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‘Support to MIPAS Level 2 Product Validation’

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“Support to MIPAS Level 2 Validation with the Scientific Prototype Processor ORM”

Technical Note on

Quality of the MIPAS Level 2 validation datasets generated with the ORM_PDS scientific processors V1.0 and V2.0

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1 Reference documents

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[RD3] S. Ceccherini, Belotti, C. Carli, B.P. Raspollini, M. Ridolfi, Technical Note: Regularization performances with the error consistency method in the case of retrieved atmospheric proles. Atmos. Chem. Phys. 7, 1435-1440 (2007). http://www.atmos-chem-phys.net/7/1435/2007/acp-7-1435-2007.html

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2 Acronyms

AKs	Averaging Kernels
CCN	Contract Change Notice
CM	Covariance Matrix (characterizing the retrieval error)
ECMWF	European Centre for Medium-range Weather Forecast
ESA	European Space Agency
ESD	Estimated Standard Deviation
FR	Full-Resolution (MIPAS measurements acquired in the years from 2002 to 2004).
IG	Initial Guess
IPF	Instrument Processing Facilities
L1b	Level 1b
L2	Level 2
MA	Middle Atmosphere (special measurement mode of MIPAS)
ML2PP	MIPAS Level 2 Prototype Processor (industrial prototype for the IPF)
MSS	Measurement Space Solution
MWs	MicroWindows, spectral intervals used for the Level 2 retrievals
NLTE	Non-Local Thermodynamic Equilibrium
NOM	NOMinal MIPAS measurement mode
NRT	Near Real Time (ESA routine retrievals)
OFL	Off-Line (ESA retrievals)
OM	Occupation Matrix, defining which MWs at which altitudes are used in the inversion
OR	Optimized Resolution (MIPAS measurements acquired from Jan. 2004 onward)
ORM	Optimized Retrieval Model
ORM_PDS	ORM version including the capability of generating PDS-formatted outputs
PCS	Product Control Service (service offered by ESA)
PDS	Payload Data Segment
QWG	Quality Working Group (relating to MIPAS)
SZA	Solar Zenith Angle
UA	Upper Atmosphere (special measurement mode of MIPAS)
VMR	Volume Mixing Ratio (always expressed in ppmv)

3 Background

Due to mechanical problems in the interferometer slides, starting from January 2005 MIPAS is being operated at 0.0625 cm^{-1} spectral resolution, the original resolution used in the first two years of the instrument operations was 0.025 cm^{-1}. The acquisition scenario of the instrument has been optimized for the new spectral resolution, resulting in a significant vertical oversampling of the atmosphere. The Level 2 analysis of the measurements acquired in this new optimized configuration (denoted as *optimized resolution*, OR) required some updates of the retrieval algorithm. The scientific prototype of the ESA L2 processor, the so called Optimized Retrieval Model (ORM), was quickly updated and tested to cope with the modified instrument configuration. Some technical problems with the industrial partners, however, prevented a quick and efficient update of the official ESA MIPAS ground processor (IPF). In order to avoid additional delays caused by the lack of official MIPAS L2 products and let progressing the validation activities, it was decided to process with the ORM a significant set of MIPAS measurements to be provided in short time to the validation community and to the users.

The validation community selected a set of approximately 4000 orbits of MIPAS data acquired in the time frame from January 2005 to June 2008, in coincidence with validation measurements. An additional set of about 500 orbits was selected by the MIPAS Quality Working Group (QWG) to achieve a "minimal" time coverage requirement for Level 2 of at least 14 contiguous orbits processed (1 day) per month, from January 2005 to November 2009. These selected measurements were

processed up to Level 1b with the latest version of the L1b processor (V5.0.1). Subsequently, at University of Bologna and IFAC, the data were processed up to L2, using the ORM_PDS code, a ORM version specifically modified and complemented with a tool that allows to generate outputs in the standard format adopted by the Payload Data Segment (PDS).
More specifically, two different L2 datasets were produced with the ORM_PDS: the first one was obtained using the ORM_PDS Version 1.0 aligned with the IPF processor Version 5.0.5. The second one was obtained using the ORM_PDS Version 2.0 aligned with the forthcoming IPF Version 6.0. The differences between the two ORM_PDS processor versions and the related IPF releases are analyzed in RD1 and RD10.

