Technical Note on

Results of WP8300 and WP8500

Draft
29 June, 2001

Delivery of WPs 8300 and 8500 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

Prepared by:

Name	Institute
M. Carlotti	University of Bologna
L. Magnani	University of Bologna

WP8300

1. Objectives

The activity connected with WP8300 is finalized to provide performance predictions and definition of initial in-flight auxiliary data for MIPAS retrieval analyses. Some steps required within WP8300 have been used also to check the decoding procedure that will be applied to level-1b MIPAS spectra as they will be provided in the ESA distribution format.

The core of this WP was based on blind tests in which the Optimized Retrieval Model (ORM) was used to operate retrieval analyses on MIPAS observations that were simulated for four different atmospheric scenarios. In simulating these observations the Reference Forward Model (RFM) introduced a few physical effects that are not modeled by the forward model built in the ORM system. These effects are expected to act as a source of systematic errors whose impact will be evaluated comparing the altitude profiles that have been retrieved, with the reference profiles (unknown to the operator of ORM) that were used to produce the simulated observations.

A further objective of this WP was to determine optimal values for the setup parameters that control the evolution of the retrieval.

2. Inputs

The following inputs were used for this WP, all coming from activities carried out in previous WPs:

1. Occupation Matrices (OM) for all target quantities supplied with cross-section Look-Up-Tables and Irregular Grid definitions
2. A database of altitude profiles to be used as initial guess (IG) for the target quantities and to model spectral features of molecular species contaminating the analyzed observations.
3. Broad-band MIPAS calibrated spectra simulated for four atmospheric scenarios corresponding to:
   - Mid-latitude day (denoted as Day)
   - Polar winter (denoted as Win)
   - Polar winter with presence of thin PSC (denoted as PSC1)
   - Polar winter with presence of thick PSC (denoted as PSC2)

3. Preliminary data processing

Broad-band spectra corresponding to the four atmospheric scenarios were downloaded from the ESA ftp site in the standard L1B format. Two processing steps were applied to these data in order to translate them in ASCII files that can be handled by our ORM interface-software. The steps are:

- Export L1B spectra to HDF-product file using the ENVIVIEW (12 October 2000 release) version for Windows.
- Translate HDF file into ASCII file using the JHV Java HDF viewer.

An ORM interface-software system has been written on purpose in order to:

- Apodize broad band spectra using the “Norton-Beer strong” apodisation function.
- Extract from broad-band spectra the spectral intervals that correspond to the MicroWindows (MW) defined in the OM files.
- Calculate the Apodized Instrument Line Shape (AILS) function corresponding to the central frequency of each MW. The “comp_ils” tool provided by ESA has been used for this purpose.
- Merge all input data needed in the *ORM input file of the observations* and write the observ_xx files in the ORM format.

Another software tool has been written to sort a desired atmospheric model from the database of altitude profiles (see Sect.2) and to write the corresponding input files in the ORM format.

4. Evaluation criteria

A set of “qualifiers” was identified that characterize the performance of a retrieval. They are needed to evaluate the quality of a retrieval in the process leading to determine the value of setup parameters (“settings” file of ORM) that provide the best performance of the analyses. These qualifiers are:

- value of χ-test at convergence and its evolution in the iterative process.
- number of macro iterations.
- number of (Marquardt) micro iterations.
- percent value of the Estimated Standard Deviation (ESD) of the retrieved quantities.
- altitude oscillation of the retrieved profile.

5. Tuning of setup parameters

At the time when the ORM system was developed, setup parameters were optimized by means of retrievals on MIPAS observations that were simulated by a forward model identical to the one built in the ORM algorithm. Within WP8300 a further tuning of these parameters was operated exploiting the availability of simulated observations that are more realistic because are generated by a different forward model (RFM) and contain the effect of systematic error sources. In this tuning process, particular attention has been given to the parameters that control:

- layering of the atmosphere
- convergence criteria
- Marquardt parameter λ

Tuning of setup parameters was first operated on the “mid-latitude day” atmospheric scenario. Different values were tested for some parameters when operating on the other three scenarios, however it resulted that the optimal set of parameters determined for the Day is also valid for the other scenarios. The exception is the convergence criterion on “maximum allowed relative difference between linear and real chi-square” that has a different value in the PSC2 scenario [see parameter rconvc(1) in appendix A].

Appendix A reports the full set of setup parameters that has been adopted for p,T retrievals (“settings_pt.dat” *ORM input file*). For the retrieval of the Volume Mixing Ratio (VMR) of the target species the same setup parameters have been adopted as for p,T retrievals apart from the parameters controlling convergence criteria. The adopted values of these parameters are reported in appendix B for each molecular species. In general, we can say that no major changes were introduced to setup parameters after this tuning exercise.

Tests with different values of the λ Marquardt parameter have shown that, in some cases, higher values of this parameter provide better performance of the retrieval. However, considering that λ acts as a constraint that limits the corrections to the initial guess profile, what we have observed could be due to the occasional vicinity of the initial guess with the true profile. For this reason we decided to adopt for λ a value which is safe even in the unfavorable cases.

6. Retrieval results

The atmospheric model relative to the month of October was adopted to feed the retrieval system with initial guess profiles of the target quantities and with the profiles of molecular species contaminating the analyzed observations. For this month the profiles relative to the latitude -45^o were adopted for the analysis of the mid-latitude day scenario while the latitude -75^o was selected for the analysis of the other three scenarios.

Table 1 reports the number of Gauss-Newton iterations and the χ-test value at convergence for all target quantities in the four retrieval scenarios. We notice that convergence was not reached in three retrievals relative to PSC2 scenario and in the HNO_3 retrieval relative to the Day scenario. However, in this last case, the χ-test value and the result of the retrieval (see table 3 and figure 6 below) should be considered satisfactory.

Table 1 - χ-test and number of iterations for all retrievals

	Day		Win		PSC1		PSC2	
	χ-test	N^o iter.	χ-test	N^o iter.	χ-test	N^o iter.	χ-test	N^o iter.
P,T	3.7	9	1.9	10	1.6	3	1.8	7
H_2O	7.3	4	4.8	10	4.6	3	4.7	7
O_3	3.0	1	1.5	1	1.2	2	1.2	10^*
HNO_3	1.5	10^*	1.2	5	1.0	2	1.1	10^*
CH_4	1.5	2	0.9	4	0.6	2	0.5	9
N_2O	3.5	4	1.1	7	0.6	2	0.5	10^*
NO_2	5.1	1	4.6	1	4.5	1	4.5	7

* no convergence after maximum number of allowed iterations

2.1. Day scenario

Figures from 1 to 9 refer to the Day scenario; they show plots of the retrieved quantities, together with their ESDs, and of the profiles used as first guess in the retrieval process. In the case of water these quantities are reported with both linear and log scale. Figures from 10 to 17 provide more details about errors; in these figures, for all target quantities but temperature, is reported (as function of altitude) the percent value of:

1. ESD;
2. p,T propagated error;
3. systematic components as provided by the OM-associated database (not including the p,T propagated error);
4. quadratic summation of components 1, 2, and 3;
5. total error obtained by the quadratic summation of components 1 and 2 with the systematic error quantifiers associated to each MW and combined with a layer-by-layer budget.

In the figure referring to temperature the errors are represented in K; in this case, as well as in the case referring to pressure, error component 2 is (of course) not present on plots.

Tables from 2 to 4 report the numerical values of the retrieved quantities. In these tables only ESDs and total error 4 are reported for each target quantity.

2.2. Other scenarios

Figures from 18 to 26 refer to the Win scenario, figures from 27 to 35 to the PSC1 scenario, and figures from 36 to 43 to the PSC2 scenario. These figures report, for all target species, the same quantities as those reported in figures from 1 to 9 for the Day scenario. In the PSC2 case the quantities relative to water are plotted only with a linear scale (see below for the explanation). Figures detailing individual error components are not reported for these three scenarios. The reason for this choice is that: errors 2 and 3 (see Sect.2.1) are considered invariant with respect to the atmospheric scenario as well as the systematic error quantifiers, associated to each MW, that enter in the computation of error 5.

Tables from 5 to 7 refer to the Win scenario, tables from 8 to 10 to the PSC1 scenario, and tables from 11 to 13 to the PSC2 scenario. These tables report, for all target species, the same quantities as those reported in tables from 2 to 4 for the Day scenario.

The results of the analysis of the PSC2 scenario deserve the following comments. At low altitudes the p,T retrieval provides results that are of lower quality with respect to those of the other three scenarios but still appear usable. In the case of VMR retrievals no meaningful results can be obtained below 24 km. In several cases the singular value decomposition (that is used by ORM for the matrix inversion in the Gauss-Newton formula) determines eigenvalues, relative to VMR at low altitudes, that are equal to zero. When this happen the table relative to PSC2-results reports the symbol: – in the corresponding entry. For this reason the figures that represent the VMR results for the PSC2 scenario do not extend below 24 km.

