MIPAS OZONE VALIDATION BY SATELLITE INTERCOMPARISONS

B.J.Kerridge⁽¹⁾, F.Goutail⁽²⁾, A.Bazureau⁽²⁾, D.-Y.Wang⁽³⁾, A.Bracher⁽⁴⁾, M.Weber⁽⁴⁾, K.Bramstedt⁽⁴⁾, R.Siddans⁽¹⁾, B.G.Latter⁽¹⁾, W.J.Reburn⁽¹⁾, V.L.Jay⁽¹⁾, A.Dethof⁽⁵⁾, V.H.Payne⁽⁶⁾

⁽¹⁾ Rutherford Appleton Laboratory, Chilton Didcot, OX11 0QX, UK, Email : B.J.Kerridge@rl.ac.uk ⁽²⁾ Service d'Aeronomie CNRS/IPSL, BP 3, 91371 Verrieres-le-Buisson, France, Email : Florence.Goutail@aerov.jussieu.fr

⁽³⁾ IMK/FZK, Postfach 3640,76021, Karlsruhe, Germany, Email : ding-yi.wang@imk.fzk.de

⁽⁴⁾ IUP, University of Bremen, P.O. Box 330440, D-28334 Bremen, Germany, Email : bracher@uni-bremen.de

⁽⁵⁾ ECMWF, Shinfield Park, Reading, RG2 9AX, UK, Email : Antje.Dethof@ecmwf.int

⁽⁶⁾ AOPP, University of Oxford, Parks Road, Oxford, OX1 3PU, UK, Email : payne@atm.ox.ac.uk

ABSTRACT

MIPAS ozone data has been compared with that from different satellite instruments, for the period July-December 2002. The MIPAS O₃ profiles have been intercompared systematically with co-located data from HALOE, SAGE-II, POAM-III, ODIN SMR, GOME, URAP climatology, and IMK independent MIPAS retrievals. At pressures less than 50hPa, results showed generally good agreement. The largest discrepancies were found to occur at pressures greater than 50 hPa, and in tropical and polar latitudes. Estimates of precision and accuracy of MIPAS O₃ are reported on the basis of the conducted comparisons.

1. INTRODUCTION

As part of the ENVISAT atmospheric chemistry validation, the aim of this paper was to intercompare MIPAS ozone against other satellite measurements. Satellite intercomparisons allow the data quality to be assessed globally, including latitudinal and longitudinal variations as well as vertical structure. Another advantage is the large number of profile coincidences which can be incorporated in the ensemble. However, atmospheric variability due to imperfect co-location inevitably enters into satellite-satellite direct comparisons as it does for satellite-ground comparisons. Although this variability will tend to average out in the assessment of bias, it will contribute to the assessment of precision.

The work reported in this paper has been conducted by six different institutes, who have compared MIPAS O_3 profiles directly with those from five other satellite instruments. In addition, the total column ozone field generated through assimilation of MIPAS O_3 profiles has been compared to a TOMS total ozone field, and MIPAS monthly-mean O_3 data has been compared with the UARS Reference Atmosphere Project O_3 climatology.

Most attention has been given to the data processed "off-line" (MIPAS OL data version 4.61), although comparisons are also reported with data produced operationally in near real time (NL data) covering a longer timespan. The near real time processor is optimised for accuracy and speed, and the NL data included here represent the Level 1 and Level 2 processor versions that were active at the time of measurement. A number of key differences exist between the off-line and near real time processors : the off-line uses consolidated level 1B data (which should correspond to improved calibration) and different parameter settings in Level 2 processing, including more stringent convergence criteria and an extended altitude range (down to 6km instead of 12km for NL data).

The attributes of correlative satellite data sets used in these intercomparisons have already been established. Instruments considered include occultation sensors (HALOE, SAGE-II, POAM-III), nadir sounders (GOME, TOMS) and another limb sounder (Sub-Millimetre Radiometer (SMR) on Odin). An independent retrieval (by IMK) from MIPAS itself is also reported.

In this paper, MIPAS OL (v4.61) O_3 is compared with: HALOE (IMK, University of Bremen), SAGE II (U.Bremen), POAM III (CNRS), Odin SMR (IMK), GOME (RAL), TOMS (ECMWF) and MIPAS in-house retrievals (IMK). MIPAS NL O_3 data are compared with: GOME (RAL) and UARS Reference Atmosphere (University of Oxford).

