

VALIDATION OF MIPAS-ENVISAT VERSION 4.61 OPERATIONAL DATA: NO₂

G. Wetzel⁽¹⁾, T. Blumenstock⁽¹⁾, H. Oelhaf⁽¹⁾, G.P. Stiller⁽¹⁾, D.-Y. Wang⁽¹⁾, G. Zhang⁽¹⁾, M. Pirre⁽²⁾, F. Goutail⁽³⁾,
A. Bazureau⁽³⁾, J.-P. Pommereau⁽³⁾, A. Bracher⁽⁴⁾, M. Sinnhuber⁽⁴⁾, M. Weber⁽⁴⁾, K. Bramstedt⁽⁴⁾,
B. Funke⁽⁵⁾, M. López-Puertas⁽⁵⁾, I. Kostadinov⁽⁶⁾, A. Petritoli⁽⁶⁾, A. Alfaro⁽⁷⁾,
F. Hendrick⁽⁸⁾, M. Van Roozendaal⁽⁸⁾, M. De Mazière⁽⁸⁾

⁽¹⁾IMK-ASF, Forschungszentrum Karlsruhe, Karlsruhe, Germany, Email: gerald.wetzel@imk.fzk.de

⁽²⁾Laboratoire de Physique et Chimie de l'Environnement/CNRS and Université d'Orléans, France

⁽³⁾Service d'Aéronomie, CNRS/IPSL, France

⁽⁴⁾Institute of Environmental Physics, University of Bremen, Germany

⁽⁵⁾Instituto de Astrofísica de Andalucía (IAA), Granada, Spain

⁽⁶⁾ISAC-CNR, Bologna, Italy

⁽⁷⁾ERS-Srl, Florence, Italy

⁽⁸⁾Belgian Institute for Space Aeronomy (IASB-BIRA), Brussels, Belgium

ABSTRACT

Embedded in the ENVISAT validation programme of the chemistry instruments GOMOS, MIPAS, and SCIAMACHY a large number of balloon-borne, aircraft and ground-based measurements were successfully carried out in the years 2002 and 2003 in the Arctic and at mid-latitudes. Unfortunately, re-analyzed operational MIPAS data were only available for the year 2002 limiting the number of validation matches with the new version 4.61 data significantly. Apart from retrieval instabilities in the operational MIPAS profiles balloon-borne observations are in good agreement with the MIPAS satellite measurements. The same holds also for a satellite inter-comparison with HALOE (version 19) data. Compared to POAM III, MIPAS exhibits a low bias of about 20% in the middle and lower stratosphere. While aircraft measurements are not quantitatively rateable due to non-overlapping measurement altitudes, ground-based inter-comparisons show a high bias in the measured MIPAS partial columns compared to FTIR observations in Kiruna and, in contrary, a low bias compared to UV-vis measurements in Harestua. Further validation coincidences have to be considered before a final quantitative assessment on the quality of the MIPAS operational NO₂ data is possible. Potential mismatches between two different sensors in terms of time and space need to be corrected with the help of photochemical model calculations taking into account the diurnal variation of the target species NO₂.

1. INTRODUCTION

The absolute necessity of validating satellite instrument products is obvious from experience with prior space instruments (as, e.g., described in [1]). Increasing complexity of space instruments and enhanced diversity of products expected from instruments like

MIPAS on ENVISAT (MIPAS-E) demand for even increased efforts in validation. Apart from satellite measurements, balloon-borne observations are a very useful tool to obtain distributions of a large number of molecules with sufficiently high vertical resolution over most of the stratospheric altitude region. However, due to a large logistical effort the number of these flights will be very limited. This holds also for aircraft observations which may cover larger horizontal regions compared to balloons taking, however, measurements from a distinctly lower flight altitude. Ground-based measurements can be carried out routinely all over the year but, apart from LIDAR observations, the vertical resolution is generally very low. The use of independent satellite measurements to validate trace gas products of these instruments has the great advantage that pole-to-pole coverage for all seasons is available and that validation activities are not limited to a certain period and location. Both instruments, HALOE (since 1991) and POAM III (since 1998), are successfully operating since many years and their NO₂ product has been comprehensively validated [2], [3].

