Technical Note on:

ORM for Commissioning Phase

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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"

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

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CONTENTS

1. Reference documents

[RD1] TN-IROE-GS0104, Draft
Title: Description of Statistical Tool

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

[RD3] TN-IROE-GS0102**,** Issue: 1 - Revision: 1
Title: Pre-flight modifications to the ORM_ABC code

[RD4] TN-IROE-GS0101, Issue: 1 - Revision: A
Title: Level 2 Algorithm Characterization & Validation Plan

[RD5] TN-UNIBO, Issue: - Revision: Update
Title: Results of WP 8300 and WP 8500

[RD6] PO-MA-DOG-GS-0001, Issue: 2 - Revision: A
Title: ML2PP Software User Manual

[RD7] Draft:
Title: 'New functionalities implemented in ORM_ABC_1.2.3' ,
M. Ridolfi (16 November 2001)

[RD8] Title: 'MIPAS-B Retrieval residuals analysis', V. Jay and A. Dudhia
(23 Jan. 01)

2. Introduction

In the frame of ESA contract 11717/95/NL/CN an Optimized forward /retrieval Model (ORM) was 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 [RD2], [RD3] and [RD6]) is the scientific reference for the Retrieval Component Library of MIPAS Level 2 NRT processor.
So far, in absence of MIPAS measurements, this code has been validated only on the basis of simulations and, whenever possible, on the basis of available measurements acquired by instruments similar to the ENVISAT version of MIPAS.
When the first MIPAS measurements will be available, the impact of the most critical approximations implemented in the ORM must be adequately characterized.
All the procedures planned for validating ORM during the Commissioning Phase, as well as the requirements of the software tools needed for performing this cal./val. activity, were described in [RD4]. The required software tools consist in both a modificated ORM with added functionalities and a dedicated software tool for the analysis of ORM products (Statistical Tool) [RD1].
Objective of this TN is to describe the new functionalities introduced in ORM with respect to ORM_ABC_1.2.3, the run procedures, the method to switch on/off the different options, and its interfaces with Level 1 products.

3. Definitions

- ORM_ABC (ORM Algorithm Baseline Code) is the scientific reference code for the Retrieval Component Library of MIPAS Level 2 NRT processor.
- ORM_ABC version 1.2.3 is the latest version of ORM_ABC described in[RD2], [RD3] and [RD6]. Its input/output files are organised for performing the analysis of a single scan.
- ORM_SDC (ORM Software Development Code) contains new functionalities for development purpose.
- ORM_SDC version 1.2.3 is the latest version of ORM_SDC developed for validating the ORM during the Commissioning Phase, consisting in ORM_ABC_1.2.3 with some added functionalities. It is described herewith in Sect. 4. Like the program ORM_ABC, its input/output files are organised for performing the analysis of a single scan. The required input files are described in Sect. 5.
- ORM_ORB version 1.0.1 is a program capable of performing the sequential analysis of a given number of sequences of the orbit. The core of this program is ORM_SDC_1.2.3. The structure of this program is described in Sect. 6.

For simplicity, since in the rest of this document only version 1.2.3 of the ORM_ABC and ORM_SDC codes will be mentioned, in the subsequent sections they will be indicated with the acronyms 'ORM_ABC' and 'ORM_SDC' respectively.

4 New functionalities implemented in ORM_SDC

The functionalities introduced in ORM_SDC are listed below:

- Change in the definition of the state vector, i.e. the vector of the parameters to be fitted
- Additional fit of ILS broadening parameter
- Additional fit of frequency scaling parameter
- Additional fit of intensity scaling parameter
- Additional fit of Instrumental offset dependent on both MW and tangent altitude (for a set of user-selected MWs)
- Interface with Statistical Tool
- Interface with REC analysis
- Option for excluding from the analysis a user-selected set of microwindows and/or line of sights.

4.1 Definition of the state vector

In ORM_ABC the definition of the state vector is rather rigid: according to the input variable *ifco*, it is possible to chose among one of the following three sets of fitted parameters:

- atmospheric parameters (either pressure-temperature or VMR profile), atmospheric continuum and offset
- atmospheric parameters (either pressure-temperature or VMR) and atmospheric continuum
- atmospheric parameters (either pressure-temperature or VMR).