1.1. Spatial and temporal sampling

A variety of sampling approaches have been adopted in the intercomparisons presented here. In general, data between July and December 2002 have been used, with a particular focus on September 2002: a period of intense scientific attention due to unusual behaviour of the southern polar vortex.

Proceedings of the Second Workshop on the Atmospheric Chemistry Validation of ENVISAT (ACVE-2) ESA-ESRIN, Frascati, Italy, 3-7 May 2004 (ESA SP-562, August 2004) EMI01BK Different co-location criteria have been used in the various comparisons. These are described for each case in the following sections. As mentioned previously, over a large ensemble of satellite-satellite co-locations, differences in co-location criteria between sensors are likely to influence variance rather than biases in the *MIPAS-correlative sensor* apparent differences.

Diverse vertical profile representations have been adopted: e.g. volume mixing ratio (VMR), number density ($[O_3]$), partial pressure, along with different approaches to interpolation and layer averaging. Some of the discrepancies between data sets may therefore be due to the choices made in binning, averaging, interpolating and presenting the data.

For MIPAS vertical profile registration, the pressure coordinate has been used in all cases except for the POAM-III comparison. Tangent point pressure is retrieved by MIPAS from the measured spectra, so comparisons on pressure coordinates should minimise effects due to differences in pressure/altitude registration between instruments. (Although the geometric altitudes reported in MIPAS OL data are derived from the retrieved tangent-pressures, the need to fix the geometric altitude of a reference pressure level introduces the possibility for offset in absolute geometric heights assigned.)

HALOE, SAGE-II and POAM-III are solar occultation sensors with very particular sampling characteristics. Since measurements are made at only at sunrise and/or sunset, their geographical and temporal coverage differs substantially from that of MIPAS. In the comparisons with HALOE and SMR carried out by IMK, the MIPAS ascending and descending nodes are separated.

GOME data are acquired only in sunlight, so the colocations are mainly with MIPAS in descending node.

2. OCCULTATION SENSORS

MIPAS data have been intercompared with measurements from the following occulation sensors:

The *Halogen Occultation Experiment* (HALOE), on board UARS launched in 1991, is an infrared (2.45 to 10.0 μ m) radiometer with a dedicated O₃ filter channel [1].

The Stratospheric Aerosol and Gas Experiment II (SAGE II), on ERBS launched in 1984, is a UV-VIS-NIR (0.385 to 1.02 μ m) radiometer, with a filter dedicated to O₃ [2].

The *Polar Ozone and Aerosol Measurement* III (POAM III), on SPOT-4 since 1998, measures solar extinction in

nine narrow bands, covering the spectral range from approximately 350 to 1060 nm, with a filter dedicated to O_3 [3].

2.1. HALOE (IMK)

Comparisons between MIPAS and HALOE were carried out by IMK for the period 18 to 28 September, and the co-location criteria were: 5° in latitude, 10° in longitude and 12 hours in time. Ascending and descending (dark and sunlit respectively) node comparisons are shown separately in figures 1 and 2. The percentage difference between HALOE and MIPAS is shown: $100\times(MIPAS-HALOE)/HALOE$. HALOE data used for comparison are taken from the Level 2-version 19 database through BADC. The solar occultation measurements tend to be in two distinct latitude bands for a given day and to sweep across the full longitude range. The HALOE ozone profiles are retrieved between 25 and 90 km at ~2 km vertical spacing.



Figure 1, Zonal mean comparison (% difference) of MIPAS with HALOE, descending node (sunlit)



Figure 2, Zonal mean comparison (% difference) of MIPAS with HALOE, ascending node (dark)

Above 0.4 hPa, a positive bias can be seen in the ascending node comparison. Between 0.4 and 40 hPa the bias is less than 10%, but an increasing bias is seen below 40hPa, especially in the tropics.

The pronounced difference in apparent bias between descending and ascending node comparisons in the mesosphere is due to atomic oxygen recombination occurring after sunset, and should therefore not be interpreted as an error in MIPAS ascending node.

