Atmos. Meas. Tech. Discuss., 8, 5565–5590, 2015
www.atmos-meas-tech-discuss.net/8/5565/2015/
doi:10.5194/amtd-8-5565-2015

Atmospheric Measurement Techniques Discussions
Open Access

Validation of MIPAS IMK/IAA methane profiles

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Received: 2 May 2015 – Accepted: 22 May 2015 – Published: 4 June 2015

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Published by Copernicus Publications on behalf of the European Geosciences Union.

Abstract

The Michelson Interferometer for Passive Atmospheric Sounding (MIPAS) was an infrared (IR) limb emission spectrometer on the Envisat platform. It measured during day and night, pole-to-pole, over an altitude range from 6 to 70 km in nominal mode and up to 170 km in special modes, depending on the measurement mode, producing more than 1000 profiles day^{-1}. We present the results of a validation study of methane version V5R_CH4_222 retrieved with the IMK/IAA MIPAS scientific level 2 processor. The level 1 spectra are provided by ESA, the version 5 was used. The time period covered corresponds to the period when MIPAS measured at reduced spectral resolution, i.e. 2005–2012. The comparison with satellite instruments includes the Atmospheric Chemistry Experiment Fourier Transform Spectrometer (ACE-FTS), the HALogen Occultation Experiment (HALOE), the Solar Occultation For Ice Experiment (SOFIE) and the SCanning Imaging Absorption spectroMeter for Atmospheric CHartographY (SCIAMACHY). Furthermore, comparisons with MkIV balloon-borne solar occultation measurements and with air sampling measurements performed by the University of Frankfurt are presented. The validation activities include bias determination, in selected cases, assessment of histograms and comparison of corresponding climatologies. Above 50 km altitude, MIPAS methane mixing ratios agree within 3 % with ACE-FTS and SOFIE. Between 30 and 40 km an agreement within 3 % with SCIAMACHY has been found. In the middle stratosphere, there is no clear indication of a MIPAS bias since comparisons with various instruments contradict each other. In the lower stratosphere (below about 25–30 km) MIPAS CH_4 is biased high with respect to satellite instruments, and the most likely estimate of this bias is 14 %. However, in the comparison with CH_4 data obtained from cryosampler measurements, there is no evidence of a MIPAS high bias between 20 and 25 km altitude. Precision validation is performed on collocated MIPAS-MIPAS pairs and suggests a slight underestimation of its errors by a factor of 1.2. A parametric model consisting of constant, linear, QBO and several sine and cosine terms with different periods has been fitted to the temporal variation

of differences of stratospheric CH_4 measurements by MIPAS and ACE-FTS for all 10° latitude/1–2 km altitude bins. Only few significant drifts can be calculated, due to the lack of data. Significant drifts with respect to ACE-FTS tend to have higher absolute values in the Northern Hemisphere, have no pronounced tendency in the sign, and do not exceed 0.2 ppmv per decade in absolute value.

1 Introduction

The Michelson Interferometer for Passive Atmospheric Sounding (MIPAS) is a high resolution limb emission Fourier transform spectrometer designed to measure trace gas distributions from the upper troposphere to the mesosphere at global coverage during day and night (Fischer et al., 2008). Institut für Meteorologie und Klimaforschung (IMK) operates a scientific data processor (von Clarmann et al., 2003b) which relies on ESA level 1B spectra. The MIPAS IMK methane data product covers mixing ratio profiles of the period 2002–2004 when MIPAS operated in its original high spectral resolution mode (Glatthor et al., 2005), as well as data from 2005–2012 when MIPAS measured at reduced spectral resolution (Chauhan et al., 2009; von Clarmann et al., 2009b). MIPAS reduced resolution nominal mode data are sampled along the orbit every 410 km, and a vertical profile contains information from up to 27 tangent altitudes, while reduced resolution UTLS-1 mode data are sampled along the orbit every 290 km, and a vertical profile contains information from up to 19 tangent altitudes. This paper reports the validation of the most recently released methane data retrieved from reduced spectral resolution measurements in nominal mode, which is version number V5R_CH4_222. The analysis is restrained on the reduced resolution measurements only because the corresponding baseline was developed for reduced resolution only. Detailed descriptions of the inversion algorithm used by the MIPAS IMK/IAA scientific retrieval processor can be found in von Clarmann et al. (2003b, 2009b) and Laeng et al. (2015). Its first application to stratospheric CH_4 is documented in Glatthor et al. (2006).

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IMK-IAA MIPAS results are characterized by error estimates, as well as vertical averaging kernels. The latter is used to estimate the altitude resolution of the retrievals. In addition, the horizontal smoothing information is calculated for sample cases on the basis of the 2-dimensional averaging kernels, computed from 2-dimensional Jacobians (von Clarmann et al., 2009a). The random error covariance matrices of the retrieved quantities are provided. The vertical resolution of a typical MIPAS IMK methane retrieval, derived from the full width at half maximum (FWHM) of the rows of averaging kernel matrix, varies between 2 and 5 km, see Fig. 1.

