Technical Note on:

Pre-flight modifications to the ORM_ABC code

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Delivery of WP 4100 of the CCN#5 of the study:

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

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1. Reference documents

[RD1] TN-IROE-RSA9601**,** Issue: 2A
Title: High level algorithm definition and physical and mathematical optimisations

[RD2] TN-IROE-RSA9603**,** Issue: 3A
Title: Software Architecture and Algorithm Definition

[RD3] TN-ISM-0001, Issue: 1
Title: Implementation of balloon geometry option and MIPAS_B data analysis

2. Introduction

Version 1.21 of the ORM_ABC code (described in [RD2]) is the scientific reference for the Retrieval Component Library of MIPAS Level 2 NRT processor. Tests performed with this code using numerical simulation and the new microwindow database provided by the Oxford team, as well as the analysis of MIPAS-B balloon measurements [RD3] have pointed out the need for some modifications in the code. These modifications could either be introduced before the flight or after further tests performed during the commissioning phase.
The modifications that could be introduced in the ORM_ABC_1.21 code before the flight deal with the following issues:

- calculation of the VCM of the observations in the case of reduced spectral resolution;
- definition of the lowest level of the 'base' grid;
- calculation of continuum derivatives;
- band dependent FOV;
- maximum altitude used in the 'mod' grid
- molecule dependent measurement grid.

All the listed modifications affect the Retrieval Component Library of MIPAS Level 2 NRT processor except the last one.

In Section 3 the high level description of these modifications is provided, with the indication of the changes in the routines affected.

Other issues are still under discussion and could lead to further modifications during the commissioning phase. A list of these issues is provided in Section 4.

3. Pre-flight modifications

3.1 Calculation of the VCM of the observations in the case of reduced spectral resolution

The Variance Covariance Matrix of the observations takes into account the correlation that exists between the spectral points. Correlations are introduced by apodisation and by zero-filling. The first effect is always present, the second is present only in the case of measurements with reduced spectral resolution.
In the case of zero-filling, the following operations are performed in the ORM. The points of the apodisation function in the interferogram domain corresponding to the zero-filled points are set to 0, and the NESR is scaled with the square root of the ratio between the measured Maximum Path Difference (MPD) and the zero-filled MPD (this ratio is identified in the code by the variable *rzerof*).
The VCM is assumed to be a block-diagonal matrix, constituted of as many blocks as many microwindows are considered. Each block is computed multiplying the diagonal VCM associated to the unapodised spectrum by the product of $\mathbf{J}\ \mathbf{J}^T$, where **J** is the Jacobian matrix associated to the convolution of the spectrum with the apodisation function [RD1].
The inverse of the VCM is obtained inverting each block.

The analysis of MIPAS-B balloon measurements[RD3], which are characterised by a reduced spectral resolution respect to MIPAS-ENVISAT (the measured MPD of the balloon instrument is about 14 cm), has pointed out that the inversion of the VCM is not properly computed by the algorithm that inverts not singular matrices. The problem is due to the fact that a value of *rzerof* smaller than one implies that the "rank" of the VCM matrix is smaller than its dimension. This fact would be evident in the case in which the VCM is calculated in a sufficiently broad spectral range. However in the ORM, where microwindows are used and correlation are calculated in a limited spectral range, the truncations make the determinant different from zero even if the number of independent pieces of information is less than the dimension of the matrix.
The problem can be solved by modifying the routine that inverts the VCM : the VCM is inverted with the Singular Value Decomposition (SVD) method also when the determinant is different from zero and a number of the smallest eigenvalues are set equal to 0. The number of the eigenvalues set to 0 is given by the number of dependent points in the spectrum (*1-rzerof*)**n1*, where *n1* is the number of the not masked sampling points of the microwindow.

Code modifications

Module **sinvcal_mw_(pt/vmr)**

- The variable *rzerof* has been added at the interface of the routine
- In the case of nominal spectral resolution, the inversion of each block of the VCM is performed, as in ORM_ABC_1.21 code, by the routine **vinvcal**. In the case of

reduced spectral resolution (*rzerof* ≤ 0.99) the inversion of each block of the VCM of the observations, relative to one microwindow and one tangent altitude, is performed by the new module **svdcmp_(pt/vmr)**