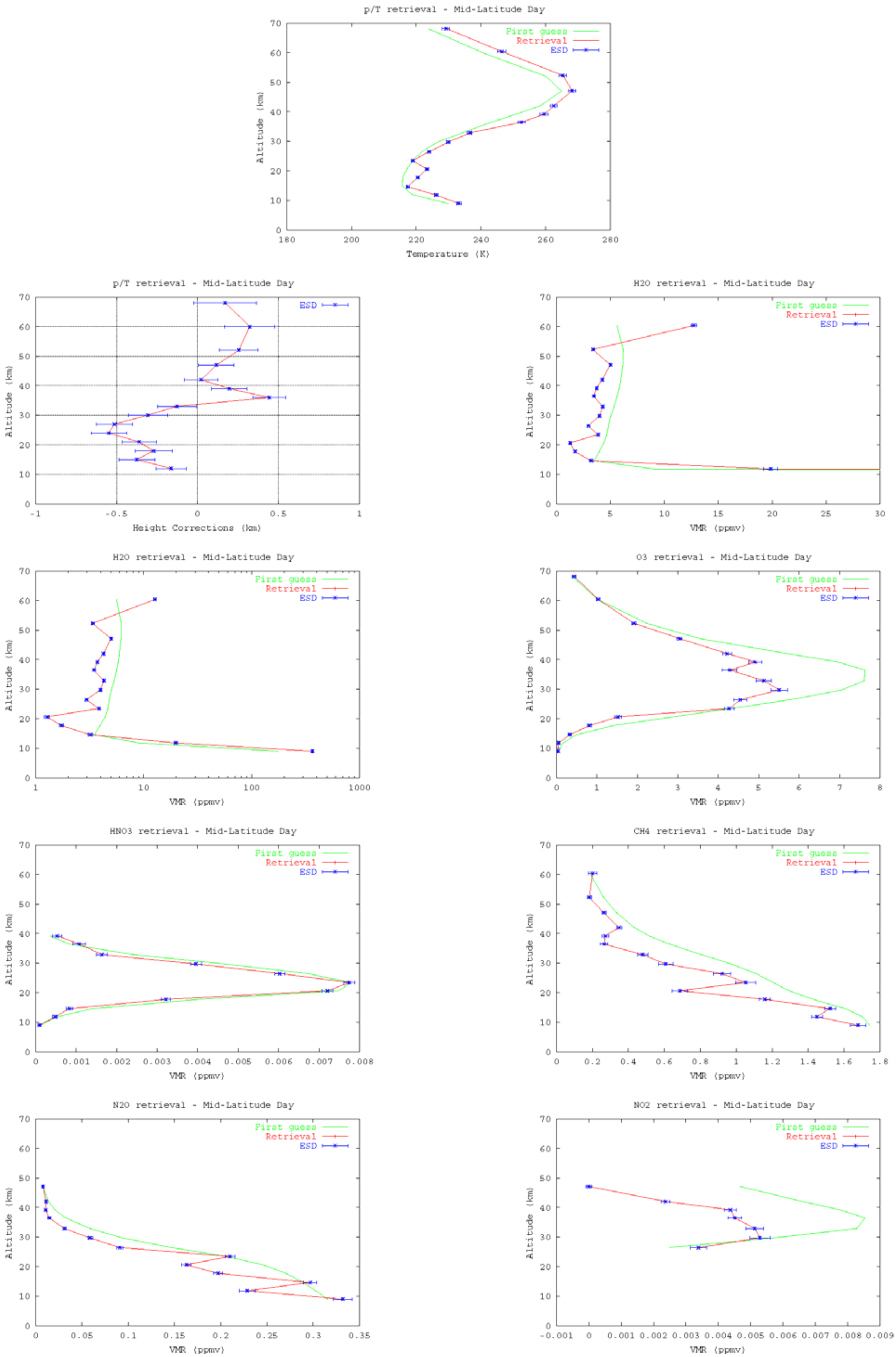

Figure from 1 to 9: plots that report the first guess profile (green curve) and the retrieved quantities (red curve), together with their total errors (blue lines), for the Day scenario.

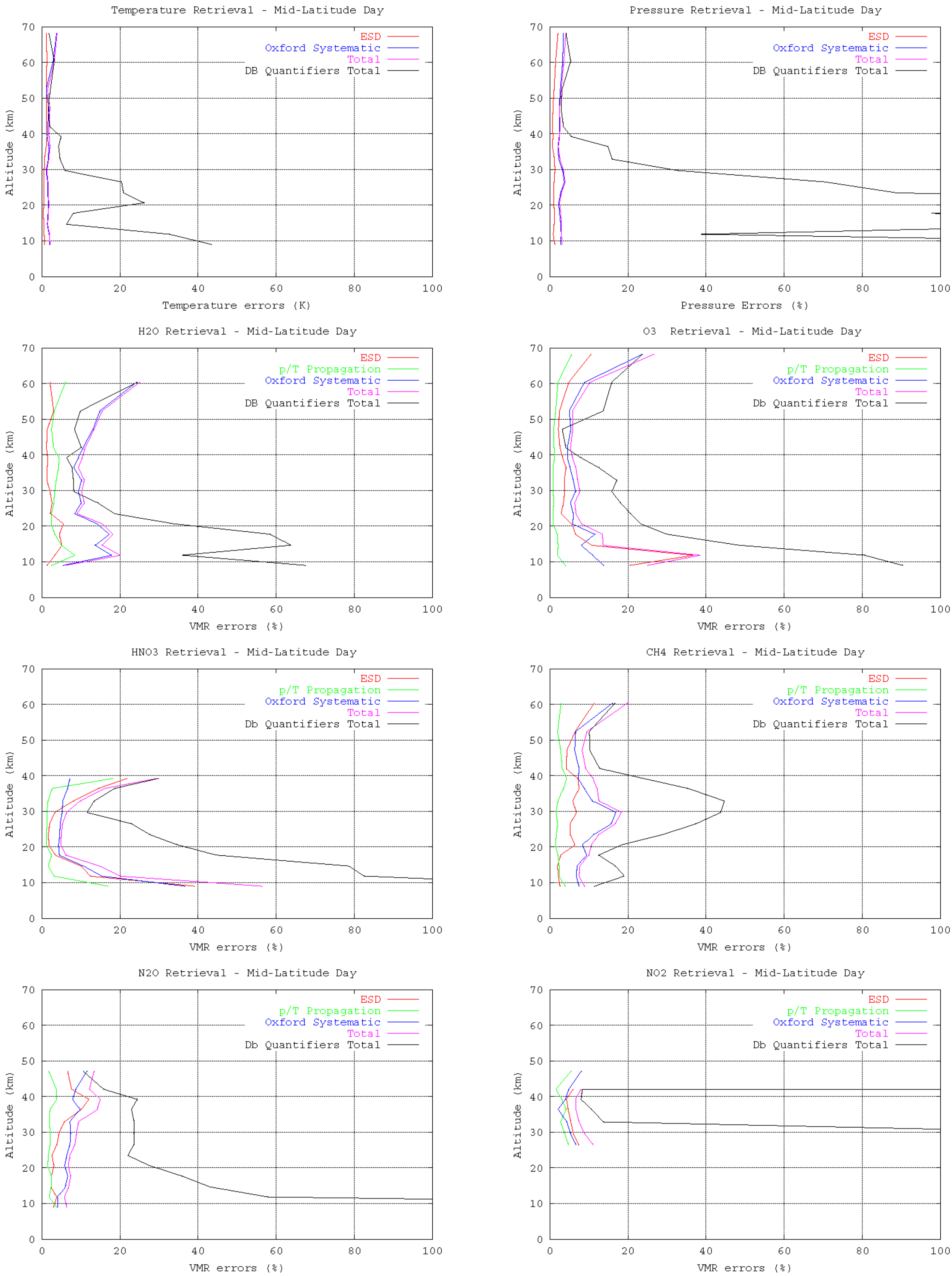

Figure from 10 to 17: plots reporting the ESD (red curve), the p,T propagated error (green curve), the systematic components (blue curve), the total error (purple curve) and the total error obtained using the systematic error quantifiers associated to each MW (black curve), for the Day scenario.

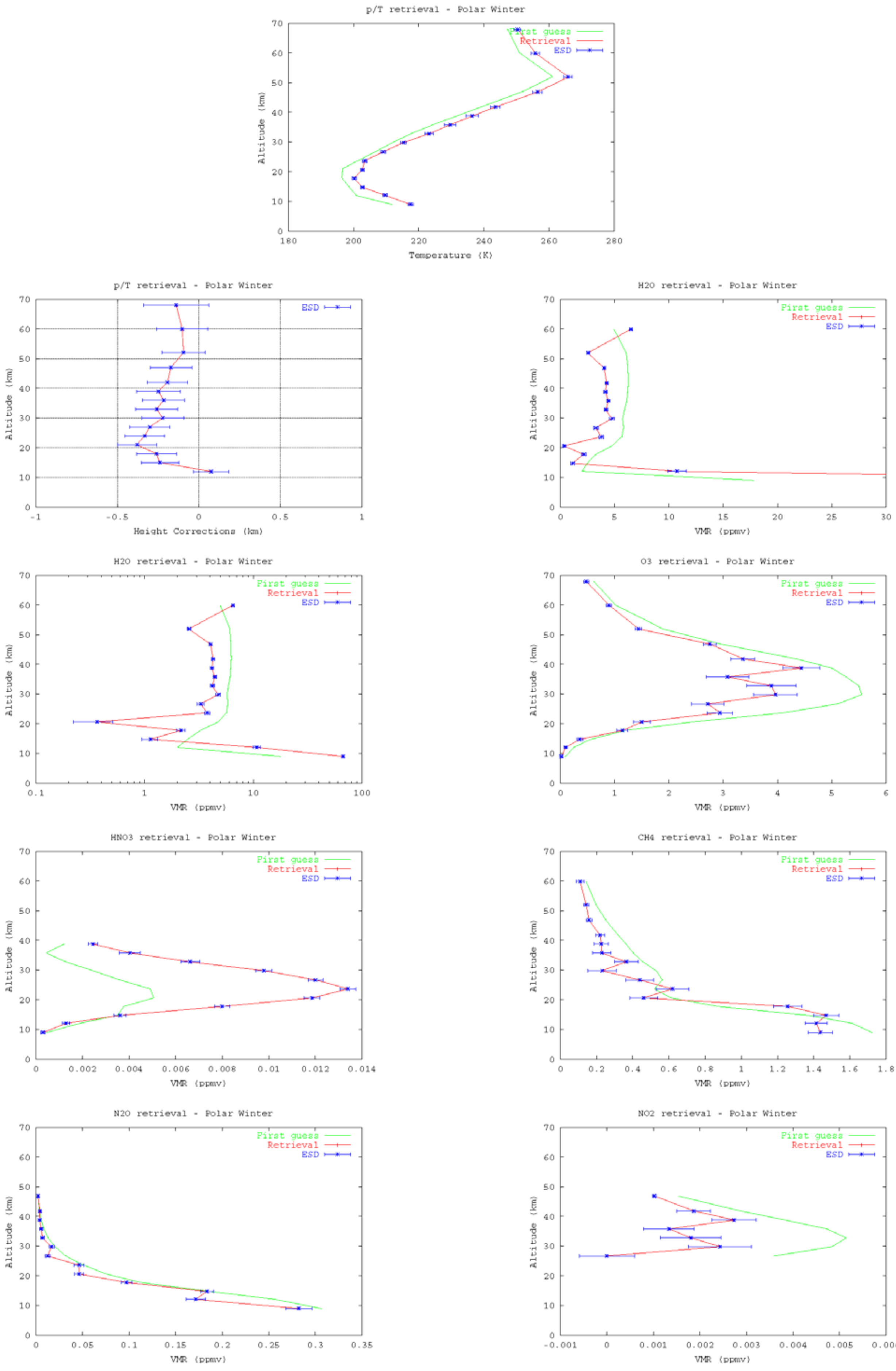

Figure from 18 to 26: plots that report the first guess profile (green curve) and the retrieved quantities (red curve), together with their total errors (blue lines), for the Winter scenario.