2 Reference instruments and comparison methodology

The MIPAS reduced resolution period covers the years 2005–2012. During this time, only five other satellite instuments measured the vertical profiles of methane: the Atmospheric Chemistry Experiment Fourier Transform Spectrometer (ACE-FTS), the Halogen Occultation Experiment (HALOE), the Scanning Imaging Spectrometer for Atmospheric Chartography (SCIAMACHY), the Solar Occultation For Ice Experiment (SOFIE), and the Tropospheric Emission Spectrometer (TES) (see for example, the list of trace gases measured by atmospheric sensors collected at the BIRA website Network for the Detection of Atmospheric Composition Change, NDACC). The comparison with four of these instruments is presented here. TES data were not used because its coarse vertical resolution makes it less suited for validation of a limb dataset. No ground-based FTIR measurements were used because of low upper limit of the profiles (30 km) and coarse (10 km) vertical resolution. Also, we have used two balloon-borne instruments: the MkIV solar occultation interferometer and cryosampler.

For the satellite instruments ACE-FTS the collocation criteria were chosen to be 9 h and 800 km. This was a result of the trade off between the collocations being as close as possible and the resulting sample being sufficiently big. For SCIAMACHY and SOFIE, which have a denser sampling pattern, these were tightened to 5 h and 500 km. For HALOE, whose time overlap with MIPAS reduced resolution period is less

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than eight months, the criteria were relaxed to 24 h and 1000 km. This led to the number of matched pairs as listed in Table 1. Figure 2 shows the latitudinal distributions over months of collocated measurements of MIPAS with satellite reference instrument. Figure 2 suggests that even an initial assessment of precision of pairs MIPAS/reference instrument can not be performed here. Indeed, it is usually done by comparing the standard deviation of the differences with the combined estimated random error (von Clarmann, 2006). Here in all cases except HALOE, most collocations are concentrated at high latitudes, where the atmospheric variability contribution into the standard deviation of the differences is significant. To assess the quality of uncertainty estimates of MIPAS CH_4 data, the structure functions as in Laeng et al. (2015) will be constructed in Sect. 5. The matched pairs were chosen in such a way that none of the MIPAS (or reference instrument) measurements participated in two pairs. Such a choice reduces the number of matches, but produces pairs that are independent. For MkIV and cryosampler measurements, the collocation criteria were also relaxed and chosen to be 24 h and 1000 km. In cases where no MIPAS data were available around the flight within the collocation criteria, zonal mean of MIPAS data for the corresponding month, season and latitude range were compared with the reference instrument profiles.

All profiles were interpolated to the MIPAS grid for intercomparison. Rodgers and Connor (1999) suggest application of averaging kernels of the poorer resolved profiles to the better resolved profiles during the regridding of atmospheric profiles. However, for any of the comparison instruments, the vertical resolution of typical MIPAS IMK methane profiles differs fromthe vertical resolution of reference instrument profiles by less than a factor of 2–2.5 and often is close to 1. Thus the application of averaging kernels appears unnecessary. To be on the safe side, sensitivity studies were performed to assess the impact of the application of the averaging kernels. When no averaging kernels were available for the coarser resolved reference instrument, the smoothing was done with a Gaussian of corresponding width. After this application, the profiles were changing by less than 2 % in the middle, where the MIPAS averaging kernel values are close to 1, and an artificial 300 % bias appeared on the extremities of the profile, where the MIPAS averaging kernel values are close to zero. Hence, the differences in vertical resolution were chosen to be neglected and no averaging kernels were applied.

3 Bias assessment

3.1 Comparison with satellite reference instruments

Figure 3 represents the percentage bias of MIPAS CH_4 retrievals with respect to the satellite reference instruments. We should keep in mind that the percentage bias is tricky to interpret when the reference values are low, which is the case for methane at the heights above 40–45 km.

The agreement with ACE-FTS at 20–65 km height is within 12 %, while in the lower stratosphere MIPAS volume mixing rations (vmrs) are consistently higher than those of ACE-FTS. The largest bias found is 15 % at 17 km altitude. A secondary maximum of the differences is found at 38 km altitude, where MIPAS methane mixing are higher by 12 %. The standard deviations of MIPAS and ACE-FTS in different seasons were studied. They have a pronounced maximum at about 30 km altitude in autumn, winter and spring, when the polar vortex is formed, persists, and breaks down, respectively, which causes enhanced variability. One might speculate that different viewing geometries (with a larger north-south component for MIPAS and a larger east west component for ACE-FTS) or different sensitivity to along-line-of-sight temperature variation might turn the enhanced random variability into a bias. The reduced variability actually leads to a smaller bias between MIPAS and ACE-FTS. In summer, when the meteorological situation in the stratosphere is quite calm, no such enhanced variability is observed. Another region of enhanced variability is the lowermost altitudes: the large variability there is attributed to tropopause height fluctuations.

Between 30–40 km altitude, the agreement between the global mean MIPAS and SCIAMACHY CH_4 profiles is within 3 %. Below, MIPAS methane mixing ratios are

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higher than those of SCIAMACHY. The largest bias found is 17 % at the lowest SCIAMACHY altitude, 20 km.

HALOE data are considered as a reference in the atmospheric science community and have been extensively used for scientific analysis (Ruth et al., 1997). Unfortunately the time overlap between MIPAS reduced resolution period and HALOE operations is only eight months, during which there were gaps in the MIPAS data. Even after relaxing the collocation criteria to 24 h and 1000 km, only 244 independent matched pairs were found. The blue curve on Fig. 3 exposes the agreement within 10 % of MIPAS and HALOE at 20–30 km. Over almost the whole height range, the bias does not change sign and stays positive. Below 25 km, the high bias of MIPAS methane is confirmed. Largest mean relative differences are about 20 %.

