Technical Note on:

ORM Cal. Val. Analysis
Part 1: Summary Sheets

Draft

Prog. Doc. N.: TN-IFAC-OST-0301 Part 1

28 April 2003

Delivery of WPs 9130 & 9500 of the CCN#5 of the study:

"Development of an Optimised Algorithm for Routine p, T and VMR Retrieval from MIPAS Limb Emission Spectra"

Contract No: **11717/95/NL/CN**

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Contents

1 Reference documents

[RD1] TN-IROE-RSA9603**,** Issue: 3A
Title: Software Architecture and Algorithm Definition

[RD2] TN-IROE-GS0102**,** Issue: 1 - Revision: 1
Title: Pre-flight modifications to the ORM_ABC code

[RD3] Draft:
Title: 'New functionalities implemented in ORM_ABC_1.2.3' ,
M. Ridolfi (16 November 2001)

[RD4] PO-MA-DOG-GS-0001, Issue: 2 - Revision: A
Title: ML2PP Software User Manual

[RD5] TN-IROE-GS0101, Issue: 1 - Revision: A
Title: Level 2 Algorithm Characterization & Validation Plan

[RD6] TN-IROE-GS0103, Draft Revision A
Title: ORM for Commissioning Phase (18 April 2002)

[RD7] TN-IROE-GS0104, Draft
Title: Description of Statistical Tool

[RD8] PO-PL-ESA-GS-1124, Issue 1B, Title: Implementation pf MIPAS post-launch calibration and validation tasks, (March 2002)

[RD9] Title: 'MIPAS-B Retrieval residuals analysis', V. Jay and A. Dudhia (23 Jan. 01)

[RD10] Title: 'REC Analysis of MIPAS data', Draft, A. Dudhia (22 April 2003)

2 Introduction

In the frame of ESA contract 11717/95/NL/CN an Optimized forward /retrieval Model (ORM) has been developed, suitable for implementation in MIPAS near real-time Level 2 Processor. In particular, version 1.2.3 of the ORM_ABC code (described in [RD1], [RD2] and [RD3]) is the scientific reference for the Retrieval Component Library of MIPAS Level 2 NRT processor [RD4]. Before the ENVISAT launch, the most critical input parameters and the most critical baselines used in the ORM were identified and a list of tests to be performed during the Commissioning Phase for both optimising the input parameters and verifying the impact of the code approximations were described in [RD5]. In order to perform these tests a modified ORM with added functionalities [RD6] and a dedicated software tool for the analysis of ORM products (Statistical Tool) [RD7] were developed.
The tests described in [RD5] have been included in the overall calibration and validation activities of the early in-flight operation of MIPAS, described in [RD8].
These tests have been performed using first one of the first orbit detected by MIPAS, i.e. orbit #504 (acquired on the 5^{th} April 2002) with unconsolidated Level1 data and then using orbit #2081 (acquired on the 24^{th} July 2002) with improved Level1 data.

This TN reports the results of the tests performed on orbit #2081 following the order of presentation used in [RD5]. It is divided in two parts. The first part is a collection of the summary sheets of all performed tests according to the template provided by ESA and provides the summary of the results and the recommendations for ESA.
The second part contains, for each test, the rationale, the used procedure (if different to the one described in [RD5]), the results and the conclusions. It is meant to collect details that justify the recommendations to ESA given in the first part.
The results of the tests described in [RD5] performed with the REC analysis are reported in [RD10].
This introduction is repeated in both parts of the report in order to make possible to consult them as independent documents.

3 Tuning of input parameters

The first group of the tests deals with the tuning of critical processing set-up parameters. The outputs of these tests consist in modified Level2 auxiliary data (PS_FRAME.DAT, PS_PT.DAT, PS_H2O.DAT, PS_O3.DAT, PS_HNO3.DAT, PS_CH4.DAT, PS_N2O.DAT, PS_NO2.DAT) that are used to generate the file MIP_PS2_AX file. The modified auxiliary files were delivered to ESA on 31st October 2002 and were implemented in the Payload data Segment (PDS) on the 13th of November.

The following input parameters have been tuned:

Tuned parameter	Sheet
Atmospheric continuum related parameters	MIP_PS_2_5 & MIP_PS_2_6 /1
Marquardt dumping factors	MIP_PS_2_5 & MIP_PS_2_6 /2
Regularization parameter	MIP_PS_2_5 & MIP_PS_2_6 /3
Convergence criteria thresholds	MIP_PS_2_5 & MIP_PS_2_6 /4
Retrieval grid	MIP_PS_2_5 & MIP_PS_2_6 /5
Layering in the forward model	MIP_PS_2_5 & MIP_PS_2_6 /6
Tropopause altitude	MIP_PS_2_5 & MIP_PS_2_6 /7
Field of view related parameters	MIP_PS_2_5 & MIP_PS_2_6 /8
Line of Sight Variance Covariance Matrix	MIP_PS_2_5 & MIP_PS_2_6 – AX2.1
Initial Guess Variance Covariance Matrix	MIP_PS_2_5 & MIP_PS_2_6 /9
Second order polynomial coefficients for the spectral correction	MIP_PS_2_3-MV_2_15

CalVal Analysis Summary Sheet	Sheet MIP_PS_2_5 & MIP_PS_2_6 /1	Page 1 of 2
	Issue: Draft	**Date** 23/06/2003
ENVISAT CARING FOR THE EARTH — *MIPAS*	**Prepared by:** Piera Raspollini	**Processing site:** IFAC-CNR
	CalVal Plan Ref: po_pl_esa_gs_1124, issue 1B, PS_2_5 & PS_2_6 **Other Ref: Sect 1.1 of 2nd Part of this TN, TN-IROE-GS0101 Issue 1 A Sect. 4.1.1,**	

Subject: :

Tuning of atmospheric continuum related parameters
PS2 , GADS#2 and 3 (#26-27.5)

AO / ESL Ref.: 11717/95/NL/CN

Inputs

PDS

Orbit 2081 data, i.e. MIP_NL__1P020724_112130_M1_2081_020801
ORM input files generated by ML2PP with quadratic frequency correction to the ILS, without cloud filtering.

Others

Outputs

Post launch version of the files : PS_PT.DAT, PS_H2O.DAT, PS_O3.DAT, PS_HNO3.DAT, PS_CH4.DAT, PS_N2O.DAT, PS_NO2.DAT and MIP_PS2_AX

File delivered to ESA by E-mail from P. Raspollini to H.Nett, 31 October 2002, Subject: New PS2, delivery of WP 9130.

Location/Access (ftp, ...)

CD

Tools

ML2PP (with patches up to 24 April 2002) for generating ORM inputs

ORM_ORB_1.0.1 (version 03.09.2002)
ST (version 0.98)

Recommendations

Accept modified parameters in PS_'SPECIE'.DAT as new default.

Repeat tuning in case of volcanic eruptions, and in general repeat tuning once /year.

Problem Areas

Summary

The fit of atmospheric continuum cross-section profiles is important for properly fitting simulations to observations, but increases significantly the number of unknown parameters.
If a big number of continuum parameters are fitted, the retrieval is weakly constrained and the final χ^2 values are expected to be small. On the other hand, in case that spectra do not contain enough information to retrieve all of them, retrieval stability decreases. Instability can induce oscillations in the retrieved profiles and can increase the number of iterations needed to reach convergence.

The minimum number of continuum parameters has to be searched that allows to properly fit the simulations to the observations (and hence to obtain a low χ^2) in a 'stable' retrieval.

In this test the following continuum related parameters have been tuned:

*Ruc*l: indicating the altitude below which continuum cross-sections are fitted;

Rzc0: altitude above which continuum is set to 0;

Dfact_cont: scaling factor of continuum parameters in the state vector (to reduce the dynamics of eigenvalues in the VCM of the state vector). The tuning of this parameter replaces the tuning of threshold for the eigenvalues in the inversion of the VCM of the retrieved parameters (see Sect. 4.1.4 in TN-GS0101, Issue 1 A).

The most critical parameter is the first one, since determines the number of the continuum fitted parameters. Complete runs of orbit #2081 were performed for different values of this parameter, from very conservative values (e.g. 50 km) to very small values (e.g. 20 km). The trade-off between low values of χ^2 and fast convergence of the retrieval (measured in term of mean number of Gauss/Marquardt iteration per scan, POQ and number of scans reaching convergence) was optimized. It was found that the average χ^2 is weakly dependent on the number of continuum fitted parameters, while fast convergence of the retrieval, expecially pT retrieval, is strongly dependent on that.
Therefore, the choice of *rucl* is driven by 'fast convergence' considerations.
The results of the tuning of rucl are reported in Table 1.

Table 1 – Values of *rucl* selected for the different retrievals:

PT	H_2O	O_3	HNO_3	CH_4	N_2O	NO_2
20 km	25 km	30 km	30 km	30 km	30 km	30 km

These results are adequate for normal atmospheric continuum conditions. In case of volcanic eruptions the level of atmospheric continuum in the stratosphere can increase significantly. In that case a re-tuning of this parameter is needed, but, if a fast action that cannot wait for the retuning process is needed, the value *rucl* = 36 km can be used, since good performances are obtained also for this value.
In order to tune the parameter *rzc0, r*uns of the complete orbit were repeated for *rzc0*=80 and *rzc0*=50 km. No modifications in the results were found in terms of both stability and final χ^2 for both these values. Since stability is not affected by this parameter, it was decided to use a conservative value, i.e. *rzc0*=80 km.Finally, runs were performed using both the hardwired value dfact_cont=10^{30} and a customized *dfact_cont* for each specie, chosen to minimise the dynamic of the eigenvalues of VCM of the retrieved quantities, i.e. pt: 10^{27}, h2o: 10^{28}, o3: 10^{28}, hno3: 10^{26}, ch4:10^{30}, n2o: 10^{27}, no2: 10^{25}. Also in this case, no modifications were obtained in terms of both stability and final χ^2.As a consequence, the final choice for *fact_cont* was to take the hardwired value, i.e. *fact_cont*=10^{30}.
These results are very similar to the ones obtained with orbit #504.

CalVal Analysis Summary Sheet		**Sheet** MIP_PS_2.5 - MIP_PS_2.6 /2	**Page 1 of 2**
		Issue: Draft	**Date** 23/06/2003
ENVISAT CARING FOR THE EARTH	***MIPAS***	**Prepared by:** Marco Ridolfi	**Processing site:** Dept. of Physical and Inorganic Chemistry - Univ. of Bologna
		CalVal Plan Ref: PO-PL-ESA-GS-1124 Issue 1A - PS 2.5 - 2.6 **Other Ref:** Sect 1.2 of 2nd Part of this TN, TN-IROE-GS0101 Issue 1A - Sect. 4.1.2	

Subject: **Tuning of parameters linked to Levenberg-Marquardt algorithm** GADS # 2 and 3 (#71, 73, 74)	**AO / ESL Ref.:** 11717/95/NL/CN

Inputs

PDS	**Others**
Orbit 2081 data, i.e. MIP_NL__1P020724_112130_M1_2081_020801 ORM input files generated by ML2PP with quadratic frequency correction to the AILS, no cloud filtering.	