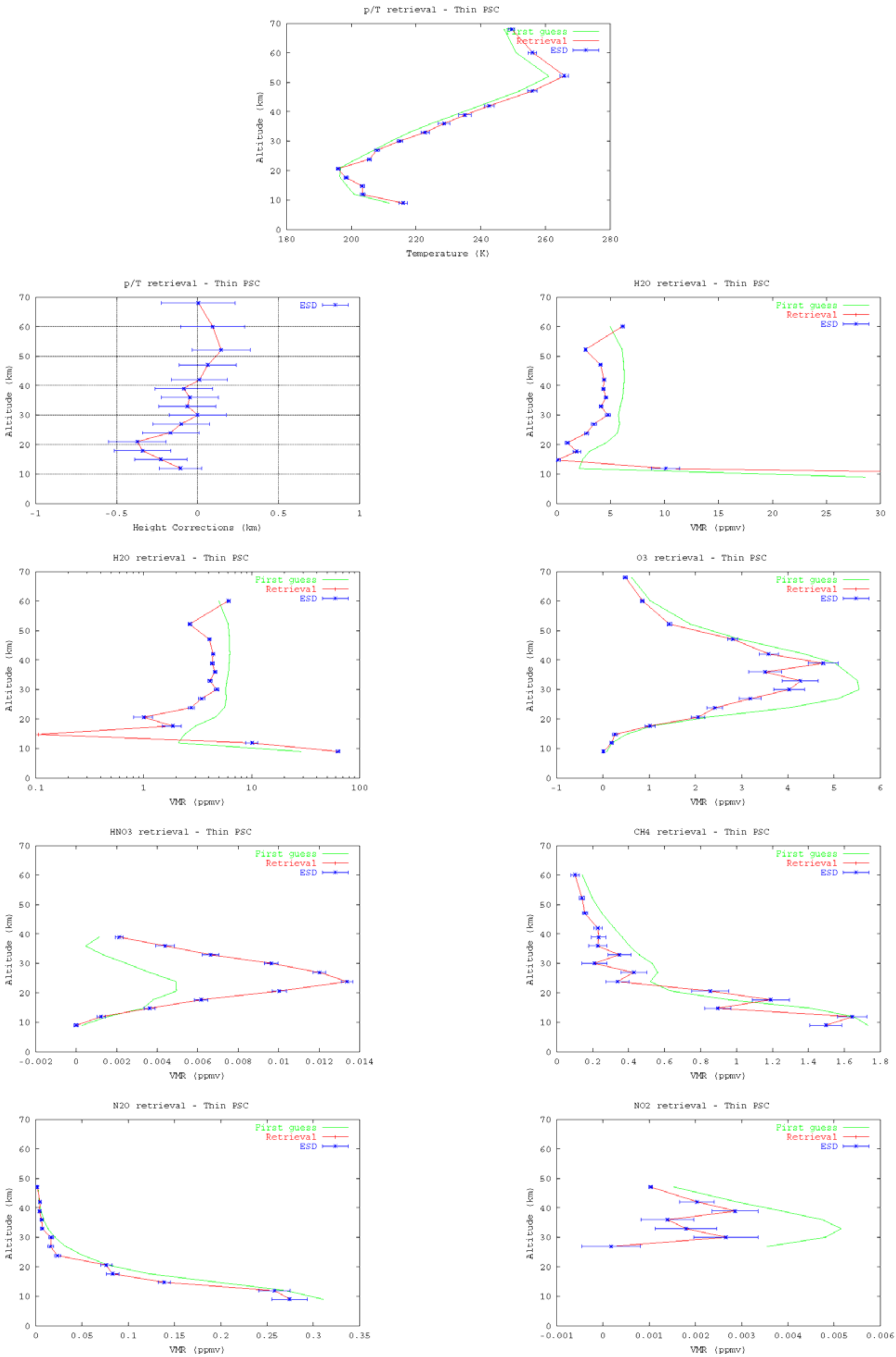

Figure from 27 to 35: plots that report the first guess profile (green curve) and the retrieved quantities (red curve), together with their total errors (blue lines), for the PSC1 scenario.

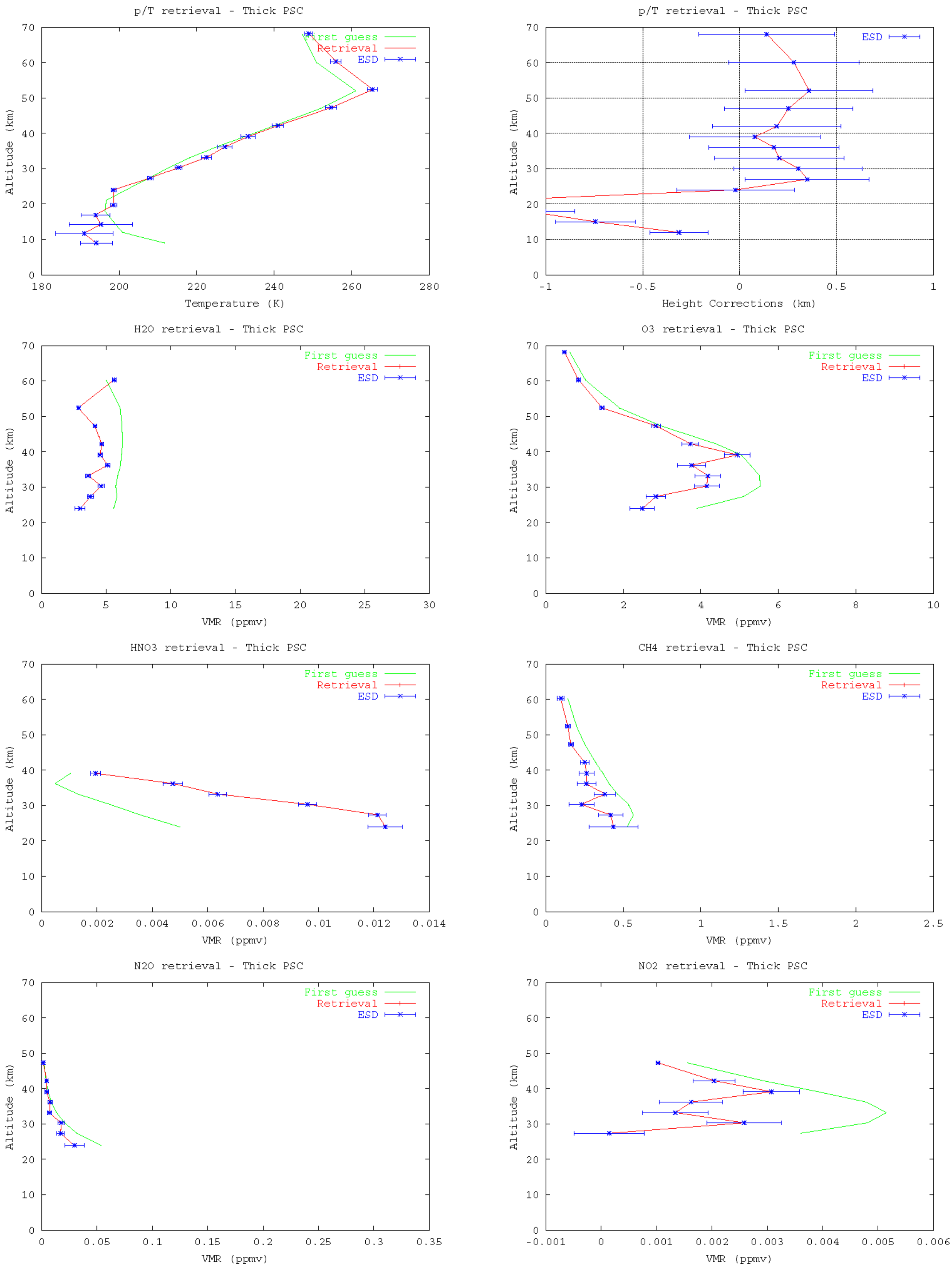

Figure from 36 to 43: plots that report the first guess profile (green curve) and the retrieved quantities (red curve), together with their total errors (blue lines), for the PSC2 scenario.

Table 2 – results of the retrievals operated on the Mid-Latitude Day atmospheric scenario

	Pressure			Temperature			Height Correction	
Altitude (km)	p (hPa)	ESD(%)	Total Error (%)	T (K)	ESD (K)	Total Error (K)	(km)	ESD (km)
68.2	7.4E-02	2.1	4.1	229.2	1.2	3.9	0.17	0.19
60.3	2.2E-01	1.5	3.6	246.4	1.3	3.2	0.32	0.15
52.3	6.4E-01	1.1	2.9	265.3	1.1	1.5	0.25	0.12
47.1	1.2E+00	0.8	2.5	268.2	1.1	2.1	0.12	0.11
42.0	2.3E+00	0.7	2.6	262.5	1.1	1.8	0.02	0.10
39.2	3.4E+00	0.8	2.5	259.5	1.3	1.9	0.20	0.11
36.4	4.8E+00	0.7	2.2	252.5	1.1	2.1	0.44	0.10
32.9	7.9E+00	1.2	2.6	236.5	0.7	1.8	-0.13	0.12
29.7	1.3E+01	1.3	3.5	229.9	0.6	1.3	-0.31	0.12
26.5	2.0E+01	1.1	3.9	224.0	0.5	1.6	-0.51	0.11
23.5	3.2E+01	1.0	3.0	218.9	0.6	1.6	-0.55	0.11
20.6	5.0E+01	1.0	2.5	223.4	0.5	1.8	-0.36	0.11
17.7	7.8E+01	1.2	2.8	220.5	0.4	1.7	-0.27	0.11
14.6	1.3E+02	1.1	3.0	217.4	0.5	1.5	-0.37	0.11
11.8	1.9E+02	0.9	3.0	226.2	0.6	2.0	-0.16	0.09
9.0	2.9E+02	1.3	3.1	233.2	0.7	2.1		

Table 3 – results of the retrievals operated on the Mid-Latitude Day atmospheric scenario

	H_2O			O_3			HNO_3		
Altitude (km)	VMR (ppmV)	ESD (%)	Total Error (%)	VMR (ppmV)	ESD (%)	Total Error (%)	VMR (ppmV)	ESD (%)	Total Error (%)
68.2				4.4E-01	10.6	26.70			
60.3	1.3E+01	2.1	25.1	1.0E+00	4.9	10.30			
52.3	3.4E+00	3.0	15.5	1.9E+00	2.5	5.80			
47.1	5.0E+00	1.4	13.4	3.0E+00	2.2	5.90			
42.0	4.3E+00	1.2	11.1	4.2E+00	2.6	5.30			
39.2	3.7E+00	1.5	10.4	4.9E+00	3.3	5.80	5.3E-04	21.9	29.5
36.4	3.5E+00	1.4	9.4	4.3E+00	4.2	6.70	1.1E-03	14.5	16.1
32.9	4.3E+00	1.3	10.9	5.1E+00	3.7	7.10	1.6E-03	8.1	9.9
29.7	4.0E+00	2.1	10.2	5.5E+00	3.8	7.70	4.0E-03	3.4	6.4
26.5	3.0E+00	2.6	10.9	4.5E+00	3.5	6.40	6.0E-03	2.0	5.3
23.5	3.9E+00	2.2	9.1	4.3E+00	2.9	6.70	7.8E-03	1.7	5.0
20.6	1.3E+00	5.5	15.4	1.5E+00	5.7	8.20	7.2E-03	1.8	4.9
17.7	1.7E+00	4.5	18.1	8.2E-01	6.6	13.50	3.2E-03	3.5	6.2
14.6	3.2E+00	5.1	15.4	3.3E-01	10.8	13.60	8.3E-04	10.2	15.0
11.8	2.0E+01	3.3	20.0	5.2E-02	36.7	38.40	4.8E-04	12.5	20.1
9.0	3.7E+02	1.3	6.1	4.0E-02	20.5	25.00	9.4E-05	39.2	56.4

