VALIDATION OF THE MIPAS LEVEL 2 PRODUCTS USING REFERENCE ATMOSPHERES

A.M. Waterfall(1), J.J Remedios(1), R. Spang(2), and H. Sembhi(1)
(1) EOS, Department of Physics and Astronomy, University of Leicester, UK, amw24@le.ac.uk
(2) ICGI, Forschungszentrum Julich, Germany

ABSTRACT

In this paper, MIPAS level 2 products have been compared against two related reference atmosphere data sets derived for use in MIPAS studies. Such comparisons can highlight areas of difference which may be indicative of problems either with the MIPAS data products, or in the reference atmosphere data sets. A key feature of many of the comparisons is the large scatter of individual profiles which can be seen in certain locations, particularly near the top and bottom altitudes of the retrieved profile, and which can lie well beyond the expected limits from atmospheric variability. Additionally, such comparisons are a good opportunity to investigate the performance of the current cloud clearing of the MIPAS data, and it will be shown that a number of cloud contaminated profiles appear to be present in the MIPAS data set.

1. INTRODUCTION

A first order test of any data set is to compare it to reference states and to evaluate the similarities and differences. In this study, the Version 4.61, reprocessed, level 2 data products for the Michelson Interferometer for Passive Atmospheric Sounding (MIPAS) are compared to reference atmospheres in both standard profile and seasonal climatology forms. The reference atmospheres, developed specifically for use in MIPAS studies, are unique in that they contain maximum, minimum and one sigma variability profiles (standard atmospheres only). The comparisons for the MIPAS products (only H$_2$O, O$_3$, CH$_4$, N$_2$O, HNO$_3$, and temperature are discussed here) provide critical tests of geophysical behaviour of the MIPAS data sets and indicate areas of special investigation. The current performance of the MIPAS data is described here and areas highlighted where discrepancies may be ascribed to MIPAS data products, problems with the reference profiles, or atmospheric variability. In addition, the comparisons provide an excellent opportunity to investigate the performance of the current cloud clearing algorithm and its implementation in the current processor.

2. REFERENCE ATMOSPHERES

The reference atmospheres employed in this study have been developed in the frame of the MIPAS Expert Support Laboratory and Quality Working Group calibration and retrieval activities. Two types of reference have been constructed: 1) standard atmospheres for five typical geophysical regimes (polar summer, polar winter, mid-latitude day, midlatitude night and tropical); 2) seasonal climatologies (the IG2 database). The former have been exploited in the set-up for MIPAS operational processing, e.g., in microwindow selection tests, in calculating transmittance tables and in setting initial values for the variance-covariance matrices required in the processing. The seasonal climatologies provide the initial guess and contaminant profiles required for the level 2 retrievals in the operational processor; ECMWF data supercede the climatologies where available. There could therefore, in principle, be some dependence of the MIPAS retrieved mixing ratio on the initial guess and hence on the seasonal climatologies. However, this is anticipated to be small since in the operational processor, it is only the first retrieved profile in a section of retrievals that involves the seasonal climatology as the initial guess. Subsequent retrievals routinely employ the previous retrieved profiles as the initial guess.

For the level 2 products considered here, i.e., H$_2$O, O$_3$, CH$_4$, N$_2$O, HNO$_3$ and temperature, the standard atmospheres and seasonal climatologies are largely based on the same data sets. For the stratosphere, monthly mean climatologies derived from data for the Upper Atmosphere Research Satellite (UARS) were exploited and supplemented by model data from the TOMCAT model. The satellite data are mostly available through the UARS Reference Atmosphere Projects (URAP) web-site [1]. For the well mixed tropospheric source gases, such as methane and nitrous oxide, the troposphere is set to measured surface values. For water vapour, the tropospheric datasets are derived from averages of ECMWF data combined with a climatology of SAGE II data. For other gases, tropospheric model data from the MOZART model is included, supplemented for ozone by the climatology of Foruin and Kelder.