Outputs	**Location/Access (ftp, ...)**
Post launch version of the files : PS_PT.DAT, PS_H2O.DAT, PS_O3.DAT, PS_HNO3.DAT, PS_CH4.DAT, PS_N2O.DAT, PS_NO2.DAT and MIP_PS2_AX File delivered to ESA by E-mail from P. Raspollini to H.Nett, 31 October 2002, Subject: New PS2, delivery of WP 9130.	

Tools

- ORM_SDC
- Statistical Tool

Recommendations

It would be advisable (but not necessary) to re-tune Levenberg - Marquardt parameters when cloud-detection filter is activated in the PDS.

Periodical (once / year) check / re-tuning of Levenberg - Marquardt parameters is recommended.

Problem Areas

Continuation Sheet	**Sheet:** MIP_PS_2.5 - MIP_PS_2.6 /2	**Page 2 of 2**
	Issue: Draft	**Date 23/06/2003**

Summary

- <u>Background:</u> Levenberg-Marquardt (LM) parameters to be tuned are: the initial value of the damping factor (λ_{in}), the number that multiplies the damping factor at each micro-iteration (λ_X) and the number that divides the damping factor at each macro-iteration ($\lambda_/$).The goal is to find values for these parameters so that the number of retrieval iterations is minimal, compatibly with a low final chi-square test.
- <u>Procedure:</u> we started from a "reference" set (Version 3, obtained from tuning on the basis of orbit 504 data with cloud filtering) of settings and we checked the variation of the performance of the ORM for various (8) combinations of the values of the three LM parameters. The performance of the ORM was evaluated in terms of: N. of iterations, final chi-square test and, with lowest priority, profile oscillations (Profile Oscillation Quantifier = POQ, defined in TN-IROE-GS0101 Issue 1A, Sect. 4.1.3).
- <u>Results:</u> as a result of this optimization procedure we have obtained the following values for the LM parameters:

ORBIT # 2081- NO CD - SUMMARY LEVENBERG-MARQUARDT

All PS2 Vers. 3 but LM Vers.4								
TARGET	Li	L/	Lx	CNVCRIT	Niter/retr	Nlm/retr	AVG(chi2)	POQ(*)
PT	0.02	2	16	0.144	2.56	0.19	1.99	2.11
H2O	0.05	4	8	0.055	2.12	0.22	1.24	31.06
O3	0.05	4	8	0.070	3.37	1.19	2.71	36.02
HNO3	0.02	2	8	0.025	4.06	1.04	1.42	71.84
CH4	0.05	4	8	0.050	2.66	0.74	1.90	33.06
N2O	0.1	2	8	0.064	2.44	0.53	1.82	45.51
NO2	0.05	4	8	0.040	2.74	0.46	1.18	31.85
AVERAGES					2.85	0.62	1.75	35.92

(*) POQ = Profile Oscillation Quantifier

- <u>Conclusions:</u>
  - Optimal LM parameters Vers.3 (optimized on the basis of orbit 504 data with cloud filtering) produce stable results also on orbit 2081.
  - LM parameters Vers. 4 differ from Vers.3 only for the initial value assigned to λ: Vers4 = Vers3 / 2
  - It would be advisable (but not necessary) to re-tune LM parameters when cloud filter is activated in the PDS.
  - It is recommended to check / re-optimize LM parameters once per year.

CalVal Analysis Summary Sheet	**Sheet** MIP_PS_2.5 - MIP_PS_2.6 /3	**Page 1 of 2**
	Issue: Draft	**Date** 23/06/2003
ENVISAT CARING FOR THE EARTH — *MIPAS*	**Prepared by:** Marco Ridolfi	**Processing site:** Dept. of Physical and Inorganic Chemistry - Univ. of Bologna
	CalVal Plan Ref: PO-PL-ESA-GS-1124 Issue 1A - PS 2.5 - 2.6 **Other Ref:** TN-IROE-GS0101 Issue 1A - Sect. 4.1.3	

Subject:

Tuning of regularization parameters
GADS # 2 and 3 (#95)

AO / ESL Ref.: 11717/95/NL/CN

Inputs

PDS

Orbit 2081 data, i.e. MIP_NL__1P020724_112130_M1_2081_020801
ORM input files generated by ML2PP with quadratic frequency correction to the AILS, no cloud filtering.

Others

Outputs

Post launch version of the files : PS_PT.DAT, PS_H2O.DAT, PS_O3.DAT, PS_HNO3.DAT, PS_CH4.DAT, PS_N2O.DAT, PS_NO2.DAT and MIP_PS2_AX

File delivered to ESA by E-mail from P. Raspollini to H.Nett, 31 October 2002, Subject: New PS2, delivery of WP 9130.

Location/Access (ftp, ...)

Tools

- ORM_SDC
- Statistical Tool

Recommendations

No significant oscillations were detected in the retrieved profiles. This is attributed to the regularizing effect of the Levenberg - Marquardt damping that is made significant by the relatively relaxed convergence criteria that are being used (Vers. 4).

Therefore regularization was switched-off. Regularization must be re-considered if more stringent convergence criteria will be adopted in the future.

Problem Areas

The retrieved profiles of some species (i.e h2o, ch4 and n2o) present some oscillations. It has to be understood how these oscillations are related to the oscillations present in Level 1 radiance (see test MIP_newtest).

<table>
<tr><td rowspan="2">Continuation Sheet</td><td>Sheet: MIP_PS_2.5 - MIP_PS_2.6 /3</td><td>Page 2 of 2</td></tr>
<tr><td>Issue: Draft</td><td>Date
23/06/2003</td></tr>
</table>

Summary

Regularization is implemented in the Level 2 processor as an option to be used in case significant oscillations are detected in the retrieved profiles. If used, regularization requires the optimization of the parameters defining its strenght. However no significant oscillations were detected in the retrieved profiles so far, therefore regularization is presently disabled.
Lack of significant oscillations in the retrieved profiles is presently attributed to the regularizing effect of the Levenberg - Marquardt damping (that is still present at the final iteration of the retrievals) that is made significant by the relatively relaxed convergence criteria that are presently being used (Vers. 4). Regularization must be re-considered if more stringent convergence criteria will be adopted in the future.

<table>
<tr><td colspan="2">CalVal Analysis
Summary Sheet</td><td>Sheet MIP_PS_2.5 - MIP_PS_2.6 /4</td><td colspan="2">Page 1 of 2</td></tr>
<tr><td colspan="2"></td><td>Issue: Draft</td><td colspan="2">Date 23/06/2003</td></tr>
<tr><td rowspan="2">ENVISAT</td><td rowspan="2">MIPAS</td><td>Prepared by: Marco Ridolfi</td><td colspan="2">Processing site: Dept. of Physical and Inorganic Chemistry - Univ. of Bologna</td></tr>
<tr><td colspan="3">CalVal Plan Ref: PO-PL-ESA-GS-1124 Issue 1A - PS 2.5 - 2.6
Other Ref: Sect 1.3 of 2nd Part of this TN,
TN-IROE-GS0101 Issue 1A - Sect. 4.1.11,</td></tr>
<tr><td colspan="4">Subject:
Tuning of convergence criteria
PS2, GADS#2 (#11, 12, 12.5) and GADS#3 (#11, 12)</td><td>AO / ESL Ref.:
11717/95/NL/CN</td></tr>
</table>

Inputs

PDS	Others
Orbit 2081 data, i.e. MIP_NL__1P020724_112130_M1_2081_020801 ORM input files generated by ML2PP with quadratic frequency correction to the AILS, no cloud filtering.	

Outputs	Location/Access (ftp, ...)
Post launch version of the files : PS_PT.DAT, PS_H2O.DAT, PS_O3.DAT, PS_HNO3.DAT, PS_CH4.DAT, PS_N2O.DAT, PS_NO2.DAT and MIP_PS2_AX File delivered to ESA by E-mail from P. Raspollini to H.Nett, 31 October 2002, Subject: New PS2, delivery of WP 9130.	

Tools

- ORM_SDC
- Statistical Tool

Recommendations

To implement convergence criteria Version 4.

For the future it is recommended to check if it is possible to use more stringent convergence criteria at the expenses of computing time.

Problem Areas

The convergence criteria deriving from this analysis, even if rather stable with respect to the data set used for the optimisation, are not conservative and induce a convergence error of the same order of magnitude of the profiles random error.

Continuation Sheet	**Sheet:** MIP_PS_2.5 - MIP_PS_2.6 /4	**Page 2 of 2**
	Issue: Draft	**Date** 23/06/2003

Summary

Background:
Convergence criteria are used by MIPAS Level 2 processor to stop the Gauss-Newton iterations of the inversion procedure. The convergence criteria are subject to tuning. Stringent convergence criteria lead to precise results but require long computing time, therefore a compromise between convergence error and computing time must be found.

Procedure:
Convergence criteria were tuned on the basis of statistical considerations about retrieval accuracy. The detail procedure is described in TN-IROE-GS0101 Issue 1A - Sect. 4.1.5 and in part II of this TN.

Results:
The following optimal thresholds were established for the relative difference between attained chi-square and chi-square computed in the linear approximation:

- PT 0.118
- H2O 0.083
- O3 0.131
- HNO3 0.143
- CH4 0.041
- N2O 0.055
- NO2 0.047

These are the so called convergence criteria Version 4.

Conclusion:
The convergence criteria deriving from this analysis, proved to be rather stable with respect to the data set used for the optimisation. However these are not conservative criteria and induce a convergence error of the same order of magnitude of the profiles random error. For the future it is recommended to check if it is possible to use more stringent convergence criteria at the expenses of computing time.

CalVal Analysis Summary Sheet	Sheet MIP_PS_2_5, MIP_PS_2_6 /5	Page 1 of 2
	Issue: Draft	**Date** 23/06/2003
ENVISAT CARING FOR THE EARTH — *MIPAS*	**Prepared by:** Piera Raspollini	**Processing site:** IFAC-CNR
	CalVal Plan Ref: po_pl_esa_gs_1124, issue 1B, PS_2_3 & MV_2_15 **Other Ref: Sect 1.4 of 2nd Part of this TN,** **TN-IROE-GS0101 Issue 1 A Sect. 4.2.6,**	

Subject: :

Retrieval grid

AO / ESL Ref.: 11717/95/NL/CN

Inputs

PDS	**Others**
Orbit 2081 data, i.e. MIP_NL__1P020724_112130_M1_2081_020801 ORM input files generated by ML2PP with quadratic frequency correction to the ILS and with cloud filtering.	