4 Objective of the document

Objective of the present document is to provide a preliminary characterization of the quality of the Level 2 datasets produced with the ORM_PDS. The results of the validation activities, however, are not included in this report. For the results of validation activities the reader should refer to both the general ESA ENVISAT validation web page (http://envisat.esa.int/m-s/envisat_mission_2001/CalVal/) and the web page of the VALID project carried-out at RIVM (https://secure.rivm.nl/wgo/valid).
The document is organized as follows: in Sect. 5 we provide a very general overview of the ORM_PDS validation datasets. In Sect. 6 we present the results of the investigations carried-out so far with the aim of characterizing the quality of the produced datasets. Finally, in Sect. 7 we summarize the conclusions of the work.

5 Outline of the ORM_PDS_V1.0 and V2.0 generated datasets

In this Section we provide some general information regarding the two Level 2 datasets generated with the ORM_PDS_V1.0 and ORM_PDS_V2.0.

5.1 The Level 2 dataset produced with the ORM_PDS_V1.0

The ORM_PDS_V1.0 algorithm baseline corresponds to the operational processor IPF 5.0.5, whose NRT and OFL operations were resumed in June 2010. This algorithm is able to process to Level 2 the MIPAS measurements of the OR scenario (measurements from Jan 2005 onward). Compared to the previous IPF V4, the upgrades of this version allow to solve the ill-conditioning of the retrieval induced by the increased vertical sampling by means of a regularization approach. In particular, the following upgrades are included with respect to the previous MIPAS IPF 4 version:

- **A-posteriori regularization.** An a-posteriori regularization is applied to the main target parameters (temperature, O3, HNO3, CH4, N2O and NO2) except for pressure and H2O profiles. The regularization approach is the one described in RD2 and RD3.
- **Averaging Kernels** (AKs). The AKs of the regularized profiles are included in the new Level 2 products. The condition number of the matrix inverted in the retrieval is also provided. It provides information if the matrix is nearly singular and if its inversion can cause instabilities in the results.
- **Miscellaneous**. Some bugs and algorithm improvements were implemented. Namely, some errors in the computation of the continuum and temperature / VMR derivatives were corrected.

5.2 The Level 2 dataset produced with the ORM_PDS_V2.0

The ORM_PDS_V2.0 is an updated version of the Level 2 scientific prototype algorithm which corresponds to the future operational processor baseline (IPF V6.0), not the operational processor version 5.0.5 activated in June 2010. This new processor baseline implements significant upgrades with respect to the ORM_PDS_V1.0. The upgrades affect both the algorithm baseline as well as the retrieval input files and settings. The details of the differences are described in RD1, here is a summary for the reader's convenience.

Additional species. The VMR of four additional species: CFC-11, CFC-12, ClONO2 and N2O5 is retrieved. For these species the retrieval grid is adapted for each species as specified in Table 1.

The retrieval outputs regarding these additional species processed by the ORM_PDS_V2.0 are not included in the standard MIPAS Level 2 PDS-formatted files. The results regarding these species are provided in ASCII files stored in a sub-directory named `Additional_species`. In this directory the ASCII files are arranged in different directories, one for each orbit. The convention used for naming the directories is: `<orbit number>_<measurement mode>_002.` The `measurement modes` range from: NOM (Nominal Mode), UTLS1 (Upper Troposphere, Lower Stratosphere), MA (Middle Atmosphere), UA (Upper Atmosphere) and NOMADD. This latter indicates the nominal measurements of the ADDitional orbits, not included in the initial list of the validation dataset. Within each orbit-directory there are four ASCII files, one for each additional species. The file name is: `xxx_results.dat` where `xxx` denotes the gas name (F11, F12, ClONO2 and N2O5). In these ASCII files, the following information is provided for each retrieved profile:

- Scan number (same convention as in the L1b products), final normalized chi-square, convergence flag (True or False depending on whether the convergence criterion is met), mean Solar Zenith Angle and mean latitude (the mean is performed over all sweeps processed).
- Profiles of VMR (ppmv) with associated Estimated Standard Deviation (ESD, in ppmv) and corresponding values of latitude, longitude, altitude, sensing time (provided in both UTC and Julian date formats) and pressure in hPa. Captions regarding the meaning of the reported fields are included in each ASCII file.

