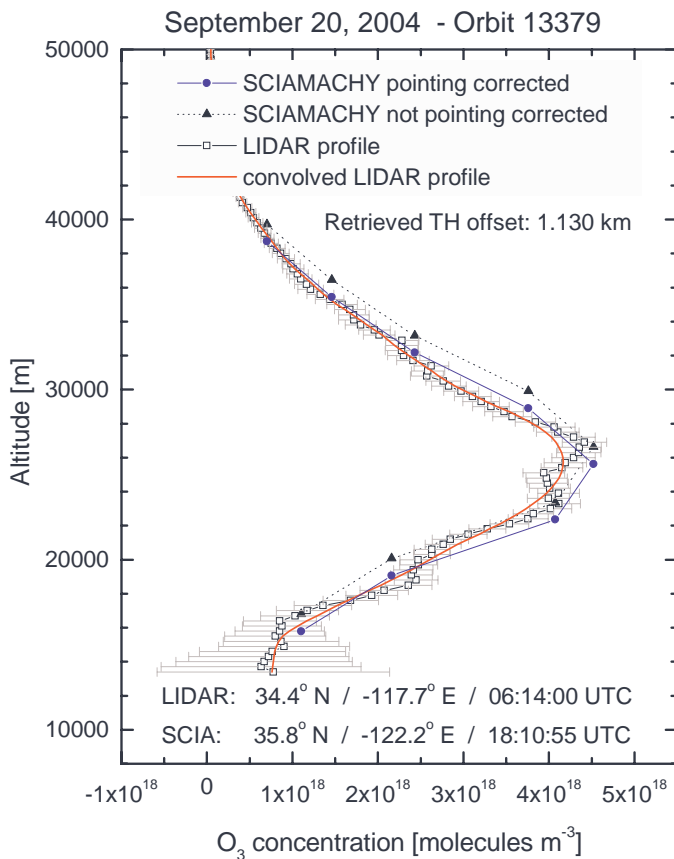


Fig. 5. Comparison between SCIAMACHY O₃ profile retrievals with collocated LIDAR measurement on 20 September 2004. SCIAMACHY retrievals were performed with and without the retrieved TH correction of 1.13 km. The red solid line shows the LIDAR profile convolved with the SCIAMACHY averaging kernels. The pointing correction significantly improves the agreement between the LIDAR and SCIAMACHY.

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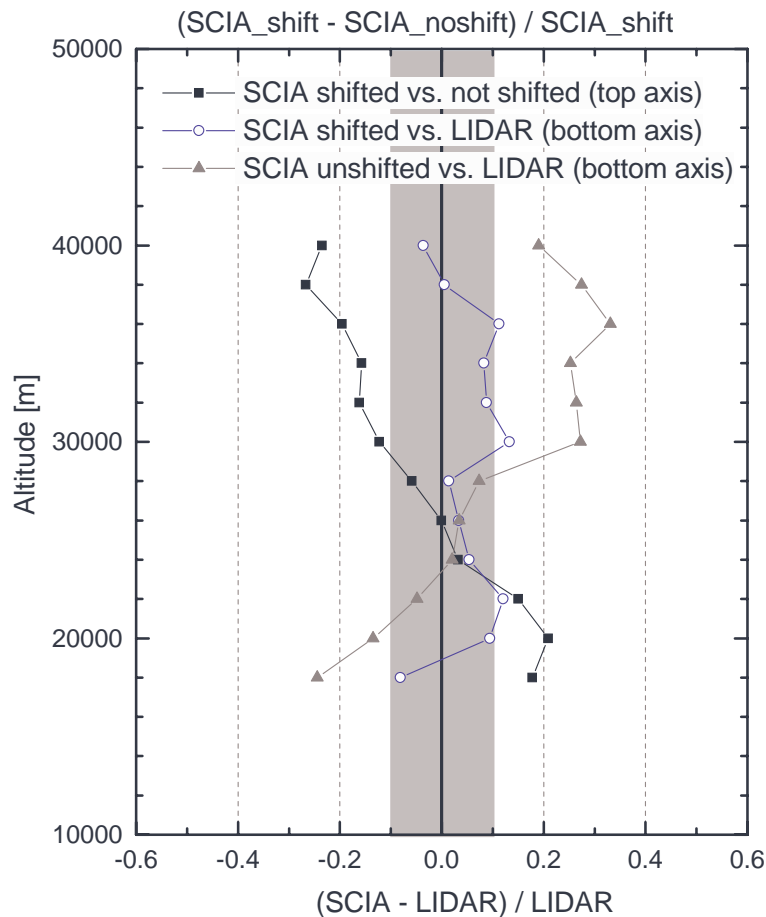


Fig. 6. Relative differences between the SCIAMACHY retrievals and the LIDAR measurement and between the pointing corrected and uncorrected SCIAMACHY profiles. The grey shaded area indicates the $\pm 10\%$ range.

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