At the heights between 45 and 60 km, the agreement between MIPAS and SOFIE is within 8 %. The maximum differences of 15 % are observed at 63 km. Let us recall that the relative differences become difficult to interpret when the reference values are getting small. This is particularly true for SOFIE whose delievered methane profiles start at 45 km height.

3.2 Comparison with MkIV balloon interferometer profiles

Figure 4 presents the three MkIV balloon profiles recorded within the MIPAS reduced resolution period. The first two MkIV profiles, from 20 September 2005 and 22 September 2007, were measured when MIPAS was temporary inactive and no matches were found within 24 h and 1000 km. The MkIV profiles were hence compared to the monthly (September) and seasonal (September–October–November, SON) means of MIPAS in [30;40] latitudes. For the profile from 20 September 2005, the agreement is very good from 20 to 24 and 28 to 31 km, while a positive MIPAS bias in the order of 0.2 ppmv is present at 12–20 and 31–37 km heights. For the profile from the sunset of 22 September 2007, the agreement is very good at 23–36 km, while a positive MIPAS bias in the order of 0.1 ppmv is present at 14–18 km heights and a negative MIPAS bias of the same order is present at 18–23 km heights.

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For the profile from the sunrise of 23 September 2007, three collocated MIPAS profiles were found (gray lines). Maximum deviation of those three profiles from the MkIV profile is 0.3 ppmv. Note that the positive MIPAS bias under 25 km, shown in the comparison with satellite instruments, is less pronounced in the comparison with MkIV profiles.

3.3 Comparison with cryosampler profiles

Cryosampler measurements do not provide continuous profiles but a series of independent point measurements. This means that not even smeared information about the atmospheric state between two sampling points is available. Thus no regridding has been performed; instead, these data have been used as they are and on the height where they were measured.

In Fig. 5 the comparison of MIPAS methane and the cryosampler measurements is shown. Besides the closest MIPAS profile (orange line) and the set of all MIPAS profiles meeting the coincidence criteria (grey lines; mean value: green line) also the climatological mean of the season and latitude is shown (green line). For the first two flights (upper panel of Fig. 5) the agreement between 23 and 32 km heights is excellent. As expected, the individual collocated profiles agree better than the corresponding means. Below 20 km, the high MIPAS bias of about 0.2 ppmv is present. Let us point out that on 20–25 km height, unlike in the satellite-satellite comparisons, the MIPAS measurements agree very well with the cryosampler measurements.

The third flight (bottom left panel of Fig. 5) of the cryosampler instrument gave rise to only four measurements, none of which is situated between 18 and 32 km. The two measurements over 32 km agree well with MIPAS. The two data points below 18 km reveal that the MIPAS CH_4 vmr is larger by 0.1 and 0.2 ppmv than the cryosampler measurement.

The last flight (bottom right panel of Fig. 5) stands out by a pronounced CH_4 minimum in the cryosampler data at approximately 22 and 24 km, which is not reproduced by the MIPAS data. This suggests that the cryosampler, which performs point measure-

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ments, samples a very localized phenomenon which is not resolved by MIPAS whose measurements represent for each profile point an air parcel of about 400 km in length times 30 km in width times 3 km in height. At the other altitudes, the cryosampler profile agrees reasonably well with both the collocated and the zonal mean MIPAS profiles. Below 20 km the tendency of MIPAS towards higher CH_4 mixing ratios is confirmed also here.

4 Temporal evolution of the bias

Based on the monthly distribution of coincident measurements (see Fig. 2) and altitude coverage (see Table 1), only ACE-FTS collocations could eventually provide enough of data for studying the stability of MIPAS CH_4 data in some latitude bands. Note however, that the stability of ACE-FTS itself has not yet been investigated. As to MIPAS, recent study by Kiefer et al. (2013) showed that the way the detector non-linearity is corrected in Level 1B spectra (up to version 5) could be a potential source for the drift in MIPAS data products.

To assess the temporal evolution of the bias of MIPAS with respect to ACE-FTS (i.e. drifts), the monthly means of differences MIPAS-ACE were calculated, then the multilinear parametric trend model from von Clarmann et al. (2010) with extensions by Stiller et al. (2012) and Eckert et al. (2014) was applied. Most of the obtained drift estimates were found to be insignificant at 2σ level due to the small number of months for which collocations were found. Figure 6 shows an example of significant drift. Generally the significant drifts tends to be higher at the Nothern Hemisphere, have no pronounced tendency in the sign, and do not exceed 0.2 ppmv per decade in absolute value.