Table 4 – results of the retrievals operated on the Mid-Latitude Day atmospheric scenario

	CH_4			N_2O			NO_2		
Altitude (km)	VMR (ppmV)	ESD (%)	Total Error (%)	VMR (ppmV)	ESD (%)	Total Error (%)	VMR (ppmV)	ESD (%)	Total Error (%)
68.2									
60.3	2.0E-01	11.4	19.9						
52.3	1.8E-01	6.5	9.5						
47.1	2.6E-01	4.4	8.3	8.0E-03	6.6	13.40	1.0E-10	8.6E+08	8.6E+08
42.0	3.5E-01	4.2	9.2	1.1E-02	7.6	12.20	2.4E-03	6.0	8.0
39.2	2.7E-01	7.2	11.1	1.1E-02	12.0	14.90	4.4E-03	4.3	6.6
36.4	2.7E-01	7.5	12.1	1.5E-02	10.0	14.20	4.5E-03	4.7	6.7
32.9	4.8E-01	5.9	12.6	3.1E-02	5.7	9.40	5.1E-03	5.4	7.5
29.7	6.1E-01	6.8	18.3	5.9E-02	4.4	8.90	5.3E-03	6.0	8.9
26.5	9.2E-01	5.2	16.7	9.1E-02	3.9	8.50	3.4E-03	7.4	11.1
23.5	1.1E+00	5.2	12.5	2.1E-01	2.6	7.20			
20.6	6.9E-01	6.4	10.7	1.6E-01	3.1	6.80			
17.7	1.2E+00	2.8	10.0	2.0E-01	2.5	7.40			
14.6	1.5E+00	2.0	7.7	3.0E-01	2.4	6.90			
11.8	1.5E+00	2.2	7.5	2.3E-01	3.8	5.80			
9.0	1.7E+00	2.6	8.9	3.3E-01	3.0	6.40			

Table 5 – results of the retrievals operated on the Polar Winter atmospheric scenario

	Pressure			Temperature			Height Correction	
Altitude (km)	p (hPa)	ESD(%)	Total Error (%)	T (K)	ESD (K)	Total Error (K)	(km)	ESD (km)
67.9	4.4E-02	2.2	4.1	250.4	1.0	3.9	-0.14	0.20
59.9	1.3E-01	1.6	3.7	255.8	1.3	3.2	-0.10	0.16
51.9	3.5E-01	1.3	3.0	265.8	1.3	1.6	-0.09	0.13
46.8	6.8E-01	1.2	2.7	256.4	1.4	2.3	-0.17	0.13
41.8	1.3E+00	1.3	2.8	243.5	1.5	2.1	-0.19	0.12
38.8	2.1E+00	1.5	2.8	236.4	1.9	2.4	-0.25	0.13
35.8	3.2E+00	1.4	2.5	229.7	1.8	2.5	-0.22	0.13
32.7	5.0E+00	1.5	2.7	223.2	1.3	2.1	-0.26	0.13
29.8	7.9E+00	1.5	3.6	215.4	0.9	1.5	-0.22	0.13
26.7	1.3E+01	1.4	4.0	209.1	0.8	1.7	-0.30	0.12
23.7	2.1E+01	1.4	3.1	203.4	0.7	1.6	-0.33	0.12
20.6	3.5E+01	1.5	2.7	202.7	0.6	1.8	-0.38	0.12
17.7	5.8E+01	1.5	2.9	200.2	0.6	1.7	-0.26	0.12
14.8	9.5E+01	1.4	3.1	202.8	0.6	1.5	-0.24	0.11
12.1	1.5E+02	1.4	3.2	209.7	0.8	2.1	0.08	0.11
9.0	2.4E+02	1.5	3.2	217.5	0.8	2.1		

Table 6 – results of the retrievals operated on the Polar Winter atmospheric scenario

	H_2O			O_3			HNO_3		
Altitude (km)	VMR (ppmV)	ESD (%)	Total Error (%)	VMR (ppmV)	ESD (%)	Total Error (%)	VMR (ppmV)	ESD (%)	Total Error (%)
67.9				4.8E-01	10.1	26.90			
59.9	6.5E+00	2.3	25.9	9.0E-01	5.5	10.80			
51.9	2.6E+00	3.9	15.9	1.4E+00	4.0	6.70			
46.8	4.1E+00	3.1	14.0	2.8E+00	4.1	6.90			
41.8	4.3E+00	3.1	12.0	3.4E+00	6.5	8.10			
38.8	4.2E+00	3.7	12.0	4.4E+00	7.6	9.10	2.5E-03	8.1	23.5
35.8	4.4E+00	3.3	11.8	3.1E+00	12.7	13.80	3.9E-03	11.6	13.4
32.7	4.2E+00	4.3	12.8	3.9E+00	11.8	13.30	6.7E-03	6.1	8.4
29.8	4.8E+00	5.1	11.9	4.0E+00	10.2	12.20	9.8E-03	3.6	6.5
26.7	3.3E+00	6.9	13.1	2.7E+00	11.0	12.30	1.2E-02	2.6	5.6
23.7	3.8E+00	5.7	10.9	2.9E+00	8.0	10.10	1.3E-02	2.5	5.5
20.6	3.7E-01	39.4	42.1	1.5E+00	10.3	11.90	1.2E-02	2.9	5.5
17.7	2.2E+00	9.3	20.0	1.1E+00	8.7	14.70	8.2E-03	4.1	6.7
14.8	1.1E+00	16.8	22.1	3.6E-01	16.1	18.20	3.6E-03	7.1	13.0
12.1	1.1E+01	7.7	21.8	9.8E-02	30.3	32.40	1.3E-03	13.3	20.5
9.0	6.7E+01	2.3	6.3	1.8E-02	71.8	73.30	3.2E-04	29.5	52.0

Table 7 – results of the retrievals operated on the Polar Winter atmospheric scenario

	CH_4			N_2O			NO_2		
Altitude (km)	VMR (ppmV)	ESD (%)	Total Error (%)	VMR (ppmV)	ESD (%)	Total Error (%)	VMR (ppmV)	ESD (%)	Total Error (%)
67.9									
59.9	1.1E-01	20.6	26.5						
51.9	1.4E-01	10.2	12.4						
46.8	1.6E-01	9.7	12.3	2.3E-03	30.2	32.40	1.0E-03	3.6E+00	1.1E+01
41.8	2.2E-01	10.9	14.1	4.4E-03	25.5	27.60	1.9E-03	19.4	20.2
38.8	2.3E-01	17.8	20.4	4.1E-03	35.3	36.70	2.7E-03	17.5	18.5
35.8	2.3E-01	22.1	24.7	5.7E-03	29.1	31.00	1.3E-03	40.7	41.3
32.7	3.7E-01	18.1	21.5	7.1E-03	26.4	27.50	1.8E-03	36.1	36.7
29.8	2.3E-01	34.0	38.0	1.7E-02	15.9	17.80	2.4E-03	28.0	29.0
26.7	4.4E-01	17.7	23.8	1.3E-02	24.2	25.40	1.0E-10	6.0E+08	6.0E+08
23.7	6.2E-01	14.5	18.5	4.6E-02	11.4	13.40			
20.6	4.6E-01	16.7	18.9	4.6E-02	10.6	12.30			
17.7	1.3E+00	6.3	11.6	9.7E-02	5.8	9.20			
14.8	1.5E+00	4.7	8.7	1.8E-01	3.7	7.50			
12.1	1.4E+00	4.3	8.7	1.7E-01	6.0	7.60			
9.0	1.4E+00	4.7	10.0	2.8E-01	5.1	8.00			

Table 8 – results of the retrievals operated on the presence of Thin PSC atmospheric scenario

	Pressure			Temperature			Height Correction	
Altitude (km)	p (hPa)	ESD(%)	Total Error (%)	T (K)	ESD (K)	Total Error (K)	(km)	ESD (km)
68.0	4.4E-02	2.2	4.1	249.5	1.0	3.9	0.00	0.23
60.1	1.3E-01	1.6	3.7	256.0	1.3	3.2	0.09	0.20
52.2	3.5E-01	1.3	3.0	265.8	1.3	1.6	0.14	0.18
47.1	6.8E-01	1.2	2.7	256.0	1.4	2.3	0.06	0.18
42.0	1.3E+00	1.3	2.8	242.6	1.5	2.1	0.01	0.17
38.9	2.1E+00	1.5	2.8	235.1	1.9	2.4	-0.09	0.18
36.0	3.2E+00	1.5	2.6	228.7	1.8	2.5	-0.05	0.18
32.9	5.1E+00	1.5	2.7	222.8	1.3	2.1	-0.06	0.18
30.0	8.0E+00	1.5	3.6	215.0	0.9	1.5	0.00	0.18
26.9	1.3E+01	1.5	4.0	207.9	0.8	1.7	-0.10	0.17
23.8	2.2E+01	1.6	3.2	205.6	0.6	1.6	-0.16	0.17
20.6	3.7E+01	1.8	2.9	195.9	0.5	1.8	-0.37	0.18
17.7	6.2E+01	1.8	3.1	198.4	0.6	1.8	-0.33	0.17
14.8	1.0E+02	1.9	3.4	203.4	0.6	1.5	-0.22	0.16
11.9	1.6E+02	2.0	3.5	203.6	0.7	2.0	-0.10	0.13
9.0	2.6E+02	2.7	3.9	216.0	1.3	2.4		

Table 9 – results of the retrievals operated on the presence of Thin PSC atmospheric scenario

