Long-term validation of MIPAS ESA operational products using MIPAS-B measurements

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- Experimental details and data analysis
- Intercomparison method
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MIPAS-B experimental details

MIPAS-B (Michelson Interferometer for Passive Atmospheric Sounding - Balloon version)

- Cryogenic limb emission FTIR spectrometer\(^1\) (-55°C, liquid nitrogen).
- Spectral coverage: 4-14 µm (four channels), unapodized spectral resolution: 0.0345 cm\(^{-1}\) (OPD\(_{\text{max}}\) = 14.5 cm); apodized NESR (single spectrum) \(\approx\) 1-7 nW/(cm\(^2\) sr cm\(^{-1}\)).

**Averaging of ~ 2 to 20 spectra per elevation scan improves signal to noise ratio (big advantage of balloon observations compared to satellite measurements).**

- INS/GPS-based pointing system plus star camera for absolute reference with an after all knowledge of \(z_{\text{min}}\) better than 50 m (1 \(\sigma\)).
- Profiles (limb mode) from UT up to float altitude; vertical resolution: 1.5 - 3 km, horizontal resolution: > 100 km along track and < 30 km cross track.

MIPAS-B data analysis

- **Radiative transfer**: Calculated with KOPRA\(^1\) (Karlsruhe Optimized and Precise Radiative transfer Algorithm) line-by-line and layer-by-layer model. Spectroscopic parameters originate from HITRAN\(^2\) and a MIPAS dedicated spectroscopic database\(^3\).

- **Retrieval calculations**: Least squares fitting procedure KOPRA\_FIT\(^4\) using a Tikhonov-Phillips regularization approach which was constrained with respect to a first derivative a priori profile \(x_a\) of the target species; state parameters \(x_i\) for iteration \(i+1\):

  \[ x_{i+1} = x_i + [K_i^T S_y^{-1} K_i + R]^{-1} [K_i^T S_y^{-1} (y_{\text{meas}} - y(x_i)) - R(x_i - x_a)] \]

  where: \(y_{\text{meas}}\) measured radiance vector; \(y(x_i)\) calculated radiance (forward) vector; \(K\) Jacobian matrix \((\partial y(x_i)/\partial x_i)\); \(S_y^{-1}\) inverse noise measurement covariance matrix; \(R\) regularization matrix;

  \[ R = \gamma L^T L \]

  where: \(\gamma\) regularization parameter; and \(L = \begin{bmatrix} -1 & 1 & 0 & \ldots & 0 \\ 0 & -1 & 1 & \ldots & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ 0 & \ldots & 0 & -1 & 1 \end{bmatrix}\) first order finite differences operator.

- **Error estimation**: Includes random noise as well as the mutual influence (covariance) of the fitted parameters, temperature errors, pointing inaccuracies, errors of non-simultaneously fitted interfering gases, and spectroscopic data errors (1 \(\sigma\)).

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\(^3\)Raspollini et al., Atmos. Meas. Tech., 6, 2419-2439, 2013.
MIPAS-B spectral windows

Overview of MIPAS-B spectral windows used for the analysis of ESA atmospheric target parameters together with typical precision errors, total errors, and altitude resolution (new V7 species marked red).