This paper outlines the current status of the validation activities of MIPAS-E within the ACVE community concerning the molecule NO₂ as shown during the ACVE-2 meeting held in Frascati (Italy) from 3-7 May 2004. The comparisons were preferably made to the new MIPAS-E ESA operational version 4.61 data. However, unfortunately no version 4.61 data for the year 2003 were available before the ACVE-2 meeting. In this case, some comparisons to older version 4.5x data or comparisons to off-line retrieved data are shown. Due to the diurnal variation of NO₂ producing strong changes in volume mixing ratios around sunrise and sunset, the quality of coincidence in time and space between the validation measurements and the satellite observations is very crucial. In some cases model

calculations are necessary to correct mismatches between two different sensors.

2. BALLOON-BORNE OBSERVATIONS

The diode laser spectrometer SPIRALE [4] measured NO_2 during a flight from Aire-sur-l'Adour (44°N, France) on 2 October 2002. Since there was no MIPAS-E data available on this date, backward trajectory calculations were performed to match MIPAS-E on 25 and 27 September 2002. The inter-comparison shown in Figure 1 reveals a good agreement bearing in mind the small photochemical difference between both observations. Since MIPAS-E measured somewhat later in the forenoon, its NO_2 values should be up to 0.3 ppbv higher compared to those measured by SPIRALE.

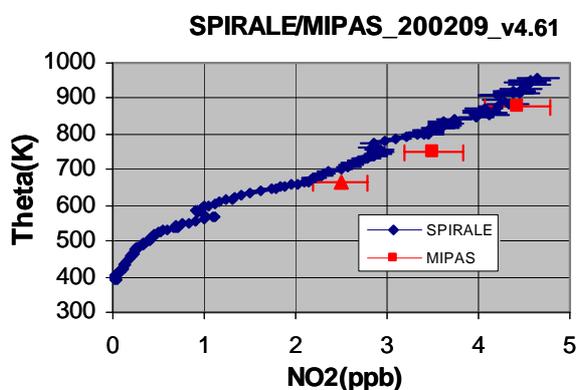


Fig. 1. Inter-comparison of SPIRALE and MIPAS-E at mid-latitudes. Due to the photochemical difference of both observations the MIPAS-E values are expected to be higher by up to 0.3 ppbv.

Another SPIRALE flight was carried out on 21 January 2003 from Kiruna (68°N, Sweden). The observation took place near the edge of the polar vortex showing a lot of vertical structures in the profile. Some of these structures can also be recognized in the MIPAS-E profile. However, this comparison to preliminary offline data from IMK is not conclusive (not shown).

A mid-latitude flight from Aire-sur-l'Adour was carried out on 24 September 2002 with the cryogenic Fourier Transform Infra-Red spectrometer MIPAS-B [5], the balloon-borne version of MIPAS on ENVISAT. For this flight a perfect coincidence in terms of time and location between MIPAS-E and MIPAS-B could be achieved. Figure 2 shows two sets of sequences measured around 47°N (seq. N3) and 40°N (seq. S) showing different profile shapes denoting to different air masses. Such differences in the profile shapes are also obvious in the MIPAS-B tracer measurements (e.g. N_2O and CH_4). Apart from

some retrieval instabilities, the MIPAS-B profiles are reproduced fairly well by the ESA operational data; differences are mostly within the combined error limits. A comparison to off-line data, processed at IMK, shows a very promising agreement also in the altitude region below about 20 hPa where no operational data have been available (not shown).

Another MIPAS-B flight was performed from Kiruna in the night from 20 to 21 March 2003 inside the polar vortex. The resulting comparison is shown in Figure 3. Since no version 4.61 data have been available so far the comparison was done for the version 4.57 data. The principal agreement is not too bad; however retrieval instabilities are very pronounced in the older MIPAS-E data version and are expected to be smaller in the new version 4.61 data.

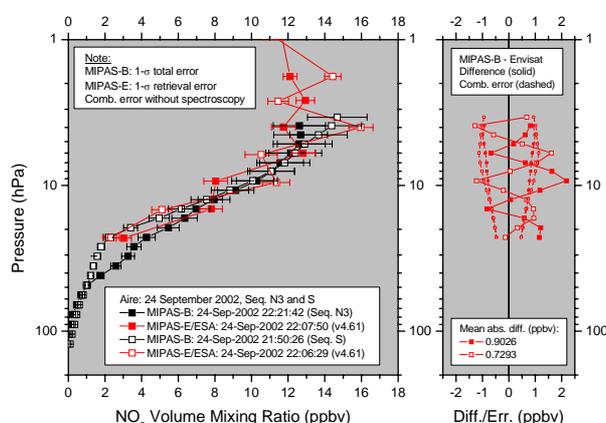


Fig. 2. Inter-comparison of MIPAS-B and MIPAS-E observations from 24 September 2002 together with differences and combined error bars (1σ).