	H_2O			O_3			HNO_3		
Altitude (km)	VMR (ppmV)	ESD (%)	Total Error (%)	VMR (ppmV)	ESD (%)	Total Error (%)	VMR (ppmV)	ESD (%)	Total Error (%)
68.0				4.8E-01	9.4	26.80			
60.1	6.1E+00	2.3	25.9	8.5E-01	5.2	10.70			
52.1	2.7E+00	3.8	15.9	1.4E+00	3.5	6.30			
47.1	4.1E+00	3.1	14.0	2.8E+00	3.9	6.80			
42.0	4.4E+00	3.1	12.0	3.6E+00	5.9	7.60			
38.9	4.3E+00	3.7	12.0	4.8E+00	6.8	8.40	2.1E-03	9.3	38.8
36.0	4.6E+00	3.3	11.8	3.5E+00	10.1	11.40	4.4E-03	10.6	13.6
32.9	4.1E+00	4.5	12.9	4.3E+00	9.2	11.00	6.6E-03	6.1	8.5
30.0	4.8E+00	5.1	12.0	4.0E+00	8.3	10.70	9.6E-03	3.5	6.5
26.9	3.4E+00	6.9	13.0	3.2E+00	7.5	9.30	1.2E-02	2.5	5.6
23.8	2.8E+00	7.0	11.8	2.4E+00	6.9	9.30	1.3E-02	2.1	5.4
20.6	1.0E+00	19.7	24.8	2.1E+00	7.1	9.40	1.0E-02	3.5	6.0
17.7	1.9E+00	19.6	26.7	1.0E+00	10.6	16.00	6.2E-03	5.5	7.8
14.8	1.1E-01	237.6	238.1	2.6E-01	23.5	25.20	3.6E-03	7.2	13.2
11.9	1.0E+01	12.9	26.1	1.9E-01	18.6	22.20	1.2E-03	16.2	23.5
9.0	6.3E+01	3.4	7.4	9.1E-03	149.9	150.70	1.0E-10	1.0E+08	1.0E+08

Table 10 – results of the retrievals operated on the presence of Thin PSC atmospheric scenario

	CH_4			N_2O			NO_2		
Altitude (km)	VMR (ppmV)	ESD (%)	Total Error (%)	VMR (ppmV)	ESD (%)	Total Error (%)	VMR (ppmV)	ESD (%)	Total Error (%)
68.0									
60.1	1.0E-01	21.9	27.5						
52.1	1.4E-01	10.3	12.5						
47.1	1.6E-01	9.6	12.2	1.9E-03	36.4	38.30	1.0E-03	3.6	13.4
42.0	2.3E-01	10.3	13.7	4.6E-03	24.4	26.60	2.0E-03	18.3	19.1
38.9	2.3E-01	17.4	20.0	4.3E-03	34.0	35.40	2.9E-03	17.3	18.4
36.0	2.3E-01	22.1	24.7	6.5E-03	26.5	28.50	1.4E-03	40.7	41.5
32.9	3.5E-01	18.1	21.5	7.1E-03	24.8	26.00	1.8E-03	37.4	38.0
30.0	2.1E-01	33.4	37.5	1.7E-02	15.1	17.10	2.7E-03	26.2	27.4
26.9	4.3E-01	16.5	23.0	1.6E-02	19.1	20.60	1.8E-04	360.5	360.7
23.8	3.4E-01	18.6	22.0	2.4E-02	14.3	16.00			
20.6	8.5E-01	12.1	15.2	7.6E-02	8.2	10.70			
17.7	1.2E+00	8.7	13.2	8.3E-02	8.3	11.30			
14.8	9.0E-01	8.0	11.2	1.4E-01	4.7	8.40			
11.9	1.6E+00	4.9	10.3	2.6E-01	6.5	8.90			
9.0	1.5E+00	5.9	12.1	2.7E-01	7.0	10.60			

Table 11 – results of the retrievals operated on the presence of Thick PSC atmospheric scenario

	Pressure			Temperature			Height Correction	
Altitude (km)	p (hPa)	ESD(%)	Total Error (%)	T (K)	ESD (K)	Total Error (K)	(km)	ESD (km)
68.1	4.5E-02	2.2	4.1	248.9	1.0	3.9	0.14	0.35
60.3	1.3E-01	1.6	3.7	255.9	1.3	3.2	0.28	0.34
52.4	3.5E-01	1.3	3.0	265.4	1.2	1.6	0.36	0.33
47.3	6.9E-01	1.3	2.7	254.7	1.4	2.3	0.25	0.33
42.2	1.4E+00	1.3	2.8	241.0	1.5	2.1	0.19	0.33
39.1	2.1E+00	1.5	2.8	233.3	1.9	2.4	0.08	0.34
36.2	3.3E+00	1.5	2.6	227.3	1.8	2.5	0.18	0.34
33.2	5.1E+00	1.5	2.8	222.5	1.3	2.1	0.20	0.33
30.3	8.0E+00	1.5	3.6	215.3	0.9	1.5	0.30	0.33
27.4	1.3E+01	1.8	4.1	208.0	0.7	1.7	0.35	0.32
24.0	2.3E+01	2.5	3.7	198.6	0.6	1.6	-0.02	0.30
19.7	4.7E+01	3.2	3.9	198.6	0.8	1.9	-1.28	0.28
16.9	7.6E+01	3.7	4.4	194.0	3.8	4.1	-1.09	0.25
14.3	1.2E+02	4.2	5.0	195.4	8.2	8.3	-0.74	0.21
11.7	1.9E+02	4.9	5.7	191.0	7.5	7.7	-0.31	0.15
9.0	3.1E+02	5.7	6.4	194.1	4.1	4.6		

Table 12 – results of the retrievals operated on the presence of Thick PSC atmospheric scenario

	H_2O			O_3			HNO_3		
Altitude (km)	VMR (ppmV)	ESD (%)	Total Error (%)	VMR (ppmV)	ESD (%)	Total Error (%)	VMR (ppmV)	ESD (%)	Total Error (%)
68.1				4.8E-01	9.4	37.60			
60.3	5.6E+00	2.4	26.7	8.4E-01	5.2	14.10			
52.4	2.9E+00	3.5	15.9	1.5E+00	3.5	6.70			
47.3	4.1E+00	3.1	14.0	2.8E+00	3.9	7.00			
42.2	4.7E+00	3.0	12.0	3.7E+00	5.8	7.70			
39.1	4.5E+00	3.7	12.2	4.9E+00	6.8	8.50	2.0E-03	8.9	78.9
36.2	5.1E+00	3.3	12.4	3.8E+00	9.6	11.10	4.7E-03	7.2	15.0
33.2	3.6E+00	5.0	13.2	4.2E+00	7.8	10.00	6.4E-03	5.0	8.0
30.3	4.6E+00	5.1	12.0	4.2E+00	7.9	10.40	9.6E-03	3.5	6.5
27.3	3.8E+00	6.3	13.1	2.8E+00	8.7	10.40	1.2E-02	2.6	5.8
24.0	3.0E+00	13.1	17.0	2.5E+00	12.8	14.50	1.2E-02	5.0	7.4
19.7	1.0E-10	1.0E+12	1.0E+12	1.0E-10	1.0E+12	1.0E+12	1.0E-10	1.0E+11	1.0E+11
16.9	1.5E+01	44.1	64.6	1.0E-10	1.0E+12	1.0E+12	1.0E-10	1.0E+11	1.0E+11
14.3	1.0E-10	1.0E+12	1.0E+12	1.0E-10	1.0E+12	1.0E+12	1.0E-10	1.0E+11	1.0E+11
11.7	6.8E+01	133.0	142.8	5.4E+02	1.0E+03	1.0E+03	-	-	-
9.0	1.0E-10	1.0E+13	1.0E+13	-	-	-	-	-	-

Table 13 – results of the retrievals operated on the presence of Thick PSC atmospheric scenario

	CH_4			N_2O			NO_2		
Altitude (km)	VMR (ppmV)	ESD (%)	Total Error (%)	VMR (ppmV)	ESD (%)	Total Error (%)	VMR (ppmV)	ESD (%)	Total Error (%)
68.1									
60.3	9.7E-02	22.9	28.7						
52.4	1.4E-01	10.2	12.6						
47.3	1.6E-01	9.9	13.0	1.7E-03	41.9	43.60	1.0E-03	3.6	19.8
42.2	2.5E-01	10.6	14.8	4.7E-03	24.3	26.60	2.0E-03	18.6	19.7
39.1	2.6E-01	18.0	21.1	4.7E-03	32.9	34.50	3.1E-03	16.5	17.8
36.2	2.6E-01	22.9	26.0	7.8E-03	25.7	28.10	1.6E-03	35.3	37.4
33.2	3.8E-01	18.2	22.2	7.2E-03	28.7	29.80	1.3E-03	44.3	45.0
30.3	2.3E-01	34.7	39.4	1.8E-02	15.7	17.80	2.6E-03	25.9	28.5
27.3	4.2E-01	18.9	25.0	1.7E-02	19.8	21.40	1.4E-04	443.7	443.8
24.0	4.4E-01	36.0	38.2	3.0E-02	29.2	30.50			
19.7	1.0E-10	1.0E+11	1.0E+11	1.0E-10	1.0E+10	1.0E+10			
16.9	2.4E+00	129.5	131.5	3.4E-02	397.6	398.40			
14.3	1.0E-10	1.0E+12	1.0E+12	1.0E-10	1.0E+11	1.0E+11			
11.7	-	-	-	-	-	-			
9.0	-	-	-	-	-	-			

WP8500

1. Introduction

Similarly to WP8300, the activities involved in WP8400 and WP8500 were finalized to provide performance predictions for MIPAS retrieval analyses. In this case the performance has been evaluated on a set of retrievals that analyze observations covering a full orbit that is 75 limb-scanning sequences. The output of WP8500 will then permit to evaluate the quality of level-2 products in a statistically significant number of different atmospheric scenarios.

The simulated observations that have been used in this WP have been generated by the Optimized Forward Model (OFM) which implements an algorithm similar to the one built in the retrieval system (ORM), the main difference being the Look-Up-tables and Irregular Grids that are not used by OFM.

2. Inputs

The following inputs have been used for WPs 8400 and 8500:

1. Occupation Matrices (OM) for all target quantities supplied with cross-section Look-Up-Tables and Irregular Grid definitions.
2. A database of altitude profiles to be used as initial guess (IG) for the target quantities and to model spectral features of molecular species contaminating the analyzed observations.
3. Geo-location of tangent point of the observation geometries over a full orbit.
4. A database of altitude profiles to be used by OFM to simulate MIPAS observations.
5. Setup parameters as determined in WP8300.

Inputs 1 and 2 are the same as for WP8300. Input 3 was provided by ESA; figure 44 show the geo-location of the mid point of each sequence. Input 4 derives from calculations performed with the SLIMCAT chemical model [1]; details about these calculations are reported in Table 10.