<table>
<thead>
<tr>
<th>Target parameter</th>
<th>Spectral range (cm⁻¹)</th>
<th>Precision error</th>
<th>Total error</th>
<th>Alt. resolution</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature</td>
<td>801.1 – 813.2</td>
<td>0.2 – 0.3 K</td>
<td>0.5 – 1.0 K</td>
<td>2 – 3 km</td>
</tr>
<tr>
<td></td>
<td>941.3 – 956.7</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>H₂O</td>
<td>808.0 – 825.3</td>
<td>1 – 2 %</td>
<td>8 – 11 %</td>
<td>3 – 4 km</td>
</tr>
<tr>
<td></td>
<td>1210.2 – 1244.5</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>1585.0 – 1615.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>O₃</td>
<td>763.5 – 824.4</td>
<td>0.1 – 1 %</td>
<td>8 – 10 %</td>
<td>2 – 3 km</td>
</tr>
<tr>
<td></td>
<td>964.9 – 969.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>1140.1 – 1195.6</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>HNO₃</td>
<td>864.0 – 874.0</td>
<td>0.2 – 2 %</td>
<td>8 – 9 %</td>
<td>2 – 4 km</td>
</tr>
<tr>
<td>CH₄ &amp; N₂O</td>
<td>1161.9 – 1229.8</td>
<td>1 – 3 %</td>
<td>6 – 10 %</td>
<td>2 – 4 km</td>
</tr>
<tr>
<td>NO₂</td>
<td>1585.0 – 1615.0</td>
<td>1 – 3 %</td>
<td>10 – 12 %</td>
<td>2 – 3 km</td>
</tr>
<tr>
<td>N₂O₅</td>
<td>1220.0 – 1270.0</td>
<td>0.4 – 2 %</td>
<td>5 – 7 %</td>
<td>2 – 4 km</td>
</tr>
<tr>
<td>ClONO₂</td>
<td>779.7 – 780.7</td>
<td>2 – 3 %</td>
<td>5 – 6 %</td>
<td>2 – 3 km</td>
</tr>
<tr>
<td>CFC-11</td>
<td>840.0 – 860.0</td>
<td>2 – 3 %</td>
<td>5 – 6 %</td>
<td>3 – 4 km</td>
</tr>
<tr>
<td>CFC-12</td>
<td>918.0 – 924.0</td>
<td>2 – 3 %</td>
<td>5 – 6 %</td>
<td>3 – 4 km</td>
</tr>
<tr>
<td>HCFC-22</td>
<td>828.0 – 830.0</td>
<td>3 – 6 %</td>
<td>9 – 12 %</td>
<td>3 – 4 km</td>
</tr>
<tr>
<td>CCl₄</td>
<td>786.0 – 806.0</td>
<td>5 – 10 %</td>
<td>11 – 15 %</td>
<td>3 – 5 km</td>
</tr>
<tr>
<td>CF₄</td>
<td>1274.3 – 1288.0</td>
<td>2 – 6 %</td>
<td>6 – 11 %</td>
<td>3 – 5 km</td>
</tr>
<tr>
<td>COF₂</td>
<td>750.0 – 776.0</td>
<td>1 – 3 %</td>
<td>10 – 12 %</td>
<td>3 – 4 km</td>
</tr>
<tr>
<td>HCN</td>
<td>750.0 – 776.0</td>
<td>4 – 8 %</td>
<td>9 – 12 %</td>
<td>3 – 4 km</td>
</tr>
</tbody>
</table>

(new V7 species marked red)
# MIPAS-B validation flights

Overview of MIPAS balloon flights used for intercomparison with MIPAS-E (FR and OR time period). Distances and times between closest trace gas profile pairs observed by MIPAS-E and the validation instrument refer to an altitude of 20 km (Kiruna) and 30 km (Aire sur l’Adour and Teresina).

<table>
<thead>
<tr>
<th>Location</th>
<th>Date</th>
<th>Distance (km)</th>
<th>Time difference (min)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Kiruna (Sweden, 68 °N)</strong></td>
<td>20 Mar 2003</td>
<td>16 / 546</td>
<td>14 / 15</td>
</tr>
<tr>
<td></td>
<td>03 Jul 2003</td>
<td>Trajectories only</td>
<td></td>
</tr>
<tr>
<td></td>
<td>11 Mar 2009</td>
<td>187 / 248</td>
<td>5 / 6</td>
</tr>
<tr>
<td></td>
<td>24 Jan 2010</td>
<td>109 / 302</td>
<td>5 / 6</td>
</tr>
<tr>
<td></td>
<td>31 Mar 2011</td>
<td>Trajectories only</td>
<td></td>
</tr>
<tr>
<td><strong>Aire sur l’Adour (France, 44 °N)</strong></td>
<td>24 Sep 2002</td>
<td>21 / 588 / 410 / 146</td>
<td>12 /13 / 15/16</td>
</tr>
<tr>
<td><strong>Teresina (Brazil, 5 °S)</strong></td>
<td>14 Jun 2005</td>
<td>109 / 497 / 184 / 338</td>
<td>228 / 229 / 268 / 269</td>
</tr>
<tr>
<td></td>
<td>06 Jun 2008</td>
<td>224 / 284 / 600 / 194</td>
<td>157 / 158 / 169 /170</td>
</tr>
</tbody>
</table>

- **2-day forw./backw. trajectories** (FU Berlin trajectory model\(^1\), ECMWF 1.25°x1.25° analyses) were calculated at different altitudes of each MIPAS-B observation to search for matches (1 h, 500 km) with the satellite sensor.