In order to read these files a FORTRAN routine is made available to the users. This routine can be downloaded from the following link:
http://www2.fci.unibo.it/~ridolfi/hak/read_additional_species.tgz. This gzipped tar file contains the Fortran routine together with some sample ASCII files and a quick guide on how to compile and run the program.

New method used for computation of Covariance Matrix (CM) and AKs. The computation of the CM and of the AKs is performed using a new method described in RD4. With this new approach, both the CM and AKs are accurate also if the final Levenberg-Marquardt damping parameter is not small.

Optimized convergence criteria. New and optimized convergence conditions are checked in order to reduce the number of iterations. The new convergence criteria are described in RD5.

No constraints for negative VMR. The VMR of the retrieved profiles is not constrained to be positive. This modification was implemented in order to avoid positive biases when performing statistical analysis and long term averaging of VMR profiles.

Bug correction. A problem in the Levenberg-Marquardt loop of pT retrieval was fixed. This correction leads to an increase in the number of convergent pT retrievals.

Measurement Space Solution (MSS). In addition to the usual vertical VMR profiles, the ORM_PDS_V2.0 provides also the so called Measurement Space Solution (MSS). The theoretical basis for the MSS is described in RD6. The ORM_PDS_V2.0 outputs relating to the MSS are distributed by IFAC (not by ESA) because these products are intended only for scientific development purposes, not for operational use. For further instructions on how to use the MSS solution and how to download the data, the reader should refer to RD7. The MSS solution is supplied only for the main MIPAS target gases: H2O, O3, HNO3, CH4, N2O and NO2.

5.3 Information common to both the ORM_PDS_V1.0 and V2.0 datasets

ESA summary reports. The ESA Product Control Service (PCS) provides the users with summary daily reports regarding ORM_PDS products. The reports are available at the following web pages:

- ORM_PDS_V1.0: http://earth.eo.esa.int/pcs/envisat/mipas/reports/daily/Level_2_ORM/
- ORM_PDS_V2.0: http://earth.eo.esa.int/pcs/envisat/mipas/reports/daily/Level_2_ORM_V2/

These reports specify the time coverage of the ORM_PDS products as well as the behavior of several key parameters characterizing the L2 retrievals. Although the sets of L1b measurements processed with the ORM_PDS_V1.0 and V2.0 are identical, there is no exact one-to-one correspondence between the L2 products Version 1.0 and 2.0. In fact the ORM_PDS processor Version 2.0 is generally more stable than Version 1.0, therefore, as it will be shown below, the V.2.0 processor is able to recover also a few difficult / anomalous situations in which the ORM_PDS_V1.0 ends-up with no products generated. The above mentioned summary reports do not include information regarding the additional species retrieved by the ORM_PDS_V2.0.

Product Format and Tools The new MIPAS Level 2 products have an updated format. The updated Product Specification that accounts for the new format is RD8. The BEAT Software version 6.3.0 has been aligned to the new specification. This tool can be downloaded from the following link: http://www.stcorp.nl/beat/. The BEAT data dictionary corresponding to the new Level 2 product format can be found at the following link: http://www.stcorp.nl/beat/documentation/codadef/ENVISAT_MIPAS/products/MIP_NL__2P_v2.html. The latest Enviview version (2.8.1) is aligned to the new Level 2 MIPAS products format. This version can be downloaded from the following link: http://envisat.esa.int/enviview/enviviewdownload.html

Download of the ORM_PDS Level 2 datasets. The ORM_PDS L2 data can be downloaded from the following ESA ftp server: ftp-ops-dp.eo.esa.int. The reader should contact Dr. Thorsten Fehr (Thorsten.Fehr[at]esa.int) at ESA-ESRIN to obtain the login credentials.

6 Performance analysis

In this report we include only a preliminary analysis of performance and quality of the Level 2 datasets produced with the ORM_PDS_V1.0 and V2.0 processors. Routine analysis of the quality of these products will however continue as part of the normal QWG activities. In particular, a comprehensive characterization of the error components associated with these products will be an output of the extensive and still ongoing geophysical validation activities. In this report we focus on the following four aspects relevant for the characterization of the products quality.

