

Results of the tests for the optimisation of convergence criteria thresholds and retrieval altitude range

Issue 1

By: Piera Raspollini, Claudio Belotti, Simone Ceccherini and Maria Prosperi

Checked by: Bruno Carli

IFAC - CNR

Date: 31 July 2003

Objectives of the tests

These tests are aimed to improve the quality of MIPAS Level 2 products by means of the following modification in the auxiliary data:

- A. Extension of the retrieval range to the whole MIPAS measurement range. This would allow to reduce the error at the boundaries of the retrieval range due to the wrong assumption of the profile outside the retrieval range.
- B. Definition of new thresholds for the convergence criteria. This would allow to reduce the error in the retrieved profiles due to the fact the real convergence is not reached (this error will be referred in the text as 'convergence error').
- C. Tuning of the variance of the ECMWF profiles.

The outputs of these tests are new OM_s (included in MIP_AX_OM2 file), new convergence thresholds and new variance for ECMWF profiles (included in MIP_AX_PS2 file), that will be contained in V3.2 of the MIPAS Level 2 auxiliary data.

Data used for the tests

The orbits that were analysed for these tests are # 2081 and # 6646. The input files for ORM were generated by ML2PP (V4.28, with cloud filtering activated). Also ECMWF files were used by ML2PP for the computation of the Initial Guess profiles.

A. Extension of the retrieval range

The auxiliary data that have been used are the same as for V3.1, with the only exception of the OM_s. Indeed, OM_s that allow to retrieve profiles in an extended altitude retrieval range have been used. Some preliminary tests showed that an extension of all retrieval to the full measurement range of 6-68 km lead to unnecessary calculations.

N₂O was not extended above 60 km and HNO₃ was not extended above 42 km, because this would have required the use of additional microwindows in the nominal OM with a consequent increase in the computing time and without a significant increase of information in the results. NO₂ was not extended at low altitudes because previous tests have proved that NO₂ retrieval is very unstable at low altitudes.

A customized retrieval range with an extension down to 6 km was therefore identified and tested. In this case a significant extra computing time was observed and another customized retrieval range, limited to 9 km altitude, was considered.

The retrieval altitude ranges for the different species are listed in Table 1 for the nominal case (V3.1), the 6 km extension and the 9 km extension (V3.2):

Table 1 Altitude retrieval range for the different retrievals in both nominal and extended cases

	Nominal case (V3.1)	6 km extension	9 km extension (V3.2)
PT	12-68 km	6-68 km	9-68 km
H2O	12-60 km	6-68 km	9-68 km
O3	12-60 km	6-68 km	9-68 km
HNO3	12-42 km	9-42 km	9-42 km
CH4	12-60 km	6-68 km	9-68 km
N2O	12-47 km	6-60 km	9-60 km
NO2	24-47 km	24-68 km	24-68 km

It must be stressed that the extension of the retrieval range does not imply the extension of useful data, but indeed improves the quality of the profiles in the nominal range.

We have tried to assess the amplitude of the errors that is removed with the extended range. To this purpose we can calculate the difference between the two retrievals as an estimate of the involved error. In table 2 the r.m.s. of the differences in the profile between nominal case and 9 km extension, normalised with respect to the random errors, is reported. The cases in which the extrapolation error is greater than 3 times the random error have been highlighted in the table.

Table 2 r.m.s. of the differences normalised with respect to the random errors

Species	Altitudes [km]	r. m. s.	
		#2081	#6646
Temperature	12	1.5	2.3
Pressure	12	1.1	3.4
H2O	12	15.2	9.2
H2O	60	16.8	10.1
O3	12	1.4	3.4
O3	60	1.7	4.0
HNO3	12	1.8	4.1
CH4	12	1.2	5.2
CH4	60	2.4	2.0
N2O	12	16.1	3.0
N2O	47	1.2	1.4
NO2	47	8.6	34.9

The extension of the retrieval range at low altitudes is also the cause of some instabilities that are responsible for lack of convergence or occasional errors in the program for some scans. Furthermore, the number of iterations needed to reach convergence increases.

In Table 3 the results of orbits #2081 and #6646 with the nominal ranges and the extended ranges are compared in term of percentage of scans not reaching convergence and computing time.