The standard atmospheres contain maximum, minimum and one sigma values as well as reference profiles for temperature and trace gases. These are based on the same data sets with adjustments to historical reports of low or high values, for example, minimum values for ozone in the Antarctic ozone hole. One sigma profiles are derived from the statistical variability of global data sets wherever possible, i.e. the satellite and model data sets described above. Where necessary, these are supplemented by measurements of latitudinal and seasonal gradients, for example, those observed by tropospheric trace gas surface networks.
3. CLOUD DETECTION

Recent versions of the ESA operational processor for MIPAS utilise a cloud detection method based on the use of a cloud index, defined by the ratio of the mean radiances in two spectral regions, as is described in [2]. Pairs of spectral windows have been selected for three of the MIPAS bands (Bands A, B, and D), and a threshold value for the cloud index defined in each case. An index value below the threshold is indicative of the presence of a cloud that is significant enough to cause errors in the retrieval, whilst spectra with indices above the threshold value may still contain some cloud influence, but in theory this should not be great enough to cause the retrieval problems. The most commonly used ratio pair, and that which has been utilised in this work, is that located in band A (788.2-796.25, 832.3-834.4 cm$^{-1}$), with a threshold value of 1.8. It should be noted that there has been a problem with the implementation of this cloud detection into the operational processor, which has resulted in the presence of cloud contaminated profiles in the current level 2 near-real-time (NRT) data sets. In addition, it is possible that the currently selected cloud detection threshold could allow some cloudy profiles through that may still have an influence on the retrieval. As will be shown here it seems likely that the reprocessed V4.61 data set, although improved in this respect over previous versions, contains a number of these cloud contaminated scans.

For all data points used in this comparison, the associated cloud index value has been derived from the MIPAS level 1b spectra using the same cloud index approach, described above, as should occur in the operational processor. These cloud indices have then been used to determine whether cloud contamination can still be observed in the reprocessed V4.61 level 2 data set. (Where the cloud index data was not available profiles have not been included in this analysis). As the associated reprocessed level 1b data was not available to us at the time of writing this cloud index had to be derived from the earlier near-real-time level 1b data, and therefore it is possible that the reprocessed cloud index will differ somewhat from that used here.

4. COMPARISONS

In the following sections, comparisons between selected months of MIPAS V4.61 reprocessed offline data (September 2002, January 2003, April 2003, and July 2003) and the relevant profiles from the two reference data sets are considered. The results for two latitude bands, the northern hemisphere tropical region (0 - 20 N), and the southern hemisphere midlatitudes (20 - 60 S), are shown. No comparisons of the polar regions have been discussed here due to potential problems with the reference atmospheres in this region, along with the difficulty of comparing widely different dynamical conditions, such as can be found inside and outside the polar vortex, to one single reference profile. Additionally, there is no discussion of NO$_2$ due to the added complexity of its diurnal variation.

All figures that will be shown subsequently follow an identical format, with the black dots indicating individual values measured by the MIPAS instrument. As mentioned above, only those profiles where cloud index values were available were included in this comparison, and any profiles flagged as cloudy by this method are instead shown by the small red crosses. (A red cross indicates a cloud index below the designated threshold at that level, whilst red indicates a cloud at another level within the profile). Unless otherwise stated the limit for cloud detection was that used in the ESA processor, with the caveat mentioned above that the cloud indices, taken from the original NRT data, may have changed in the reprocessed data shown here. Mean values of the retrievals in each altitude bin are given by the red diamonds (all profiles) and green crosses (removing cloud flagged profiles) respectively. The reference profiles from the correct season and latitude band from the IG2 database (shown by the light blue solid line) and the most relevant of the five standard atmospheres (given by the darker blue dot dashed lines) are overplotted. In a number of cases these two profiles are identical due to the similar sources from which the two datasets were compiled. Also shown on the plot are the maximum and minimum profiles given in the five standard atmospheres.

4.1 Water Vapour

There is generally observed to be good agreement between the monthly mean MIPAS water vapour values and the reference profiles (Fig. 1), particularly within the stratosphere, although there is a tendency for slightly higher water vapour values in the MIPAS data at the higher altitudes (between approximately 40 and 60 km). Conversely the data at the highest altitude is often low and shows a large spread of values, which may be indicative of a retrieval effect. In general within the stratosphere individual retrieved profiles lies within the expected maximum and minimum variability from the standard atmospheres; however at low altitudes (below approximately 20 km), particularly around the tropopause region, the MIPAS retrieval can sometimes give extremely low and often unrealistic mixing ratios for water vapour, including values off the scale of these plots. In the southern hemisphere in July 2003, an increase in the variability of the profiles at all altitudes can be observed, with extreme values occasionally occurring at all altitudes. The reasons for this increased variability need to be explored further.