- Statistics of the normalized chi-square. We define chi-square (CHI2) the summation of the squared residuals (observed minus simulated spectrum) weighted with the inverse CM of the measurement noise. We define “normalized chi-square” (CHI2N) the chi-square divided by the number of degrees of freedom of the retrieval, i.e. the number of observed data points used for the inversion, minus the number of retrieved parameters. The expectation value for CHI2N is 1. Therefore, the study of the obtained statistical distribution of CHI2N provides insight regarding the capability of the forward model internal to the retrieval of simulating the observed spectra for varying atmospheric conditions along the orbit. In practice, CHI2N is a proxy useful for identification and characterization of the systematic errors of the retrieval.

- Computation time / number of iterations. The ORM_PDS_V2.0 processor uses renewed convergence criteria with respect to V1.0. The performance of the new criteria is to be assessed. In particular, we have to assess the computing time savings and verify the impact on the minimum CHI2N achieved. Assessing the computing time savings is not straightforward because, globally, due to additional tasks such as retrieval of additional species and calculation of the MSS, the ORM_PDS_V2.0 computation time is approximately a factor of 3 greater than that of the ORM_PDS_V1.0. For this reason, for the evaluation of the efficiency of the new convergence criteria we focus on the behavior of the number iterations required to reach the convergence. The calculation of the MSS will not be included in the routine ESA retrievals, therefore, in that case, the computing time will be roughly proportional to the number of iterations.

- Analysis of tangent height corrections. A preliminary inspection of the ESA summary reports mentioned in Sect. 5.3, highlighted that the tangent height corrections derived by the ORM_PDS processors are by far larger than those obtained from the IPF processor when Full-Resolution (FR) MIPAS measurements are analyzed. Since such a large degradation of the MIPAS elevation pointing is not expected, an investigation was carried-out to understand the cause of the large height corrections obtained with the ORM_PDS.
- Consistency with the Full-Resolution MIPAS measurements. Due to the changed spectral resolution, the retrievals from OR measurements use different spectral intervals (microwindows, MWs) compared to the retrievals from FR measurements acquired in the first two years of MIPAS operations (from July 2002 to March 2004). Different MWs imply different systematic errors in the retrieved profiles, therefore a systematic difference may exist between the FR and OR datasets. For use of MIPAS L2 products in scientific applications this difference must be carefully assessed.

The first two aspects listed above are dealt with in sub-section 6.1. The third and fourth aspects are discussed in sub-sections 6.2 and 6.3 respectively.

6.1 Statistics of normalized chi-square and number of iterations

In Figures from 1 to 11 we report the histograms of the final CHI2N obtained in the retrievals. Each of the figures refers to a specific target quantity retrieved and consists of four plots. Each plot refers to a measurement mode: NOM (top left), UTLS1 (top right), MA (bottom left) and UA (bottom right). The vertical retrieval ranges of HNO3 and ClONO2 overlap very little with the vertical scanning range of the UA mode, therefore these species are not retrieved in the UA mode. When applicable, in each plot we show the histograms of both ORM_PDS_V1.0 (green line) and V2.0 (blue line) retrievals. The additional species (N2O5, ClONO2, F11 and F12) are retrieved only by version 2.0 of the ORM_PDS, therefore the histograms relating to ORM_PDS_V1.0 do not exist for these species. The height of the histogram bars represents the relative frequency, i.e. the number of samples with value within the bin divided by the total number of samples. The plot key reports the value of some quantifiers relevant for the characterization of the CHI2N distribution, namely: the number of samples (SIZE), the average (AVG) and the standard deviation (ST.DEV). These quantifiers are evaluated after removal of the few outliers with CHI2N > 7.0. The plot key reports also the percentage of non-converging retrievals over the total number of retrievals, i.e. without removal of outliers. Note that we consider as “anomalous” or “lost” the retrievals with CHI2N > 7.0. This is why for the calculation of AVG and ST.DEV we first remove these outliers. AVG and ST.DEV should quantify the position and the width of the main lobe of the CHI2N distribution, we do not want them to be influenced by a few outlying samples with too large and anomalous values.
Given the large size of the samples considered, the histograms provide a realistic representation of the CHI2N statistical distributions. For this reason the terms “histogram” and “statistical distribution” or simply “distribution” are considered equivalent in this document.

