Technical Note: Use of MIPAS vertical averaging kernels in validation activities

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1 Background and objective

In the frame of the ongoing activities for the validation of MIPAS Level 2 products generated by the ORM scientific processor (files `MIP_NL__2PSORM200*`), it is crucial for the validation team to reach a common understanding on how to handle the averaging kernels (AKs) included in the MIPAS Level 2 product files themselves. This Technical Note (TN) is intended to provide some guidelines for the use of the vertical AKs in comparisons with correlative validation measurements. Horizontal AKs will not be dealt with here. For the use of horizontal AKs the user should refer to [1].

The present TN will be updated on the basis of questions that will arise from the validation team during the activities. Updates of this document will be available from the following WEB link: `http://www2.fci.unibo.it/~ridolfi/hak/mipas_tn_use_vertak_v1.pdf`.

2 Why and when to use AKs

As already pointed out by several authors (see e.g. [2, 3, 4]), the intercomparison of measurements acquired by instruments that use different techniques, and therefore have different response functions to the real state of the atmosphere, is not a trivial task and sometimes may require specific methods to be used.

Remote emission measurements operated from satellites offer the great advantage of providing measurements with very good geographical and time coverage. Remote measurements, however, show characteristics that are intrinsically different from those of in-situ sounders that provide *local* and often *direct* measurements of the quantities of interest, as e.g. temperature or Volume Mixing Ratio (VMR) of atmospheric constituents. Remote sensors do not measure directly the geophysical quantities of interest, but a complicated function of them (the limb-emission spectrum in the case of MIPAS); therefore these measurements must undergo an inversion process to extract the desired information. Both the characteristics of the inversion algorithm and instrument-specific features such as the instantaneous field of view, the sampling grid and the spectral resolution contribute to making the shape of the measurement spatial response a complex function.

Assuming the availability of well characterized correlative *reference* measurements, the intercomparison provides insight at two different levels:

a) firstly, the statistical analysis of the discrepancies between MIPAS and reference measurements can be used to characterize both the bias and the precision of MIPAS [5]. The bias and precision estimates obtained from the intercomparison can be then compared with the available estimates based on error propagation analyses, hence corroborating them or raising question marks regarding their reliability.

b) Secondly, if the intercomparison is carried out by avoiding or minimizing the known discrepancies due to the differences in the response functions of the intercompared measurements [2, 3, 4], the error budget of the profile differences is significantly reduced and it is then possible to investigate the remaining discrepancies with improved accuracy.

Unfortunately, in several cases the intercomparison cannot proceed up to this second level because the spatial response functions, or *averaging kernels* (AKs), which are the linear approximation [6] of the considered measurements, are not accurately known. There also might be cases in which AKs are accurately known but the instrument response function is strongly nonlinear. In this case the AKs may not provide an accurate description of the response function itself [7], if the discrepancies between the compared profiles are large enough.

The experience accumulated in the validation of MIPAS full-resolution (FR) measurements in the years 2006-2007 [8] has shown that correlative measurements often belong to one of these two categories:

1. Measurements with a vertical resolution much finer than that of MIPAS ($\approx$ 2 to 3 km in the range from 6 to 42 km). For example, radiosonde and in-situ measured profiles have very high vertical resolutions and fine sampling steps (of the order of 100 m). Lidar measurements may also have a very good vertical resolution (ranging from 150 m up to 1-2 km).

2. Measurements with a vertical resolution comparable to that of MIPAS. For example balloon or satellite limb-sounding measurements, or analyses from the European Centre for Medium-Range Weather Forecasts [10] belong to this group.

Different spatial response functions of the measurements considered induce a significant *smoothing error* [6, 2, 4] on the difference profile. In the intercomparisons we want to check if this difference is statistically consistent with zero. The smoothing error of the difference and the other error components add up quadratically to form the total error of the difference.