Module **svdcmp_(pt/vmr)**

- This new module is similar to the module **ainvcal. ainvcal** performs the inversion of a singular matrix using the SVD approach. In **svdcmp** a predetermined fraction (*nint(1-rzerof)*n1*) of the smallest eigenvalues is set to 0 before the inversion.
- Interface: *rcjdp, n1, rcinvdp, rzerof*
  rcjdp(imxi,imxi) real*8: compressed VCM relative to a given microwindow and a given tangent altitude, obtained eliminating rows and columns relative to the masked spectral points
  n1 integer*4: number of not masked spectral points in the microwindow
  rcinvdp(imxi,imxi) real*8: inverse of *rcjdp* (output)
  rzerof real*8: ratio between measured MPD and nominal MPD

Module **retr_(pt/vmr)**

- Changed interface with module **sinvcal_mw_(pt/vmr)**

3.2 Definition of the lowest level of the 'base' grid

The ORM 'base' grid is defined by the following set of points: the tangent altitudes of the measurements, all the levels of the grid of the first-guess profile above the highest measured tangent altitude and one level below the lowest measured tangent altitude (coincident with a given level of the grid of the first-guess profile). In version 1.21 of the ORM_ABC the latter level of the 'base' grid is set to be a fixed valued defined by the hardwired variable *istart*, indicating the *istart*-th level in the grid of the first-guess profile. In practice, large differences may occur between the lowest tangent altitude and this hardwired value leading to a layer of non-optimum size in the base grid.
In order to eliminate this problem in the reconstruction of the profiles, the code should be modified as follows: the lowest point of the retrieval grid is defined in correspondence of the level of the first-guess grid coincident or just below the altitude *rztang (ilimb) - rintup* , where *rztang (ilimb)* is the lowest measured tangent altitude, *rintup* is an already existing input parameter indicating the vertical amplitude of the FOV pattern.

Code modifications

Module **chbase_(pt /vmr)**

- The level of the first guess profile coincident or just below the altitude *max(rzprof(ipro), (rztang (ilimb) - rintup))* is searched. The corresponding altitude is assigned to the lowest level of the base grid.
- The variable *rintup* has been added in the interface of this module.

Module **retr_(pt/vmr)**

- Changed interface with module **chbase_(pt/vmr)**.

3.3 Modification in the calculation of continuum derivatives

Tests of the ORM performed using the microwindows selected by the Oxford team have pointed out the need to drop an approximation in the calculation of the derivatives of the spectrum with respect to continuum. This approximation deals with the continuum derivative in correspondence with the value of the continuum fitted at the lowest tangent altitude. Furthermore, inconsistencies in the continuum derivatives have also been found in the case that the fit is performed in correspondence of a sub-set of the actual measurement tangent altitudes (this sub-set is defined in the code by the logical variable *lfit*).

In order to eliminate both problems, a major modification in the calculation of the continuum derivatives is required.

The derivatives of the spectrum with respect to the fitted continuum values are computed as the product of

(1) the derivative of the spectrum with respect to the mean value of the continuum in each layer (computed in routine **spectrum_**)

(2) the derivative of the mean continuum value in each layer with respect to the continuum values on the levels of the base grid (computed in routine **conlay_**)

(3) the derivative of the continuum values on the base grid with respect to the fitted continuum parameters (computed by routine **ficarra_**).

In version 1.21 of the ORM_ABC code, derivatives (2), instead of being computed with respect to all values of the base grid, are wrongly computed with respect to the levels of the retrieval grid (that is a subset of the base grid).

The modification to be implemented consists in computing derivatives (2) for all the points of the base grid.

Code modifications

Module **retr_(pt/vmr)**

- Changed interface with modules **chbase_(pt/vmr)**, **gcgeo_vmr (tcgeo_pt**), **fwdmdl_(pt/vmr)** (see module description)
- Exchanged order of calls to modules **chbase_(pt/vmr)** and **tcgeo_pt (gcgeo_vmr)**: firstly module **chbase_(pt/vmr)**, then module **tcgeo_pt (gcgeo_vmr)** are called.

Module **chbase_(pt/vmr)**

- Added definition of the variable *nucl1* indicating the highest level of the base grid with respect to which derivatives (2) have to be computed. In theory, *nucl1* should be given by the highest level of the base grid (*nucl2*)whose altitude is smaller than *rzc0* (altitude above which atmospheric continuum is set to 0). In practice, it is sufficient to define *nucl1* as max(*nucl2, nucl0-5*), where *nucl0* is the highest level of the base grid whose altitude is smaller than *rucl* (equal to the altitude above which atmospheric continuum is not fitted)
- The variables *rucl* , *rzc0* and *nucl1* have been added in the interface.