In order to increase flexibility in the selection of the parameters to be fitted, and also considering the increased number of quantities to be fitted, ORM_SDC is organised so that any possible combination of parameters can be fitted. To this purpose, a switch is used for each type of variable in the state vector. ORM_SDC is able to fit any combination of the following quantities:

- atmospheric parameters (tangent pressures and temperature profile for pT retrieval and VMR profile for VMR retrievals)
- atmospheric continuum
- either tangent altitude independent offset or tangent altitude dependent offset
- altitude independent, band dependent ILS broadening
- altitude independent, band dependent frequency shift
- altitude independent, band dependent intensity calibration

These parameters can be included in the state vector setting the corresponding switch to .true. .

4.2 Fit of ILS broadening parameter

ILS broadening strongly affects tangent pressure and temperature retrieval, as well as VMR retrievals. The fit of an ILS broadening parameter can identify possible errors in the ILS function provided by Level 1. The switch identifying this fit is LILS.
The width of the ILS function is varied multiplying the ILS, in the interferogram domain, by a rectangular trapezium defined as follows:
trapezium(x)= (1-K) rectangle $_L$ (x) + K triangle $_L$ (x) ,
where:

$$\text{rectangle}_{\,L}\,(x) = \begin{cases} 1 & |x| \le \text{MPD} \\ 0 & |x| \ge \text{MPD} \end{cases}$$

and:

$$\text{triangle}_{\,L}\,(x) = \begin{cases} 1 - x / MPD & |x| \le \text{MPD} \\ 0 & |x| \ge \text{MPD} \end{cases}$$

MPD identify the Maximum Path Difference.

The multiplying factor K, allowed to take values between -1 and 1, represents the ILS broadening parameter. The ILS broadening increases as K increases, a “sharpening” of the ILS occurs when K<0. In the spectral domain the multiplication of the ILS function by the Trapezium function becomes the convolution of the ILS function (in the spectral domain) with the following function:

$$Broad(\sigma) = (1 - K) \cdot \text{MPD} \cdot s\text{inc}\left(2\,\pi\,\sigma\,\text{MPD}\right) + \frac{\text{K} \cdot \text{MPD}}{2} \cdot s\text{inc}^2\left(\pi\,\sigma\,\text{MPD} / 2\right)$$

A different ILS broadening parameter is fitted for each MIPAS spectral band.
When the fit of ILS broadening is active, the AILS relative to each microwindow is obtained by convolving the AILS provided by Level 1 for each microwindow with the function *Broad (σ)*.
Derivatives of the spectrum with respect to the ILS broadening parameter of each band are performed numerically, by convolving the high resolution spectrum once with the broaded AILS function computed as described above, once with a perturbed broaded AILS, obtained as the previous one, but with a perturbed K parameter.
Since the result of convolution of a given finite vector **a** with a finite vector **b** is a vector whose length is (length_**a** - length_**b**), when the fit of ILS broadening is activated an extended AILS function is expected as input of the program (default AILS function length equal to 0.375 cm^{-1}). A control has been inserted in the code to check the length of input AILS function when ILS broadening fit is active.
When ILS broadening is fitted, ORM_SDC must be compiled with the option 'fitils'.

4.3 Fit of frequency scaling parameter

If an imperfect frequency calibration is performed by Level 1, retrieval results are expected to improve if a frequency scaling parameter is fitted. This option is activated by setting the switch LSHIFT to true.
A different frequency shift parameter for each MIPAS spectral band is fitted. A shift in the frequency calibration is applied as a modification of the AILS function of each microwindow. The AILS of each microwindow is obtained by convoluting the AILS provided by Level 1 with a "shifted" sinc function. Th "shifted" sinc function is sampled at the MIPAS nominal resolution (0.025 cm^{-1}), but its zero position is shifted of a frequency interval equal to the product of the central frequency of the microwindow times the frequency shift parameter relative to the band of microwindow itself.
As in the case of the fit of ILS broadening parameter, derivatives of the spectrum with respect to frequency shift parameter of each band are performed numerically and when the fit of frequency shift is activated an extended AILS function is expected as input of the program. A control has been inserted in the code to check the length of input AILS function when the fit of frequency shift is actived.
When frequency shift parameters are fitted, ORM_SDC must be compiled with the option 'fitils'.

4.4 Fit of intensity scaling parameter

Error in the intensity calibration of spectra consists in a scaling factor applied to the spectrum. If the intensity calibration performed by Level 1 is imperfect (in particular different spectral bands are characterised by different intensity calibration errors) the fit of the intensity calibration parameter provides an indication of the errors in the calibration.
This option is activated with the switch LINTCAL.
Two fitting modes are foreseen: either only one parameter per band is fitted, or two parameters per band are fitted, one for the reverse sweeps and one for the forward sweeps. This latter choice is selectable with the switch LONE: if LONE is true, only one parameter per band is fitted, if LONE is FALSE, two parameters per band are fitted.