2.2. HALOE AND SAGE-II (U.Bremen)

University of Bremen carried out comparisons with HALOE version 19 and SAGE-II version 6.2. The colocation criteria were: within 250 km and on the same day. For HALOE, 79 co-locations were included between 22 July and 14 December 2002. Most were at $30^{\circ}N - 60^{\circ}N$ (56) and $60^{\circ}N - 90^{\circ}N$ (13). Only 8 profiles were located in the tropics and only 6 in southern latitudes. Examples of co-located profiles at two latitudes are shown in figures 3 and 4.

The stated accuracy for HALOE profiles is 6% over 30-60km and 20% over 15-30km [4].

For SAGE-II, 137 co-locations were included between 18 July and 15 December 2002. Most profiles were located between $60^{\circ}N - 90^{\circ}N$ (66), $30^{\circ}N - 60^{\circ}N$ (28) and $60^{\circ}S - 90^{\circ}S$ (24). Only 13 profiles were located in the tropics, and only 6 between $30^{\circ}S - 60^{\circ}S$. The accuracy of SAGE-II profiles over 10-50km is 10% [5]. Some example profile intercomparisons are shown in figures 5 and 6.



Figure 3, Example co-located profiles from MIPAS and HALOE (high southern latitude)



Figure 4, Example co-located profiles from MIPAS and HALOE (subtropics)



Figure 5 Example co-located profiles from MIPAS and SAGE-II (Southern mid-latitude)



Figure 6, Example co-located profiles from MIPAS and SAGE-II (tropics)

Figures 7 and 8 show the mean and RMS deviation for the ensemble of co-locations, with the deviation calculated as (MIPAS-HALOE)/HALOE and (MIPAS-SAGE-II)/SAGE-II.



Figure 7, MIPAS/HALOE intercomparison showing ensemble mean and RMS deviations



Figure 8, MIPAS/SAGE-II intercomparison showing mean deviations and RMS

For HALOE, the mean deviations between 0.5 and 50 hPa are between +5 and +15% (\pm 5-15%). For SAGE-II, the mean deviations between 0.5 and 60 hPa are between -5 and +5% (\pm 7 – 15%). It should be noted that the 10% difference in bias between HALOE and SAGE may partly reflect differences in latitude sampling of the two ensembles.

At pressures greater than 50 hPa, positive biases and large increases in RMS can be seen, especially with respect to HALOE, for which sampling is weighted to northern mid-latitudes rather than high-latitudes.

2.3. POAM-III (CNRS)

CNRS/IPSL carried out intercomparisons with POAM-III data. Two latitude bands are covered: 60-70°N, and 62-87°S. Data were included between August and December 2002 and the coincidence criteria were: within 600 km and within 24 hours. This gives 168 coincidences in the northern hemisphere and 194 coincidences in the southern hemisphere. The stated precision of POAM-III is 5-10% over 13-60 km.

Figures 9 and 10 show the resulting mean relative differences and RMS, in percent, for each hemisphere.



Figure 9, POAM-II/MIPAS intercomparison for Northern hemisphere, showing mean relative difference and RMS

In the northern hemisphere, good agreement is found for all profiles and the altitude co-registration is found to be reasonable. Between 20 and 35 km the bias is less than 3% and between 35 and 55 km the bias is between -5 and +7%.

In the southern hemisphere, an offset correction was arbitrarily applied to the MIPAS geometric altitudes (+1km). Prior to this, a positive MIPAS O_3 bias (<12%) was seen between 25 and 35 km, and a negative bias (-7 to -9%) between 35 and 55 km. After applying the altitude correction, much better agreement is obtained, with a small positive bias (<5%) between 25 and 60 km.



Figure 10, POAM-III/MIPAS intercomparison for Southern hemisphere (after +1km altitude correction), showing mean relative difference and RMS

2.4. Summary of Occultation Sensors

Taking into account the different latitude weightings in the ensembles, the comparisons with HALOE, SAGE-II and POAM-III appear to present a quite consistent picture. The quality of MIPAS O₃ data in the upper and middle stratosphere appears to be good, and the height range of good quality data extends to progressively lower altitudes with increasing latitude in the sunlit hemisphere.

3. LIMB SOUNDER

The *SubMillimetre Radiometer* (SMR) on the Odin satellite, launched in 2001, is a limb-viewing heterodyne radiometer with receivers in five frequency bands. Four bands near 500 GHz measure thermal emission from rotation lines of O_3 and other trace gases, and one near 119 GHz measures an O_2 line, to determine pressure/temperature [6].