5 Assessment of quality of uncertainty estimates of MIPAS methane profiles

The uncertainty usually provided with a dataset is the random component of the error (random error). In order to evaluate how realistic these uncertainties are, one compares

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the square of the mean uncertainty σ_{noise} provided with the dataset with the variance of a sample derived from the dataset, performed in a region with low natural variability σ_{nat}. We work with the sample which is composed of differences of closed profiles, with converging collocation criteria. This approach was used in Sofieva et al. (2014) and Laeng et al. (2015). Then the variance S^2_{diff} reflects the variability of (MIPAS-MIPAS) for collocated MIPAS pairs; the natural variability included in this variance is the small-scale natural variability:

$$2\sigma^2_{\text{noise}} + \sigma^2_{\text{nat}} = S^2_{\text{diff}}.$$

We expect that the smaller the separation distance, the smaller is the discrepancy between σ_{noise} and $S_{\text{diff}}/\sqrt{2}$. In particularly, when the separation distance tends to zero, $S_{\text{diff}}/\sqrt{2}$ should approach σ_{noise}, if the latter is realistic (recall that the atmospheric variability in the selected regions is small). The parameter $S_{\text{diff}}/\sqrt{2}$ is a direct analogue of the integral of the structure function from the theory of random functions. More details can be found in Sofieva et al. (2014) and Laeng et al. (2015). In Fig. 7, we construct structure functions for MIPAS methane retrieval. The colored lines in Fig. 7 (ex-post) correspond to $S_{\text{diff}}/\sqrt{2}$ for converging distance r between the air parcels, and the red line (ex-ante) shows σ_{noise}. As observed in Fig. 7, $S_{\text{diff}}/\sqrt{2}$ nicely converges with decreasing separation distance, but does not approach σ_{noise}, the values on the limit curve of $S_{\text{diff}}/\sqrt{2}$'s being approximatively 1.2 bigger than σ_{noise} values. This indicates at a slight (by a factor of about 1.2) underestimation of error estimates in CH_4 MIPAS IMK retrievals.

6 Climatologies and histograms comparisons

Figure 8 represents the temporal evolution of methane monthly zonal means of SCIAMACHY (top panel), MIPAS (middle panel), and the relative difference (bottom panel). The SCIAMANY instrument was choosen for this study because of its best agreement

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in the stratosphere with MIPAS methane profiles. The bin [50° N, 70° N] is restricted by the measuring mode of SCIAMACHY, from which vertical profiles of methane are retrieved (Noël et al., 2011). As dynamical tracer, CH_4 is expected to follow the transport patterns. As one can see at the Fig. 8, MIPAS and SCIAMACHY instruments see a similar morphology in the structure of atmospheric variation of methane, in particular a pronounced annual cycle. In the springs of the years 2005 and 2007, MIPAS methane distribution present secondary peaks at 25–27 km. The strong red parts in the lower panel of Fig. 8 occur mostly in winter time and are most probably due to the polat fortex edge, i.e. the studied air masses are not always comparable.

Figure 9 shows the histograms of measured CH_4 mixing ratios at 45 and 60 km heights on the MIPAS-SOFIE co-incidences. In each column, frequency polygons of both histograms are supposed to imitate the distribution function of the same random variable, which is the value of methane vmr at a given height independent of location. Hence top and bottom distributions in each column should look similar, with the same number and position of local maxima. The corresponding MIPAS and SOFIE histograms agree with respect to the approximate position of the main mode, their approximate width, and their skewness. The SOFIE histograms, however, presents several chaotic secondary modes. Such a structure is not seen in any comparison of MIPAS with other instruments, which hints at some systematic or retrieval-related effect causing the numerous positive and negative outliers, e.g. turning-points of onion-peeling related profile oscillations.

7 Conclusions

The MIPAS IMK V5R_CH4_222 data were compared to the data from four satellite instruments and two balloon-borne instruments. Below 25 km, MIPAS methane is biased high. The magnitude of this bias cannot unambigouosly be inferred from the comparisons because results are not fully consistent, but 14 % seems to be a reasonable estimate. In the middle stratosphere, the bias analysis is a little ambiguous but MIPAS

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seems to have a slight tendency towards higher values. In the upper stratosphere and above, excellent agreement with the other instruments is found, except for altitudes near 70 km, at the upper end of the MIPAS profiles, where MIPAS tends towards lower values. A high bias in MIPAS methane in the lower stratosphere has also been reported for the operational MIPAS data product provided by ESA (Payan et al., 2009). Interestingly, in the comparison with CH_4 data obtained from cryosampler measurements, there is no evidence of a MIPAS high bias between 20 and 25 km altitude. Precision validation was performed on collocated MIPAS-MIPAS pairs and suggested a slight underestimation of uncertainties provided with the data by a factor of 1.2. Significant drifts with respect to ACE-FTS tend to have higher absolute values in the Nothern Hemisphere, have no pronounced tendency in the sign, and do not exceed 0.2 ppmv per decade in absolute value. Overall, this MIPAS data set has a reasonable bias with respect to standard methane data records and can be used for climatological studies in an altitude range from 10 to 60 km.

Acknowledgements. The first author is grateful to Viktoria Sofieva for numerous helpful conversations. This work was performed in the framework of the European Space Agency Climate Change Initiative Greenhouse Gases Project. MIPAS level 1 data are provided by the European Space Agency. The ACE mission is supported primarily by the Canadian Space Agency. Part of this research was performed at the Jet Propulsion Laboratory, California Institute of Technology, under contract with NASA. We thank the Columbia Scientific Balloon Facility (CSBF) for performing the launches of the JPL MkIV instrument.

We acknowledge support by Deutsche Forschungsgemeinschaft and Open Access Publishing Fund of Karlsruhe Institute of Technology.

The article processing charges for this open-access publication were covered by a Research Centre of the Helmholtz Association.

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Table 1. Reference datasets.