Tests with simulated observations have confirmed our expectation of strong correlation between the intensity scaling parameter and the VMR profile.

4.5 Fit of altitude dependent instrumental offset

In ORM_ABC the fit of a limb scanning angle independent offset can be performed for each microwindow. In order to increase flexibility in the code the option for fitting an altitude dependent offset has been inserted in ORM_SDC. In the file settings_***.dat two switchs have been added, one for fitting an altitude independent offset (as in ORM_ABC) and one for fitting an altitude dependent offset. Of course these two switchs cannot be activated at the same time. (The code performs a check to avoid this inconsistency).
In the case of the fit of an altitude dependent offset, it is also possible to select the microwindows for which an altitude dependent offset is fitted, for the others (expected to contain not enough information to discriminate between offset and atmospheric continuum) only one offset parameter is fitted for all the altitudes. This selection is made via a logical vector contained in the file settings_***.dat.

4.6 Recursive pT -H2O retrieval in case of unsuccessful pT or H2O retrieval

Tests performed with observations simulated on the whole orbit have shown [RD5] that whenever the input atmospheric model has the tropopause at a "wrong" altitude H2O retrieval is likely not to succeed.
An initial guess for water wrong by some orders of magnitude causes large errors in the p,T retrieval. The water retrieval that follows (in the ORM sequence) suffers for both a poor first guess of the target molecule and for poor inputs from the results of p,T retrieval.
In order to overcome the problem, the flow of operations can be modified so that, after the retrieval of water, the ORM sequence is repeated from the beginning if either p,T or water retrievals have not satisfied the convergence criteria (i.e. either the maximum number of micro-iterations or the maximum number of macro-iterations have been reached). In this case both pT and water retrieved profiles determined at the end of the unsuccessful step are fed as input to the new run.
This option was originally present only in the ORM_ORB program, then it has been implemented also in ORM_ABC code (see [RD7]).
The maximum number of allowed repetitions of pT - h_2o retrievals is given by the user-selected parameter *maxloop* (contained in script *orm_orbit*). If the maximum number of allowed repetitions is reached and pT is not successful, the retrieval of the scan is interrupted, if h_2o is not successful, the dump file containing h2o retrieved profile is cancelled and the other VMR retrievals of the sequence are performed.
Recursive pT-h_2o retrieval is performed in ORM_ORB_1.0.1 program only if the switch *lpt_h2O_recursive* (contained in file settings_pt.f) is true.

4.7 Option for excluding a user-selected set of microwindows and /or lines of sight from the analysis

The set of microwindows used for the retrieval of each specie and the measurement range is defined by the occupation matrix selected for each retrieval.
The possibility of excluding a user-selected set of microwindows and/or lines of sight from the analysis can be very useful during the interpretation of the results, for example it could be useful to repeat the analysis excluding microwindow characterised by very high partial chi-square values or microwindows belonging to a particular band.
In order to avoid the re-generation of the input files for each new test, two logical vectors have been added in the files settings_*.dat, i.e. vectors *lusedmw(imxmw)* and *lusedlos(imxlmb),* where the 'T' values provide the indication of respectively what microwindows and what lines of sight, among the ones contained in the selected occupation matrix, are included in the analysis.
If some 'F' values are contained in either *lusedmw* or *lusedlos*, the compression of all variables dependent on the microwindows and/or lines of sight is performed by the new routine compress_*.f.

4.8 Interface with Statistical Tool

ORM_SDC generates also the input files for the Statistical Tool [RD1], consisting of a different binary file for each analysed scan containing ORM products and house-keeping data.

4.8.1 Data exchanged with Statistical Tool.

The structure of exchanged data file is reported below.
The first Block of data (HEADER) is coded in ASCII character in order to be visible with any text editor. Appended blocks are coded in binary format in order to be compacted. Those data are divided in:

- *General Information, containing data referred to the sequence and to the initial guess;*
- *Data referred to p,T retrieval*
- *General Data*
- *Spectral Data*
- *Retrieval Data*
- *Variance – Covariance Matrix Data*
- *Data referred to VMR retrievals*
- *General Data*
- *Spectral Data*
- *Retrieval Data*
- *Variance – Covariance Matrix Data*
- *Control of End of File*