Outputs	**Location/Access (ftp, ...)**
This report	**CD**

Tools

ML2PP (with patches up to 24 April 2002) for generating ORM inputs

ORM_ORB_1.0.1 (version 03.09.2002) with fit of frequency shift scaling parameter activated
ST (version 0.98)

Recommendations

Stay with current retrieval grid

Problem Areas

Summary
The vertical resolution and the accuracy with which the retrieved profiles are determined are strongly dependent on the altitude grid where the retrieved points are represented (retrieval grid).
This test is meant to assess the impact on the retrieved profile of a specie dependent degradation of the vertical resolution at the altitudes (in the nominal range) characterised by large random noise.

The altitude that is characterised by the greatest random noise is identified, and the retrieval is performed excluding that altitude from the fit (*lfit* is set to F in correspondence of that altitude).
The retrieved profiles obtained in the two cases are compared.
The results are that in most cases a degradation of the vertical resolution succeeds in reducing the oscillations in the retrieved profile, but the retrieved profile with a reduced vertical resolution could be obtained from the other just drawing a line through the two points contiguous to the altitude that is not retrieved in one case. Therefore a degradation of the vertical resolution in the nominal range does not lead to an improvement of the profile.

CalVal Analysis Summary Sheet	**Sheet** MIP_PS_2_5 - MIP_PS_2_6 /6	**Page 1 of 2**
	Issue: Draft	**Date** 23/06/2003
ENVISAT CARING FOR THE EARTH / ***MIPAS***	**Prepared by:** Marco Ridolfi	**Processing site:** Dept. of Physical and Inorganic Chemistry - Univ. of Bologna
	CalVal Plan Ref: PO-PL-ESA-GS-1124 Issue 1A - PS 2.5 - 2.6 **Other Ref:** Sect 1.5 of 2nd Part of this TN, TN-IROE-GS0101 Issue 1A - Sect. 4.1.7	

Subject: **Tuning of the layering used in the forward model (linear-in-tau approx.)** GADS # 2 and 3	**AO / ESL Ref.:** 11717/95/NL/CN

Inputs

PDS	**Others**
Orbit 2081 data, i.e. MIP_NL__1P020724_112130_M1_2081_020801 ORM input files generated by ML2PP with quadratic frequency correction to the AILS, no cloud filtering.	

Outputs	**Location/Access (ftp, ...)**
Post launch version of the files : PS_PT.DAT, PS_H2O.DAT, PS_O3.DAT, PS_HNO3.DAT, PS_CH4.DAT, PS_N2O.DAT, PS_NO2.DAT and MIP_PS2_AX File delivered to ESA by E-mail from P. Raspollini to H.Nett, 31 October 2002, Subject: New PS2, delivery of WP 9130.	

Tools

- ORM_SDC
- Statistical Tool

Recommendations

The accuracy obtained with the optimized layering determined on the basis of synthetic data proved to be satisfactory also for the real atmosphere encountered along MIPAS orbit 2081.

We therefore recommend to use the optimized layering determined before launch also for retrievals from real MIPAS data.

Problem Areas

<table>
<tr><td rowspan="2">Continuation Sheet</td><td>Sheet: MIP_PS_2.5 - MIP_PS_2.6 /6</td><td>Page 2 of 2</td></tr>
<tr><td>Issue: Draft</td><td>Date 23/06/2003</td></tr>
</table>

Summary

Background: The atmospheric layering used for the calculation of the radiative transfer integral had already been tuned before launch on the basis of synthetic data. However real atmospheres more opaque than theoretically anticipated could have caused a degradation of the accuracy of the radiative transfer calculation. For this reason a further check of the layering was carried-out on the basis of the real atmosphere measured by MIPAS along orbit 2081.

Procedure: the profiles retrieved on the basis of the layering determined before launch (43 levels) were compared with profiles retrieved using a very fine layering (80 levels). The differences between profiles determined in the two cases were compared with the profile ESD. For some scans the use of different layerings causes a different number of iterations required for convergence. Therefore in these cases differences between profiles would be due to different number of iterations rather than different layerings. For this reason it was decided, for this test, to stop the retrievals after three iterations. No constrains were applied to micro-iterations.

Results: the observed discrepancies between the profiles retrieved with the layering determined before launch (43 levels) and the profiles retrieved using a fine layering (80 levels) are generally well below the random error associated with the retrieved profiles. Discrepancies above the random errors were detected only in correspondence of cloudy sweeps.

Conclusions: Since the retrieval performance is degraded in any case whenever cloudy sweeps are included in the analysis, it was decided to keep using the layering determined before launch (on the basis of synthetic data) also for the analysis of real observations.
Frequent checks of the adequacy of the used layering are not considered necessary. A new check of the layering will be required only in case of special events having significant impact on the opacity of the atmosphere.

CalVal Analysis Summary Sheet		**Sheet MIP_PS_2_5, MIP_PS_2_6 /7**	**Page 1 of 2**
		Issue: Draft	**Date 23/06/2003**
ENVISAT CARING FOR THE EARTH	***MIPAS***	**Prepared by Simone Ceccherini**	**Processing site IFAC-CNR**
		CalVal Plan Ref: PS_2_5, PS_2_6 **Other Ref: TN-IROE-GS0101 Issue 1 A Sect. 4.1.8**	

Subject:
‘Tropopause’ altitude
GADS #2 and GADS#3 (#91-92)

AO / ESL Ref.:11717/95/ NL/CN

Inputs

PDS	**Others**
Orbit 2081 data, i.e. MIP_NL__1P020724_112130_M1_2081_020801 ORM input files generated by ML2PP with quadratic frequency correction to the ILS, without cloud filtering.	

Outputs	**Location/Access (ftp, ...)**
Post launch version of the files : PS_PT.DAT, PS_H2O.DAT, PS_O3.DAT, PS_HNO3.DAT, PS_CH4.DAT, PS_N2O.DAT, PS_NO2.DAT and MIP_PS2_AX File delivered to ESA by E-mail from P. Raspollini to H.Nett, 31 October 2002, Subject: New PS2, delivery of WP 9130.	**CD**

Tools

ML2PP (with patches up to 24 April 2002) for generating ORM inputs

ORM_ORB_1.0.1 (version 03.09.2002)

ST (version 0.98)

Recommendations

Accept modified ‘tropopause’ altitude values in PS_’SPECIE’.DAT as new default.

Problem Areas

Continuation Sheet	Sheet MIP_PS_2_5, MIP_PS_2_6 /7	Page 2 of 2
	Issue: Draft	Date 23/06/2003

Summary

FOV modelling is more critical at low altitudes, where the pressure is higher and where sharp changes in the atmospheric gradients occur. In order to model FOV accurately, a greater number of simulated spectra are generally necessary at low altitudes. The altitude delimiting the part of the atmosphere where FOV convolution is more critical is called ‘tropopause’, even if this altitude does not necessarily coincide with the physical tropopause.
A value of “tropopause” too low would imply a not precise calculation of the convolution of the spectrum with the FOV, while a too high value would lead to an increase of computing time.

This altitude depends on latitude and is determined by two user-defined parameters:
- “tropopause” altitude at poles
- difference between “tropopause” altitude at equator and at poles.

The visual inspection of the maps of retrieved profiles of temperature and water vapor has indicated that reasonable values of these two parameters are 15 km and 2 km. The use of these values has proven not to introduce errors in FOV convolution.

CalVal Analysis Summary Sheet		**Sheet MIP_PS_2_5, MIP_PS_2_6 /8**	**Page 1 of 2**
		Issue: Draft	**Date 23/06/2003**
ENVISAT	***MIPAS***	**Prepared by Simone Ceccherini**	**Processing site IFAC-CNR**
		CalVal Plan Ref: PS_2_5, PS_2_6 **Other Ref: Sect 1.6 of 2nd Part of this TN, TN-IROE-GS0101 Issue 1 A Sect. 4.1.9**	

Subject: **Tuning of field of view related parameters** **for Level 2 aux PS2 GADS #2 (#93), GADS #3 (#93)**	**AO / ESL Ref.:11717/95/ NL/CN**

Inputs

PDS	**Others**
Orbit 2081 data, i.e. MIP_NL__1P020724_112130_M1_2081_020801 ORM input files generated by ML2PP with quadratic frequency correction to the ILS, without cloud filtering.	

Outputs	**Location/Access (ftp, ...)**
Post launch version of the files : PS_PT.DAT, PS_H2O.DAT, PS_O3.DAT, PS_HNO3.DAT, PS_CH4.DAT, PS_N2O.DAT, PS_NO2.DAT and MIP_PS2_AX File delivered to ESA by E-mail from P. Raspollini to H.Nett, 31 October 2002, Subject: New PS2, delivery of WP 9130.	**CD**

Tools

ML2PP (with patches up to 24 April 2002) for generating ORM inputs

ORM_ORB_1.0.1 (version 03.09.2002) with fit of frequency shift scaling parameter activated

ST (version 0.98)

Recommendations

Accept modified values in PS_'SPECIE'.DAT as new default.
In case that we decide to extend the retrievals below 12 km new values of “rint” have to be adopted.

Problem Areas

Continuation Sheet	Sheet MIP_PS_2_5, MIP_PS_2_6 /8	Page 2 of 2
	Issue: Draft	Date 23/06/2003

Summary

The effect of finite FOV is taken into account in the ORM by convolving the tangent altitude dependent spectrum with the FOV pattern. The forward model calculates spectra for a number of lines of sight that span the vertical range of the FOV around the tangent altitude. The continuous variation of the spectrum as a function of tangent altitude is determined by interpolation of a polynomial through the calculated spectra. The shape of the FOV is a piecewise linear altitude distribution tabulated in the processor input files. It is a measured instrument parameter.

The FOV convolution parameter that is subject to tuning is “rint”, i.e. the maximum separation between simulated spectra below a certain altitude (named tropopause altitude), chosen above the sharp vertical gradients of water vapor and temperature. The smaller is the tangent altitude separation between the simulated spectra, the smaller are the discretisation errors. However, a too large number of simulated spectra in the FOV convolution implies a too high order of the interpolating polynomial with another type of error source. Furthermore, the smaller is the tangent altitude separation between the simulated spectra the longer is the time requested to perform the calculation.

A retrieval in which the forward model calculates a spectrum every 200 metres below 20 km and uses a linear interpolation in between for the FOV convolution was performed. The profiles obtained from this retrieval are considered not affected by problems of FOV convolution and are used as reference truth to estimate the correctness of the calculation performed by ORM. The tuning was performed for the scans not affected by clouds of the orbit #2081.

The root mean square of deviation of the profiles, calculated with “rint”=1 km, 2 km, 4 km, with respect to the reference truth is compared with the averaged random error.

Another parameter to take into account for the choice of the “rint” values is the calculation time:
- the use of rint=2 km instead of rint=1 km allows to save about 15% of the calculation time

- the use of rint=4 km instead of rint=1 km allows to save about 20% of the calculation time.