Modules **gcgeo_vmr** and **tcgeo_pt**

- Changes in the interface: the variable *nucl* has been replaced by *nucl1*, and variables *rzsi*, *ibase* and *rzbase* have been added.
- Modifications in the determination of the variable *igeocder*:
  igeocder(jgeo,1): for each simulated geometry, this variable indicates the highest level of the base grid, affecting the spectrum: this is set equal to *nucl1* for all the geometries.
  igeocder(jgeo,2): the lowest level of the base grid affecting the spectrum *jgeo* if FOV convolution is not considered. This is set equal to the greatest value between *nucl1* and the highest level of the 'base' grid whose altitude is lower than the tangent altitude *jgeo*.
  igeocder(jgeo,3): the lowest level of the base grid affecting the spectrum if FOV convolution is considered . This is set equal to the greatest value between *nucl1* and the highest level of the 'base' grid whose altitude is lower than the tangent altitude *jgeo – rintup/2*.

Module **fwdmdl_(pt/vmr)**

- Changes in the interface: variable *nucl* has been replaced by variable *nucl1*
- Changed interface with modules **mkplev_(pt/vmr)**, **conlay_(pt/vmr)**, **spectrum_(pt/vmr)**, **jacsetmw_(pt/vmr)**

Module **mkplev_(pt/vmr)**

- Changes in the interface: added variables *iderlayc* and *nucl1*.
- Determination of the new variable *iderlayc(imxpro,2)*: this variable is analogous to *iderlay(imxlmb,3)*, but for continuum derivatives: the parameters with respect to which continuum derivatives have to be computed are all the points of the 'base' grid instead of only the fitted points. The variable *iderlay* is computed using the assumption that the grid of the 'model' is finer than the 'base' grid: this is correct because in the range of the tangent altitudes, where *iderlay* works, this assumption is always verified. In general this assumption is not verified above the highest tangent altitude. Since *iderlayc* has to be computed for all the base grid points, a different algorithm has to be used for its determination. i*derlayc(jbase,1(2))* indicates, for each point *jbase* of the base grid, the highest (lowest) layer whose average pressure is included either between *rpbase(jbase)* and *rpbase(jbase+1)* or between *rpbase(jbase-1)* and *rpbase(jbase)*. The determination of *iderlayc* is performed in two steps: first for each layer, the levels of the base grid whose pressure is just above and below the layer average pressure are searched. Then, for each level of the base grid *jbase*, the highest (lowest) layer affected by level *jbase* is determined and assigned to *iderlayc(jbase,1(2))* . For the levels of the base grid that do not affect any layer, *iderlayc(jbase,1)* is set equal to *imxpro*, while *iderlayc(jbase,2)* is set to *imxpro -1*.

Module **conlay_(vmr/pt)**

- Changes in the interface: *iderlay(imxlmb,3)* has been replaced by variable *iderlayc(imxpro,2)*. Variable *nucl1* has been added.
- Derivatives of the mean continuum value in each layer with respect to the continuum values on the base grid (*rpartcder(imxlay,imxlmb,imxmw)* becomes

rpartcder(imxlay,imxpro,imxmw)) are computed for all the points of the 'base' grid instead of only the points of the base grid corresponding to 'fitted' points.

Module **jacsetmw_(vmr/pt)**

- Changes in the interface: variable *nucl* has been replaced by variable *nucl1*, variable *lparbase* has been dropped
- The product of derivatives (2) times derivatives (3) is performed without the check on *lparbase*.

Module **spectrum_(pt/vmr)**

- Added variable *ibase* in the interface
- Modified computation of internal variable *iderlay1*: *iderlay1* is set equal to *iderlayc(igeocder(jgeo,1),1)* : if this is equal to *imxpro*, it means that *igeocder(jgeo,1)* is a level of the base grid that do not affect any layer. In this case *iderlay1* is given by the first level of the base grid *jbase* below *igeocder(jgeo,1)* such that *iderlayc(jbase)* is different from *imxpro*.

Module **updprof_(pt/vmr)**

- Added variable *nucl1* in the interface
- Changed interface with sub-module **tcgeo_pt**

3.4 Band dependent FOV

The current version of the ORM code assumes a band independent FOV pattern and foresees the option of using for the FOV pattern either a pre-defined shape (trapezium shape) or a tabulated function for a piecewise linear representation. The information on the FOV pattern is contained in the input files *settings_*.dat*.
In order to allow for possible instrument complications, it was decided to foresee the possibility of using a band dependent modelling of the FOV. Furthermore, since the use of a pre-defined trapezium shape does not lead to a significant reduction in computing time and the tabulated function provides the trapezium shape as particular case, it was decided to simplify the code dropping the possibility of using the trapezium option.
Modification are performed in the input files *settings_*.dat*, in the module **finput_**, where the vector that associates with each microwindow the corresponding band is determined, and in module **fov_**, where convolution is performed, for each microwindow, using the appropriate FOV pattern.