HEADER visible data concerning identification pointers

Format	*Type*	*	*Size [Bytes]*	*Name*	*Description*
ASCII	Character	1	80	Title	Data file presentation
ASCII	Character	1	80	Subtitle	Info and Pointer to documentation
ASCII	Character	1	10	Cnserie	Serial number
ASCII	Character	1	80	DataSource	Source of measurement
ASCII	Character	1	40	Code	Name ad version of retrieval code
ASCII	Character	1	40	Host	HostType – environmental variable
ASCII	Character	1	40	AcqTime	Date and Hour of retrieval
ASCII	Character	1	40	SunE	Sun Elevation

GENERAL INFORMATION referred to scan and ORM initial guess

Format	*Type*	*	*Size [Bytes]*	*Name*	*Description*
BIN	Integer	4	1	hit_code	Hitran Code: Retrieval Identifier
BIN	Integer	4	1	Ilimb	Number of lines of sight used
BIN	Real	4	1	Rlat	Average latitude related to the scan
BIN	Real	4	1	Rlong	Average longitude related to the scan
BIN	Real	4	Ilimb	Rztanginit	Initial values for tangent altitude
BIN	Real	4	Ilimb	Rztang	Corrected values of tangent altitude
BIN	Real	4	Ilimb*ilimb	Rvchcorr	Tangent altitude corrections
BIN	Real	4	Ilimb*ilimb	Rinvclos	
BIN	Integer	4	1	Ilimb	Control Flag
BIN	Integer	4	1	Ipro	Number of points for initial guess profile
BIN	Integer	4	1	Igas	Number of initial guess profiles
BIN	Real	4	Ipro	Rzprof	Tangent altitude profile of initial guess
BIN	Real	4	Ipro	Rtprof	Temperature profile of initial guess
BIN	Real	4	Ipro	Rpprof	Pressure profile of initial guess
BIN	Real	4	Ipro*igas	Rvmrprof	Gas Profiles of initial guess
BIN	Integer	4	1	Ipro	Control Flag

DATA BLOCKS – FOR p,T RETRIEVAL

GENERAL DATA referred to result of ORM Procedure

Format	*Type*	*	*Size [Bytes]*	*Name*	*Description*
BIN	Integer	4	1	Ibase	Number of points for calculated profile
BIN	Real	4	ibase	Rzbase	Calculated Tangent altitude profile
BIN	Real	4	ibase	Iparbase	Points used for retrieval
BIN	Real	4	ibase	Rtbase	Calculated Temperature profile
BIN	Integer	4	ibase	Rpbase	Calculated Pressure profile
BIN	Integer	4	1	Iconverg	Retrieval convergence
BIN	Integer	4	1	Ipt	Switch for fitting pT profile
BIN	Integer	4	1	Iatmcont	Switch for fitting atm. Continuum
BIN	Integer	4	1	Ioffsetconst	Switch for fitting constant zero-level calibration
BIN	Integer	4	1	Ioffsetad	Switch for fitting altitude dependent zero-level calibration
BIN	Integer	4	1	Iils	Switch for fitting ILS width
BIN	Integer	4	1	Ishift	Switch for fitting frequency shift
BIN	Integer	4	1	Iintcal	Switch for fitting intensity calibration parameters
BIN	Integer	4	1	Ione	Switch for fitting only 1 intensity calibration parameters
BIN	Integer	4	1	Iorm_again	
BIN	Real	4	5	ralpha	
BIN	Real	4	5	kappa	Frequency shift
BIN	Real	4	5*2	rintcal	Intensity calibration
BIN	Integer	4	1	Nselmw	Number of selected MicroWindows

SPECTRAL DATA referred to Occupation Matrix

Format	*Type*	*	*Size [Bytes]*	*Name*	*Description*
BIN	Integer	4	1	j	Index of line of sight
BIN	Integer	4	1	i	Index of MicroWindow
BIN	Character	1	12	Smw	MicroWindow code
BIN	Integer	4	1	Ifspmw	Index related to frequency start point of the selected MicroWindow
BIN	Real	4	1	Rchisqp	Square χ for selected MicroWindow
BIN	Real	4	1	Rnoise	Indicator of Noise related to
BIN	Integer	4	1	Nsam	Number of samples in selected MicroWindow
BIN	Real	4	Nsam	Robs	Values of observed data
BIN	Real	4	Nsam	Rspfov	Values of calculated data
BIN	Integer	4	Nsam	Imask	Points used for retrieval

Format	*Type*	*	*Size [Bytes]*	*Name*	*Description*
BIN	Real	4	Nelmw*ibase	Rcbase	Retrieved Continuum
BIN	Integer	4	Nelmw	ioffsetadmw	Switch for fitting offset altitude dependent
BIN	Real	4	Nelmw*ilimb	Roffs	Offset
BIN	Integer	4	ilimb	iusedlos	Switch for used LOS