From the analysis described above we have seen that a reduction of the differences with the reference profile is obtained with small values of “rint”.
The chosen values of “rint” on the basis of a compromise between accuracy and saving calculation time are:

T	rint = 2 km
H_2O	rint = 2 km
O_3	rint = 2 km
HNO_3	rint = 2 km
CH_4	rint = 4 km
N_2O	rint = 4 km

For NO_2 the minimum tangent altitude for which the retrieval is performed is 24 km that is above the “rint” altitude. So for the NO_2 retrieval the tuning of “rint” is not necessary.

<table>
<tr><td colspan="2" rowspan="2">CalVal Analysis Summary Sheet</td><td colspan="2">Sheet MIP_PS_2.5 – MIP_PS_2.6 - AX2.1</td><td>Page 1 of 2</td></tr>
<tr><td>Issue: Draft</td><td colspan="3">Date 23/06/2003</td></tr>
<tr><td rowspan="2">ENVISAT
CARING FOR THE EARTH</td><td rowspan="2">MIPAS</td><td>Prepared by: Marco Ridolfi</td><td colspan="2">Processing site: Dept. of Physical and Inorganic Chemistry - Univ. of Bologna</td></tr>
<tr><td colspan="3">CalVal Plan Ref: PO-PL-ESA-GS-1124 Issue 1A - PS 2.5 - 2.6
Other Ref: Sect 1.7 of 2nd Part of this TN,
TN-IROE-GS0101 Issue 1A - Sect. 4.1.11</td></tr>
<tr><td colspan="4">Subject:
Tuning of the error associated with engineering LOS information</td><td>AO / ESL Ref.:
11717/95/NL/CN</td></tr>
<tr><td colspan="5">Inputs</td></tr>
<tr><td colspan="4">PDS
Orbit 2081 data, i.e. MIP_NL__1P020724_112130_M1_2081_020801
ORM input files generated by ML2PP with quadratic frequency correction to the AILS, cloud filtering applied.</td><td>Others</td></tr>
<tr><td colspan="4">Outputs
Output is only a report. The related AX2 file “PI_VCM.DAT” was not updated as a consequence of this tuning procedure.</td><td>Location/Access (ftp, ...)</td></tr>
<tr><td colspan="5">Tools
➢ ORM_SDC
➢ Statistical Tool</td></tr>
<tr><td colspan="5">Recommendations
Given the large uncertainty on the estimated total error of the retrieved profiles, it is not possible to derive from this test constraining considerations about the covariance matrix of the engineering pointing information. Therefore we do not recommend any modification of the covariance matrix of the engineering pointing information on the basis of this test.</td></tr>
<tr><td colspan="5">Problem Areas</td></tr>
</table>

Continuation Sheet	**Sheet:** MIP_PS_2.5 - MIP_PS_2.6 AX2.1	**Page 2 of 2**
	Issue: Draft	**Date 23/06/2003**

Summary

Background: MIPAS Level 2 processor uses the engineering LOS (pointing) information as an a-priori data source to constrain pT retrieval with the optimal estimation method. The knowledge of the accuracy of the engineering pointing data is therefore a crucial issue in Level 2 processing. Hence the pointing covariance matrix initially estimated on the basis of theoretical pointing specifications is subject to tuning and verification.

Procedure:
- Statistical analysis of tangent height corrections when no LOS info is used (see TN-IROE-GS0101 Issue 1A - Sect. 4.1.11 and appendix to this template). This test provides insight on pointing jitter and drift, but no indication about offset.
- Comparison of MIPAS retrieved profiles with co-located ECMWF measurements. This test provides indication about pointing offsets.

Results / conclusion:
It is difficult to assess MIPAS pointing errors on the basis of inspection of Level 2 results. Nevertheless, the tests performed so far on Level 2 results pointed-out that:
- the tool simulating MIPAS pointing performance produces realistic estimates of MIPAS pointing error (correct order of magnitude). However it is not clear whether this tool underestimates the pointing drift + jitter (≈ 150 m) or we underestimate the systematic components of the error on retrieved pointing when no LOS info is used (not easy to discriminate from inspection of Level 2 results).
- The analyzed data-set suffers of a pointing offset of about -1.1km. This is confirmed by the results of pointing characterization carried-out by ESA on the basis of dedicated measurements (see e.g E-mail from H.Nett to MICT group:

Date: Tue, 12 Nov 2002 15:37:23 +0100 (MET)
From: Herbert Nett <hnett@jw.estec.esa.nl>
To: mict@jw.estec.esa.nl
Subject: [ENVISAT:mict] MIPAS auxiliary data update

CalVal Analysis Summary Sheet		**Sheet MIP_PS_2_5 and MIP_PS_2_6 /9**		**Page 1 of 2**
		Issue: Draft	**Date** 23/06/2003	
ENVISAT CARING FOR THE EARTH	***MIPAS***	**Prepared by:** Maria Prosperi	**Processing site:** IFAC-CNR	
		CalVal Plan Ref: po_pl_esa_gs_1124, issue 1B, PS_2_5 , PS_2_6 (82-90) **Other Ref: Sect 1.8 of 2nd Part of this TN,** **TN-IROE-GS0101 Issue 1 A Sect. 4.2.14**		

Subject: :

VCM of a-priori profiles for the computation of the IG profiles
PS2 file,GADS 2-3 (field 82-90)

AO / ESL Ref.: 11717/95/NL/CN

Inputs

PDS

Orbit 2081 data, i.e. MIP_NL__1P020724_112130_oldNL_M3_2081_020918.

ORM input files generated by ML2PP with quadratic frequency correction to the ILS, with cloud filtering.

Others

Outputs

Post launch version of the files : PS_FRAME, PS_PT.DAT, PS_H2O.DAT, PS_O3.DAT, PS_HNO3.DAT, PS_CH4.DAT, PS_N2O.DAT, PS_NO2.DAT and MIP_PS2_AX

File delivered to ESA by E-mail from P. Raspollini to H.Nett, 31 October 2002, Subject: New PS2, delivery of WP 9130.

Location/Access (ftp, ...)

CD

Tools

ML2PP (with patches up to 24 April) for generating ORM inputs

ORM_ORB_1.0.1 (version 03.09.2002)
ST (version 0.98)

Tool for the computation of the variance of the retrieved profiles on each latitude band.

Tool for the computation of the weighted mean between retrieved profile and a-priori profile.

Recommendations

Realistic variances of climatological profiles from the team of University of Leicester are needed for the PS2 file.

Accept modified parameters relative to the correlation of the VCM of the a-priori profiles in PS_'SPECIE'.DAT as new default.

Problem Areas

Continuation Sheet	**Sheet:** MIP_PS_2.5 - MIP_PS_2.6 /9	**Page 2 of 2**
	Issue: Draft	**Date 23/06/2003**

Summary

Initial guess profiles are an important element in the inversion procedure: they are required to be as close as possible to the real atmosphere, in order to reduce the number of iterations needed to reach convergence, and smooth, because in this case the Marquardt method used in the retrieval algorithm provides also a mild ‘regularisation’. In order to choice the best Initial Guess (IG) profile, the Level 2 operational processor computes the weighted mean between the retrieved profile in the previous scan and the ‘a-priori’ profile (obtained by merging climatological and -if available- ECMWF profiles). The weight is provided by the VCM of each profile. The parameters used for the computation of the VCM of the climatological profiles have to be defined correctly in order to obtain IG profile that are as close as possible to the reality and as smooth as possible

The objectives of this test are the following ones:

- to verify the correctness of the diagonal values of the VCM associated to the a-priori profiles, by comparing the variance of the retrieved profiles computed in all the latitude bands with the variance associated to the climatological profiles;
- to investigate which is the most appropriate value and sign of the non-diagonal terms in order to have an non-oscillating IG profile.

The validation of the correctness of the diagonal values of the VCM associated to the a-priori profiles has been performed comparing, for each latitude band and each specie, the variance of the retrieved profiles with the variance of the climatological profile. The climatological variance is expected to be much greater than the one associated with the retrieved profiles, since the latter has been computed on the base of only one orbit, while the other is meant to take into account the seasonal variation; against this expectation the climatological variance is in most cases much smaller than the one associated with the retrieved profiles. For this reason we believe that the climatogical variances supplied in the PS2 file are not very realistic and so new realistic atmospheric variances have to be provides by the University of Leicester team.

In order to determine the most appropriate value and sign of the non-diagonal terms of the VCM of the climatological profiles, a small program has been developed that computes the weighted mean between the retrieved profile and the a-priori one. All the cases of positive, negative and 0 correlations in the VCM of the climatological profile have been considered. A very oscillating retrieved profile has been used for this test. Both negative and positive correlations increase the oscillations of the resulting profile. On the contrary, the resulting profile in case of correlations equal to 0 is a profile with oscillations smaller than the ones in the retrieved profile. Therefore, even if in a smooth profile (as it is the a-priori profile) correlations are expected to be positive, the most appropriate value for correlations in the VCM of the a-priori profile is 0.

Subject: :

Verification of frequency calibration & determination of coefficients for second order polynomial frequency correction
PS2 , GADS#1 (#74-76)

AO / ESL Ref.: 11717/95/NL/CN

Inputs

PDS	**Others**
Orbit 2081 data, i.e. MIP_NL__1P020724_112130_M1_2081_020801 ORM input files generated by ML2PP with and without quadratic frequency correction to the ILS, with cloud filtering.	

Outputs	**Location/Access (ftp, ...)**
Outputs included in PS2 file Vers. 4 (post launch version). File delivered to ESA by E-mail from P. Raspollini to H.Nett, 31 October 2002, Subject: New PS2, delivery of WP 9130. PS_FRAME.DAT	**CD**

Tools

ML2PP (with patches up to 24 April 2002) for generating ORM inputs

ORM_ORB_1.0.1 (version 03.09.2002) with fit of frequency shift scaling parameter activated
ST (version 0.98)

Recommendations

Accept modified parameters in PS_FRAME.DAT as new default.

Repeat analysis with new full orbit Level1 data periodically (every three months at the beginning, then once/year).

Repeat analysis for band D (this band was not included in the analysis, since no microwindows in that band are used).

Problem Areas

Requirements for frequency calibration accuracy $\Delta\omega / \omega$ are 1.e-6. However, a frequency calibration better than the requirements seems possible in MIPAS spectra.

Even if retrieved profiles are not significantly affected by the frequency shift, frequency shift in MIPAS spectra induces big residuals and hence big χ^2. Since χ^2 is used as an indicator of the presence of systematic errors, an improvement in frequency calibration is useful to eliminate the contribution of this error in the residuals and to investigate the effect of other systematic errors.