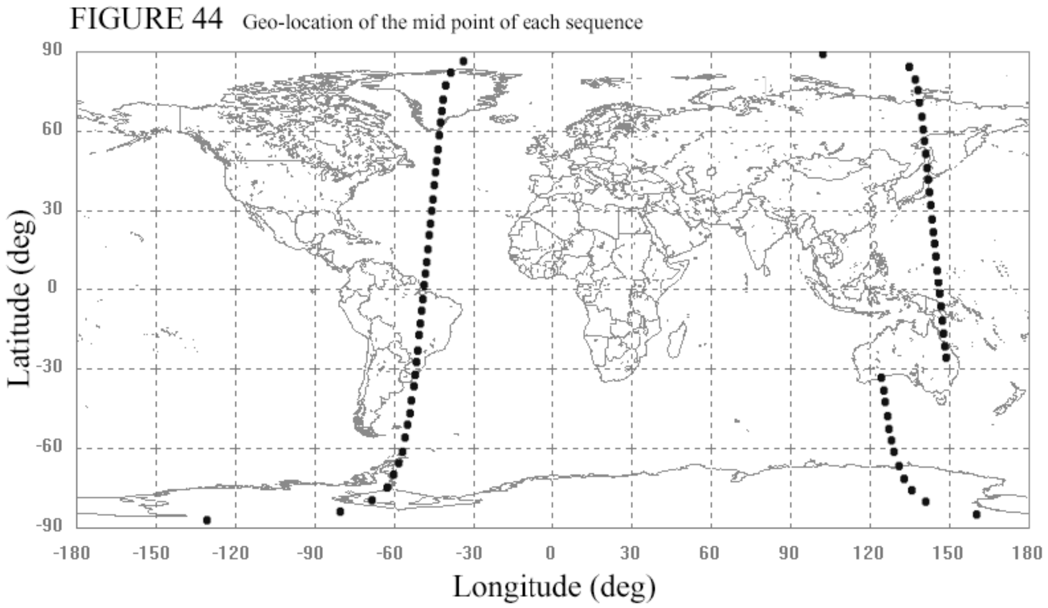

Figure 44: Geo-location of the mid point of each limb-scanning sequence.

Table 10. Characteristics of SLIMCAT calculation

3-D chemical transport model
Latitude grid: 5^o , 4.5^o in polar regions
Longitude grid: 7.5^o
Altitude grid: 8-57 km irregular steps of ≈ 2, 4, 5 km
Day: 27 September 1996 (ozone hole conditions)
Calculated quantities: p, T, VMR of H_2O, O_3, N_2O, CO, CH_4, NO, NO_2, HNO_3, OH, HF, HCl, HBr, ClO, CH_2O, HOCl, H_2O_2, COF_2, HO_2, O, $ClONO_2$

3. Sequence of the operations

For each limb-scanning sequence the SLIMCAT profiles were interpolated on the geo-location of the mid point of the sequence itself. Since the SLIMCAT profiles cover an altitude range which is limited with respect to the required range, an extension of the profiles was operated upward and downward applying a scaling factor to the IG profiles of the corresponding species in that latitudinal strip. IG database was also used to complement SLIMCAT atmospheres with a few molecular species missing in this atmospheric model. Figures from 45 to 51 show the distribution of the target quantities along the considered orbit. In these maps, as well as in those that will be reported in the following of this report, we adopt on the *x*-axis an orbital coordinate that is equal to zero in correspondence of north pole.

For each limb-scanning sequence the retrieval chain was started building the input atmosphere with the profiles retrieved by the analysis on the previous sequence; the only exception being the first limb-scanning sequence for which the nearest IG profiles were used for p,T and all molecular species. With this exception the following flow diagram shows the operations applied to each of the limb-scanning sequences that cover the full orbit.

Geo-location of tg points

↓

Geo-location of mid point $\mathbf{P_m}$

↓

SLIMCAT model → Interpolation of SLIMCAT on $\mathbf{P_m}$
$\mathbf{S_i}$ atmosphere

↓

Altitude extension + missing species in $\mathbf{S_i}$ with IG
$\mathbf{S_{ext}}$ atmosphere

↓

Standard OMs → Simulation of observations with OFM on $\mathbf{S_{ext}}$

↓

Contaminant's from nearest IG → Retrieval with ORM ← Initial guess + target contam. from previous retrieval

↓ ↑

Retrieved profiles of target quantities →→→→→→→→→ ↑

4. Results and discussion

An overall picture of the result of the retrievals is provided, for each target quantity, in figures from 52 to 58 in which the χ-test value at convergence and the number of iterations is reported for each limb-scanning sequence (the position of equator, north pole, and south pole are marked in all figures with EQ, NP, and SP respectively).

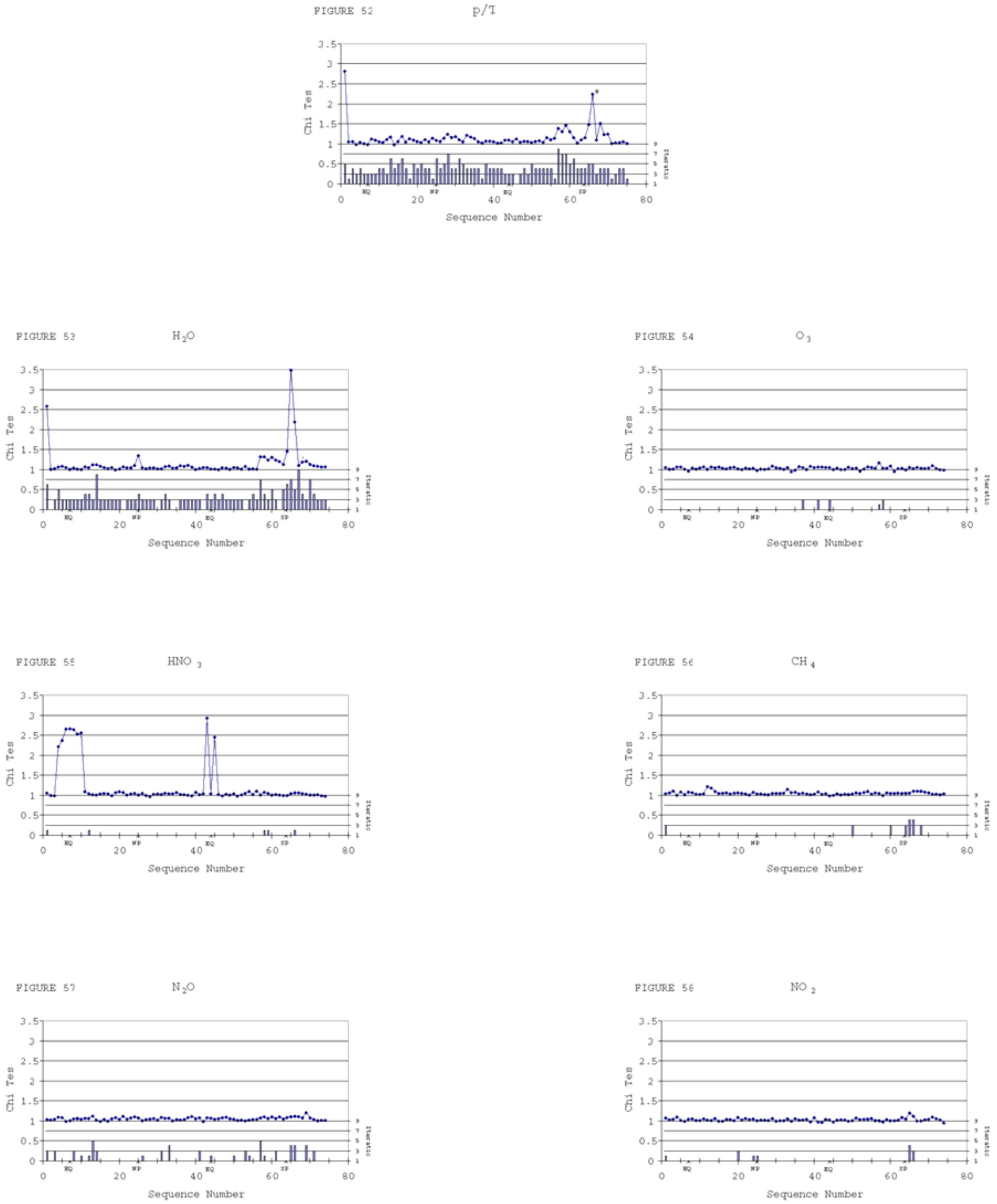

Figure from 52 to 58: plot reporting the χ-test value at convergence and number of iterations for each limb-scanning sequence.

In order to better interpret these figures we describe in more detail a few steps that led to the reported results. In some of the p,T and water retrievals, the convergence criteria were not satisfied after the maximum number of allowed iterations was reached. This occurrence depends on the random distribution of spectral noise on the simulated observations in the sense that, repeating the full orbit simulation with a different distribution of spectral noise, the convergence may be reached at a sequence where it was not before and vice-versa. In most cases the lack of convergence was at the starting limb-scanning sequence where, as stated above, the initial guess profiles need to be taken from the IG database. At first sight this behavior cannot be explained by the difference between the IG and the SLIMCAT profiles (that are used to simulate the observations) because they seem quite similar. However the apparent similarity is misleading in the case of water VMR. In fact, we must consider the water behavior below the tropopause, and that the SLIMCAT profiles are extended in altitude applying a scaling factor to the nearest IG profile. Figure 59 reports, for the starting sequence, the IG profile together with the extended SLIMCAT profile. It can be seen, in figure 59, that the SLIMCAT profile refers to a tropopause which differs in altitude by a few kilometers with respect to the tropopause of the IG profile. The consequence is that the resulting scaling factor applied to the SLIMCAT profile is very high (109 in this particular case). An initial guess for water which is wrong by two orders of magnitude has a negative effect on the p,T retrieval (that operates with a wrong water continuum). The water retrieval that follows (in the ORM sequence) suffers of both a poor first guess of the target molecule and of poor inputs from the results of the p,T retrieval.

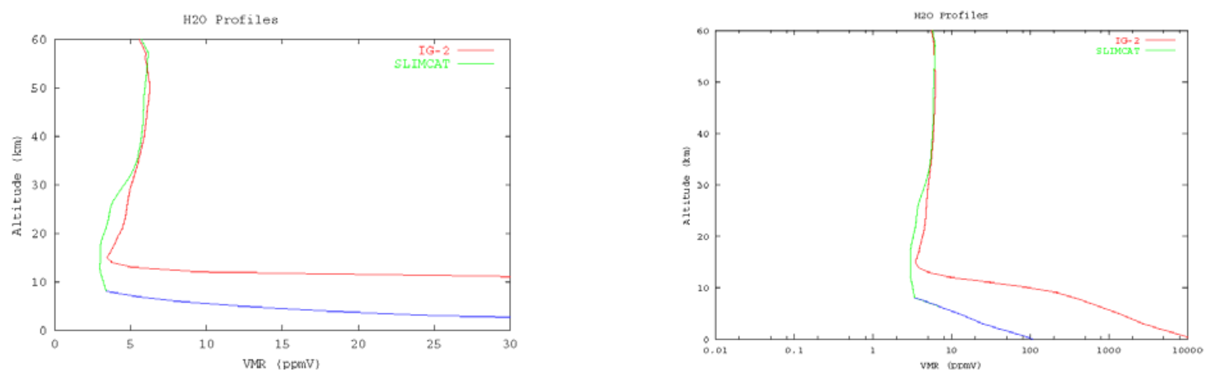

Figure 59: Comparison between the IG profile (red curve) end the extended SLIMCAT profile (blue curve), for the starting sequence. Both linear (left) and logarithmic (right) scale are reported.