Reference instrument	Version	Viewing geometry	Time overlap	Collocation criteria	Number of matches	Reference	Recent validation
ACE-FTS	v3.5	solar occultation	2005–2012	9 h – 800 km	14 200	Boone et al. (2013)	Waymark et al. (2013)
HALOE	v19	solar occultation	Jan–Aug 2005	24 h – 1000 km	783	Russell III et al. (1993)	Park et al. (1996)
SCIAMACHY	v3.3.6	solar occultation	2005–2010	5 h – 500 km	5636	Noël et al. (2011)	Noël et al. (2011)
SOFIE	v1.2	solar occultation	2007–2012	5 h – 500 km	29 124	Gordley et al. (2009)	
MkIV	n/a	solar occultation	2005–2007	24 h – 1000 km	3	Toon (1991)	Toon et al. (1999)
Cryosampler	n/a	n/a	n/a	24 h – 1000 km	n/a	Engel et al. (1997); Levin et al. (1999)	

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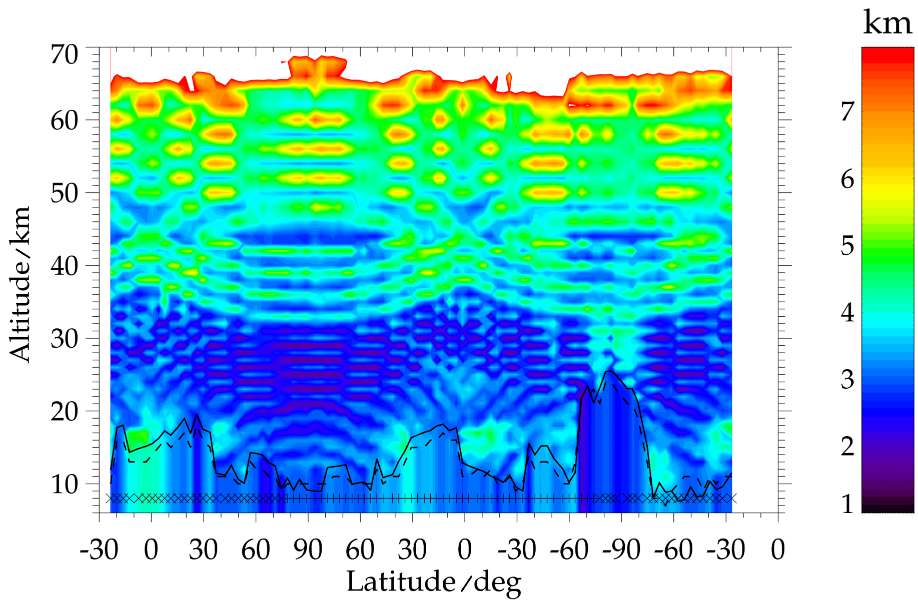

Figure 1. Vertical resolution of CH_4 profiles along one orbit.

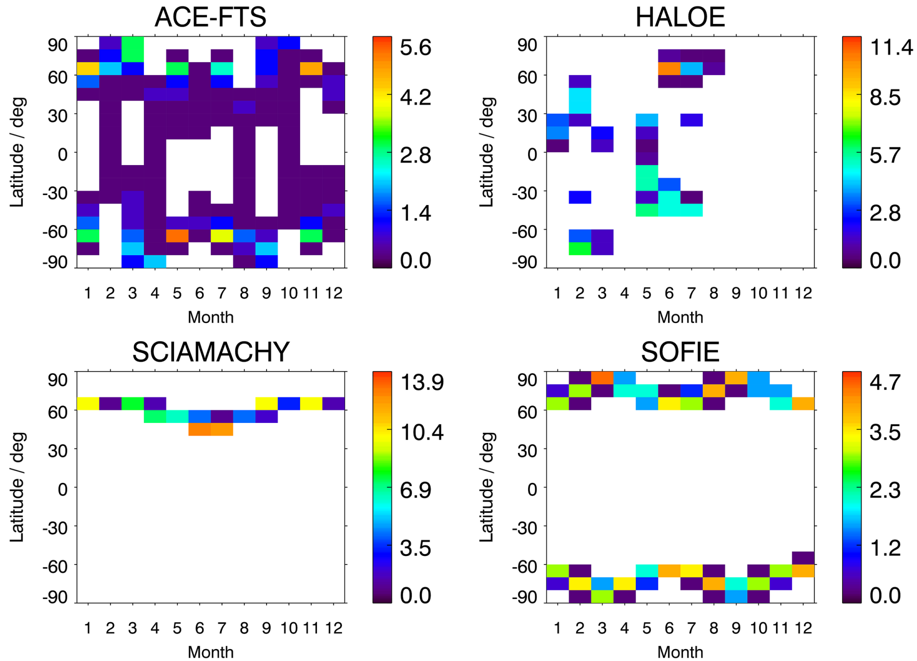

Figure 2. Monthly latitudinal distributions of collocated measurements of MIPAS with reference instruments, in percent.