4.2 Ozone

In Fig. 2 the results of the comparisons between the MIPAS ozone product and the reference data sets are shown. It can be observed that above the altitude of the ozone peak, retrieved mixing ratios are slightly greater than the IG2 reference profile, whilst for values for altitudes below the peak (down to around 20 km), the retrieved values are often slightly lower, although they are then often in agreement with the profiles from the 5 standard atmospheres. These differences between MIPAS and the
Figure 1. Comparisons of MIPAS H\textsubscript{2}O values to ref. atmospheres for 2 latitude bands (going across: 0-20 N and 20-60 S) and 4 months (going down: Sept 2002, Jan 2003, April 2003, and July 2003). In each plot, the black dots represent individual MIPAS retrieved values, whilst small crosses represent MIPAS profiles flagged as cloud contaminated using a threshold value of 1.8 [Red indicates a cloud at that altitude, whilst blue indicates a cloud at another altitude in the same profile]. The mean of the MIPAS value is given by red diamonds (all data), and the green crosses (removing cloud contaminated profiles). The seasonal climatology from the IG2 database (light blue solid line), the most relevant profile from the 5 standard atmospheres (dark blue dot dashed line), and the associated maximum and minimum profiles (blue dashed lines) are also illustrated.
Figure 2. Comparisons of MIPAS ozone values to ref. atmospheres for 2 latitude bands (going across: (0-20 N) and (20-60 S)) and 4 months (going down: Sept 2002, Jan 2003, April 2003, and July 2003). In each plot, the black dots represent individual MIPAS retrieved values, whilst small crosses represent MIPAS profiles flagged as cloud contaminated using a threshold value of 1.8 [Red indicates a cloud at that altitude, whilst blue indicates a cloud at another altitude in the same profile]. The mean of the MIPAS value is given by red diamonds (all data), and the green crosses (removing cloud contaminated profiles). The seasonal climatology from the IG2 database (light blue solid line), the most relevant profile from the 5 standard atmospheres (dark blue dot dashed line), and the associated maximum and minimum profiles (blue dashed lines) are also illustrated.
IG2 database could be explained by a shift in the altitude of the peak, and it should be investigated if this remains when plotted against the more accurate retrieved pressure rather than altitude. At 68 km diurnal variation can be observed in the MIPAS ozone values, which has not been adequately represented in either of the reference atmosphere data sets. Below 20 km, many very low individual values can be observed in the MIPAS data, well below the expected minimum from the reference values. In addition in the southern hemisphere mid-latitude comparisons a number of unexpectedly high ozone values occur. These high values are generally associated with profiles which have been flagged as cloud contaminated.

4.3 Methane

Results of the comparisons between the methane product from MIPAS and the reference data sets indicate that in general, mean CH₄ concentrations are slightly higher than either of our reference atmosphere profiles (Fig. 3). This is particularly apparent at the lower altitude levels where the variability of our reference atmosphere is believed to be very small and the mean vmrs lie outside the expected maximum and minimum values. Exceptions to this tendency occur at the highest altitude where the mean CH₄ value is generally too low, and in the July southern hemisphere mid-latitude comparison where values lower than the reference profile are seen between 40 and 60 km. In both the July 2003 and September 2002 profiles a scatter of very low methane values (reaching down to below 0.01 ppmv) can be seen around 30 km in the southern hemisphere mid-latitudes. This is well below the expected CH₄ minimum profile, and warrants further investigation.

In addition at altitudes below 20 km, there is typically a large scatter of concentrations, with mixing ratios retrieved that lie both above and below the expected range of values, including in some cases points beyond the limits of the plots shown here. In many of these plots it can be seen that a number of these values correspond to points with cloud index values below the cloud index threshold of 1.8, and which (if the original cloud ratios still hold) should have been removed from the level 2 data. Even if the presence of these low cloud index profiles can be explained by changes in the reprocessed level 1b MIPAS spectra in comparison to the near-real-time data, rather than a fault in the performance of the cloud detection in the operational processor, the fact that so many of these points have very large deviations from the expected values indicates that cloud contamination is still occurring in these cases. In addition, when a increased cloud index threshold value of 2.2 was utilised it was found that many of the other points in the scatter were also flagged. This is shown in Figure 4. The removal of such values improves the mean mixing ratios in the UTLS region, although the high bias in comparison to the reference atmosphere still occurs.