Input/output files modifications

Files ***settings_***.dat***

The fields dealing with the greater base of the trapezium (*rbase*) and the half difference between the greater and smaller base (*rsl*), together with the logical variable *lfovtab* have been dropped.

A tabulated function is provided for each spectral band in sequence, starting from band A, and continuing with bands AB, B, C, D. . The tabulated function for the *i*-th band is defined by the following variables:

- *nfovinc(i)* (integer*4) , equal to the number of points used for tabulating FOV pattern
- *rfov(i,1→nfovinv(i))* (Real*8): vector containing the y-values of FOV tabulated function
- *ranginc(i,1→nfovinc(i))* (Real*8): vector containing the x-values of FOV tabulated function, relative to the centre of FOV pattern

Code modifications

Module **finput_(pt/vmr)**

- Modified reading of file settings_***.dat
- Modified common setting_(p/v): deleted variable *rbase*, *rsl* and *lfovtab* and added variable *iband(imxmw)*
- Modified submodule **uplimit_(pt/vmr)**, that changes the value of variable *rulatm* (equal to the boundary of the atmosphere) if this is lower than the highest tangent altitude + *2 * rintup* (in the previous version of the code *rulatm* was imposed to be higher or equal to *rztang(1)+ 2 * rbase*)
- Added subroutine **r_band_(pt/vmr)** that computes the vector indicating what band each microwindow belongs to, using the MIPAS band limits hardwired in a datablock. The band limits are defined in such a way to cover the whole MIPAS spectral range without gaps.

Module **retr_(pt/vmr)**

- Modified interface with module **fwdmdl_**.
- Modified commons settings_(p/v)

Module **fwdmdl_(pt/vmr)**

- Modified interface: dropped variables *rbase*, *rsl* and *lfovtab* and added variable *iband(imxmw)*
- Modified call to module **fov_(pt/vmr)**

Module **fov_(pt/vmr)**

- Modified interface: dropped variables *rbase*, *rsl* and *lfovtab* and added variable *iband(imxmw)*
- Modified call to submodule **fovn_(pt/vmr)**: dropped variables *rbase, rsl, lfovtab* and *rarea* and added variable *iband(imw)*
- Submodule **fovn_(pt/vmr)**: modified call to submodule **intcon_(pt/vmr)**, dropped variables *rbase, rsl, lfovtab* and *rarea* and added variable *iband(imw)*
- Submodule **intcon_(pt/vmr)**: dropped computation of convolution in the case of trapezium FOV pattern. The convolution is performed using the appropriate FOV pattern, i.e. the one relative to the band the given microwindow belongs to.

3.5 Maximum altitude used in the 'mod' grid

A minor change has been introduced in the module **mkplev_(pt/vmr)** that builds the grid 'mod', defining the layering used by the Radiative Transfer.
This modification takes into account the fact that the highest altitude considered in the modelling of the atmosphere is not only limited by the top of the atmosphere, but also by the base grid.

Code modification
Module **mkplev_(pt/vmr)**
Between the highest tangent altitude and the limit of the atmosphere (*rulatm*) a new level *j* at altitude *rz(j)=rz(j-1)+rincz* is added to the grid only if the following condition is not fulfilled: *(rz2.gt.rulatm .or. rz2 .gt. rzbase(1)).* In version ORM_ABC_1.21 the condition was: *(rz2.gt.(rulatm+rincz))*

3.6 Molecule dependent measurement grid

The current version of the ORM_ABC assumes that all the retrievals of a sequence use the same measurement grid, that is the grid of the tangent altitudes that identifies the spectra used in the retrieval. The retrieval grid of each retrieval (that identifies the tangent altitudes at which the atmospheric quantities are retrieved) is then defined as a user-defined sub-set of the measurement grid. In the case that in a sequence a retrieval uses a measurement grid different from the one used by previous retrievals, the program stops.
The new microwindows provided by the Oxford team have been defined only in the altitude range corresponding to the retrieval range of the considered molecule. This means that for each molecule the measurement grid coincides with the retrieval grid. Since different molecules are characterised by different retrieval ranges, we have a molecule dependent measurement grid and the approach used in the ORM has to be changed accordingly.
The modifications involve the part of the program that writes the retrieved profiles (in the files *dump*****) and interpolates them on the 'base' grid of the subsequent retrievals.
This modification of the ORM_ABC does not affect the Retrieval Component Library of the Level 2 NRT processor.