For comparison with measurements of type 1 the smoothing error of the difference profile can be avoided, or at least reduced, by applying the MIPAS AK to the high vertical resolution correlative measurement profile. A method to accomplish this task is described in Sect. 3.

In case of comparison with measurements of type 2, two alternatives are possible:

- The differences in the instrument spatial response functions are neglected. In this case a smoothing error component affects the difference profile. This error component is very hard or even impossible to estimate. The related covariance matrix $\mathbf{S}_s$ can be calculated as:

$$\mathbf{S}_s = (\mathbf{A}_2 - \mathbf{A}_1)\, \mathbf{S}_{\rm a}\, (\mathbf{A}_2 - \mathbf{A}_1)^t . \tag{1}$$

  However, even if the AKs $\mathbf{A}_1$ and $\mathbf{A}_2$ of the two compared measurements are known, it is difficult to estimate the covariance matrix $\mathbf{S}_{\rm a}$ representing the variability in the atmosphere of the target profile considered.

- The smoothing error of the difference profile can be reduced using an appropriate interpolation rule to match the altitude / pressure grids of the two intercompared profiles. This approach is proposed in [4], however, to the best of our knowledge, it was never applied to real intercomparisons, most likely due to the unavailability of accurate estimates of the AKs of the compared profiles.

Note that in the past validation of MIPAS FR measurements [8] AKs were used only rarely. This is because at that time accurate AKs were not available for MIPAS profiles. For FR MIPAS measurements AKs were evaluated only for a set of standard atmospheric conditions, as outlined in [9].

3 Convolution of profiles with MIPAS AKs

For profiles retrieved from MIPAS optimized resolution (OR) measurements (acquired from January 2005 onward), either with the ORM or the ESA Level 2 processor (IPF), AKs are calculated specifically for each profile. Therefore these AKs are expected to be more accurate than those available in the past for FR profiles.

Whenever comparing a MIPAS profile $\mathbf{x}_{\rm m}$ to a high-vertical resolution reference profile $\mathbf{x}_{\rm r}$ (see type 1. profiles mentioned in Sect. 2), the smoothing error of the difference profile can be avoided by downgrading $\mathbf{x}_{\rm r}$ to the MIPAS vertical resolution prior to the intercomparison. The objective is then to compare $\mathbf{x}_{\rm m}$ with the downgraded version of the reference profile ($\mathbf{x}_{\rm cr}$) calculated as:

$$\mathbf{x}_{\rm cr} = \mathbf{x}_0 + \mathbf{A}\,(\mathbf{x}_{\rm r} - \mathbf{x}_0)\,, \tag{2}$$

where $\mathbf{A}$ is the MIPAS AK relating to profile $\mathbf{x}_{\rm m}$ and $\mathbf{x}_0$ is the atmospheric state vector assumed for the calculation of the AK elements, that are defined as:

$$\mathbf{A}_{ij} = \left[\frac{\partial \mathbf{x}_{\rm m}(i)}{\partial \mathbf{x}(j)}\right]_{\mathbf{x}=\mathbf{x}_0} \tag{3}$$

where $\mathbf{x}_{\rm m}(i)$ is the $i-$th component of $\mathbf{x}_{\rm m}$ and $\mathbf{x}(j)$ is the $j-$th component of the atmospheric real state $\mathbf{x}$. The derivatives are evaluated for $\mathbf{x} = \mathbf{x}_0$. In the ORM/IPF calculations $\mathbf{x}_0$ is the profile evaluated at the second last iteration of the retrieval. Since the convergence criteria adopted in the retrieval are rather conservative, in the first order approximation the profile can be assumed to have changed very little at the last iteration, i.e. we can assume $\mathbf{x}_0 \approx \mathbf{x}_{\rm m}$. With this assumption Eq.(2) becomes:

$$\mathbf{x}_{\rm cr} = \mathbf{x}_{\rm m} + \mathbf{A}\,(\mathbf{x}_{\rm r} - \mathbf{x}_{\rm m})\,. \tag{4}$$