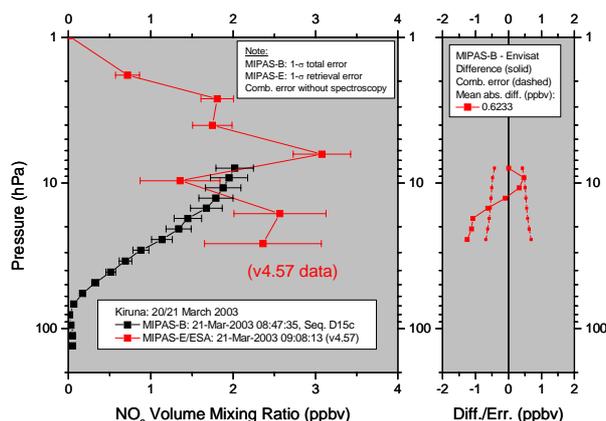


Fig. 3. MIPAS-B measurements from the March 2003 flight compared to MIPAS-E (version 4.57) data.

In the period between August 2002 and February 2004 a number of SAOZ (UV-vis sun occultation spectroscopy) balloon flights have been performed but

only one appropriate coincidence was found with MIPAS-E using a coincidence criterion of 600 km and 4 hours. The precision of SAOZ is about 10% between 10 and 30 km altitude [6]. This flight was carried out from Vanscoy (52°N, Canada). The MIPAS-E profile, observed in the late forenoon lies in between the sunrise and sunset measurement from SAOZ yielding to a qualitatively good agreement with the SAOZ profiles (see Figure 4). However, a photochemical correction is necessary in this case for a more quantitative validation.

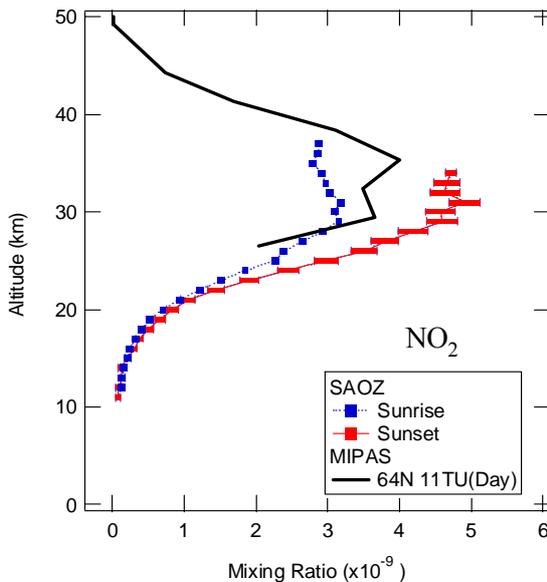


Fig. 4. SAOZ sunrise and sunset observations from 4 September 2002, compared to MIPAS-E.

3. SATELLITE INTER-COMPARISONS

A comparison between the solar occultation instrument POAM III aboard the SPOT-4 satellite and MIPAS-ENVISAT was performed in two periods from August to September 2002 and from October until December 2002 using a coincidence criterion of 600 km and 4 hours. The POAM III precision is less than 10% between 20 and 45 km altitude [3].

While for the first period the agreement of the sensors was mostly poor, in the second period some examples for a fair agreement could be found (see Figure 5). The mean difference of the profiles with fair agreement shows a low bias of MIPAS-E compared to POAM III by about 20% between 27 and 40 km altitude (see Figure 6).

Another inter-comparison was carried out for the newest data release (version 19) of the HALOE solar occultation sensor aboard UARS to MIPAS-E (data version 4.61). Figure 7 shows an example for observations from October 2002. The coincidence

criterion was 250 km during the same day. The HALOE NO₂ mixing ratios were taken as input for a 1-dimensional photochemical model and scaled to the MIPAS-E solar zenith angle (SZA) [7]. The accuracy of HALOE NO₂ profiles is about 15% between 25 and 45 km altitude [2].

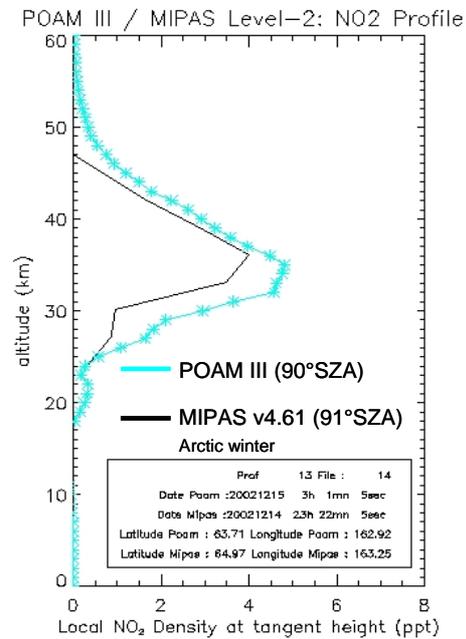


Fig. 5. Example of a fair agreement between MIPAS-E and POAM III from mid-December 2002 around the short daylight period near 64°N.