3.1. ODIN SMR (IMK)

Comparisons with ODIN SMR have been performed by zonally-averaging MIPAS-SMR percentage differences between 19 and 28 September 2002. The criteria used for co-location were: less than 5° in latitude, 10° in longitude, and less than 6 hours in time. Separate comparisons have been made for MIPAS descending

and ascending node data, i.e. sunlit and dark side respectively. Results are shown in figures 11 and 12, as $100\times(MIPAS-SMR)/SMR$. The Odin SMR O₃ data are mainly derived from the two frequency bands around 501 and 544 GHz. The data used here (Version V1.2) were obtained from the O₃ weak line at 501.45 GHz, which allows retrieval between ~20 km and ~55 km with a vertical resolution of ~2 km. It is important to note that, at altitudes above and below this range, the SMR data are reflecting *a priori* information, which does not include mesospheric diurnal variation.



Figure 11, Zonal mean comparison (% difference) of MIPAS with ODIN SMR O₃, descending node (sunlit)



Figure 12, Zonal mean comparison (% difference) of ODIN SMR with MIPAS O₃, ascending node (dark)

Features <0.4hPa in these plots should be ignored, since they are due to differences between MIPAS data and the (diurnally invariant) *a priori* used for Odin SMR retrievals. Between 0.4 and 20 hPa, where Odin SMR offers good quality data, the MIPAS bias is generally less than 10%. At latitudes greater than 60°, a bias can be seen between 20 and 40 hPa, which may be due to contamination of MIPAS data by polar stratospheric clouds (PSCs). In the tropics, there is a positive bias below 30 hPa, where there are particularly steep vertical gradients in O₃ and temperature. Upward propagation of errors from cirrus contaminated heights near the tropopause might also be a contributing factor.

4. NADIR SOUNDERS

The following nadir sounders have been used in MIPAS intercomparisons:

The Global Ozone Monitoring Experiment (GOME) was launched on board ERS-2 in 1995 and measures in nadir viewing geometry in the wavelength range of 240 - 790 nm [7]. The RAL GOME O₃ retrievals are described in [8].

The *Total Ozone Mapping Spectrometer* (TOMS), launched on Earth Probe in 1996, is a nadir-viewing UV spectrometer [9].

4.1. GOME (RAL)

RAL carried out comparisons with in-house retrievals of O_3 profiles from GOME. MIPAS data from September 2002 were considered, both off-line (OL v4.61) and near real time. The co-location criteria were: within 500 km and on the same day, which selects MIPAS data mostly from the descending node, but also some from the ascending node. The MIPAS and GOME O_3 number densities from co-located profiles were averaged between fixed pressure levels (~4km spacing), and the mean and standard deviation were calculated in 10° latitude bins for GOME, MIPAS and MIPAS-GOME.

Figure 13 and 14 show the zonal mean and standard deviations over a 3 day period (19-21 September 2002). The standard deviation in MIPAS data is high between 16 and 24 km at latitudes greater than 60° S, which may be due to PSCs. High MIPAS standard deviations are also seen below 20 km in the tropics, perhaps due to cirrus contamination. The threshold altitude above which MIPAS O₃ data quality appears good decreases steadily with increasing latitude in the autumn hemisphere; the same progression with latitude as that found in the intercomparison with solar occultation sensors.

The standard deviation in the difference between MIPAS and GOME is seen to be smaller than the standard deviation of the MIPAS O_3 data alone, which confirms MIPAS and GOME to be observing similar airmasses.

The GOME profile bias has been established in independent comparisons with ozone sondes and other satellite sensors to be less than 10% in the 12 - 40km range.



Figure 13, GOME and MIPAS mean and standard deviation in 10° latitude and ~4km altitude bins.



Figure 14, MIPAS-GOME mean and standard deviation in 100 latitude and ~4km altitude bins.

Figure 15 shows means and standard deviations for the entire September ensemble, split into latitude bands: >60S, 60-30S, 30S-30N, 30N-60N, >60N. The picture from the whole month average is quite consistent with that for the 3-day period. The MIPAS-GOME bias is seen to be less than 10% everywhere, except between 34 and 38 km for $30^{\circ}S-30^{\circ}N$, where it is greater than 15%, and between 30 and $60^{\circ}N^{1}$.