The lack of convergence that has been verified in the tests of this WP should be expected whenever the input atmospheric model has the tropopause at a "wrong" altitude. In order to support this hypothesis and to test a possible solution to the problem we have modified the flow of operations within ORM in such a way 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. In this case the profiles determined at the end of the unsuccessful step are fed as input to the new run. With this modification we have verified that one repetition of the ORM sequence is sufficient to obtain convergence in all cases in which the problem occurs. The results shown in the figures of this report, refer to a distribution of spectral noise for which the problem of convergence occurs for p,T at sequence 67. Asterisks on plots mark the values of χ-test after the unsuccessful run. In this test it can be noted that, despite the high χ-test values, the convergence criteria are satisfied at the first run on the starting sequence.

For each target quantity we report, In figures from 60 to 75, maps that represent, along the whole orbit,:

- ESD of the retrieved quantity,
- difference between the retrieved and the reference value of the target quantity (in module).

All maps report % values apart from those relative to temperature that report the absolute values in K.

No figures including systematic error components are reported for this WP. The reason for this is that, for a given OM, these components do not depend (in a first order approximation) from the atmospheric scenario, therefore their combination applies as a constant offset over the ESD random component. An estimate of this offset is provided in Figs. from 10 to 17 for each target quantity. Actually, the p,T propagated error depends on the altitude profile of the target quantities, however it has been verified that this dependence can be considered a second order effect.

[1] M.P. Chipperfield, “Multiannual Simulations with a Three-Dimensional Chemical Transport Model”, *J. Geophys. Res.*, **104**, 1781-1805 (1999).

FIGURE 60 Temperature ESD

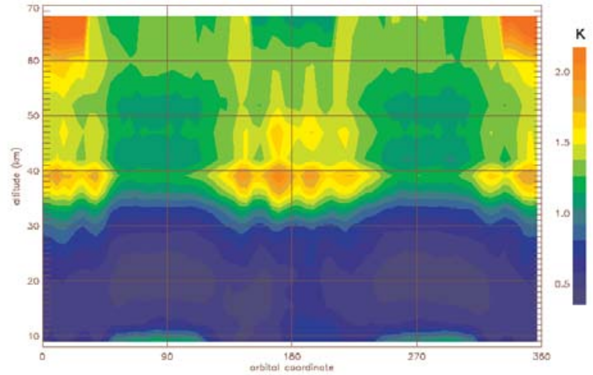

FIGURE 61 Temperature |Retr - Ref|

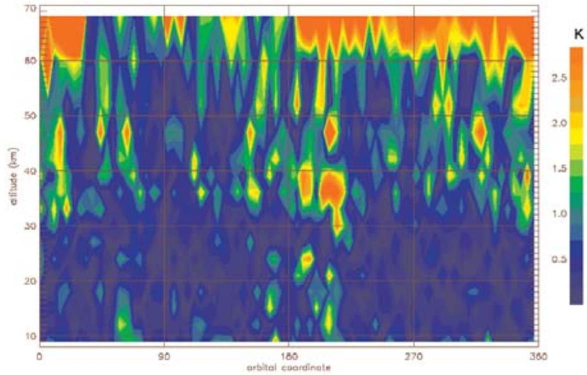

FIGURE 62 Tangent Pressure ESD

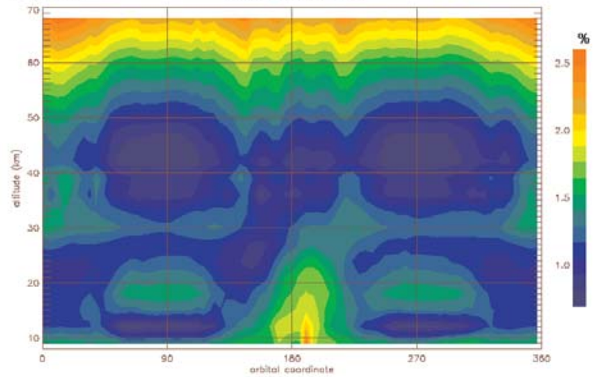

FIGURE 63 Tangent Pressure |Retr - Ref|

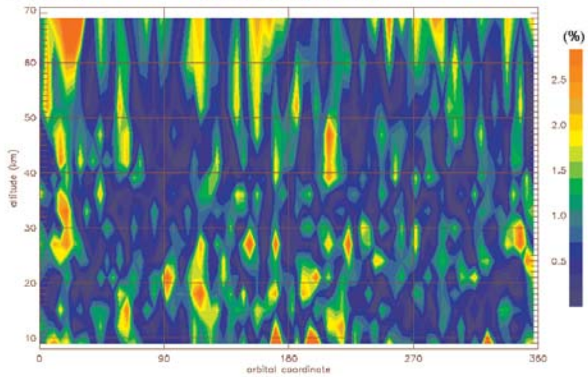

FIGURE 64 H2O ESD

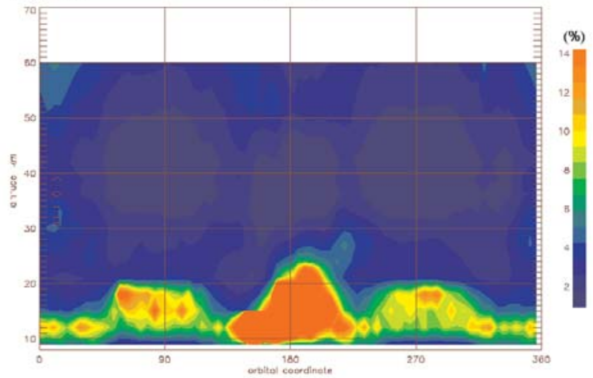

FIGURE 65 H2O |Retr - Ref|

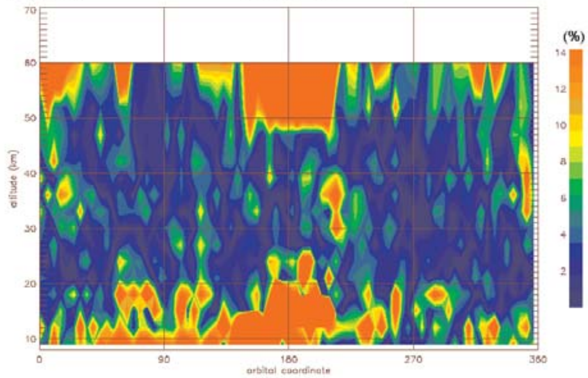

FIGURE 66 O3 ESD

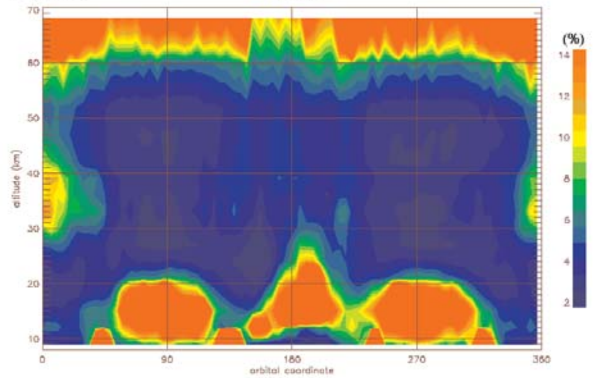

FIGURE 67 O3 |Retr - Ref|

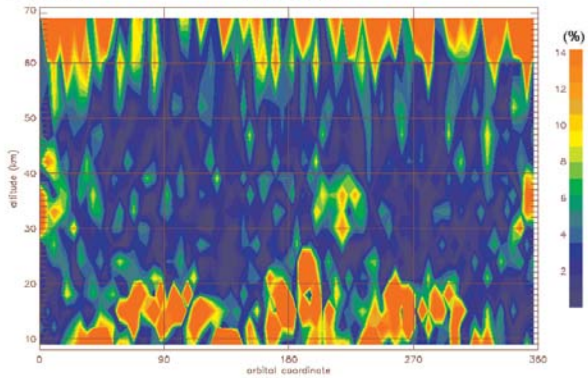

Figure from 60 to 67: maps reporting the ESDs of the retrieved quantity and the difference between the retrieved and the reference value of the target quantity (in module).