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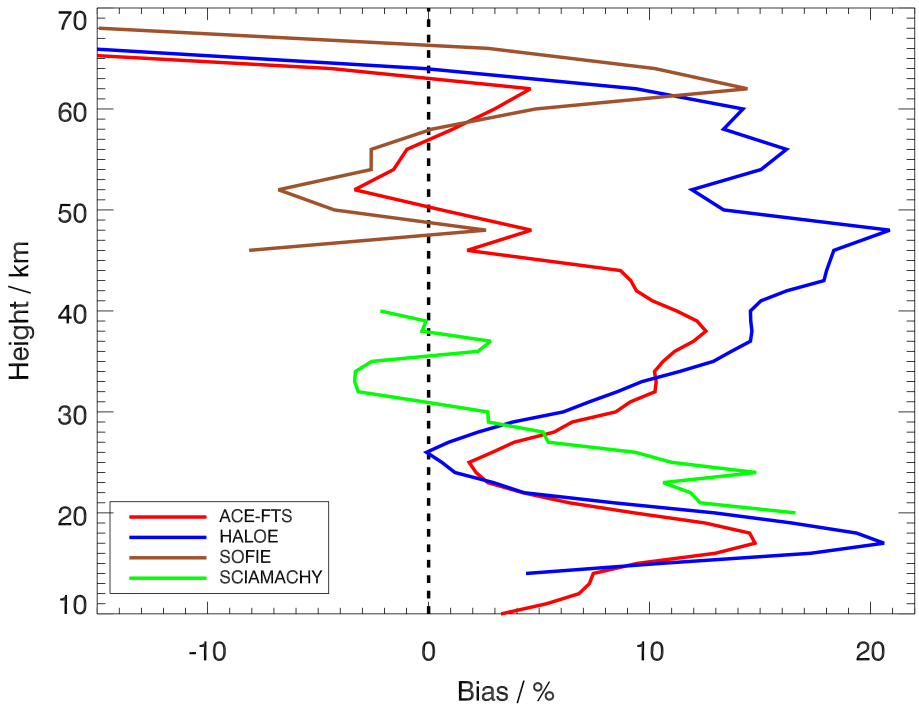

Figure 3. Bias estimation of MIPAS methane retrievals with respect to satellite reference instruments. The quantity showed is the mean estimate over all latitudes of $\frac{\text{MIPAS}-\text{REF}}{\text{REF}} \times 100\,\%$.

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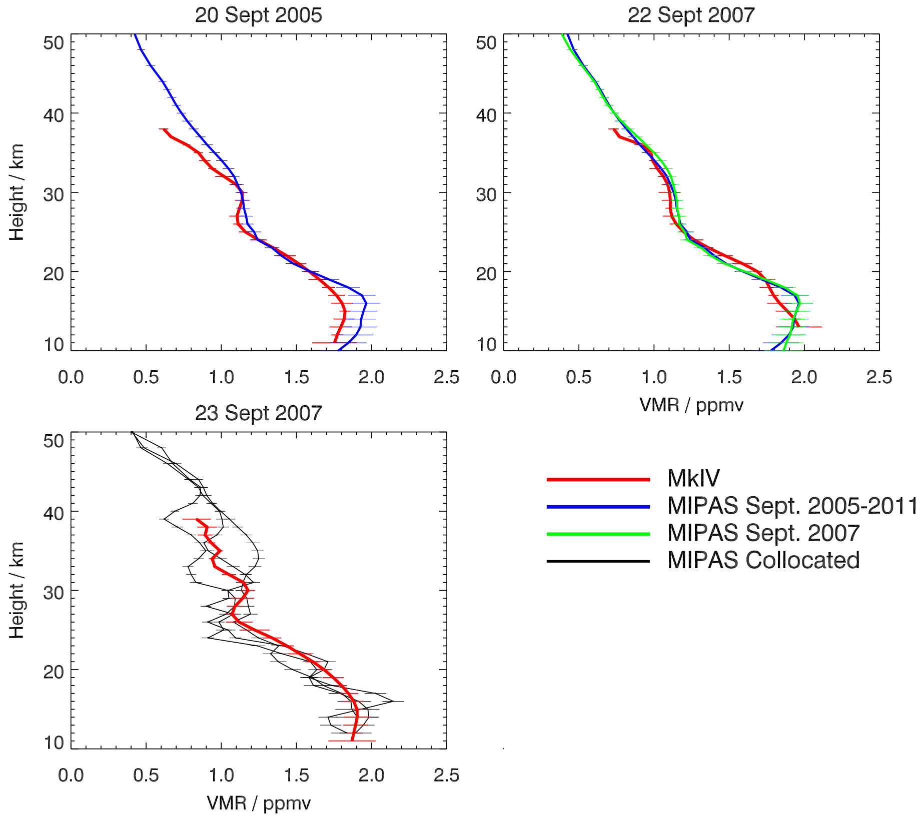

Figure 4. MkIV profiles and MIPAS CH4 vmr vertical profiles – collocated profiles when they exist, otherwise mean profiles in September 2007 and Septembers 2005–2011 in the [30° N, 40° N] latitude band where the three balloon flights took place.