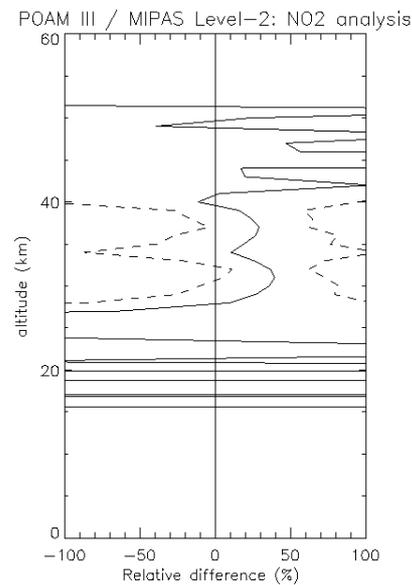


Fig. 6. Statistical difference between POAM III and MIPAS-E for selected profiles with fair agreement.

91 collocations have been taken for the validation between 30°S and 90°N from July to December 2002. An example for the statistics of 14 collocations

between 94 and 120° SZA is given in Figure 8. The mean relative difference varies between -15 and +25% between 1.5 and 25 hPa pressure altitude and the root of mean squares (RMS) range lies between 10 and 25% in this altitude region. For other SZA classifications, differences are similar.

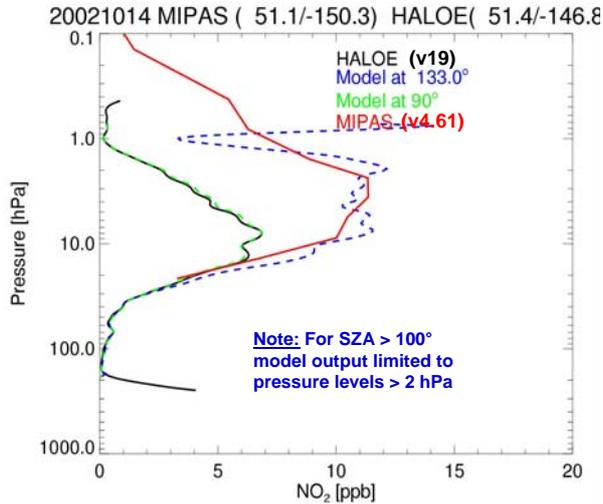


Fig. 7. Comparison of HALOE (v. 19) and MIPAS-E (v. 4.61) data. A 1-dimensional model was used to correct photochemical differences of both sensors.

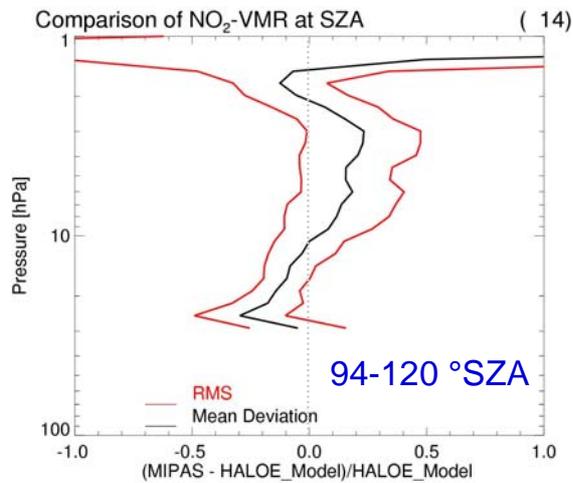


Fig. 8. Statistics for comparisons of MIPAS-E (v. 4.61) data) to model-corrected HALOE data at MIPAS-E SZAs from 94 to 120°.

A retrieval/processor comparison is shown in Figure 9. Here, differences of mean daily profiles over all latitudes between the ESA operational data (version 4.61) and the NO₂ results [8] inferred with the IMK/IAA scientific processor [9] (based on the version 4.55 level 1b data, considering non-LTE effects) are shown in the period from 18 September to 13 October 2002. Between 20 and 0.2 hPa pressure altitude the agreement of both data sets is very promising. Small

differences in this altitude region could at least partly be caused by different level 1b data used for the processing. The low bias of IMK/IAA data compared to the ESA data around 0.1 hPa cannot be explained by inclusion of non-LTE in the IMK/IAA retrieval which generally results in derived NO₂ profiles 10-30% higher than LTE in this altitude region. Hence, the reason for this large deviation is not yet clear.