BIN	Integer	4	nselmw	Iusedmw	Switch for used MW
BIN	Integer	4	1	Nselmw	Control Flag

RETRIEVAL DATA referred to ORM procedure

Format	*Type*	*	*Size [Bytes]*	*Name*	*Description*
BIN	Integer	4	1	Ntot_it	Number of total iteration
BIN	Real	4	1	Rchisq_0	Initial Chi Square
BIN	Integer	4	Ntot_it	indx_g	Index of Gauss Iteration
BIN	Integer	4	Ntot_it	indx_m	Index of micro iteration
BIN	Real	4	Ntot_it	rtime_it	Iteration time
BIN	Real	4	Ntot_it	rlambda_it	Marquardt indicator
BIN	Real	4	Ntot_it	rchisq_it	Square χ of iteration
BIN	Real	4	Ntot_it	rmaxp_it	Maximum variation of parameter used for p
BIN	Real	4	Ntot_it	rmaxt_it	Maximum variation of parameter used for T
BIN	Integer	4	1	Ntot_it	Control Flag

VARIANCE – COVARIANCE MATRIX DATA referred to ORM procedure

Format	*Type*	*	*Size [Bytes]*	*Name*	*Description*
BIN	Integer	4	1	Itop	Rank of Variance-Covariance Matrix
BIN	Integer	4	1	Icontpar	Number of contiuum parameters
BIN	Real	4	itop*itop	Rainv	Elements of
BIN	Real	4	Itop	Rw	Elements of
BIN	Integer	4	1	Itop	Control Flag

DATA BLOCKS – FOR VMR RETIREVAL

GENERAL DATA referred to result of ORM Procedure

Format	*Type*	*	*Size [Bytes]*	*Name*	*Description*
BIN	Integer	4	1	hit_code	Hitran Code: Retrieval Identifier
BIN	Integer	4	1	Ilimb	Number of lines of sight used
BIN	Integer	4	1	ipro	Number of points for initial guess profile
BIN	Real	4	Ilimb	Rztang	Corrected values of tangent altitude
BIN	Integer	4	1	Ilimb	Control flag
BIN	Integer	4	1	ipro	Number of points for initial guess profile
BIN	Real	4	Ipro	Rzprof	Tangent altitude profile of initial guess
BIN	Real	4	Ipro	Rvmrprof	profile of initial guess
BIN	Integer	4	1	ipro	Control flag
BIN	Integer	4	1	Ibase	Number of points for calculated profile
BIN	Real	4	ibase	Rzbase4	Calculated Tangent altitude profile
BIN	Real	4	ibase	Iparbase	Points used for retrieval
BIN	Integer	4	ibase	Rvmrbase4	Calculated VMR profile
BIN	Integer	4	1	Iifptret	Identifier related to the use of initial guess
BIN	Integer	4	1	Iifvmret	Identifier related to the use of initial guess

BIN	Integer	4	1	Ibase	Control Flag
BIN	Integer	4	1	Iconverg	Retrieval convergence
BIN	Integer	4	1	Ipt	Switch for fitting pT profile
BIN	Integer	4	1	Iatmcont	Switch for fitting atm. Continuum
BIN	Integer	4	1	Ioffsetconst	Switch for fitting constant zero-level calibration
BIN	Integer	4	1	Ioffsetad	Switch for fitting altitude dependent zero-level calibration
BIN	Integer	4	1	Iils	Switch for fitting ILS width
BIN	Integer	4	1	Ishift	Switch for fitting frequency shift
BIN	Integer	4	1	Iintcal	Switch for fitting intensity calibration parameters
BIN	Integer	4	1	Ione	Switch for fitting only 1 intensity calibration parameters
BIN	Integer	4	1	Iorm_again	
BIN	Real	4	5	ralpha	
BIN	Real	4	5	kappa	Frequency shift
BIN	Real	4	5*2	rintcal	Intensity calibration
BIN	Integer	4	1	Nselmw	Number of selected MicroWindows