MIPAS O_3 is systematically lower than GOME in the tropics below 18 km, but higher than HALOE and SAGE-II (see earlier sections). This progression is in the sense that might be expected from the vertical resolutions of the respective sensors and the structure of the O_3 profile in the tropical lower stratosphere.

¹ Part of this discrepancy may lie on the GOME side. Residual error from an empirical correction for degradation in uv reflectance of the scan-mirror may propagate downwards to these altitudes, yielding error on retrieved O_3 of ~few %.



Figure 15, MIPAS-GOME zonal mean in latitude bands for September 2002

4.2. TOMS and assimilated GOME (ECMWF)

ECMWF has performed several 6 hour 4D-var assimilation experiments to assess the data quality of MIPAS O_3 .



Figure 16, total column O₃ in DU on 25 September 2002, top panels: ECMWF 4D-var assimilation with GOME, middle panels: ECMWF 4D-var assimilation with MIPAS, bottom panels: TOMS data

In two separate experiments, GOME O_3 profiles from RAL retrievals and MIPAS O_3 profiles (version 4.61) have been assimilated. T159 horizontal resolution was used, and 60 vertical levels, with the top level at 0.1

hPa. The experiments covered the period 12-28 September 2002. The results were compared with TOMS total column ozone data. Example synoptic maps from each experiment, and the TOMS ozone field are shown in figure 16 for 25th September 2002.

The structure and absolute values agree well between the assimilated MIPAS and GOME, and the TOMS observations.

5. IMK MIPAS SCHEME AND URAP

MIPAS O₃ data have also been intercompared with IMK in-house MIPAS retrievals, and the UARS Reference Atmosphere Project (URAP) climatology.

The IMK MIPAS processor is fully independent from the operational ESA processor, using a different forward model, different spectral microwindows and a different retrieval set-up. A description can be found in e.g. [10].

The UARS Reference Atmosphere Project (URAP) provided a reference climatology for the stratosphere from data recorded by instruments on the Upper Atmosphere Research Satellite (UARS). The 'extended standard' O_3 data has been used, which is based on HALOE and MLS data [11].

5.1. IMK MIPAS (IMK)

MIPAS profiles retrieved by the ESA processor have been intercompared with retrievals from IMK's inhouse MIPAS processor. The MIPAS IMK data version V1.0 have been used. The IMK data are retrieved based on the operational ESA level-1B data (IPF V4.59). The retrieval is done between 6 and 70 km on a 1-km grid below 44 km and 2-km above.

Comparisons have been made covering the period 18 September – 13 October 2002. Figures 17 and 18 show comparisons between MIPAS v4.61 and IMK MIPAS retrieved O_3 . The figures show zonally averaged percentage differences : $100\times(ESA-IMK)/IMK$. The data are split into ascending and descending node.

The ESA ozone VMR between 6 and 68 km tend to be higher than those of the IMK by \sim 0.2 ppmv, except for the region around 40 km where the ESA data are lower by \sim 0.2 ppmv. The largest discrepancies of ozone VMR between the two MIPAS data sets are observed in the tropical and polar regions.



Figure 17, Comparisons MIPAS v4.61/IMK MIPAS: zonal mean differences, descending node



Figure 18, Comparisons MIPAS v4.61/IMK MIPAS, zonal mean differences, ascending node

5.2. URAP climatology (University of Oxford)

Oxford University made comparisons between MIPAS near real time retrieved profiles and URAP ozone climatology (see figure 19).

Monthly mean MIPAS ozone profiles are included from July 2002 to February 2004. The MIPAS data were divided into 6 latitude bands (90S-65S, 65S-20S, 20S-0, 0-20N, 20N-65N, and 65N-90N). It should be noted that these L2 data are from the near-real-time processor, and the processor version is the one that was running at any particular month. This allowed assessment of a relatively long-term dataset with many profiles with which to calculate means.

The URAP data were split into the same latitude bands, and interpolated onto the MIPAS monthly mean pressure profiles for each month. The figure shows the percentage difference between the MIPAS and URAP O_3 data: 100× ((MIPAS-URAP)/URAP).

It can be seen from these plots that the MIPAS ozone peak occurs higher in altitude than the peak in the climatology. MIPAS also has larger ozone VMR peak values than URAP in the mid-latitudes and tropics (particularly in the tropics).