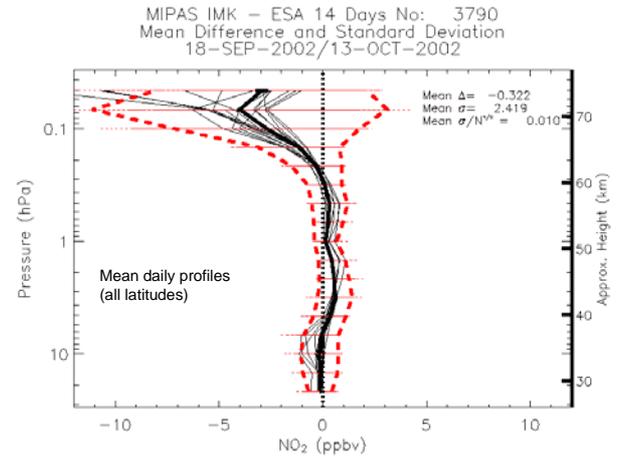


Fig. 9. Mean differences (black) and standard deviation (red) of MIPAS-E operational version 4.61 data and MIPAS-E NO₂ retrieved with the scientific processor at IMK/IAA (V1/4.55 data). Bold line represents the average over all days.

4. AIRCRAFT OBSERVATIONS

The only NO₂ data available so far for an inter-comparison were measured by the GASCOD quasi in-situ instrument [10] aboard the Geophysica high-altitude aircraft.

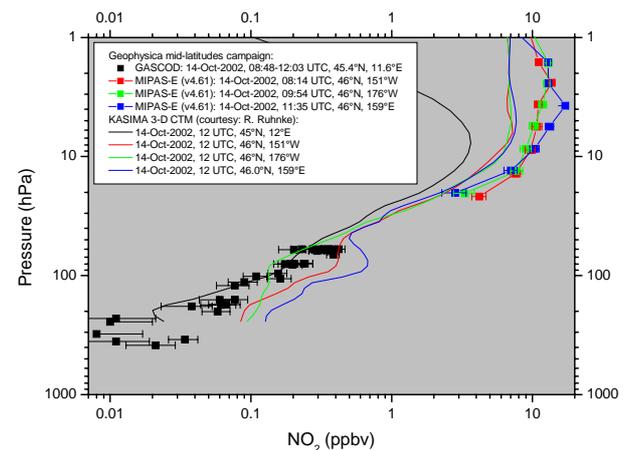


Fig. 10. Inter-comparison of aircraft quasi in-situ and MIPAS-E observations. 3-dimensional CTM KASIMA calculations (courtesy: R. Ruhnke) have been used to close the “altitude gap” between the measurements of both sensors.

Figure 10 displays NO₂ volume mixing ratios as measured during a mid-latitude Geophysica campaign in October 2002 compared to MIPAS-E measurements in the same latitudinal region. Due to the constraint of the maximum cruising altitude of the aircraft and the fact that the MIPAS-E NO₂ retrieval was not performed below about 20 hPa pressure altitude a vertical mismatch (“altitude gap”) is obvious between both observations. However, calculations with the 3-dimensional chemistry transport model (CTM) KASIMA [11] can help to close this “altitude gap” and seem to confirm at least qualitatively the agreement of both sensors.

5. GROUND-BASED OBSERVATIONS

Inter-comparisons of ground-based measurements to MIPAS-E are available from two NDSC (Network for the Detection of Stratospheric Change) stations located in Kiruna (68°N, Sweden) and Harestua (60°N, Norway).

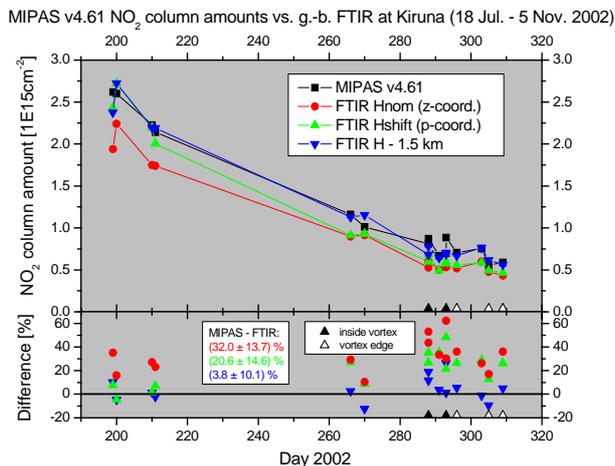


Fig. 11. Inter-comparison of stratospheric NO₂ column amounts to integrated MIPAS-E columns (for details see text).