We found that the extra retrieval time is reduced from 70% and 103% (in the case of the extension down to 6 km) to 40% and 50% (in the case of the extension down to 9 km), respectively for the #2081 and #6646 analysed orbits. This large reduction for a small change of retrieved altitudes means that we have correctly removed the "critical altitudes". Also the number of sequences that do not reach convergence is reduced.

We think that the improvement in the quality of MIPAS Level 2 data induced by the extension of the retrieval range makes it worthwhile to extend the profiles, also at the cost of losing some occasional profiles. The 9 km extension provides a better compromise between improvements and computing time with respect to the 6 km extension and is the one implemented in the V3.2 of MIPAS level 2 auxiliary data.

Table 3 Comparison between nominal and extended altitude range, with nominal convergence criteria

	# 2081						# 6646					
	Nominal range		6 km extension		9 km extension		Nominal range		6 km extension		9 km extension	
	% scan with errors in ML2PP	% scans that do not reach conv.	% scan with errors in ML2PP	% scans that do not reach conv.	% scan with errors in ML2PP	% scans that do not reach conv.	% scan with errors in ML2PP	% scans that do not reach conv.	% scan with errors in ML2PP	% scans that do not reach conv.	% scan with errors in ML2PP	% scans that do not reach conv.
PT	0	0	1.4	0	0	0	0	0	1.4	0	0	0
H2O	0	0	0	10.4	0	2.9	0	0	0	11.1	0	5.6
O3	0	0	0	1.5	0	0	0	0	0	11.3	0	2.8
HNO3	0	0	0	3	0	0	0	1.4	0	7	0	4.2
CH4	0	0	0	0	0	1.5	0	0	0	11.3	0	2.8
N2O	0	0	0	3	0	0	0	0	0	7	0	0
NO2	0	0	0	0	0	0	0	2.8	0	1.4	0	1.4
Increase in computing time with respect to the nominal range	-		70 %		40 %		-		103 %		50 %	

B. Optimisation of convergence criteria thresholds

Introduction

The approach currently used by the Level 2 prototype for deciding if the convergence has been reached is the following one: convergence is reached at the iteration for which one of the following two criteria is fulfilled:

- a) the relative difference between χ^2 and linear χ^2 is smaller than a given retrieval dependent threshold;
- b) the maximum variation of the profile at a given iteration with respect to the previous iteration is smaller than a given retrieval dependent threshold.

Retrieval is stopped without reaching convergence in case that none of the two criteria listed above is fulfilled either after 10 Gauss iterations or after 10 Marquardt iterations.

In the current approach the threshold for the maximum variation of the profile is set to very relaxed values, so that in general convergence is reached when the criteria for the linear variation of the χ^2 is fulfilled. The thresholds for linear variation of the χ^2 is set to values that are rather conservative in term of computing time. This makes the convergence error significant, and hence an optimisation is required in order to reduce this error.

The tests for the optimisation of the convergence thresholds that are presented in the following section have been performed using the 9 km extension range as described in the previous paragraph. Similar results have been obtained with the 6 km extension range.

Test procedure

A reference profile is obtained from the result of a run where 10 Gauss iterations are performed. As check that these results can be used as a reference, they are compared with those obtained imposing that the convergence criterion b) is satisfied within the following very conservative thresholds (a maximum number of 20 Gauss iterations is allowed in this case):

p	0.1 %
T	0.5 K
H2O	1 %
O3	1 %
HNO3	1 %
CH4	1 %
N2O	1 %
NO2	1 %

This comparison has shown that the result of the run where 10 Gauss iterations are performed is a correct reference profile.

In order to find the appropriate convergence criteria some runs of ORM have been performed with different convergence criteria and the results have been compared with the reference profile.

The comparison is done with both the visual inspection of the profiles and by comparing for the different cases the fraction of the convergence error with respect to the random error. This quantity is computed as follows:

$$\frac{\text{conv}}{\text{random}} = \sqrt{\frac{1}{n_scan} \sum_{j=1}^{n_scan} \frac{1}{n_sweeps_j} \sum_{i=1}^{n_sweep_j} \frac{(\text{prof}_{,ji} - \text{prof_ref}_{,ji})^2}{\text{random}_{i,j}^2}}$$

$n_{tot_sweeps_j}$ represents the total number of sweeps analysed in the scan j in the nominal altitude range, n_{scan} is the total number of scans of the orbit, $prof_{i,j}$ and $prof_ref_{i,j}$ represent respectively the value of the profile at the altitude i^{th} of scan j .