Figure 19, comparisons MIPAS/UARS reference atmosphere, monthly means in latitude bands

6. SUMMARY AND CONCLUSIONS

MIPAS O₃ data produced by the ESA processors (v4.61 off-line and NRT) have been intercompared with satellite instruments of various types, and also with an independent retrieval method. The agreement has been found to be generally good at pressures <50hPa, except at latitudes where PSCs are likely to be present. At pressures >50hPa, agreement expressed as %O₃ is less good. This is attributed to the steep decrease in O₃ mixing ratio with increasing pressure in the lower stratosphere, which is particularly marked in the tropics, in conjunction with differences in the vertical resolution and sampling of MIPAS and the other satellite sensors. Residual contamination of MIPAS data by cirrus clouds is also likely to contribute to discrepancies found at pressures >100hPa, particularly in the tropics. Abrupt discontinuities in vertical structure (nb H₂O at the hygropause and temperature at the tropopause) are difficult to accommodate with the 3 km spacing of MIPAS limb views and retrieval levels. It is postulated that this might be an additional source of variance in the MIPAS data at pressures >50hPa.

From the comparisons reported here, it can be concluded that MIPAS v4.61 O_3 data are suitable for a range of scientific research studies, especially those focused on $O_3 < 50$ hPa. For the full potential of MIPAS observations to be exploited in future, improvements to O_3 data quality are desirable > 50 hPa and in the vicinity of PSCs.

6.1. Direct comparison of v4.61 with other heightresolved satellite O₃ data

6.1.1. Precision of MIPAS O₃:

Direct satellite comparisons will tend to underestimate MIPAS precision, due to: (a) imperfect co-location (ie differences in viewing geometry and spatial and temporal offsets cf atmospheric variability); (b) differences in representation of the O₃ vertical profile and (c) the finite precision of the correlative sensor. Comparisons with occultation sensors, which have high precision and vertical resolution suggest a MIPAS single-profile (3km retrieval grid, v4.61 regularisation) precision estimate of: 10-15% over 0.5 - 50hPa, ~25% by 100hPa but with a rapid increase >100hPa.

Comparisons with GOME show that MIPAS precision in the lower stratosphere deteriorates $>60^{\circ}$ S (probably due to PSC contamination of MIPAS measurements) and with increasing pressure >50hPa, especially in the tropics (probably due to cirrus).

6.1.2. Accuracy of MIPAS O₃:

The vertical structure of biases varies from sensor to sensor, partly reflecting their vertical resolutions. For example, MIPAS would be expected to resolve structure in the tropical lower stratosphere better than GOME (leading to an apparent negative bias with respect to GOME) but not as well as solar occultation sensors (leading to apparent positive biases with respect to these sensors).

Between 50hPa – 0.5hPa MIPAS bias with respect to other sensors is generally 5-10% (except where PSCs are present), but >50hPa larger biases are found, especially at low latitudes where the O_3 profile shape and the presence of cirrus can cause particular difficulties.

A pointing bias (1km) is inferred from POAM-III at southern high latitudes, when comparing O_3 profiles on altitude levels. Comparison with POAM-III on pressure levels would eliminate potential for discrepancy attributable to conversion from pressure to absolute geometric height.

Comparison of v4.61 with IMK in-house retrievals indicates agreement to generally within +/- 0.4ppmv. Biases of the IMK scheme with respect to HALOE and SMR differ in vertical structure to those of v4.61, but are similar in magnitude <50hPa.

6.2. Indirect comparison (via assimilation) with TOMS total column O₃ data

The geographical distribution and values in synoptic maps of total column O_3 produced from MIPAS O_3 profile assimilation by ECMWF agree well with the TOMS map, and also with that produced by assimilation of RAL GOME O_3 profiles.

6.3. Comparisons of near real time O₃ data

Comparisons of near real time data with URAP climatology (which incorporates MLS & HALOE measurements) and RAL GOME O_3 profiles show broad agreement in latitudinal and seasonal variation. Deviations vary with height, latitude and also month, in part due to discontinuities in time of the NRT processor configuration

From intercomparison with GOME, the altitude above which MIPAS O_3 data quality appears good decreases with increasing latitude in the autumn hemisphere; this is consistent with findings from the comparisons with solar occultation sensors.

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