Figure 11 shows a comparison between ground-based FTIR measurements from Kiruna [12] and MIPAS-E for the period July to November 2002. The lowest tangent altitude of MIPAS-E is located near 25 km. This means that about 40% of the total NO₂ column as measured by the ground-based FTIR has to be subtracted to compare it with the integrated MIPAS-E column amount. The resulting ground-based partial column is therefore strongly dependent on the assumed lowest tangent altitude of MIPAS-E. Columns derived on the basis of the geometric altitude (red symbols) do not match the MIPAS-E measurements while columns inferred from the lowest altitude referring to the pressure scale fit already better to the satellite observations. However, taking into account a constant

altitude shift of 1.5 km (as deduced from previously performed inter-comparisons) leaves only a small high bias of some percent in the MIPAS-E measurements. Apart from these residual deficiencies in the agreement of both sensors it should be noted that the seasonal variation of NO₂ is captured pretty well by both instruments.

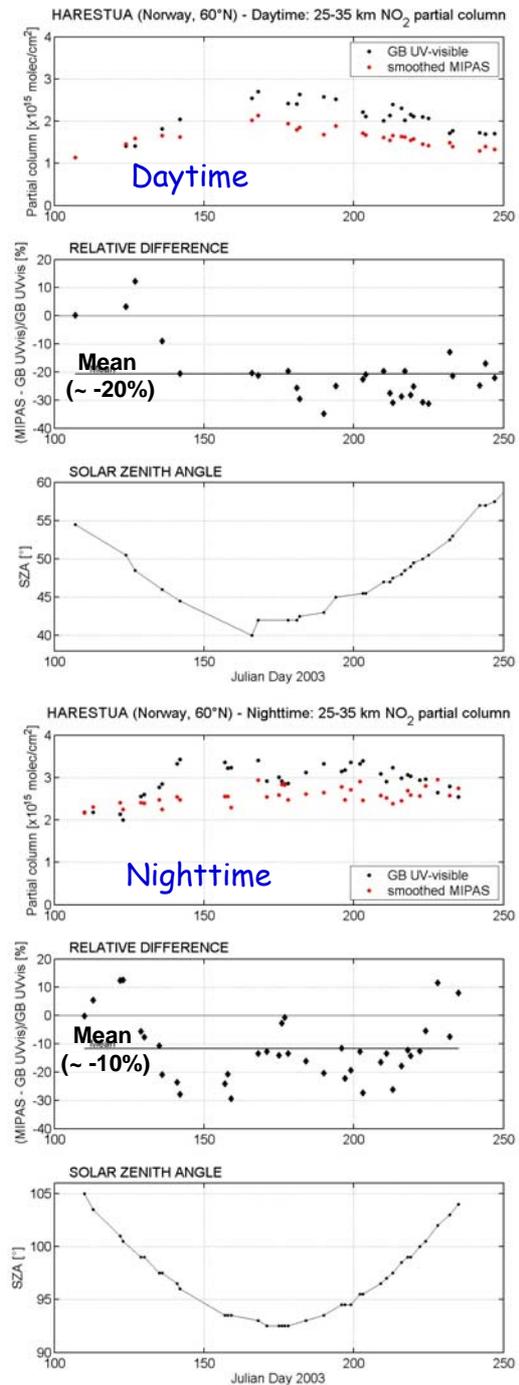


Fig. 12. Comparison of partial columns in the 25-35 km altitude region as measured by the ground-based UV-vis spectrometer in Harestua and MIPAS-E (version 4.5x data) for daytime (SZA: ~ 40-60°, top) and nighttime (SZA: ~ 95-105°, bottom) conditions.

Figure 12 displays the comparison of measurements carried out with the UV-vis spectrometer in Harestua for the period April to August 2003. The retrieval technique is based on the dependence of the mean scattering height on the solar zenith angle [13]. A stacked box photochemical model is included in the retrieval algorithm in order to reproduce the effect of the rapid variation of the NO₂ concentration at twilight. From the comparison of ground-based UV-vis and MIPAS-E averaging kernels it results that the altitude region between 25 and 35 km is most relevant for the comparison. A low bias in the MIPAS-E observations turns out during daytime (-20%) and nighttime (10%) conditions.