SPECTRAL DATA referred to Occupation Matrix

Format	*Type*	*	*Size [Bytes]*	*Name*	*Description*
BIN	Integer	4	1	j	Index of line of sight
BIN	Integer	4	1	i	Index of MicroWindow
BIN	Character	1	12	Smw	MicroWindow code
BIN	Integer	4	1	Ifspmw	Index related to frequency start point of the selected MicroWindow
BIN	Real	4	1	Rchisqp	Square χ for selected MicroWindow
BIN	Real	4	1	Rnoise	NESR
BIN	Integer	4	1	Nsam	Number of samples in selected MicroWindow
BIN	Real	4	Nsam	Robs	Values of observed data
BIN	Real	4	Nsam	Rspfov	Values of calculated data
BIN	Integer	4	nsam	Imask	Points used for retrieval
BIN	Real	4	1	Rcbase	Retrieved Continuum

Format	*Type*	*	*Size [Bytes]*	*Name*	*Description*
BIN	Real	4	Nelmw*ibase	Rcbase	Retrieved Continuum
BIN	Integer	4	Nelmw	ioffsetadmw	Switch for fitting offset altitude dependent
BIN	Real	4	Nelmw*ilimb	Roffs	Offset
BIN	Integer	4	ilimb	iusedlos	Switch for used LOS
BIN	Integer	4	nselmw	Iusedmw	Switch for used MW
BIN	Integer	4	1	Nselmw	Control Flag

RETRIEVAL DATA referred to ORM procedure

Format	*Type*	*	*Size [Bytes]*	*Name*	*Description*
BIN	Integer	4	1	Ntot_it	Number of total iteration
BIN	Real	4	1	Rchisq_0	Initial Chi Square
BIN	Integer	4	ntot_it	indx_g	Index of Gauss Iteration

BIN	Integer	4	ntot_it	indx_m	Index of micro iteration
BIN	Rela	4	ntot_it	rtime_it	Iteration time
BIN	Real	4	ntot_it	rlambda_it	Marquardt indicator
BIN	Real	4	ntot_it	rchisq_it	Square χ of iteration
BIN	Real	4	1	rmax_it	Maximum variation of parameter used for VMR
BIN	Integer	4	1	Ntot_it	Control Flag

VARIANCE – COVARIANCE MATRIX DATA referred to ORM procedure

Format	*Type*	*	*Size [Bytes]*	*Name*	*Description*
BIN	Integer	4	1	Itop	Rank of Variance-Covariance Matrix
BIN	Integer	4	1	Icontpar	Number of continuum parameters
BIN	Real	4	itop*itop	Rainv	Elements of
BIN	Real	4	Itop	Rw	Elements of
BIN	Integer	4	1	Itop	Control Flag

END OF FILE CONTROL

BIN	Integer	4	1	CloseCode	Control Flag – End of File

4.9 Interface with REC analysis

Residual and Error Correlation (REC) analysis [RD8] will analyse the residuals and compare them with the error spectra computed on the basis of pre-estimated systematic errors assumed to affect either measurements or analysis made by ORM. The REC analysis will be performed by the Oxford team using the files provided by the program ORM_ORB.
For each scan, ORM_SDC generates a file named *res_$number_of_scan.dat*, containing the residuals.

5 Input files for ORM_SDC

ORM_SDC runs using all and only the input files of ORM_ABC and only the files settings_***.dat have been modified.

Modifications introduced in files settings_*.dat:

Modifications in file settings_pt.dat:

- Added switch at the beginning for enabling the recursive pT - H2O retrieval in case of unsuccessful pT or H2O retrievals.

```
lpt_h2o_recursive = switch for performing pt+H2O retrieval recursively
                    in case that either pt or h2o retrievals are not successful
                    ('not successful' means that either the maximum number of
                            micro iterations or the maximum number of macro-iterations
                    are reached)
#
T
```

Modifications in all files settings_*.dat:

- Field containing variable *ifco* is not active any longer.
- Fields have been added containing switches for activating the fit of additional parameters (specie independent):

fit of tangent pressures and temperature profile (in file settings_pt.dat) : LPT
fit of VMR profile (in all settings_***.dat except settings_pt.dat) : LVMR
fit of atmospheric continuum : LATMCONT
fit of altitude independent zero-level calibration : LOFFSETCONST
fit of altitude dependent zero-level calibration : LOFFSETAD
fit of ILS broadening parameter: LILS
fit of frequency shift : LSHIFT
fit of intensity calibration : LINTCAL

If intensity calibration is fitted, it is possible to fit either one intensity parameter per band (if switch LONE is true), or two intensity calibration parameters for band, one for forward sweeps and one for reverse sweeps (if LONE is false)

(The new fields described above are independent on the specie and are contained in file *sw2,* see Sect. 7).