Usually $\mathbf{x}_{\mathrm{m}}$ and $\mathbf{x}_{\mathrm{r}}$ are sampled on different grids, therefore the direct calculation of the term $\mathbf{A}(\mathbf{x}_{\mathrm{r}} - \mathbf{x}_{\mathrm{m}})$ of Eq.(4) is not possible. What we can calculate is:

$$\mathbf{x}_{\mathrm{cr}} = \mathbf{x}_{\mathrm{m}} + \tilde{\mathbf{A}}(\mathbf{x}_{\mathrm{r}} - \tilde{\mathbf{x}}_{\mathrm{m}}), \tag{5}$$

where $\tilde{\mathbf{x}}_{\mathrm{m}}$ and $\tilde{\mathbf{A}}$ indicate versions of $\mathbf{x}_{\mathrm{m}}$ and $\mathbf{A}$, respectively, resampled to the pressure grid $\mathbf{p}_{\mathrm{r}}(i)$ $(i = 1, \ldots, n_{\mathrm{r}})$ of $\mathbf{x}_{\mathrm{r}}$. In particular, $\tilde{\mathbf{A}}$ is obtained from $\mathbf{A}$ by resampling only the individual rows. The AKs supplied in MIPAS Level 2 files are square matrices, their rows and columns are sampled on the retrieval grid, i.e. on the same pressure grid $\mathbf{p}_{\mathrm{m}}(i)$ $(i = 1, \ldots, n_{\mathrm{m}})$ of $\mathbf{x}_{\mathrm{m}}$. Therefore the interpolation algorithm for the calculation of $\tilde{\mathbf{x}}_{\mathrm{m}}$ and $\tilde{\mathbf{A}}$ could be implemented as follows:

for each $\mathbf{p}_{\mathrm{r}}(i)$ such that $\mathbf{p}_{\mathrm{m}}(1) \leq \mathbf{p}_{\mathrm{r}}(i) \leq \mathbf{p}_{\mathrm{m}}(n_{\mathrm{m}})$ perform the following steps (1. to 3.):

1. find j_0 that fulfills $\mathbf{p}_{\mathrm{m}}(j_0) < \mathbf{p}_{\mathrm{r}}(i) \leq \mathbf{p}_{\mathrm{m}}(j_0 + 1)$,

2. interpolate $\mathbf{x}_{\mathrm{m}}$:

$$\tilde{\mathbf{x}}_{\mathrm{m}}(i) = \mathbf{x}_{\mathrm{m}}(j_0) + \frac{\mathbf{x}_{\mathrm{m}}(j_0+1) - \mathbf{x}_{\mathrm{m}}(j_0)}{\ln(\mathbf{p}_{\mathrm{m}}(j_0+1)) - \ln(\mathbf{p}_{\mathrm{m}}(j_0))}\left(\ln(\mathbf{p}_{\mathrm{r}}(i)) - \ln(\mathbf{p}_{\mathrm{m}}(j_0))\right). \tag{6}$$

3. interpolate the rows of $\mathbf{A}$, i.e. for each $k = 1, \ldots, n_{\mathrm{m}}$, such that $\mathbf{p}_{\mathrm{r}}(1) \leq \mathbf{p}_{\mathrm{m}}(k) \leq \mathbf{p}_{\mathrm{r}}(n_{\mathrm{r}})$, compute:

$$\tilde{\mathbf{A}}(k,i) = \mathbf{A}(k,j_0) + \frac{\mathbf{A}(k,j_0+1) - \mathbf{A}(k,j_0)}{\ln(\mathbf{p}_{\mathrm{m}}(j_0+1)) - \ln(\mathbf{p}_{\mathrm{m}}(j_0))}\left(\ln(\mathbf{p}_{\mathrm{r}}(i)) - \ln(\mathbf{p}_{\mathrm{m}}(j_0))\right). \tag{7}$$