6. CONCLUSIONS AND OUTLOOK

The inter-comparison and validation of NO₂ is very much aggravated by the strong diurnal variation of this species. Changes in the volume mixing ratio may reach several ppbv within half an hour around sunrise and sunset. Consequently, the quality of coincidence in time and space between the validation measurement and the satellite observation is even more crucial than for species exhibiting only small diurnal variations. Measurements around sunrise and sunset are therefore difficult to compare and the use of a photochemical model to account for any temporal and spatial difference is in most cases absolutely essential.

Table 1. Summary of validation results.

Quality rating: ++ very good, + good, o fair, ? unclear.		
<u>Balloon:</u>		
SPIRALE	Sep./Oct. 2002, mid-lat.	++
MIPAS-B	Sep. 2002, mid-latitudes	++
SAOZ	Sep. 2002, mid/high-lat.	+?
<u>Satellite:</u>		
POAM III	Aug.-Dec. 2002, high-lat. low bias in MIPAS-E (20%, 27–40 km)	o
HALOE	Jul.-Dec. 2002, all latitudes high bias in MIPAS-E (~ 5%, 1.5-25 hPa)	++
MIPAS-E (IMK/IAA)	Sep./Oct. 2002, all latitudes between 20 and 0.2 hPa	++
<u>Aircraft:</u>		
GASCOD	Oct. 2002, mid-latitudes no altitude match, qualitatively reasonable	?
<u>Ground-based:</u>		
FTIR Kiruna	Jul.-Nov. 2002, high lat. high bias in MIPAS-E (4-20%)	+
UV-vis Harestua	Apr.-Aug. 2003, mid/high lat. low bias in MIPAS-E (v4.5x, 10-20%)	o

The validation process has been hampered due to a lack of re-processed version 4.61 operational data for the year 2003 where a lot of validation experiments

have been carried out. Meanwhile the data for 2003 are being re-processed such that inter-comparison results should be available within the near future.

Table 1 gives an overview on the validation results obtained so far. A main problem still existing for the MIPAS-E version 4.61 NO₂ data are some retrieval instabilities, although less pronounced than in the 4.5x data.

The agreement between balloon-borne observations and the satellite measurements is generally pretty good. For the SAOZ observation, a photochemical model correction is necessary to make a more quantitative conclusion. Satellite comparisons reveal a low bias in the MIPAS-E data of 20% between 27 and 40 km compared to POAM III while the agreement with HALOE is pretty good with only a small high bias in the MIPAS-E data. The statistical comparison of operationally analyzed data (ESA version 4.61) to scientifically processed data from IMK/IAA reveals high consistency between 20 and 0.2 hPa. The airborne GASCOD inter-comparison seems to be in a qualitatively agreement with MIPAS-E, however there is no altitude match available between both sensors. The comparison of ground-based FTIR observations from Kiruna to MIPAS-E exhibits a small high bias of about 4 to 20% dependent on the assumed lowest tangent altitude necessary for the calculation of the partial column of the ground-based measurements. On the other hand, MIPAS-E data show a low bias of 10 to 20% compared to the UV-vis observations performed from Harestua.

Apart from retrieval instabilities the operational MIPAS-E version 4.61 NO₂ data look reasonable. However, a final quantitative assessment on the quality of the NO₂ data is not yet possible. Low biases in MIPAS-E are visible compared to UV-vis instruments (POAM III, ground-based spectroscopy in Harestua) while on the other hand a tendency of high biases in MIPAS-E was recognized compared to IR observations (HALOE, ground-based FTIR in Kiruna). This disagreement could at least partly be caused by inaccuracies in the spectroscopic data used for the analyses.

Validation activities need to be continued with the inclusion of further validation coincidences (especially for the year 2003). Mismatches in coincidence have to be corrected with the help of photochemical model calculations. If necessary, different vertical resolutions of the sensors should also be considered during the validation processes as well as error budgets for the calculation of combined errors.

7. ACKNOWLEDGMENTS

Financial support by the DLR and ESA is gratefully acknowledged. We thank the CNES balloon launching team and the SSC Esrange people for excellent balloon operations and the Free University of Berlin (K. Grunow and B. Naujokat) for meteorological support and trajectory calculations. We thank also the Canadian CSA, NSERC and balloon launching teams (MANTRA/SAOZ flight).

8. REFERENCES

1. Gille, J.C., S.T. Massie, and W.G. Mankin, Evaluation of the UARS data, Preface to the special issue of *J. Geophys. Res.*, *101*, 9539-9540, 1996.