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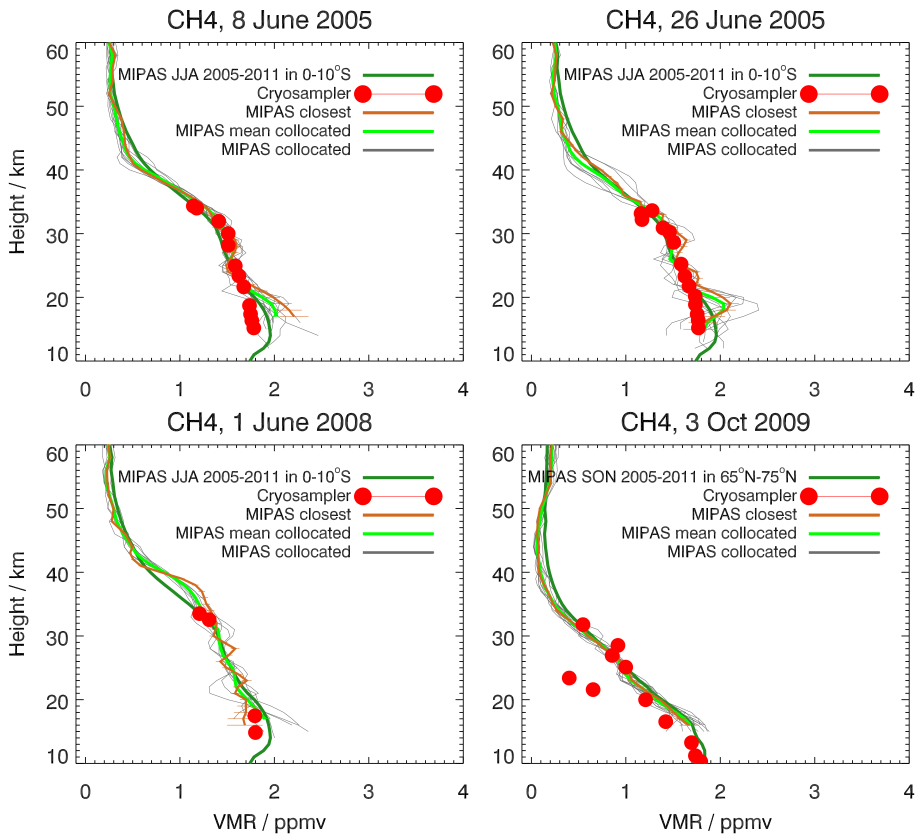

Figure 5. Four cryosampler profiles and MIPAS CH4 vmr profiles – collocated, monthly and seasonal means in corresponding latitude bands. JJA stays for June–July–August; SON stays for September–October–November.

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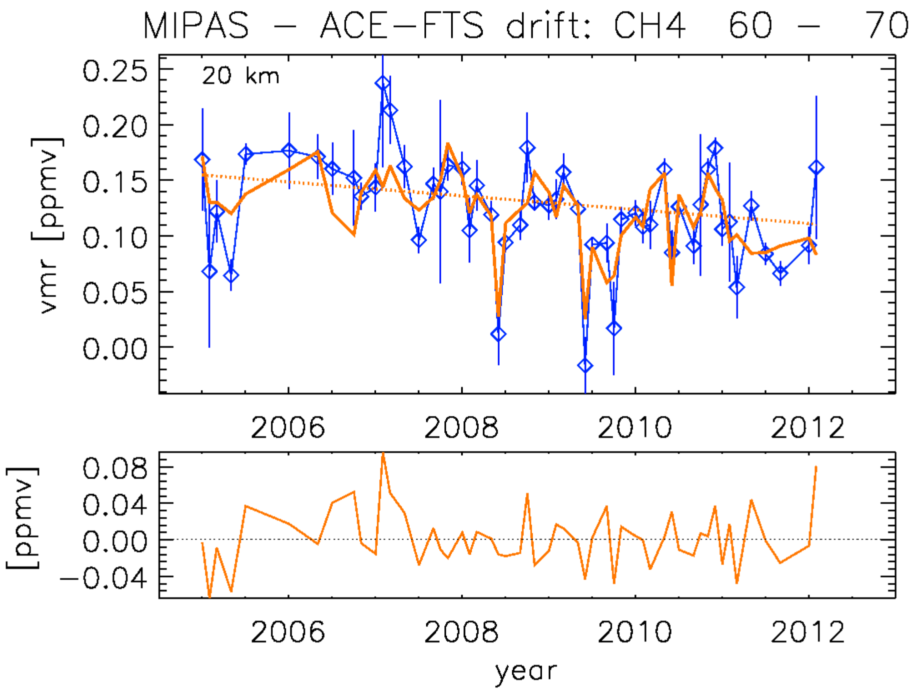

Figure 6. Drift of MIPAS methane with respect to ACE-FTS at 20 km height in [60° N; 70° N] latitudes. Upper panel: monthly means (blue diamonds), calculated fit and the related trend (orange lines) for the differences (MIPAS-ACE). The drift here is −0.06 ppmv per decade. Bottom panel: differences between the fit and the data points (the residual).