- **Diurnal variations** of photochemically reactive species (mainly NO\(_2\) and N\(_2\)O\(_5\)) were corrected taking into account differences in the SZA between the measurements of both sensors using a 1-D model\(^2\) constrained with MIPAS-B measured NO\(_y\).

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\(^2\)Bracher et al., Atmos. Chem. Phys., 5, 393-408, 2005.
**Intercomparison method**

- **Differences** between measured quantities of MIPAS-E and MIPAS-B are expressed in absolute units and relative differences. **Mean differences** $\Delta x_{mean}$ and $\Delta x_{mean,rel}$ for $N$ profile pairs of compared observations are given as:

  $$\Delta x_{mean} = \frac{1}{N} \sum_{n=1}^{N} (x_{E,n} - x_{B,n}) \quad \text{and} \quad \Delta x_{mean,rel} = \frac{\Delta x_{mean}}{\frac{1}{N} \sum_{n=1}^{N} x_{B,n}} \cdot 100\%$$

  where $x_{E}$ and $x_{B}$ are VMR values of MIPAS-E and MIPAS-B at one altitude level.

- **Combined errors** $\sigma_{comb}$ of both instruments are defined as:

  $$\sigma_{comb} = \sqrt{\sigma_{E}^2 + \sigma_{B}^2}$$

  where $\sigma_{E}$ and $\sigma_{B}$ are the precision, systematic or total errors of MIPAS-E and the validation instrument MIPAS-B, respectively.

- **Precision errors** characterize the reproducibility of a measurement and correspond, in general, to random noise errors. **Systematic errors** (MIPAS-E) of the ESA processor have been assessed in corresponding studies\textsuperscript{1,2}.

- A **bias** between both instruments is considered significant if the SEM is smaller than the bias itself. The comparison between the VMR difference and the combined systematic error (for statistical comparisons) or total error (for single comparisons) is appropriate to identify unexplained biases in the MIPAS-E data when they exceed these combined error limits.

\textsuperscript{1}Dudhia et al., Appl. Opt., 41, 3655-3673, 2002.
\textsuperscript{2}Raspollini et al., Atmos. Meas. Tech., 6, 2419–2439, 2013.
Temperature (V7) MIPAS-E – MIPAS-B

- Difference within ±2 K in the stratosphere (larger deviations below tropopause).
- Positive MIPAS-E bias (~10%) within combined systematic errors (above hygropause).
- Enhanced positive MIPAS-E bias in V7 FR period (compared to V6 FR).
H$_2$O (V6) MIPAS-E – MIPAS-B & 100 · (MIPAS-E – MIPAS-B) / MIPAS-B

FR mode (V6)

MIPAS-E - MIPAS-B (all)
ESA ML2PP V6 (FR mode)
2-days traj. (8-45 coll./alt.)
Mean diff.: 3.83 ± 2.47 ppmv
16.4 ± 8.5 %

difference ( sd)
prec.  systematic
tot. mean comb. err.

OR mode (V6)

MIPAS-E - MIPAS-B (all)
ESA ML2PP V6 (OR mode)
2-days traj. (10-258 coll./alt.)
Mean diff.: 0.65 ± 0.31 ppmv
9.6 ± 3.5 %
- Positive bias (5-10%).
- Better agreement at lower end and generally in FR period, compared to V6 data.
CH\textsubscript{4} (V6) MIPAS-E − MIPAS-B & 100 \cdot (MIPAS-E − MIPAS-B) / MIPAS-B

FR mode (V6)

OR mode (V6)
Positive bias (5-15%). Slightly better agreement of V7 data compared to V6 data).
**N$_2$O-CH$_4$ (V7) correlation**