Continuation Sheet	Sheet: MIP_PS_2_3-MV_2_15	Page 2 of 2
	Issue: Draft	Date 23/06/2003

Summary

The correctness of the frequency calibration was investigated by fitting the residual frequency shift scaling factor $\Delta\omega/\omega$ in MIPAS spectra. This fit leads in most cases to a significant reduction of the residuals suggesting the possibility for an improvement in the frequency calibration. In particular, the retrieved frequency shift presents a systematic behaviour with frequency: from negative values of the order of 10^{-6} in band A, to positive values of the same order of magnitude in band C, with 0 located somewhere between band AB and B. This behaviour with frequency indicates that the instrument has a small non-linear distortion in the frequency scale. Since this effect is not modelled in Level1 it leads to a bias in the determination of the linear scaling factor. Considering that Level 2 pre-processor has the capability of applying a frequency dependent shift to the ILS (with a second order polynomial), the optimal coefficients has been determined in order to reduce the detected frequency shift. The average along the orbit of the frequency shift scaling factors retrieved for the different spectral bands by the different retrievals has been fitted to a second order polynomial with the constant term set to 0: $f(\omega)=b\omega+c\omega^2$ The obtained second order polynomial is:

$$f(\sigma) = -2.60511 \cdot 10^{-6}\,\sigma + 2.140841 \cdot 10^{-9}\,\sigma^2,$$

with σ measured in cm^{-1}.

The second order polynomial shift of the ILS succeeds in correcting the small non-linear distortion of the instrument in the frequency scale and the residual frequency shift after this spectral correction is significantly smaller (the retrieved scaling factor is less than 5 10^{-7}).

Besides, it has been checked that the polynomial correction that has been determined by the analysis of a single orbit can be used also for the subsequent orbits.

A bias in the frequency shift calibration does not significantly affect the retrieved profiles, but increase the residuals and hence the χ^2.
Correction is necessary to eliminate from the residuals this strong contribution of systematic error that may cover other systematic errors under investigation.

4 Verification of critical baselines

The second group of tests deals with the verification of critical level2 baseline verification, and the outputs of these tests consist in recommendation for modifications in the code or suggestions for improvements of the quality of data products.

The table below associates each test with the corresponding Sheet.

Test	Sheet
Verification of extrapolation rules	MIP_MV_2_25/1
Measurement altitude range	MIP_MV_2_25/2
Local thermodynamic equilibrium	MIP_MV_2_1
Verification of horizontal homogeneity hypothesis	MIP_MV_2_2
Verification of hydrostatic equilibrium (assumption of vertical profiles)	MIP_MV_2_3
Verification of error in the VMR profiles of interfering species	MIP_MV_4
Errors in the spectroscopic parameters	MIP_MV_2_8-AX_2_3
Verification of the assumptions related to the line-mixing for CO_2 Q-branches	MIP_MV_2_10
Verification of the ILS width	MIP_MV_2_12
Verification of the intensity calibration	MIP_MV_2_16
Zero-level calibration	MIP_MV_2_17

CalVal Analysis Summary Sheet	Sheet MIP_MV_2_25/1		Page 1 of 2
	Issue: Draft	**Date** 23/06/2003	
ENVISAT — CARING FOR THE EARTH *MIPAS*	**Prepared by:** Bianca Maria Dinelli	**Processing site:** ISAC-CNR	
	Ref: Sect 2.1 of 2nd Part of this TN, TN-IROE-GS0101 Issue 1 A Sect. 4.2.12		

Subject: :

Verification of extrapolation rules

AO / ESL Ref.: 11717/95/NL/CN

Inputs

PDS	Others
Orbit 2081 data, i.e. MIP_NL__1P020724_112130_M1_2081_020801 ORM input files generated by ML2PP with quadratic frequency correction to the ILS, with cloud filtering.	**Settings version 3**

Outputs	Location/Access (ftp, ...)
This report	**CD**

Tools

ML2PP (with patches up to 24 April 2002) for generating ORM inputs

ORM_ORB_1.0.1 (version 03.09.2002) with option to modify the IG profile shape above the highest fitted altitude tool to calculate the average deviations

Recommendations

It is recommended to include the extrapolation of the assumed profile among the sources of systematic errors. (See related results of test MIP_MV_2_25/2).

Problem Areas

Continuation Sheet	Sheet: MIP_MV_2_25 /1’	Page 2 of 2
	Issue: Draft	Date 23/06/2003

Summary

In ORM the retrieved discrete values of the vertical profile are determined in correspondence of the so-called “retrieval grid”, equal to the grid of the measured tangent altitudes. However, not all the measured tangent altitudes are necessarily used for the determination of a profile and the retrieval is in general performed in a subset of points (‘retrieval grid’) that exclude some measurements at either the topmost or the lowermost altitudes. The retrieved profile above the highest tangent altitude used in the retrieval is obtained scaling the initial guess (IG) profile by the same quantity used for the highest fitted point. The assumptions made on the shape of the initial guess profiles may therefore affect the quality of the retrievals.
To assess the impact of the extrapolation rule used by ORM to handle profiles above the highest retrieved point, we have analysed the 71 sequences of orbit 2081 using different profile shapes in the IG.
The reference retrieval has been performed with the same initial guess profiles used by the ML2PP code.
Then 5 different shapes have been used for the initial guess profiles above the highest fitted altitude, in order to obtain statistically significant results.
For each altitude the resulting retrieved values have been compared with the reference value and the obtained averaged deviations have been compared with the random errors of the reference retrieval.
Results are that in general the retrieved profiles at high altitudes depend on the assumed shape of the profile above them.
Temperature and H_2O retrieved profiles are the most affected by the shape of the profile above the highest fitted altitude, with deviations bigger than 3 times the estimated standard deviation.
For the molecules whose VMR is very low above the highest retrieved point, such as HNO_3 and CH_4, these deviations are lower than the retrieval esd.
The whole NO_2 profile depends on the assumed shape above the highest retrieved altitude. This can be explained by the fact that the altitude range where NO_2 VMR is retrieved is very limited, and the assumption on the shape of the profiles weights much more on the few retrieved points.
It is, therefore, recommended to include the extrapolation of the assumed profile among the sources of systematic errors. (See related results of test MIP_MV_2_25/2).

<table>
<tr><td rowspan="2">CalVal Analysis Summary Sheet</td><td colspan="2">Sheet MIP_MV_2_25 /2</td><td>Page 1 of 2</td></tr>
<tr><td>Issue: Draft</td><td colspan="2">Date 23/06/2003</td></tr>
<tr><td rowspan="2">ENVISAT CARING FOR THE EARTH</td><td rowspan="2">MIPAS</td><td>Prepared by: Piera Raspollini</td><td colspan="2">Processing site: IFAC-CNR</td></tr>
<tr><td colspan="3">Ref: Sect 2.2 of 2nd Part of this TN,
TN-IROE-GS0101 Issue 1 A Sect. 4.1.10</td></tr>
</table>

<table>
<tr><td>Subject: :
Measurement altitude range</td><td>AO / ESL Ref.:
11717/95/NL/CN</td></tr>
</table>

Inputs

PDS	**Others**
Orbit 2081 data, i.e. MIP_NL__1P020724_112130_M1_2081_020801 ORM input files generated by ML2PP with quadratic frequency correction to the ILS, with cloud filtering. Nominal OMs extended on the whole MIPAS measurement altitude range	

Outputs	**Location/Access (ftp, ...)**
This report	**CD**

Tools

ML2PP (with patches up to 24 April 2002) for generating ORM inputs

ORM_ORB_1.0.1 (version 03.09.2002)
ST (version 0.98)

Recommendations

Extend the retrieval range to the whole MIPAS measurement range for all the species, with the only exception of NO2 at low altitudes.

Investigation has to be made in order to assess the contribution of systematic errors in the points of extended altitude range.

Problem Areas

In water profiles some differences are visible at high altitudes, but their cause has to be searched not in the upward propagation of retrieval error, but in inherent water profile oscillations, whose cause is still under investigation (see MIP_newtest).

Continuation Sheet	Sheet: MIP_MV_2_25 /2	Page 2 of 2
	Issue: Draft	Date 23/06/2003

Summary

Retrieval of profiles at very low altitudes can be affected by lack of information below a certain altitude, large horizontal gradients, extra absorption and / or scattering due to clouds that are not modelled in the ORM.
At high altitudes, retrieval of the species having low concentration can result in strongly oscillating profiles that may induce problems also in the nominal range. Besides, systematic errors can increase significantly at high altitudes due to non-LTE.
In order to avoid these problems, it was decided not to exploit all spectra of a MIPAS scan, but to perform operational retrievals only between 12 and 68 km. Furthermore, within this range, a customized retrieval range was defined for each specie, according to the information content of each specie in MIPAS measurements.

On the other hand, retrieval on the whole measurement range would allow:

_ to derive information on tropospheric profiles from MIPAS measurements;

_ to extend the height range in which the profiles are not affected by the assumption on the initial guess profile outside the retrieval range (see results on test MIP_MV_2_25/1);

_ to get information on species whose concentration is significant only for particular latitudes and seasons (ex. NO2 significant above 47 km only in the winter pole).

Tests have been done to understand whether retrievals on the whole MIPAS measurement range are advantageous.
The first test was meant to evaluate the possibility to retrieve profiles down to 6 km. The profiles obtained with two different retrieval ranges (nominal range and extended range) in the common altitude range were compared. In order to avoid problems coming from clouds in the line of sight, this test was performed with the cloud filtering activated, so that the retrieval range is extended only if clouds are not present in the line of sight. Orbit #2081, acquired on 24th July 2002, was used for this test.
Main differences above 6 km are observed in temperature and water vapor profiles, but this can be explained considering the results obtained in the test on extrapolation and the fact that water and temperature have sharp gradients in the low troposphere. The extension of the retrieval range surely reduces the error at 12 km due to the assumption of the slope of the profile below the lowest retrieved value, i.e. 12 km for the nominal range, 6km for the extended range.
In water profiles some differences are visible also at high altitudes, but their cause has to be searched not in the upward propagation of retrieval error, but in inherent water profile oscillations, whose cause is still to be explained.
For the other species the differences are smaller.
In general we can say that, whenever cloud free conditions are observed, the altitude range of the retrieval of all species can be extended to altitudes lower than 12 km: if insufficient information is present large errors are found in the retrieved values, but the errors generally do not propagate in a negative way to higher altitudes. Further investigations are needed to understand the impact of some approximations below 12 km (water independent refractive index, pressure shift, self-broadening, refraction-independent FOV) and the feasibility of the extension should not imply the validated quality of the extra retrieved points.
The second test was meant to evaluate the possibility to retrieve profiles up to 68 km.
Extension of no2 retrieval range (nominal range: 12-47 km) is very interesting. No significant differences are found in the retrieved profiles of no2 below 47 km except in the South Pole. This means that outside the polar vortex, where the concentration of n2o is low at altitudes above 47 km, the oscillations in the retrieved profile from 47 to 68 km do not affect retrieved profiles below 47 km; on the contrary, in the South Pole (in winter), where no2 concentration above 47 km is high, retrieved profiles in the range 12-47 km are strongly affected by the assumption of the profile above 47 km, if retrieval is stopped at that altitude: in this case, downward propagation of the error strongly affects the retrieved profile down to very low altitudes.
Therefore, NO2 retrieval up to 68 km is very useful in the polar vortex and does not degrade profiles in normal conditions. ESDs are acceptable, however the role of NLTE error above 47 km has to better investigated.
In general, for all species the extension of the retrieval range to the whole MIPAS measurement range does not seem to degrade the retrieved profiles in the range originally selected for the retrieval. Further investigations has to be made in order to assess the contribution of systematic errors to the total error in the extended altitude range.