4.4 Nitrous oxide

Fig. 5 shows the comparison between N₂O from MIPAS and the reference atmospheres. Reasonably good agreement between the mean of the MIPAS retrieved values and the profiles can be seen in the lower stratosphere (around 15 to 30 km). Above this the mean values show more deviation from the reference profiles, but lie well within the expected range of values indicated by the maximum and minimum. At the lowest altitudes the mean MIPAS retrieved values are somewhat higher than the reference profiles, despite the expected variability in the reference atmospheres being very small. For methane, an unexpected scatter of points can be seen at these low altitudes, a number of which are observed to be cloudy, and many more of which would be flagged if the cloud index threshold was increased slightly. In addition, there are some very low individual N₂O values observed between 20 - 40 km in September 2002 and to a lesser extent in July 2003 southern hemisphere, the same cases where anomalous behaviour was observed for methane. It is also noted that in northern hemisphere mid-latitudes in April 2003, values below the minimum profile were also observed at a similar altitude.

4.5 HNO₃

For the case of nitric acid (Figure 6), slight differences can be observed between the reference profiles from the seasonal climatology and the five standard atmospheres. The mean MIPAS nitric acid values can typically be seen to be in reasonable agreement with these profiles, although it can vary between the months and locations, and even within a given profile as to which of the two reference profiles provides the best agreement. As has been observed for many of the gases near the top and bottom retrieval altitudes, below 20 km and above about 40 km, a number of very low individual retrieved values can be observed. These are probably an artifact of the retrieval, and may have an influence on the mean HNO₃ values for these altitudes, which in some cases can be seen to deviate from the expected profile shape. In addition, a few very high nitric acid values can be observed at the lowest altitudes, particularly in the southern hemisphere mid-lat-
Figure 3. Comparisons of MIPAS methane values to ref. atmospheres for 2 latitude bands (going across: (0-20 N) and (20-60 S)) and 4 months (going down: Sept 2002, Jan 2003, April 2003, and July 2003). In each plot, the black dots represent individual MIPAS retrieved values, whilst small crosses represent MIPAS profiles flagged as cloud contaminated using a threshold value of 1.8 [Red indicates a cloud at that altitude, whilst blue indicates a cloud at another altitude in the same profile]. The mean of the MIPAS value is given by red diamonds (all data), and the green crosses (removing cloud contaminated profiles). The seasonal climatology from the IG2 database (light blue solid line), the most relevant profile from the 5 standard atmospheres (dark blue dot dashed line), and the associated maximum and minimum profiles (blue dashed lines) are also illustrated.
Figure 5. Comparisons of MIPAS N\textsubscript{2}O values to ref. atmospheres for 2 latitude bands (going across: 0-20 N and 20-60 S) and 4 months (going down: Sept 2002, Jan 2003, April 2003, and July 2003). In each plot, the black dots represent individual MIPAS retrieved values, whilst small crosses represent MIPAS profiles flagged as cloud contaminated using a threshold value of 1.8 [Red indicates a cloud at that altitude, whilst blue indicates a cloud at another altitude in the same profile]. The mean of the MIPAS value is given by red diamonds (all data), and the green crosses (removing cloud contaminated profiles). The seasonal climatology from the IG2 database (light blue solid line), the most relevant profile from the 5 standard atmospheres (dark blue dot dashed line), and the associated maximum and minimum profiles (blue dashed lines) are also illustrated.
Figure 6. Comparisons of MIPAS nitric acid values to ref. atmospheres for 2 latitude bands (going across: (0-20 N) and (20-60 S)) and 4 months (going down: Sept 2002, Jan 2003, April 2003, and July 2003). In each plot, the black dots represent individual MIPAS retrieved values, whilst small crosses represent MIPAS profiles flagged as cloud contaminated using a threshold value of 1.8 [Red indicates a cloud at that altitude, whilst blue indicates a cloud at another altitude in the same profile]. The mean of the MIPAS value is given by red diamonds (all data), and the green crosses (removing cloud contaminated profiles). The seasonal climatology from the IG2 database (light blue solid line), the most relevant profile from the 5 standard atmospheres (dark blue dot dashed line), and the associated maximum and minimum profiles (blue dashed lines) are also illustrated.
itudes in January. Again these appear to be due to the presence of cloud contaminated profiles in the spectra.