- MIPAS-E tropics correlation (middle stratosphere) slightly shifted upwards. ‘Unphysical outliers’ at LMS and UT.
Hydrogen budget: $\text{H}_2\text{O} + 2 \text{CH}_4$ (V7)

- Some (too) large MIPAS-E values are obvious in all geographical regions.
- Positive bias of up to 20% (in mid/upper stratosphere, increasing with altitude).
- Retrievals extended from 23 km down to LMS from V6 onwards.
Extreme positive biases.
CFC-11 (V7)  MIPAS-E – MIPAS-B & 100 · (MIPAS-E – MIPAS-B) / MIPAS-B

- Problem fixed (Incorrect handling of COCl₂ in the ESA V6). Agreement with MIPAS-B data significantly improved (compared to V6 data).
- Residual positive bias above ~19 km (increasing with altitude).
Differences within ±10% for all altitudes (FR mode) and below 28 km (OR mode).
- Good agreement in lower stratosphere. Positive bias above about 25 km.
- Positive (unexplained) bias in the middle stratosphere (esp. FR mode).
Differences within ±20% (within combined total error bars) in the stratosphere.
Puzzling and inconsistent results. Stratospheric positive bias (mainly in FR mode, exceeding combined errors).
MIPAS (ESA ML2PP V7 & V6) vs. MIPAS-B

Summary of MIPAS-ENVISAT validation results (trajectory comparison to eight MIPAS-B flights). Atmospheric parameter differences refer to MIPAS-ENVISAT minus the balloon instrument.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Comments (V7 data)</th>
<th>Changes from V6 to V7</th>
<th>Tendency</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temp.</td>
<td>Difference within ±2 K between 11 and 39 km</td>
<td>No significant difference</td>
<td>▶</td>
</tr>
<tr>
<td>H₂O</td>
<td>Positive bias (about 10%) between 11 and 39 km (within combined systematic errors)</td>
<td>Enhanced positive bias in FR period</td>
<td>▼</td>
</tr>
<tr>
<td>O₃</td>
<td>Difference within ±10% for all altitudes between 11 and 39 km</td>
<td>Slightly higher VMRs, reduced agreement with MIPAS-B data</td>
<td>▼</td>
</tr>
<tr>
<td>HNO₃</td>
<td>Positive bias (5-10%) between 11 and 33 km, significant negative bias above 35 km</td>
<td>Algebraic sign change in VMR difference above 35 km</td>
<td>▶</td>
</tr>
<tr>
<td>CH₄ &amp; N₂O</td>
<td>Positive bias for CH₄ (5-10%) and N₂O (5-15%)</td>
<td>Lower N₂O/CH₄ VMRs (FR period), better agreement with MIPAS-B data now</td>
<td>▲ ▲</td>
</tr>
<tr>
<td>NO₂</td>
<td>Positive bias of up to 20% (increasing with altitude and unexplained above 33 km)</td>
<td>No significant difference (but more comparison altitudes further down)</td>
<td>▶</td>
</tr>
<tr>
<td>N₂O₅</td>
<td>Differences &lt; 20% between 24 and 36 km (no significant bias)</td>
<td>Slightly lower VMRs around altitude of VMR maximum</td>
<td>▶</td>
</tr>
<tr>
<td>ClONO₂</td>
<td>Differences &lt; 10% between 17 and 33 km (no significant bias)</td>
<td>No significant difference</td>
<td>▶</td>
</tr>
<tr>
<td>CFC-11</td>
<td>Positive bias of more than 10% above 19 km (increasing with altitude)</td>
<td>Significantly lower VMRs, agreement with MIPAS-B data clearly improved</td>
<td>▲ ▲</td>
</tr>
<tr>
<td>CFC-12</td>
<td>Differences within ±10% for altitudes between 10 and 34 km (no significant bias)</td>
<td>Slightly lower VMRs (FR period), improved agreement with MIPAS-B data</td>
<td>▲</td>
</tr>
</tbody>
</table>
Summary of MIPAS-ENVISAT validation results (trajectory comparison to eight MIPAS-B flights) for new version 7 species. Atmospheric parameter differences refer to MIPAS-ENVISAT minus the balloon instrument.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Comments (V7 data)</th>
<th>Changes from V6 to V7</th>
<th>Reliability</th>
</tr>
</thead>
<tbody>
<tr>
<td>HCFC-22</td>
<td>Differences within ±10% for all altitudes (FR mode) and below 28 km (OR mode)</td>
<td>No V6 data available</td>
<td>+ (LS only)</td>
</tr>
<tr>
<td>CCI₄</td>
<td>Positive (unexplained) bias above about 25 km</td>
<td>No V6 data available</td>
<td>+ (LS only)</td>
</tr>
<tr>
<td>CF₄</td>
<td>Positive (unexplained) bias in the middle stratosphere (esp. FR mode)</td>
<td>No V6 data available</td>
<td>poor</td>
</tr>
<tr>
<td>COF₂</td>
<td>Differences within ±20% in the stratosphere; no unexplained biases</td>
<td>No V6 data available</td>
<td>o</td>
</tr>
<tr>
<td>HCN</td>
<td>Stratospheric positive bias (mainly in FR mode, exceeding combined errors)</td>
<td>No V6 data available</td>
<td>poor</td>
</tr>
</tbody>
</table>
Summary and conclusions