At the end of this interpolation process the rows of $\tilde{\mathbf{A}}$ must be re-normalized to 1. This can be done as follows. For each $k = 1, \ldots, n_{\mathrm{m}}$ fulfilling $\mathbf{p}_{\mathrm{r}}(1) \leq \mathbf{p}_{\mathrm{m}}(k) \leq \mathbf{p}_{\mathrm{r}}(n_{\mathrm{r}})$, perform the following two operations (a and b):

a) compute:

$$\alpha = \sum_{i:\mathbf{p}_{\mathrm{m}}(1) \leq \mathbf{p}_{\mathrm{r}}(i) \leq \mathbf{p}_{\mathrm{m}}(n_{\mathrm{m}})} \tilde{\mathbf{A}}(k,i) \tag{8}$$

b) for i such that $\mathbf{p}_{\mathrm{m}}(1) \leq \mathbf{p}_{\mathrm{r}}(i) \leq \mathbf{p}_{\mathrm{m}}(n_{\mathrm{m}})$, re-normalize:

$$\tilde{\mathbf{A}}(k,i) \leftarrow \frac{\tilde{\mathbf{A}}(k,i)}{\alpha} \tag{9}$$

Finally, the profile $\mathbf{x}_{\mathrm{cr}}$ of Eq.(5) can be evaluated as follows. For each $k = 1, \ldots, n_{\mathrm{m}}$ fulfilling $\mathbf{p}_{\mathrm{r}}(1) \leq \mathbf{p}_{\mathrm{m}}(k) \leq \mathbf{p}_{\mathrm{r}}(n_{\mathrm{r}})$, compute:

$$\mathbf{x}_{\mathrm{cr}}(k) = \mathbf{x}_{\mathrm{m}}(k) + \sum_{i:\mathbf{p}_{\mathrm{m}}(1) \leq \mathbf{p}_{\mathrm{r}}(i) \leq \mathbf{p}_{\mathrm{m}}(n_{\mathrm{m}})} \tilde{\mathbf{A}}(k,i) \cdot [\mathbf{x}_{\mathrm{r}}(i) - \tilde{\mathbf{x}}_{\mathrm{m}}(i)] \tag{10}$$

As mentioned earlier, the profile $\mathbf{x}_{\mathrm{cr}}$ can now be compared directly to $\mathbf{x}_{\mathrm{m}}$. The two profiles have the same vertical response function.

Note that the procedure described in this section is applicable to the MIPAS retrieved profiles of both VMR and temperature. Temperature, however, is inferred from MIPAS using a joint retrieval, together with tangent pressure. For this reason the Level 2 products contain a single *global* AK including both the pressure and temperature parts. The AK blocks related to pressure should not be used in validation experiments. If $\mathbf{A}(k,i)$ is the joint pressure-temperature AK with $k, i = 1, \ldots, n_p + n_t$, the matrix block relating to temperature is the one with $k, i = n_p + 1, \ldots, n_p + n_t$.

4 Where to find AKs

It is important to note that the averaging kernel information is only available in the `xxx_retrieval_mds` datasets and not in the `scan_information_mds`. For each `xxx_retrieval_mds` record there is a field called `avg_kernel` containing the 2-dimensional averaging kernel for the retrieved VMR profile (the profile itself is found in the `vmr` field).

BEAT specific instructions: for BEAT/CODA, the following IDL example shows how to read the VMR profile and averaging kernel for the i^{th} O3 retrieval record:

```
IDL> pf = coda_open('MIP_NL__2P_your_mipas_level_2_file.N1')
IDL> vmr = coda_fetch(pf, 'o3_retrieval_mds', i, 'vmr')
IDL> avk = coda_fetch(pf, 'o3_retrieval_mds', i, 'avg_kernel')
IDL> result = coda_close(pf)
```

The variable `avk` is then a vector where the averaging kernel matrix is stored columnwise.

Note that retrieving of AK information with BEAT-II (i.e. using the `beatl2_ingest()` function) is not supported.

References

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