4.6 Temperature

Finally, Fig. 7 shows the comparison of the MIPAS temperature retrievals against the two reference data sets. It can be seen that in general the retrieved temperatures lie within the expected maximum and minimum limits, although with a tendency to somewhat lower mean values in the stratosphere than are contained in the reference cases. This temperature difference can be seen particularly in July, which also shows increased variability, although still within the bounds of the reference maximum and minimum. Large variability is also seen in the September 2002 midlatitude profile, with a number of higher than expected values between 30 and 50 km. (It should be noted that September 2002 was characterised by the anomalous behaviour of the southern hemisphere polar vortex that year and it is possible that this could be the source of the high values in comparison to our references.) It is not possible from these comparisons alone to determine the source of the temperature differences. These may potentially come from problems with the reference profiles, biases in the MIPAS data, or from some atmospheric phenomenon.

5. CONCLUSIONS

In this paper, the ESA MIPAS version 4.61 reprocessed data set has been compared to two sets of reference atmospheres, a set of 5 standard atmospheres, and a database of seasonal climatologies. Such comparisons are a useful indication of the quality of the MIPAS data products, as well as a check for the validity of the reference atmospheres. In most of the cases examined here reasonable agreement is observed between the reference atmospheres and monthly mean profiles calculated from the MIPAS data. However in the preceding sections a number of existing differences have been highlighted, which indicate potential regions to be investigated further. It has generally not been possible to determine whether the reason for these differences in the mean profiles results from problems in the reference atmosphere data sets, biases in the MIPAS data, or from atmospheric variability from year to year.

A key feature which is observed in many of the data products is the presence of a number of retrieved values beyond the expected limits of variability from the reference atmospheres. This is particularly true at altitudes close to the top or bottom of the profiles, where the MIPAS product can sometimes contain exceptionally low values (e.g. HN$_3$, O$_3$, H$_2$O), the most likely cause of which are artifacts of the retrievals. Other increased variability is seen in specific cases, for example in the July 2003 southern hemisphere water vapour which is highly variable throughout the atmosphere, and which contains cases of unrealistic values at all altitudes. Exceedingly low values of methane and nitrous oxide are also observed between 20-40 km in the September 2002 and July 2003 southern hemisphere midlatitude comparisons.

A certain number of these anomalous points can be shown to be linked to the remaining presence of a number of cloud contaminated profiles (with near-real-time cloud index values below the detection threshold) in the MIPAS dataset. As the reprocessed level 1b data was not yet available, it is not clear whether these discrepancies result from the changes with respect to the original near-real-time data, or from problems with the implementation of the detection in the processor, but either way the removal of such profiles from the data set would be desirable. In these comparisons it appears that methane and nitrous oxide are particularly sensitive to the presence of cloud contamination. Much of the scatter seen at low altitudes for these two species would be removed if the threshold value for the cloud detection was increased slightly above the current value. However, it is not clear that such an increase would be of benefit to the other species, and further work is ongoing to determine the optimum threshold value.

REFERENCES

Figure 7. Comparisons of MIPAS nitric acid values to ref. atmospheres for 2 latitude bands (going across: (0-20 N) and (20-60 S)) and 4 months (going down: Sept 2002, Jan 2003, April 2003, and July 2003). In each plot, the black dots represent individual MIPAS retrieved values, whilst small crosses represent MIPAS profiles flagged as cloud contaminated using a threshold value of 1.8 [Red indicates a cloud at that altitude, whilst blue indicates a cloud at another altitude in the same profile]. The mean of the MIPAS value is given by red diamonds (all data), and the green crosses (removing cloud contaminated profiles). The seasonal climatology from the IG2 database (light blue solid line), the most relevant profile from the 5 standard atmospheres (dark blue dot dashed line), and the associated maximum and minimum profiles (blue dashed lines) are also illustrated.