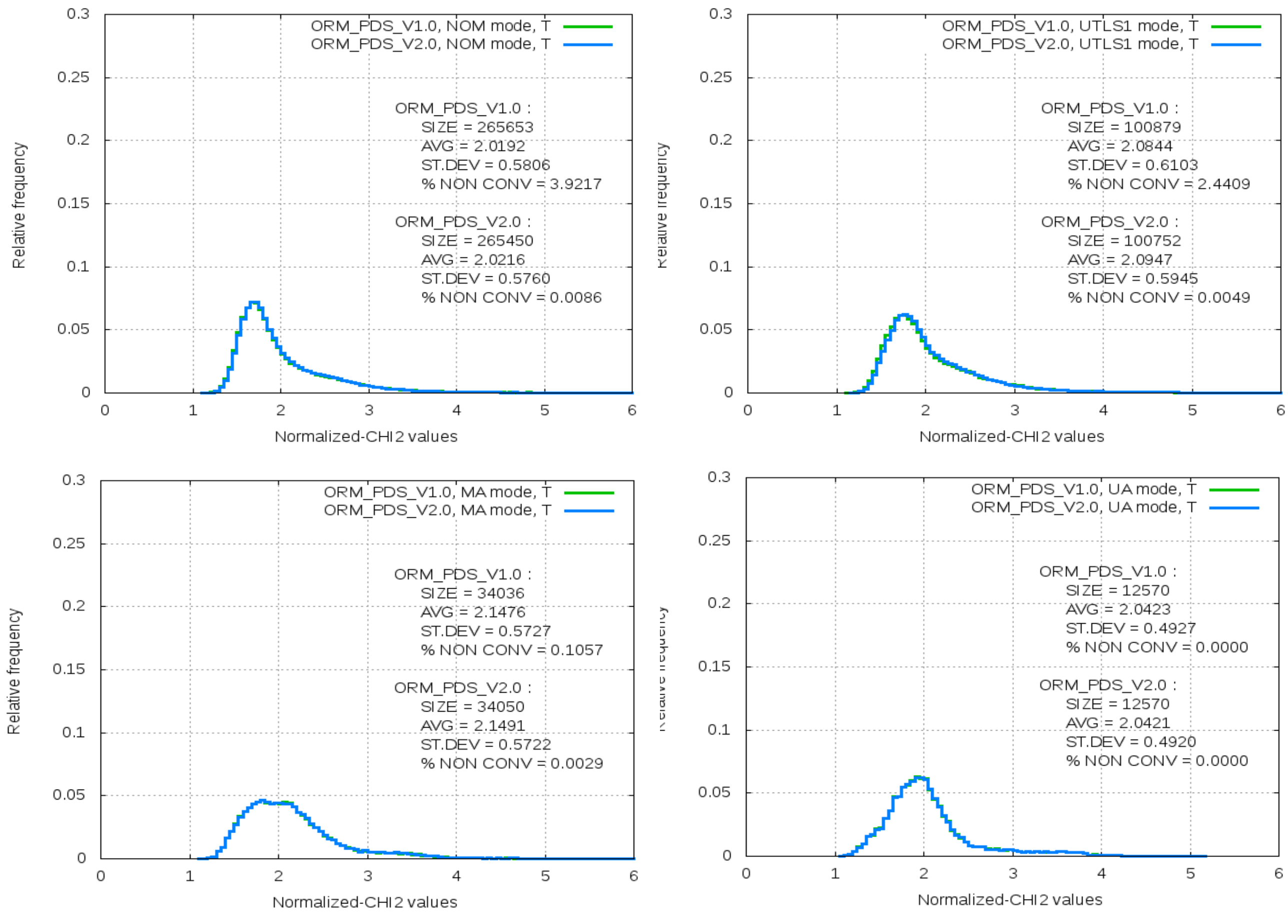


Figure 1: Histograms of the final CHI2N obtained in Temperature retrievals from NOM (top left), UTLS1 (top right), MA (bottom left) and UA (bottom right) retrievals. The green curve (exactly matching the blue curve in this case) refers to ORM_PDS_V1.0 retrievals, while the blue curve refers to ORM_PDS_V2.0 retrievals.