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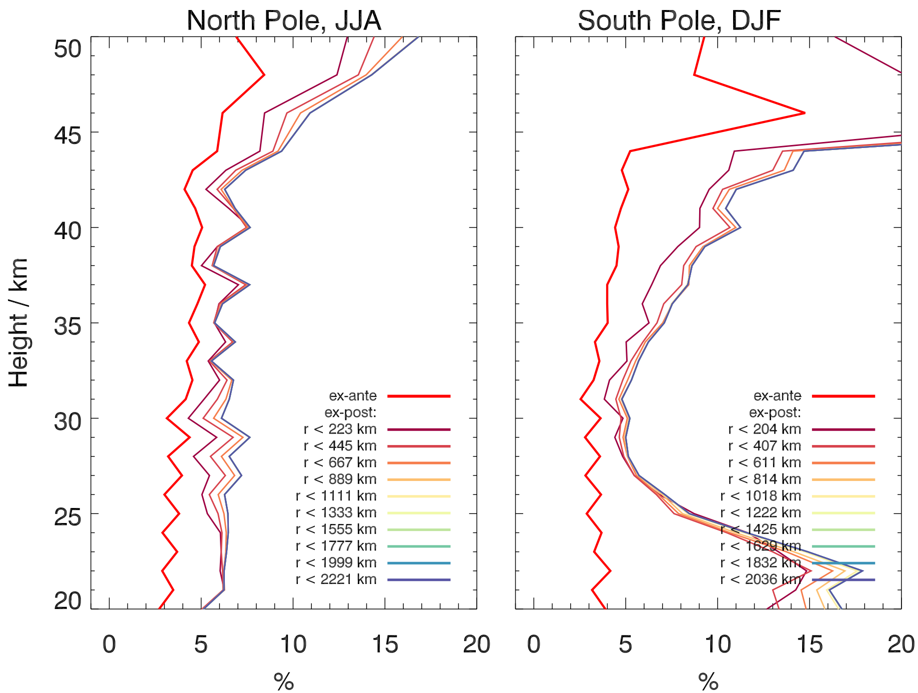

Figure 7. Structure functions of MIPAS IMK processor in two regions with low atmospheric variability: North Pole in June–July–August (JJA, left column) and South Pole in December–January–February (DJF, right column). The analysis was run on 430 pairs within 220 km, 7500 pairs within 880 km, going up to 12 400 pairs within 2000 and more km.

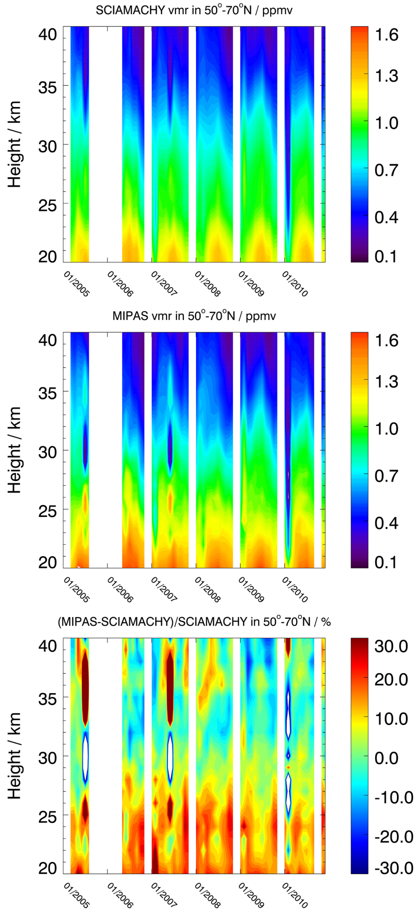

Figure 8. Monthly mean values of SCIAMACHY (top panel) and MIPAS (middle panel) and monthly means of differences (MIPAS-SCIAMACHY)/SCIAMACHY in percents (bottom panel) in 2005–2010.

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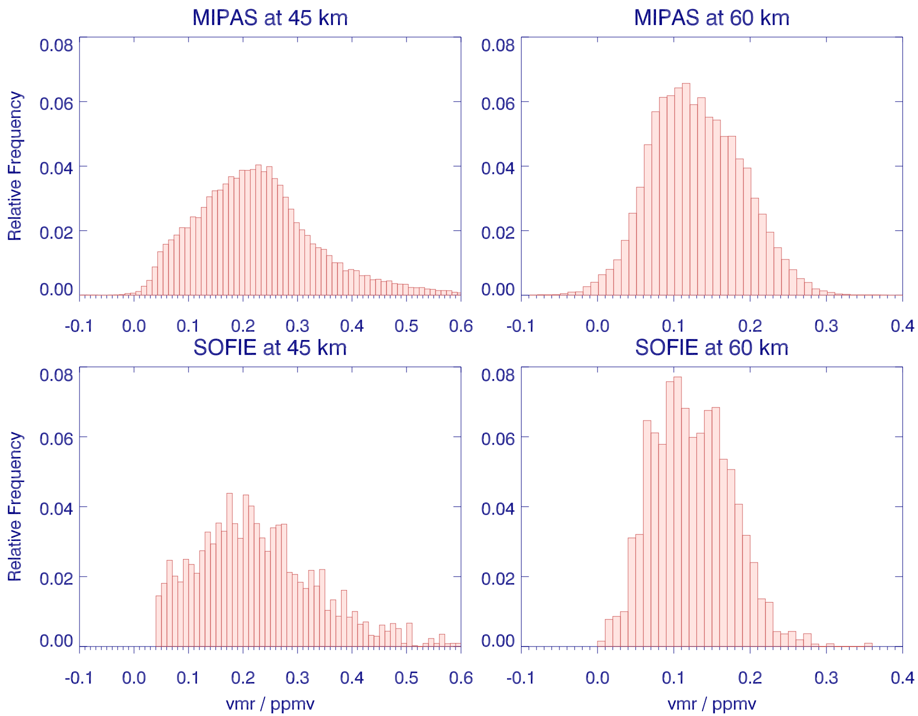

Figure 9. Relative frequency of vmr values of MIPAS (upper line) and SOFIE (bottom line) at 45 km (left column) and 60 km (right column).

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