<table>
<tr><td colspan="2">CalVal Analysis Summary Sheet</td><td colspan="2">Sheet MIP_MV_2_1</td><td>Page 1 of 2</td></tr>
<tr><td colspan="2"></td><td>Issue: Draft</td><td colspan="2">Date 23/06/2003</td></tr>
<tr><td rowspan="2">ENVISAT
CARING FOR THE EARTH</td><td rowspan="2">MIPAS</td><td>Prepared by Simone Ceccherini</td><td colspan="2">Processing site IFAC-CNR</td></tr>
<tr><td colspan="3">CalVal Plan Ref: MV_2_1

Other Ref: Sect 2.3 of 2nd Part of this TN,
TN-IROE-GS0101 Issue 1 A Sect. 4.2.1</td></tr>
<tr><td colspan="4">Subject:
Local thermodynamic equilibrium (LTE)</td><td>AO / ESL Ref.:11717/95/ NL/CN</td></tr>
<tr><td colspan="5">Inputs</td></tr>
<tr><td colspan="3">PDS
Orbit 2081 data, i.e. MIP_NL__1P020724_112130_M1_2081_020801
ORM input files generated by ML2PP with quadratic frequency correction to the ILS, with cloud filtering.</td><td colspan="2">others</td></tr>
<tr><td colspan="3">Outputs
This report</td><td colspan="2">Location/Access (ftp, ...)
CD</td></tr>
<tr><td colspan="5">Tools
ML2PP (with patches up to 24 April 2002) for generating ORM inputs
ORM_ORB_1.0.1 (version 03.09.2002) with fit of frequency shift scaling parameter activated
ST (version 0.98)</td></tr>
<tr><td colspan="5">Recommendations
The strategy adopted for NLTE is confirmed.</td></tr>
<tr><td colspan="5">Problem Areas</td></tr>
</table>

Continuation Sheet	Sheet MIP_MV_2_1	Page 2 of 2
	Issue: Draft	Date 23/06/2003

Summary

ORM assumes the atmosphere in local thermodynamic equilibrium (LTE). This means that the temperature of the Boltzmann distribution is equal to the kinetic temperature and the source function is the Planck function at the local kinetic temperature. This LTE model is usually valid at low altitudes where kinetic collisions are frequent.
Non-LTE effects cause a radiance higher or lower than that modeled in LTE, so a retrieval that does not take into account NLTE can produce wrong values of the VMR at high altitudes for the species affected by NLTE.
Non-LTE effects can sometimes be discriminated by the fact that they tend to decrease during the night.

In this test χ^2 corresponding to the day scans are compared with the χ^2 corresponding to the night scans of orbit #2081.
Partial χ^2 in correspondence of the species and altitudes which have the highest non-LTE error quantifiers are reported for day and night measurements for orbit #2081.
The comparison between χ^2 corresponding to day and night scans are reported in the table below:

	day	**night**
PT	1.71	1.70
H_2O	0.94	0.96
O_3	1.19	1.20
HNO_3	1.31	1.13
CH_4	1.06	1.06
N_2O	1.01	1.05
NO_2	1.02	1.01

The error analysis has identified significant non-LTE error for the following species and altitudes:

gas	**altitude**	**Non-LTE error**
H_2O	60 km	39.1%
CH_4	60 km	12.4 %
NO_2	47 km	62.5 %
NO_2	42 km	12.2 %

The analysis of the partial χ^2 corresponding to these species and altitudes has evidenced no significant variation between χ^2 obtained in day or night measurements. This does not necessarily mean that NLTE does not influence the retrieval, because the effect of NLTE could be compensated by wrong values of the VMR. So a deeper analysis of this problem is necessary and for it we refer to that performed by the team of Manuel Lopez Puertas.

CalVal Analysis Summary Sheet		**Sheet** MIP_MV_2_2	**Page 1 of 2**
		Issue: Draft	**Date** 23/06/2003
ENVISAT CARING FOR THE EARTH	***MIPAS***	**Prepared by:** Marco Ridolfi	**Processing site:** Dept. of Physical and Inorganic Chemistry - Univ. of Bologna
		CalVal Plan Ref: PO-PL-ESA-GS-1124 Issue 1A - MV_2_2 **Other Ref:** Sect 2.4 of 2nd Part of this TN, TN-IROE-GS0101 Issue 1A - Sect. 4.2.2	

Subject: **Verification of horizontal homogeneity hypothesis**	**AO / ESL Ref.:** 11717/95/NL/CN

Inputs

PDS	**Others**
Orbit 2081 data, i.e. MIP_NL__1P020724_112130_M1_2081_020801 ORM input files generated by ML2PP with quadratic frequency correction to the AILS, no cloud filtering applied.	

Outputs	**Location/Access (ftp, ...)**
This report.	

Tools

- ORM_SDC
- Statistical Tool

Recommendations

From this test we had no evidence of systematic errors induced by horizontal homogeneity assumption. However tests done so far are very limited. It is recommended to:

- Carry-out extensive intercomparison of Level 2 profiles with external (e.g. ECMWF) profiles and correlate discrepancies with horizontal gradients
- Compare Level 2 profiles retrieved by the Level 2 processor with profiles retrieved using a 2D retrieval algorithm (e.g. GEOFIT)

Problem Areas

Continuation Sheet	**Sheet:** MIP_MV_2_2	**Page 2 of 2**
	Issue: Draft	**Date 23/06/2003**

Summary

Background:
The forward model included in the MIPAS Level 2 processor assumes horizontal homogeneity of the atmosphere. In the geographical regions with significant horizontal variability this approximation, in principle, may cause both a systematic bias of the retrieved profiles and large residuals of the fit (i.e. the forward model could be unable to match the observed spectra within the measurement error).

Procedure:
1. Evaluate the correlation between the chi-square test and the horizontal gradient for the individual tangent altitudes measured by MIPAS.
2. Comparison of retrieved profiles with external (ECMWF) profiles

Results / conclusion:
No large correlations were detected at the individual altitudes between chi-square and horizontal gradients, therefore, if present, the effect of horizontal homogeneity assumption is expected to cause a systematic bias in the retrieved profiles (as shown in Carlotti et al., 2001). However this bias is not evident from the intercomparisons with external data (ECMWF profiles) carried-out so far. This may be due to the fact that the intercomparison with external info has not been carried-out specifically for scans corresponding to large horizontal gradients.

Reference:

M.Carlotti, B.M.Dinelli, P.Raspollini, M.Ridolfi, 'Geo-fit approach to the analysis of satellite limb-scanning measurements', *Appl. Optics*, Vol. **40**, No. 12, p. 1872 – 1875, (April 2001).

CalVal Analysis Summary Sheet		**Sheet** MIP_MV_2_3		**Page 1 of 2**
		Issue: Draft	**Date** 23/06/2003	
ENVISAT CARING FOR THE EARTH	*MIPAS*	**Prepared by:** Marco Ridolfi	**Processing site:** Dept. of Physical and Inorganic Chemistry - Univ. of Bologna	
		CalVal Plan Ref: PO-PL-ESA-GS-1124 Issue 1A - MV_2_3 **Other Ref:** Sect 2.5 of 2nd Part of this TN, TN-IROE-GS0101 Issue 1A - Sect. 4.2.3		

Subject:
Verification of hydrostatic equilibrium (assumption of vertical profiles)

AO / ESL Ref.: 11717/95/NL/CN

Inputs

PDS	**Others**
Orbit 2081 data, i.e. MIP_NL__1P020724_112130_M1_2081_020801 ORM input files generated by ML2PP with quadratic frequency correction to the AILS, cloud filtering applied.	

Outputs	**Location/Access (ftp, ...)**
This report	

Tools

- ORM_SDC
- Statistical Tool

Recommendations

There is no evidence of significant errors induced by the assumption of vertical profiles (instead of slant). Therefore it is recommended to keep using this assumption in Level 2 retrievals.

Problem Areas

Continuation Sheet	**Sheet:** MIP_MV_2_3	**Page 2 of 2**
	Issue: Draft	**Date 23/06/2003**

Summary

Background:
Hydrostatic equilibrium provides a relationship between temperature, pressure and geometrical altitude and is generally fulfilled in normal atmospheric conditions (especially in the stratosphere). However it should be noted that, with limb scanning, the profile of acquired tangent points is a slant profile. This is due both to the variation of the tangent point position with the elevation angle and because of the satellite motion (most important factor). The Level 2 algorithm assumes retrieved profiles as "vertical" to apply the hydrostatic balance and this approximation could have a significant impact on the accuracy of the retrieved tangent altitude corrections.

Procedure:
The test procedure consists in the assessment of the correlations between the horizontal temperature gradients and the tangent altitude corrections (i.e. the difference between engineering and retrieved estimates of the tangent altitude separation) obtained from p,T retrieval, when no engineering pointing information is used. A scatter plot was built correlating the horizontal temperature gradients with the tangent altitude correction at the same altitude. The plot contains as many points as many are the sweeps measured along the considered orbit (orbit #2081). The correlation between the considered quantities is quantified by the linear correlation coefficient.

Results:
Correlation between tangent altitude corrections and temperature gradients exists but is small (9%). Given the heterogeneity of the considered sample of tangent altitude corrections (considered tangent altitude corrections are different due to real differences in MIPAS pointings along the orbit rather than to horizontal variability of temperature) it is not possible to compare this empirical correlation with its theoretically expected value.

Conclusion:
The assumption of "vertical" profiles is justified and does not have significant impact on the accuracy of retrieved tangent altitude corrections.

CalVal Analysis Summary Sheet	Sheet MIP_MV_4	Page 1 of 2
	Issue: Draft	**Date** 23/06/2003
ENVISAT CARING FOR THE EARTH — *MIPAS*	**Prepared by:** Bianca Maria Dinellli	**Processing site:** ISAC-CNR
	CalVal Plan Ref: PO-PL-ESA-GS-1124 Issue 1A - MV_2_4 **Other Ref:** Sect 2.6 of 2nd Part of this TN, TN-IROE-GS0101 Issue 1A - Sect. 4.2.12	

Subject: **Verification of error in the VMR profiles of interfering species**	**AO / ESL Ref.:** 11717/95/NL/CN

Inputs

PDS	**Others**
Orbit 2081 data, i.e. MIP_NL__1P020724_112130_M1_2081_020801 ORM input files generated by ML2PP with quadratic frequency correction to the AILS, cloud filtering applied.	