Results

Tests have proved that in order to reduce the convergence error, the criterion on the maximum variation of the profile at a given iteration with respect to the previous iteration has to be used, instead of the criterion on linear variation of χ^2 . The linear χ^2 threshold was, after several tests, reduced by a factor 8 with respect to the nominal value, while the thresholds for the maximum profile variation were increased to more realistic values.

The thresholds for the maximum variation of the parameters were selected on the basis of the estimated minimum of the random error profile obtained for the nominal OM. Table 4 shows for each retrieval the minimum random error and the adopted thresholds.

Table 4 Thresholds for maximum variation of the parameters in the different retrievals (compared with the minimum of the estimated random error profile)

	Minimum of the random error profile for the nominal OM	Thresholds for maximum variation of the parameters
Temperature	0.8 K	1.2 K
Pressure	1.3 %	2%
H2O	4.9 %	8%
O3	5.7 %	8%
HNO3	3.8 %	14%
CH4	8.5 %	18%
N2O	10.3 %	12%
NO2	14.3 %	12%

We also modified the maximum number of Gauss iterations, that is now set to 8, and the maximum number of Marquardt iterations, that is now set to 5. Considering that the average number of Gauss iterations per retrieval is between 2 and 3, the reduction of the total number of Gauss iterations tries to avoid losing time in scans that have too many problems. The reduction of the maximum number of Marquardt iterations is caused from the fact that with the current Marquardt parameters, the retrieval step after 5 Marquardt iterations is small enough to make a further reduction unnecessary.

The results obtained by the ORM in the nominal case (V3.1) are compared with those obtained in the optimised one (V3.2). Table 5 shows the results obtained for the 2 analysed orbits. In particular, the fraction of the convergence error with respect to the random error and the percent of scans that do not reach convergence are reported for the different retrievals as well as the increase in computing time.

The new convergence criteria make the convergence error small enough to be neglected in the total error budget. The number of retrievals that do not reach convergence increases slightly.

In general a greater number of iterations is needed in the optimised case with respect to the nominal case, but the convergence error is strongly reduced. These new convergence criteria are implemented in the V3.2 of MIPAS level 2 auxiliary data.

Table 5 Comparison between nominal and optimised convergence criteria thresholds for the orbits #2081 and #6646

	# 2081				# 6646			
	Nominal case		Optimised case		Nominal case		Optimised case	
	conv error / random error	% scans that do not reach convergence	conv error / random error	% scans that do not reach convergence	conv error / random error	% scans that do not reach convergence	conv error / random error	% scans that do not reach convergence
P	0.77	0	0.31	0	1.03	0	0.51	4.2
T	0.53		0.34		1.69		0.62	
H2O	1.24	2.9	0.38	2.9	0.85	5.6	0.53	7.0
O3	0.97	0	0.43	4.4	0.92	2.8	0.43	4.2
HNO3	0.91	0	0.35	0	0.86	4.2	0.57	5.6
CH4	0.77	1.5	0.26	1.5	0.37	2.8	0.31	4.2
N2O	0.96	0	0.36	0	1.05	0	0.45	4.2
NO2	0.97	0	0.23	7.3	0.97	1.4	0.42	5.6
Increase in computing time with respect to the nominal case	-		32%		-		35%	

C. Effect of the variance associated to the ECMWF profiles for the definition of the Initial Guesses of the retrievals.

Tests have been performed in the following cases: variance associated to ECMWF profiles equal to 1/3 and 1/10 of the variance of the climatological profiles (provided by J.Remedios). 1/10 is the expected value for the variance of ECMWF profiles, but 1/3 provides the best results.

As a consequence, a variance equal to 1/3 of the climatological variance is chosen for the ECMWF profiles and is implemented in V3.2 of MIPAS level 2 auxiliary data.

Suggestion for possible future improvements in Level 2 codes

Considering the fact that now restrictive convergence criteria are used, it could be useful to provide Level 2 products also in case that the convergence criteria are not reached. In this case, in order to discriminate between well behaved and poorly behaved (but still useful) profiles, suitable qualifiers should be provided to assess the quality of the profiles.