FIGURE 68 HNO_3 ESD

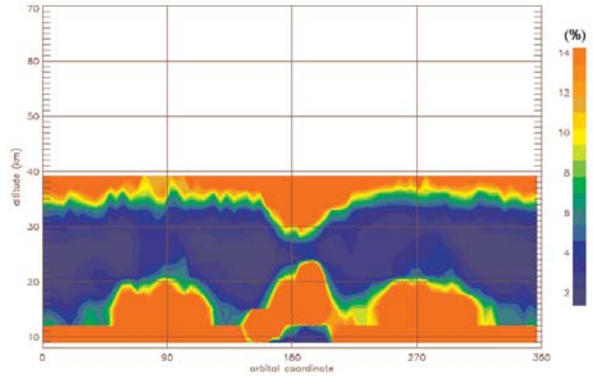

FIGURE 69 HNO_3 |Retr - Ref|

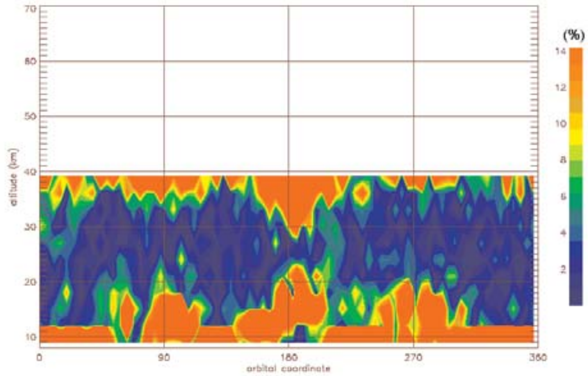

FIGURE 70 CH_4 ESD

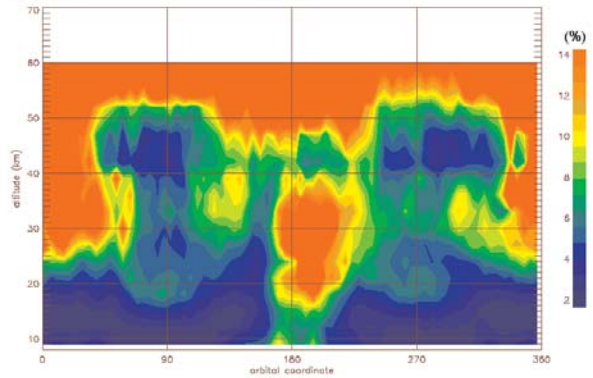

FIGURE 71 CH_4 |Retr - Ref|

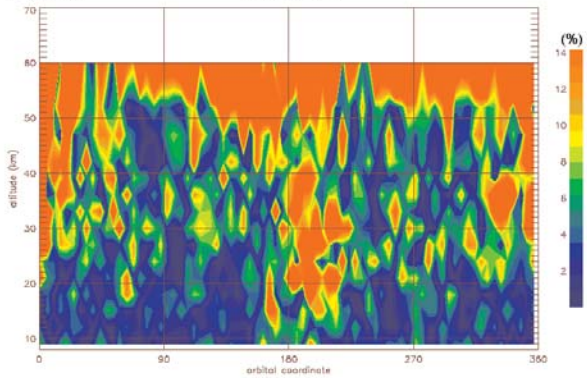

FIGURE 72 N_2O ESD

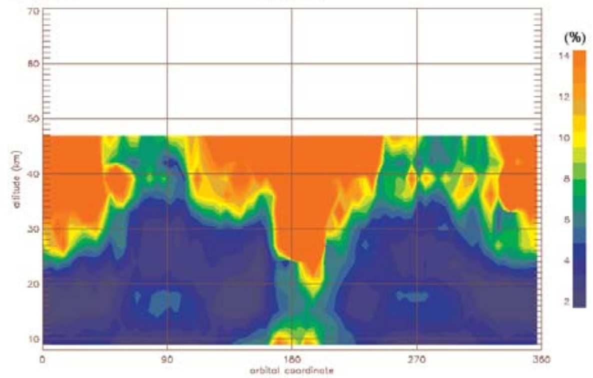

FIGURE 73 N_2O |Retr - Ref|

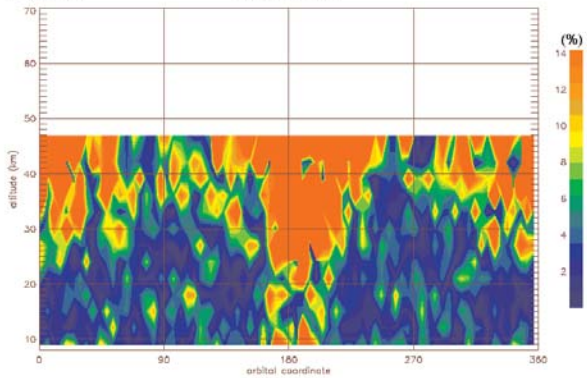

FIGURE 74 NO_2 ESD

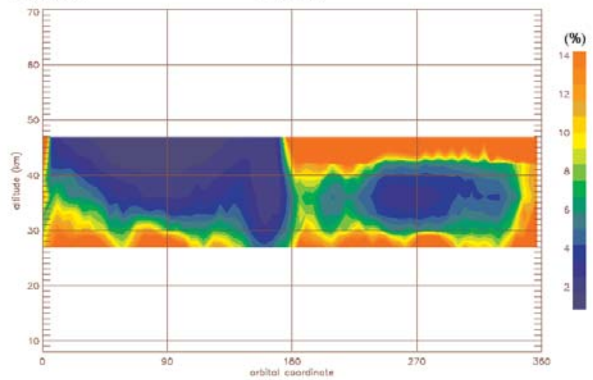

FIGURE 75 NO_2 |Retr - Ref|

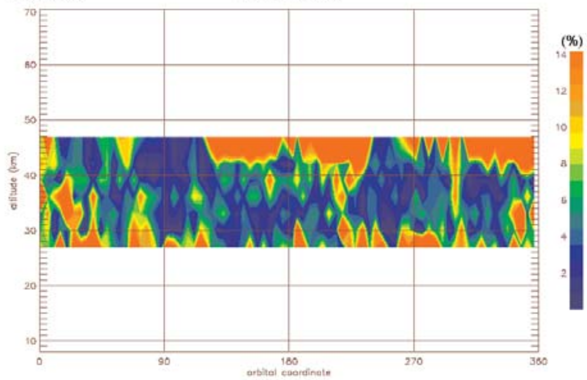

Figure from 68 to 75: maps reporting the ESDs of the retrieved quantity and the difference between the retrieved and the reference value of the target quantity (in module).

APPENDIX A

ORM input file SETTINGS_PT.DAT

```
 delta = frequency step that simulates infinitesimal spectral resolution
        in forward simulations (f10.5)
#
 0.0005

 dstep = frequency spacing between observed spectral data points (f10.5)
#
 0.025

  sdol = definition of the output level (a25)
#
 MAXIMUM DEFINITION

  rconvc = vector of convergence criteria to stop iterations (3f10.5)
  rconvc(1) = max. allowed relative differnce between lin. and real chi-square
  rconvc(2) = max. allowed relative variation of the tangent pressures
  rconvc(3) = max. allowed absolute variation of tangent temperatures

   0.1         0.003      0.1      for PSC2
#
   0.03000     0.003      0.1


  imxiterg = maximum number of Gauss-Newton macro-iterations
#
   10

  imxiterm = maximum number of Marquard micro-iterations
#
    3

  lookupc = switch for the use of cross sections look-up tables (l1)
#
T

  lextinf1 = switch for using a-priori info on LOS during the retrieval
  lifend   = switch for using a-priori info on LOS after the retrieval
  lextinf2 = switch for using a-priori info on atm. continuum
  lextinf3 = switch for using a-priori info on instr. offset
```

```
  lextinf4 = switch for using a-priori info on temperature

#
 T F F F F

  rmaxtv1,rmaxtv2,rzt12: parameters for the layering of the atmosphere (3f10.5)
  rmaxtv1 = max. allowed T variation (K) between levels: 0 < altitude < rzt12
  rmaxtv2 = max. allowed T variation (K) between levels: rzt12<altitude<rulatm
  rzt12 = altitude (km) where the thresholds rmaxtv1 and rmaxtv2 are exchanged
#
 5.0       15.0      68.0

  rhwvar = max half-width change allowed between levels for ref. transiton (f10.5)
#
 1.5

  rincz = max thickness of the layers used for modelling the atmosphere (f10.5)
#
 10.0

  redfact = reduction factor for rincz to produce thinner layers
#
 1.1

  dsigma0,rhw0ref,rexphref,rwmolref
  data relative to the transition that is used for layering criterion (4f10.5)
  dsigma0 = frequency position
  rhw0ref = half-width at the reference T and P
  rexphref = T dependence of half-width
  rwmolref = molecular weight
#
947.741977  0.0704    0.77     44.0

  rtropopause, rint, rintup
  rtropopause: altitude level delimiting troposphere
  rint: maximum separation between two contiguous tangent altitudes of
        two simulated spectra in troposphere
  rintup: maximum separation between two contiguous tangent altitudes of
          two simulated spectra above tropopause
#
 14.0, 2.0, 4.0

  rulatm = boundary of the atmosphere (km) (f10.5)
#
```

100.0

deps = convergence criterion for the C.G. integrals (f10.5)
#
1.0D-5

iept = actual number of extra paths (i5)
#
1

nswco2 = switch for the calculation of the CO2 chi factor (i5)
=0 no factor, =1 n2/o2 broadening, =2 n2 broadening only
#
1

ninterpol = switch for the interpolation on the cross-sections (i5)
= -1: no interpolation, all cross-sections recalculated
= 0: all those above the lowest geometry are interpolated
= 1: new calculation only of tangent-layer
= 2: new calculation for tangent-layer and the one above
#
-1

Tabulation of FOV pattern for the 5 MIPAS bands

Band A (685-995 cm-1)
nfovinc(1) = number of points used for tabulating FOV
rfov(1,1->nfovinc) = height of FOV function
ranginc(1,1->nfovinc) =

#
4
0.d0, 1.d0 , 1.d0, 0.d0
-2.d0, -1.4d0, 1.4d0, 2.d0

Band AB (995-1192.5 cm-1)
nfovinc(2) = number of points used for tabulating FOV
rfov(2,1->nfovinc) = height of FOV function
ranginc(2,1->nfovinc) =
#
4
0.d0, 1.d0 , 1.d0, 0.d0
-2.d0, -1.4d0, 1.4d0, 2.d0

```
  Band B (1192.5-1535 cm-1)
  nfovinc(3) = number of points used for tabulating FOV
  rfov(3,1->nfovinc) = height of FOV function
  ranginc(3,1->nfovinc) =
#
 4
  0.d0,  1.d0 , 1.d0,  0.d0
 -2.d0, -1.4d0, 1.4d0, 2.d0

  Band C (1535-1785 cm-1)
  nfovinc(4) = number of points used for tabulating FOV
  rfov(4,1->nfovinc) = height of FOV function
  ranginc(4,1->nfovinc) =
#
 4
  0.d0,  1.d0 , 1.d0,  0.d0
 -2.d0, -1.4d0, 1.4d0, 2.d0

  Band D (1785-2410 cm-1)
  nfovinc(5) = number of points used for tabulating FOV
  rfov(5,1->nfovinc) = height of FOV function
  ranginc(5,1->nfovinc) =
#
 4
  0.d0,  1.d0 , 1.d0,  0.d0
 -2.d0, -1.4d0, 1.4d0, 2.d0

  imaingas = HITRAN code of the main molecule of the retrieval (i5)
#
    2

  lfit(j),j=1,ilimb = logical vector that identifies the tangent altitudes which
  correspond to fitted parameters (40l2)
#
 T T T T T T T T T T T T T T T T T

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

Upper continuum limit (rucl): atmospheric continuum is not fitted at the
```

sweeps having tangent altitude > rucl. Units: km
#
36.0

Forces atmospheric continuum = 0 above this altitude (km):
#
80.0

Relative distance between two MWs (with respect to the umbrella radius) below which the continuum is considered the same in the two MWs:
#
0.1

Parameters controlling the evolution of Marquardt damping factor (rlmbda) during the iterations:
- initial value,
- decreasing factor at each Gauss it.
- increasing factor at each Marquardt iteration
#
0.01   1.0   10.0

Logical variable lirrgrid : if it is T, irregular grids will be used for the calculation of the spectra
#
T

Switch for enabling Temp. profile regularization (variable lifreg, format 1L2):
#
F

Parameter for tuning profile regularization (rl1):
#
5.d0

Diagonal elements of the regularization matrix: p,t,cont,offset
#
2.d0 2.d0 25.d0 2.d0

First off-diagonal elements of the regularization matrix: p,t,cont,offset
#
-1.d0 -1.d0 -1.d0 -1.d0

spare = spare field for retrieval configuration
#

APPENDIX B

vector of convergence criteria (rconvc) to stop iterations for VMR retrievals

	rconvc(1)	rconvc(2)
H_2O	0.01	0.005
O_3	0.05	0.01
HNO_3	0.15	0.01
CH_4	0.05	0.01
N_2O	0.05	0.01
NO_2	0.05	0.01

for PSC2:

H_2O	0.05	0.005

rconvc(1) = max. allowed relative difference between lin. and real chi-square
rconvc(2) = max. allowed relative variation of the fitted parameters