Outputs	**Location/Access (ftp, ...)**
Output is only this report, with appendix containing detail information on tests carried-out so far.	

Tools

ML2PP (with patches up to 24 April 2002) for generating ORM inputs

ORM_ORB_1.0.1 (version 03.09.2002) with forced pt+h2o recursive

Recommendations

We recommend:

- to use more stringent convergence criteria thresholds
- to implement p,T + H_2O loop to help ORM coping with p,T retrievals that do not converge

Problem Areas

Continuation Sheet	Sheet: MIP_MV_2_4	Page 2 of 2
	Issue: Draft	Date 23/06/2003

Summary

ORM first performs the retrieval of pressure and temperature, then the VMRs of the target species in sequence. This means that in each retrieval the VMR of the interfering species, i.e. the species whose VMR is not fitted in the current retrieval, are assumed as known, acting as a systematic error source. In particular, tests have shown that a "wrong" H_2O profile may cause problems in the p,T retrieval.

To assess the impact of the assumed H_2O profile on the p,T retrieval the following procedure has been followed

1. For each sequence, the p,T and H_2O retrievals have been performed on orbit 2081 using the initial guess profiles coming from ML2PP processor (iteration 0) with no cloud detection
2. The retrieved profiles have been used as initial guess in a new retrieval
3. The loop has been repeated until the retrieved profiles were consistent (within their error) with the profiles at the previous step.

The retrievals have been performed using version 3 of the settings.
Apart few exceptions, consistent profiles have been found after 2 p,T+H_2O loops. This means that, on average, the loops have to be repeated at least once per sequence in order to reach stable results.
This instability may be explained by either the use in the retrievals of a wrong initial guess profiles or by the fact that the adopted convergence criteria are too "weak".
In order to check if these results are due to 'weak' convergence criteria, the test was repeated using IG of ML2PP with cloud detection and forcing each p,T and H_2O retrievals to perform always 10 Gauss Newton iterations. The results of this test showed that in the majority of cases consistent results were obtained after the first loop.
This means that in general there is no need for a p,T + H_2O loop if true convergence has been reached.
We recommend to use strong convergence criteria and implement p,T + H_2O loops to help ORM coping with the exceptional cases in which p,T retrievals do not converge.

<table>
<tr><td rowspan="2">CalVal Analysis
Summary Sheet</td><td colspan="2">Sheet MIP_MV_2_8-AX_2_3</td><td>Page 1 of 2</td></tr>
<tr><td>Issue: Draft</td><td colspan="2">Date 023/06/2003</td></tr>
<tr><td rowspan="2">ENVISAT
CARING FOR THE EARTH</td><td rowspan="2">MIPAS</td><td>Prepared by:
Chiara Piccolo</td><td>Processing site: AOPP - University of Oxford</td></tr>
<tr><td colspan="2">CalVal Plan Ref: PO-PL-ESA-GS-1124 Issue 1A - MV_2_8
Other Ref: TN-IROE-GS0101 Issue 1A - Sect. 4.2.5,
TN-LPM-IFAC-02</td></tr>
<tr><td colspan="3">Subject:
Errors in the spectroscopic parameters</td><td>AO / ESL Ref.:
11717/95/NL/CN</td></tr>
<tr><td colspan="4">Inputs</td></tr>
<tr><td colspan="3">PDS
Orbit 2081 data, i.e. MIP_NL__1P020724_112130_M1_2081_020801 ORM input files generated by ML2PP with quadratic frequency correction to the AILS, cloud filtering applied.</td><td>Others
Updates of CO_2, HNO_3, CH_4, NO_2, O_3 and COF_2 parameters obtained through new laboratory studies or new calculations</td></tr>
<tr><td colspan="3">Outputs
The technical note TN-LPM-IFAC-02, the new version of the spectroscopic database called hitran_mipas_pf3.0</td><td>Location/Access (ftp, ...)</td></tr>
<tr><td colspan="4">Tools
➢ ORM_SDC
➢ Statistical Tool</td></tr>
<tr><td colspan="4">Recommendations
It is recommended to use the updated version hitran_mipas_pf3.0 of the MIPAS spectroscopic database.</td></tr>
<tr><td colspan="4">Problem Areas</td></tr>
</table>

Continuation Sheet	**Sheet:** MIP_MV_2_8-AX-2-3	**Page 1 of 2**
	Issue: Draft	**Date 23/06/2003**

Summary

Background:

The spectroscopic parameters are assumed to be known, therefore their errors cause systematic retrieval errors. The spectroscopic parameters associated with the most relevant retrieval errors are the line strength, the line position and the pressure broadening coefficients. The line position can also depend on the pressure shift. Pressure shift is included in the LUTs (only for some H_2O and CH_4 lines, for which there is the information) and it is neglected in the LBL calculation. Errors in the spectroscopic parameters can show-up with characteristic shapes of residuals (line shape, first and second dervative shape as examples of line strength, position and broadening errors respectively).

Procedure:

The test procedure consists in several steps. For each species a visual inspection in the residuals of the typical patterns of spectroscopic errors has been performed for a single sequence of orbit 2081. Identified the possible cause, a new set of spectroscopic parameters has been used to generate the atmospheric simulations (LBL calculation) for the same sequence of orbit 2081. In case of an improvement in the residuals at most altitudes of the considered sequence, the same test has been performed considering the whole orbit and averaging the residual at each altitude for which the same OM has occurred. The improvement is measured by the decrease of the averaged chi-squared values derived from retrievals using on the one hand the old spectroscopic parameters and on the other hand the new set of parameters.

For more details of the procedure and the results see TN-LPM-IFAC-02.

Results:

CO_2: New line parameters for the four most abundant isotopic species, namely $^{12}C^{16}O_2$, $^{13}C^{16}O_2$, $^{16}O^{12}C^{18}O$ and $^{16}O^{12}C^{17}O$ have been validated through p,T retrievals performed using orbit 2081. At all altitudes but 24km these new line parameters give better results.

HNO_3: Simulations of MIPAS spectra have showed an inconsistency between the spectral parameters of the hot band (24-19) and the cold bands (18-14, 21-14, 27-14 and 17-14) absorbing in the same spectral region (around 885 cm^{-1}). New line intensities of these four cold bands have been obtained by multiplying them by a factor 0.879. The consistency has been checked performing retrievals of HNO_3 using orbit 2081 and a clear improvement at all altitudes has been achieved. However, it is essential to notice that this change leads to a systematic increase of the HNO_3 abundance of about 13%.

CH_4: New pressure shift and new pressure broadening coefficients.

NO_2: Updated temperature and pressure dependence of NO2 absorption features and values for the self broadening coefficients.

O_3: Updated absolute intensities of the $\nu_1 + \nu_3$ bands of $^{16}O^{18}O^{16}O$, $^{16}O^{16}O^{18}O$, $^{16}O^{17}O^{16}O$ and $^{16}O^{16}O^{17}O$ absorbing around 4.8 μm.

COF_2: Updated line parameters in the 5.2 μm spectral region for three bands (5-1, 2-1 and 4-1).

Conclusion:

A new version of the MIPAS spectroscopic database has been generated including updated parameters of CO_2, HNO_3, CH_4, NO_2, O_3 and COF_2 parameters obtained through new laboratory studies or new calculations.

<table>
<tr><td colspan="2">CalVal Analysis Summary Sheet</td><td colspan="2">Sheet MIP_MV_2_10</td><td>Page 1 of 2</td></tr>
<tr><td colspan="2"></td><td>Issue: Draft</td><td colspan="2">Date 23/06/2003</td></tr>
<tr><td rowspan="2">ENVISAT CARING FOR THE EARTH</td><td rowspan="2">MIPAS</td><td>Prepared by Simone Ceccherini</td><td colspan="2">Processing site IFAC-CNR</td></tr>
<tr><td colspan="3">CalVal Plan Ref: MV_2_10

Other Ref: Sect 2.7 of 2nd Part of this TN,
TN-IROE-GS0101 Issue 1 A Sect. 4.2.6</td></tr>
<tr><td colspan="4">Subject:
Verification of the assumptions related to the line-mixing for CO_2 Q-branches</td><td>AO / ESL Ref.:11717/95/ NL/CN</td></tr>
<tr><td colspan="5" align="center">Inputs</td></tr>
<tr><td colspan="3">PDS
Orbit 2081 data, i.e. MIP_NL__1P020724_112130_M1_2081_020801
ORM input files generated by ML2PP with quadratic frequency correction to the ILS, with cloud filtering.</td><td colspan="2">others</td></tr>
<tr><td colspan="3">Outputs
This report.</td><td colspan="2">Location/Access (ftp, ...)
CD</td></tr>
<tr><td colspan="5">Tools
ML2PP (with patches up to 24 April 2002) for generating ORM inputs
ORM_ORB_1.0.1 (version 03.09.2002) with fit of frequency shift scaling parameter activated
ST (version 0.98)</td></tr>
<tr><td colspan="5">Recommendations
None</td></tr>
<tr><td colspan="5">Problem Areas</td></tr>
</table>

Continuation Sheet	Sheet MIP_MV_2_10	Page 2 of 2
	Issue: Draft	Date 23/06/2003

Summary

Line mixing corresponds to the deviation of measured line shape from the Voigt function. This effect occurs when collisions between a radiating molecule and the broadening gas molecules cause the transfer of population between rotational-vibrational states. Line mixing affects especially the Q-branches where transitions between rotational-vibrational energy levels closer than $K_B T$ (K_B is the Boltzmann constant, T is the temperature) are packed together. The most apparent effect of line-mixing is a reduction of the cross-section in the wings of the branch. The impact of line-mixing effects, mainly significant for CO_2 lines, is reduced in ORM by using an appropriate selection of microwindows.
By inspection of the CO_2 line mixing error spectra provided by the University of Oxford four spectral ranges (in the range measured by MIPAS) have been found where the error introduced by ignoring line mixing can be significant. In the nominal occupation matrix used by ORM there are four microwindows inside these four spectral ranges.
The averaged residuals corresponding to these four microwindows have been compared with the random error (NESR) and with the CO_2 line mixing error spectra.
A clear correlation between averaged residuals and line mixing error is noticed in particular for the following microwindows and altitudes:

PT0004	15, 18 km
PT0006	15, 18 km
PT0002	12, 15, 18, 21, 24, 27 km

We have found that the values of averaged residuals are a little smaller than the error spectra indicating an overestimation of the error spectra.
In some microwindows the error on the simulated spectrum introduced by line-mixing is comparable with the random error on the single measurement. On the basis of these results we can conclude that line-mixing error is not a major problem but is significant and can introduce a bias in analyses involving the calculation of averages of the profiles.