- Fields have been added containing the following logical vectors/settings that are specie dependent:
  - l*offsetadmw(imxmw)*: if altitude dependent zero-level calibration is fitted, this vector indicates for what microwindows an altitude dependent zero-level calibration is fitted, for the other microwindows a constant zero-level calibration is fitted
  - l*usedmw(imxmw)*: the true values of this vector indicate what microwindows, among the ones contained in the occupation matrix, are included in the analysis
  - l*usedlos(imxlmb)*: the true values of this vector indicate what lines of sight, among the ones contained in the occupation matrix, are included in the analysis
  - *dfact_cont*: factor multiplying continuum profiles in order to handle quantities in the state vector of comparable magnitudes

Old settings_*.dat files:

```
……..
Switch for fitting atmospheric continuum and offset (ifco):
    ifco = 2 -->   p,T, continuum and offset are fitted
    ifco = 1 -->   p,T and continuum are fitted
    ifco = 0 -->   only p,T are fitted
#
  2
……..
```

New settings_***.dat file

```
Switch for fitting pressure and temperature profile or VMR profile (lpt or lvmr)
#
  T

Switch for fitting atmospheric continuum (latmcont)
#
  T

Switch for fitting constant zero-level calibration (loffsetconst)
#
  T

Switch for fitting altitude dependent  zero-level calibration (loffsetad)
#
```

```
  F

Switch for fitting ILS width (lils)
#
  F

Switch for fitting frequency shift (lshift)
#
  F

Switch for fitting intensity calibration parameter (lintcal)
#
  F

Switch for fitting only 1 intensity calibration parameter (lone)
if (lone=F) two intensity calibration parameters are fitted for each band,
one for forward sweeps and one for reverse sweeps

#
  T

+
```

Specie dependent switches/settings:

```
Logical vector indicating for what microwindows an altitude dependent
zero-level calibration is fitted (for the mws with F value, a constant offset
is fitted).
This vector (named loffsetadmw(imxmw)) is used only if switch loffsetad=.T.

#
 T T F F F T F F F F F F F F F F F F F

Logical vector indicating the microwindows that have to be included
in the analysis  (lusedmw)
#
 T T T T T T T T T T T T T T T T T T T T T

Logical vector indicating the line of sights that have to be included
in the analysis (lusedlos)
 #
 T T T T T T T T T T T T T T T T T T T T T T T

Factor multiplying continuum profiles
#
1.d30
```

6 General Structure of ORM_ORB_1.0.1 and description of ORM_ORB run procedure

The program ORM_ORB_V1.0.1 performs the sequential analysis of a given number of sequences of the orbit. The core of this program is ORM_SDC, that performs the analysis of a single sequence. The interface with Level 1 products is provided by ML2PP [RD6], that, together with Level 2 products, provides also ORM_ABC dedicated input files relative to the different analysed

sequences. The files settings_*.dat as required by ORM_SDC (see Sect. 5) are modified automatically when running the program.

The scheme of the directories of the program ORM_ORB_1.0.1 is reported below:

ORM_ORB_1.0.1

- **ORM_SDC_1.2.3/** — containing source, object, executable files and makefile of the ORM_SDC program
- **ORM_SDC_1.2.3_IODIR/**
  - **0/** — containing input/output files of the first analysed scan
    - **INP_FILES/**
    - **OUT_FILES/**
  - **1/** — containing input/output files of the second analysed scan
    - **INP_FILES/**
    - **OUT_FILES/**
- **ORM_out/**
  - **$serial_number_1/**
    - **LOG/** `logfile_*, serial_number_1, ml2pp.rdf (1)`
    - **ST_out/** `input for ST`
  - **$serial_number_2/**
    - **LOG/**
    - **ST_out/**
- **REC/** — containing the input files for REC analysis

The directory ORM_ORB_1.0.1 contains the following files:
orm_inp_ex
orm_orbit
orm_seq_ex
settings.dat
start.f
sw1
sw2
sw3_pt
sw3_h2o
sw3_o3
sw3_hno3
sw3_ch4
sw3_n2o
sw3_no2
def_new_settings.f
new_settings_pt.dat
new_settings_h2o.dat
new_settings_o3.dat

new_settings_hno3.dat
new_settings_ch4.dat
new_settings_n2o.dat
new_settings_no2.dat

The script *orm_orbit* starts the sequential analysis of a given number of scans inside the orbit after the definition of the environmental variables and other variables characteristic of the whole set of scans in consideration.
It calls the program *start.f* , containing the do-loop on the sequences to be analysed (the information on the first and the last index of the scan to be analysed is contained in the file *scans.dat*). For each scan the script *orm_seq_ex* prepares the input files and runs ORM_SDC.