Code modifications

Module **retr_pt**

The nominal tangent altitudes of the analysed sweeps are written
into the *pt_dump* file

* Writing p,T retrieved values into a dump file:
*

```
      open(34,file=sodir(1:iodl)//'pt_dump.dat',
     &       form='unformatted',status='unknown')
      write(34) ibase
      write(34) imxpro
      write(34) imxgeo
      write(34) ilimb
      write(34) rpbase
      write(34) rtbase
      write(34) rzbase
      write(34) rztang
      write(34) rztanginit
      close (34)
```

Module **retr_vmr**

If the result of the p,T retrieval is to be used (*lifptret* = true) when reading the *pt_dump.dat* file we read the nominal tangent altitudes of the p,T retrieval too.
If the current VMR retrieval is not performed on the same number of sweep of the p,T retrieval, the nominal tangent altitudes of the current retrieval are compared with the nominal tangent altitudes of the p,T retrieval and corrected when they coincides.
The new initial guess profiles are calculated on the altitude grid of the p,T base profiles and the *rzprof, rpprof, rtprof,rvmrprof* are updated.

If the VMR profiles retrieved previously are to be used (*lifvmret*= true) we read the altitude grid of each profile (*rzbase_prv*) then a check is made to see if they were retrieved on a different altitude grid than the one contained in *rzprof*.
If this is the case, the retrieved profiles are recalculated on the grid of *rzprof*. If the grid in *rzprof* spans altitudes that are all within the limit of the retrieval grid, then a linear interpolation is used to recalculate the VMRs.
If some of the altitudes of the *rzprof* grid are outside this limits, we scale the initial guess profile according to the ratio between the retrieved VMR at the last altitude and the corresponding value in the initial guess profile.

In the dump file we added the instruction to write the *rzbase* vector

4. Unconsolidated issues and possible commissioning-phase modifications

The test of the ORM on real data (analysis of MIPAS-B balloon measurements) has pointed out possible problems in the retrieval. Below possible modifications to be implemented in the code after the tests performed during the commissioning phase are listed for future memory.

- **Dependence of P,T retrieval on H_2O profile.**

  Provision for iterations between the two retrievals.

- **Robustness of retrieval.**

  Physical cut-off (rather than a mathematical cut-off) for eigenvalues in the inversion of the VCM of the retrieved parameters ($\mathbf{K}^T\mathbf{S}^{-1}\mathbf{K}$). (Issue relevant for the continuum retrieval, it may imply also a change in the definition of the unknowns).

- **Interpolation of the spectrum as a function of altitude (for FOV convolution).**

  Polynomial interpolation is now used for optimum speed-accuracy compromise.

  Problem are encountered when the FOV spans large altitude ranges with steep emission gradients and when a step is present in the distribution (this always occurs in the Jacobian). A step back to linear interpolation may provide more stable results, even if more demanding from the computing time point of view.

5. Summary table of ORM modifications affecting Retrieval Component Library

#	Description of change	Affected/new ORM modules	Modified interface?	List of modified I/O files	Modified TEPs
1	Calculation of the VCM of the observations in the case of reduced spectral resolution	Retr_(pt/vmr) Sinvcal_mw_(pt/vmr) Svdcmp_(pt/vmr)	N Y	-	-
2	Definition of the lowest level of the base grid	Retr_(pt/vmr) Chbase_(pt/vmr)	N Y	-	-
3	Modification in the calculation of continuum derivatives	Retr_(pt/vmr) Chbase_(pt/vmr) Tcgeo_pt Gcgeo_vmr Fwdmdl_(pt/vmr) Mkplev_(pt/vmr) Conlay_(pt/vmr) Jacsetmw_(pt/vmr) Spectrum_(pt/vmr) Updprof_pt	N Y Y Y Y Y Y Y Y Y	-	-
4	Band dependent FOV	Finput_(pt/vmr) Retr_(pt/vmr) Fwdmdl_(pt/vmr) Fov_(pt/vmr)	N N Y Y	Settings_pt.dat Settings_h2o.dat Settings_o3.dat Settings_hno3.dat Settings_ch4.dat Settings_n2o.dat Settings_no2.dat	-
5	Maximum altitude used in the 'mod' grid	Mkplev_(pt/vmr)	N	-	-