CalVal Analysis Summary Sheet		**Sheet MIP_MV_2_12**	**Page 1 of 2**
		Issue: Draft	**Date** 23/06/2003
ENVISAT CARING FOR THE EARTH	*MIPAS*	**Prepared by:** Piera Raspollini	**Processing site:** IFAC-CNR
		CalVal Plan Ref: po_pl_esa_gs_1124, issue 1B, MV_2_12 **Other Ref: Sect 2.8 of 2nd Part of this TN,** **TN-IROE-GS0101 Issue 1 A Sect. 4.2.8**	

Subject: : **Verification of ILS width**	**AO / ESL Ref.:** 11717/95/NL/CN

Inputs

PDS	**Others**
Orbit 2081 data, i.e. MIP_NL__1P020724_112130_M1_2081_020801 ORM input files generated by ML2PP with and without quadratic frequency correction to the ILS, with cloud filtering.	

Outputs	**Location/Access (ftp, ...)**
This report	**CD**

Tools

ML2PP (with patches up to 24 April 2002) for generating ORM inputs

ORM_ORB_1.0.1 (version 03.09.2002) with fit of frequency shift scaling parameter activated
ST (version 0.98)

Recommendations

Repeat analysis with new full orbit Level1 data periodically (every three months at the beginning, then once/year).

Problem Areas

The ILS width has a high correlation with pressure retrievals. This correlation with pressure is the reason for the requirement of an accurate ILS, and is also the cause of the difficulties in the retrieval of the ILS from the atmospheric measurements.

Continuation Sheet	**Sheet:** MIP_MV_2_12	**Page 2 of 2**

Summary

The objective of this test is to verify the correctness of the width of the ILS from the analysis of the spectra by fitting a band dependent ILS broadening parameter.

The ILS width is highly correlated with pressure and this is the cause of the difficulties in the retrieval of the ILS from the atmospheric measurements. In order to avoid this problem it is necessary to limit the interference of the atmospheric broadening that is greater at low altitudes. Therefore, special sensitivity tests were made with retrieval limited at altitude above 40 km. The ILS broadening parameters were determined for all scans of orbit # 2081 for bands A, AB, B and C (no microwindows in band D have been used). These retrieved values present significant variations as a function of the scan, and on average the broadening parameter is negative, suggesting that the real ILS may be sharper than the one provided by Level 1.
The table below reports the retrieved ILS broadening parameters averaged on the whole orbit for the different spectral bands.

A	AB	B	C
-1.56e-2±4e-4	-2.59e-2±8e-4	-3.78e-2±8e-4	-4.68e-2±7e-4

The conclusion is that we obtain on average an indication for a sharper ILS, but the large variability of the results leaves the suspicion that other modelling effects may be interfering with this test.

ENVISAT CARING FOR THE EARTH	*MIPAS*	**Prepared by:** Piera Raspollini	**Processing site:** IFAC-CNR
		CalVal Plan Ref: po_pl_esa_gs_1124, issue 1B, MV_2_16 **Other Ref: Sect 2.9 of 2nd Part of this TN,** **TN-IROE-GS0101 Issue 1 A Sect. 4.2.10**	

Subject: : **Verification of intensity calibration**	**AO / ESL Ref.:** 11717/95/NL/CN

Inputs

PDS	**Others**
Orbit 2081 data, i.e. MIP_NL__1P020724_112130_M1_2081_020801 ORM input files generated by ML2PP with quadratic frequency correction to the ILS and with cloud filtering.	

Outputs	**Location/Access (ftp, ...)**
This report	**CD**

Tools

ML2PP (with patches up to 24 April 2002) for generating ORM inputs

ORM_ORB_1.0.1 (version 03.09.2002) with fit of frequency shift scaling parameter activated
ST (version 0.98)

Recommendations

No positive evidence is observed of an intensity calibration error. Better information on intensity calibration from the analysis of the spectra could be derived using dedicated selection of microwindows (with saturated signals).

Problem Areas

A systematic oscillation in Level 1 radiance between forward and reverse sweeps has been identified due to a difference in the treatment of the non-linearity correction for forward and reverse sweeps (see MIP_newtest).

Continuation Sheet	Sheet: MIP_MV_2_16	Page 2 of 2
	Issue: Draft	Date 23/06/2003

Summary

The objective of this test is to assess, from the analysis of the spectra, the correctness of the intensity calibration by fitting a band dependent and altitude independent intensity scaling parameter for each scan of the orbit and for each retrieval (pT, h2o, o3, etc.). The microwindows used for this fit are the ones selected for the nominal retrievals (no dedicated microwindows are used).
Due to the strong correlations of this parameter with temperature and VMR, it is not possible to provide an absolute verification of the intensity calibration, but whenever microwindows belonging to different bands are used in the fit, the ratio between the intensity calibration parameters of different bands is expected to provide useful information.
The fit of the intensity scaling factor varies only marginally the residuals. Furthermore, a reduction of the residuals is observed only in cases of sequences that have large errors.
No consistent results are obtained when computing the ratio between the fitted intensity calibration parameters of band A and band B, that are the bands characterised by the highest statistics.
Therefore the conclusion are that it is difficult to extract information on intensity calibration error from the analysis of the spectra and no positive evidence is observed of a intensity calibration error.

<table>
<tr><td colspan="2">CalVal Analysis Summary Sheet</td><td colspan="2">Sheet MIP_MV_2_17</td><td>Page 1 of 2</td></tr>
<tr><td colspan="2"></td><td>Issue: Draft</td><td colspan="2">Date 23/06/2003</td></tr>
<tr><td>ENVISAT
CARING FOR THE EARTH</td><td>MIPAS</td><td>Prepared by Simone Ceccherini</td><td colspan="2">Processing site IFAC-CNR</td></tr>
<tr><td></td><td></td><td colspan="3">CalVal Plan Ref: MV_2_17

Other Ref: Sect 2.10 of 2nd Part of this TN,
TN-IROE-GS0101 Issue 1 A Sect. 4.2.11</td></tr>
<tr><td colspan="4">Subject:
Zero-level calibration</td><td>AO / ESL Ref.:11717/95/ NL/CN</td></tr>
<tr><td colspan="5" align="center">Inputs</td></tr>
<tr><td colspan="3">PDS
Orbit 2081 data, i.e. MIP_NL__1P020724_112130_M1_2081_020801
ORM input files generated by ML2PP with quadratic frequency correction to the ILS, with cloud filtering.</td><td colspan="2">others</td></tr>
<tr><td colspan="3">Outputs
This report</td><td colspan="2">Location/Access (ftp, ...)
CD</td></tr>
<tr><td colspan="5">Tools
ML2PP (with patches up to 24 April 2002) for generating ORM inputs
ORM_ORB_1.0.1 (version 03.09.2002)
ST (version 0.98)</td></tr>
<tr><td colspan="5">Recommendations
The fit of an altitude dependent offset is not necessary.
The fit of an altitude independent zero-level calibration is more than appropriate.
Since the retrieved offset is very close to zero with respect to the random error, it would also be possible to avoid all together the fit of the offset. However, the retrieved offset can also be useful as a quality indicator and we recommend that for the moment the retrieval approach is not changed.</td></tr>
<tr><td colspan="5">Problem Areas</td></tr>
</table>

Continuation Sheet	Sheet MIP_MV_2_17	Page 2 of 2
	Issue: Draft	Date 23/06/2003

Summary

Causes of instrument zero level offset are internal emission of the instrument, scattering of light into the instrument or third order non-linearity of the detectors. All these causes of offset are corrected during the calibration step in Level 1b data processing.
In the ORM, a limb scanning angle independent offset is fitted for each microwindow in order to compensate for the residual uncorrected instrument offset. If the instrument has a limb angle dependent offset, the ORM corrects only partially for it.
An altitude dependent offset probably can not be seen in the residuals because cross talks are possible with intensity calibration errors and atmospheric continuum retrieval. The evidence is hidden in the inconsistency of the retrieved quantities.

A fit of the instrumental offset as a function of both tangent altitude and microwindow has been done and compared with the nominal retrieval.
A retrieval without to fit the instrumental offset has been performed and compared with the nominal retrieval.
Neglegible differences in the χ^2 are observed when an offset altitude dependent is fitted or no offset is fitted with respect to the nominal case.
The profiles obtained fitting an altitude dependent offset show significant differences with respect to those obtained with the nominal retrieval. Instead the profiles obtained without fitting the offset are very close to those obtained with the nominal retrieval.
In all the studied cases the retrieved offset is very close to zero when compared with the random error, so it would be possible to avoid to fit the offset, but it is useful to have it as a quality indicator.

CalVal Analysis Summary Sheet		Sheet MIP_newtest	Page 1 of 2
		Issue: Draft	Date 23/06/2003
ENVISAT CARING FOR THE EARTH	**MIPAS**	Prepared by Vivienne Payne	Processing site IFAC-CNR
		Other Ref: Sect 5 of 2nd Part of this TN,	

Subject: **Non-linearity correction**	**AO / ESL Ref.:11717/95/ NL/CN**

Inputs

PDS	Others
Orbit 2081: MIP_NL__1P020724_112130_M1_2081_020801 New Level 1 file for orbit #2081 supplied in January: L1_2081_NewNLCoef	

Outputs	Location/Access (ftp, ...)
This report	CD

Tools

OPTIMO (Oxford retrieval program)

Recommendations

Use the new treatment of non-linearity correction in Level1 processor.

Other investigations are needed to further reduce the oscillations in Level1 radiance.

Problem Areas

Continuation Sheet	Sheet MIP_MV_2_17	Page 2 of 2
	Issue: Draft	Date 23/06/2003

Summary

It was observed that there were oscillations in the retrieved profiles (both in the retrievals from the Oxford processor and in the ESA Level 2 product) for orbit #2081. These oscillations were anti-correlated between scans, indicating a systematic problem with the Level 1 radiances. The problem was traced back to a difference in the treatment of the non-linearity correction for forward and backward sweeps of the interferogram. New Level 1 data for orbit #2081 was supplied in January. In this new data, the difference between forward and backward sweeps is supposed to have been eliminated.

For each sweep of each scan of the orbit #2081, the mean value of the radiance over the whole of each band was calculated. Then, a weighted mean for each sweep of each scan was computed, passing along the orbit, using a weighting of 1/4, 1/2, 1/4 for the previous scan number, the present scan number and the next scan number respectively. The percentage difference between the mean radiance of each band and the weighted mean taking account of scans on either side was calculated. A regular pattern is visible along the orbit, and this could indicate a systematic difference between radiances measured during forward and backward interferogram sweeps.

After the new treatment of the non-linearity correction, this regular pattern is significantly reduced, even if not completely eliminated.

The reduction in the oscillations in the radiance induces a reduction in the oscillations in the retrieved temperature and H2O profiles. However, even if the results after the new treatment of non-linearity correction are much improved, there are still oscillations present in H2O VMR profile of the order of 5-10%.

We can conclude that the non-linearity correction used in the new Level1 file seems to be successful in reducing the oscillations in the radiance and, as a consequence, in the retrieved profiles.

However, the problem does not appear to have been entirely eliminated.