- Meanwhile 16 parameters retrieved in MIPAS V7 op. processor (cf. poster by Piera Raspollini). Overall continuous improvement with processing upgrades.

- ESA V7 data compared to MIPAS-B show improved agreement for tropospheric source gases CH₄, N₂O (at lower altitudes), CFC-11 (striking), and (to a lesser extent) CFC-12.

- V7 temperature and stratospheric species (O₃, NO₂, HNO₃, ClONO₂, N₂O₅): no significant change or slightly reduced agreement with MIPAS-B measurements.

- H₂O: enhanced positive bias in FR period in stratosphere; generally large SDs and inconsistencies for T and H₂O around tropopause/hygropause.

- Overall similar degree of agreement between MIPAS-B and MIPAS-E V7 in the OR and FR operating periods.

- **New V7 species**: HCFC-22, CCl₄, and COF₂ are in general agreement with MIPAS-B within combined systematic errors. CF₄ and HCN exhibit large differences in wide regions in the stratosphere (particularly in FR period); thus data of both species should still be used with great care (if any) in scientific studies.
Thank you for your attention

MIPAS-B-F20, 7 Sept. 2014, Timmins, Canada
Advertisement
to people interested in scientific ballooning
HEMERA:

IS-H2020-proposal: Integrated access to balloon-born platforms for innovative research and technology (1st stage successfully passed)

HEMERA will integrate a large Starting Community in the field of tropospheric and stratospheric balloon-borne research, in order to make existing balloon facilities available to all scientific teams in the European Union and associated states.

The complementarity of the HEMERA partners capabilities in the field of balloon systems and operations will allow an easy and enhanced service to the scientific community

13 partners, 7 countries in the consortium
HEMERA objectives:

HEMERA will be complementary to the national programmes and will coordinate European activities in the field of ballooning in order to:

- **Provide better and coordinated balloon access** to the troposphere and stratosphere for scientific and technological research;
- **attract new users** to enlarge the community accessing the balloon infrastructure;
- **enlarge the fields of the science and technology** research conducted with balloons;
- improve the balloon service offered to scientific and technical users;
- favour standardisation, synergy, complementarities and industrialisation through joint developments, with greater cost-effectiveness.
- provide **synergies with the EU program COPERNICUS**
- provide **complementarity and calval opportunities to the ESA satellite program**
HEMERA potential users:

- A wide range of scientific and technical themes will be addressed, such as astronomy, atmospheric and climate research, fundamental physics, biology, space research and technology.

- HEMERA potential users community is extremely large; it encompasses the scientists and engineers involved in instrument development, instrument data processing and analysis, scientists that will assimilate HEMERA data in their models, engineers and technicians that will perform in flight experiments...

- Dedicated call for proposals will be organised, with peer review group for evaluation

- Users experiments have to be funded by a national program or other funds
Points of contact:

Proposal coordinator:
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POC for scientific aspects:
Dr. Nathalie Huret, CNRS: Nathalie.Huret@cnrs-orleans.fr