Before the retrieval of each specie ('specie') the script *orm_inp_ex* is called by routines *retr_pt.F* and *retr_vmr.F* in order to change the name of the files containing the first guess profiles, namely 'in_alt_'specie'.dat' , 'in_pres_'specie'.dat', 'in_temp_'specie'.dat', 'in_vmr_prof_'specie'.dat' are renamed 'in_alt.dat' , 'in_pres.dat', 'in_temp.dat', 'in_vmr_prof.dat' respectively.

The files *sw1*, *sw2 and sw3_'specie'* contain the additional switches to be included in the file settings_*.dat (see Sect. 5) and are used by the script *orm_seq_ex* that modifies automatically the files settings_*.dat.
Different retrieval options (fit of different quantities, pT-h2o recursive retrieval, use of retrieved profiles, see Sect. 4) can be selected in the retrieval by modifying files *sw1* and /or *sw2 and /or sw3_'specie'*.

The directory **ORM_out**/ collects all the ORM outputs we want to store for the different runs. Each run is characterised by a serial number selectable by keyboard at the beginning of the run. The outputs of each run will be stored under a directory whose name is the serial number in:
- directory LOG, containing:
  - _ logfile_* for all the sequences,
  - _ file named as the serial number containing the list of the setting parameters used for the actual run
  - _ the file *.rdf, generated by ML2PP, containing the list of ML2PP input files
- directory ST_out, containing the input files for ST.

6.1 Procedure for modifying some setting parameters.

If some of the items contained in the files *settings_specie.dat* have to be changed for all the scans, it is necessary to set to 1 the environmental variable SET in the script *orm_orbit* and then to modify the files *new_settings_specie.dat* according to the description below. The structure of the file *new_settings_specie.dat* is the same as the file *settings_specie.dat* generated by ML2PP (i.e. each field is preceded by a '#'). The only difference is that after each '#' there is an additional item that can be either 0 or 1. If, for a particular field the variable after '#' is equal to 1, it means that the final *settings_specie.dat* will use, for this field, the values written in the file *new_settings_specie.dat*, if it is different of 1 it means that the final *settings_specie.dat* will use, for this field, the values contained in the file *settings_specie.dat* generated by ML2PP (i.e. this field will not be changed). As a consequence, in order to change the values of some of the fields in the file *settings_specie.dat* it is necessary to set in the file *new_settings_specie.dat* the value after the proper '#' to 1 and modify the other values of the field before the subsequent '#' , play attention to the format of the different items.
The program *def_new_settings.f* (called by the script *orm_seq_ex* if the variable SET is equal to 1) will read both the file *settings_specie.dat* generated by ML2PP and the file *new_settings_specie.dat*

and will generate a new setting file where the items of each field is taken either from the file *new_settings_specie.dat* (if the variable after '#' is equal to 1) or from the file *settings_specie.dat* (if the variable after '#' is different of 1).

6.2 Procedure for running the program

The operations to be performed for running ORM_ORB_1.0.1 program are described below:

1. go in directory ORM_ORB_1.0.1

2. modify the script *orm_orbit* as follows:
   _ define enviromental variable *home_dir* with the complete path of the directory under which ORM_ORB_1.0.1 is located
   _ define enviromental variable *ORM_auxiliary* with the complete path of the directory containing auxiliary data
   _ define enviromental variable *ORM_ML2PP* with the complete path of the directory containing files generated by ML2PP
3. modify, if necessary, files *sw1, sw2, sw3_specie*
4. modify, if necessary, files *new_settings_specie.dat*
5. run *orm_orbit*

The operator is asked to digit first the name of the person performing the test (maximum 6 digits) and then a number of 3 digits (number identifying the test). These two fields will be merged to form the serial number of the performed retrieval of the orbit and will be associated to each graph generated by the Statistical Tool. ORM_SDC will also produce a file with the name equal to the serial number containing information on the inputs used by ORM_ORB_1.0.1 for the performed retrieval.

When the fit of ILS broadening parameter and/or frequency shift parameter is performed, ORM_SDC requires input ails functions defined on a extended grid (see Sect. 4.2 and Sect. 4.3). In order to modify the AILS functions width the following modifications have to be performed in MIP_PS2_AX file used by ML2PP:
1. setting of variable: 'Requested spectral width of AILS [cm^{-1}] to 1.35
2. disabling LUT usage

It is also necessary to exclude from the microwindows database the gases whose Hitran code is greater than 36, i.e. the gases for which only cross-sections are provided.