2. Gordley, L.L., et al.: Validation of nitric oxide and nitrogen dioxide measurements made by the Halogen Occultation Experiment for UARS platform, *J. Geophys. Res.*, *101*, 10241-10266, 1996.

3. Randall, C.E., J.D. Lumpe, R.M. Bevilacqua, K.W. Hoppel, E.P. Shettle, D.W. Rusch, L.L. Gordley, K. Kreher, K. Pfeilsticker, H. Boesch, G. Toon, F. Goutail, and J.-P. Pommereau, Validation of POAM III NO₂ measurements, *J. Geophys. Res.*, *107*(D20), 4432, doi:10.1029/2001JD001520, 2002.

4. Moreau, G., et al., A new balloon-borne instrument for in situ measurements of stratospheric trace species using infrared laser diodes, *ESA SP-397*, 421-426, 1997.

5. Friedl-Vallon, F., G. Maucher, A. Kleinert, A. Lengel, C. Keim, H. Oelhaf, H. Fischer, M. Seefeldner, and O. Trieschmann, Design and characterization of the balloon-borne Michelson Interferometer for Passive Atmospheric Sounding, *Appl. Opt.*, *43*, 3335-3355, 2004.

6. Pommereau, J.-P., and J. Piquard, Ozone, nitrogen dioxide and aerosol vertical distributions by UV-visible solar occultation from balloons, *Geophys. Res. Lett.*, *21*, 1227-1230, 1994.

7. Bracher, A., M. Sinnhuber, A. Rozanov, J.P. Burrows, Using photochemical models for the validation of NO₂ satellite measurements at different solar zenith angles, *submitted to Atmos. Chem. Phys.*, 2004.

8. Funke, B., T. von Clarmann, H. Fischer, M. García-Comas, S. Gil-López, N. Glatthor, U. Grabowski, M. Höpfner, S. Kellmann, M. Kiefer, A. Linden, M. López-Puertas, M.A. López-Valverde, G. Mengistu

Tsidu, M. Milz, T. Steck, G.P. Stiller, and D.-Y. Wang, Non-LTE retrieval of NO, NO₂, and CO from MIPAS-ENVISAT, *11th International Workshop on Atmospheric Science from Space Using Fourier Transform Spectrometry (ASSFTS)*, Bad Wildbad, Germany, 8-10 October 2003.

9. von Clarmann, T., T. Chidiezie Chineke, H. Fischer, B. Funke, M. García-Comas, S. Gil-López, N. Glatthor, U. Grabowski, M. Höpfner, S. Kellmann, M. Kiefer, A. Linden, M. López-Puertas, M.A. López-Valverde, G. Mengistu Tsidu, M. Milz, T. Steck, and G.P. Stiller, Remote Sensing of the Middle Atmosphere with MIPAS, in: *Remote Sensing of Clouds and the Atmosphere VII*, K. Schäfer, O. Lado-Bordowsky, A. Comerón, and R.H. Picard (Eds.), *Proc. SPIE*, *4882*, 172-183, 2003.

10. Petritoli, A., F. Ravegnani, G. Giovanelli, D. Bortoli, U. Bonafe, I. Kostadinov, and A. Oulanovsky, Off-axis measurements of atmospheric trace gases by use of an airborne ultraviolet-visible spectrometer, *Appl. Opt.*, *41*, 5593-5599, 2002.

11. Kouker, W., I. Langbein, Th. Reddmann, and R. Ruhnke, The Karlsruhe simulation model of the middle atmosphere (KASIMA), version 2, *Rep. FZKA 6278*, Forschungszentrum Karlsruhe GmbH, Karlsruhe, Germany, 1999.

12. Blumenstock, Th., H. Fischer, A. Friedle, F. Hase, and P. Thomas: Column amounts of ClONO₂, HCl, HNO₃, and HF from ground-based FTIR measurements made near Kiruna, Sweden, in late winter 1994, *J. Atmos. Chem.* *26*, 311 - 321, 1997.

13. Hendrick, F., B. Barret, M. Van Roozendael, H. Boesch, A. Butz, M. De Mazière, F. Goutail, C. Hermans, J.-C. Lambert, K. Pfeilsticker, J.-P. Pommereau, Retrieval of nitrogen dioxide stratospheric profiles from ground-based zenith-sky UV-visible observations: validation of the technique through correlative comparisons, *Atmos. Chem. Phys. Discussions*, *4*, 2867-2904, 2004.