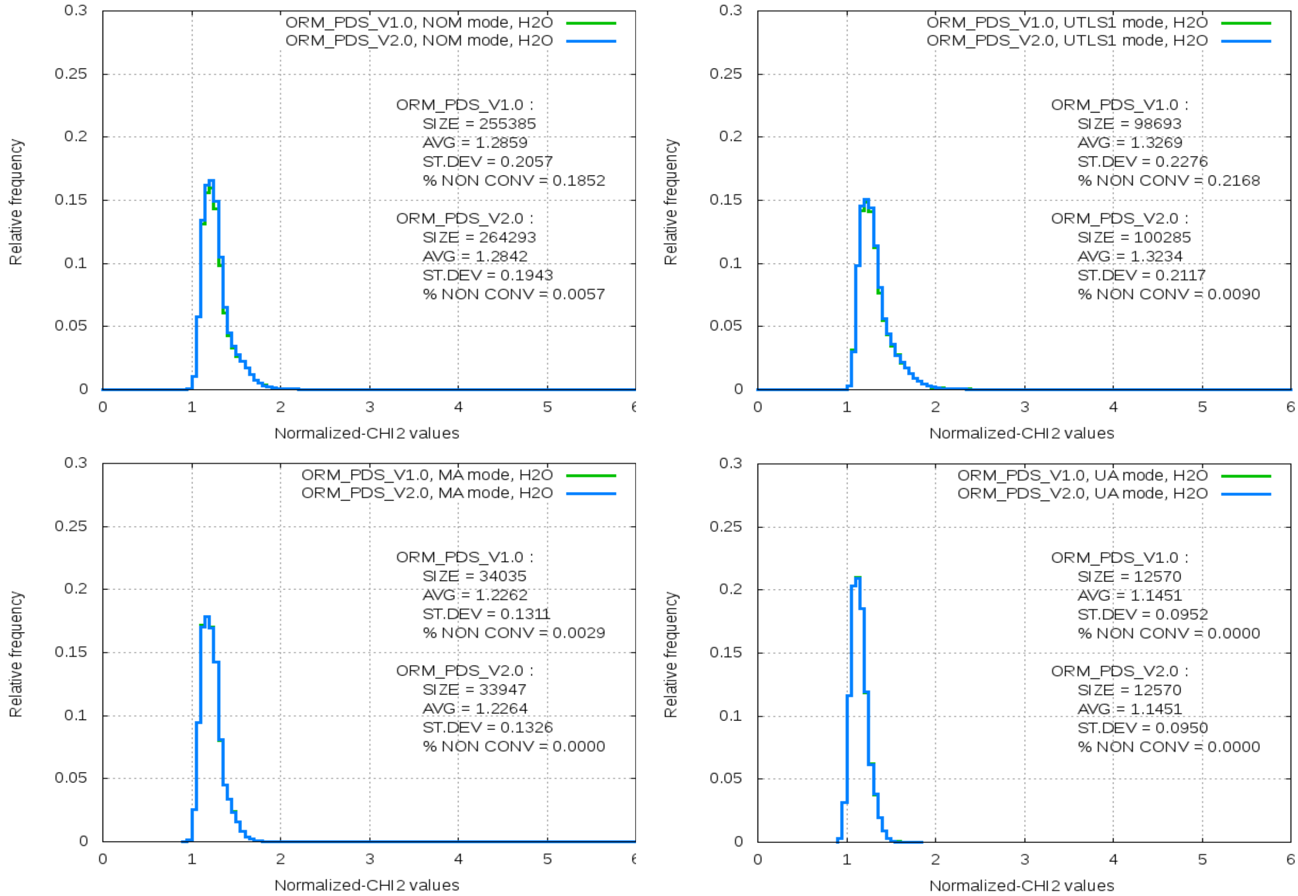


Figure 2: Same as Figure 1 but relating to H2O retrievals.

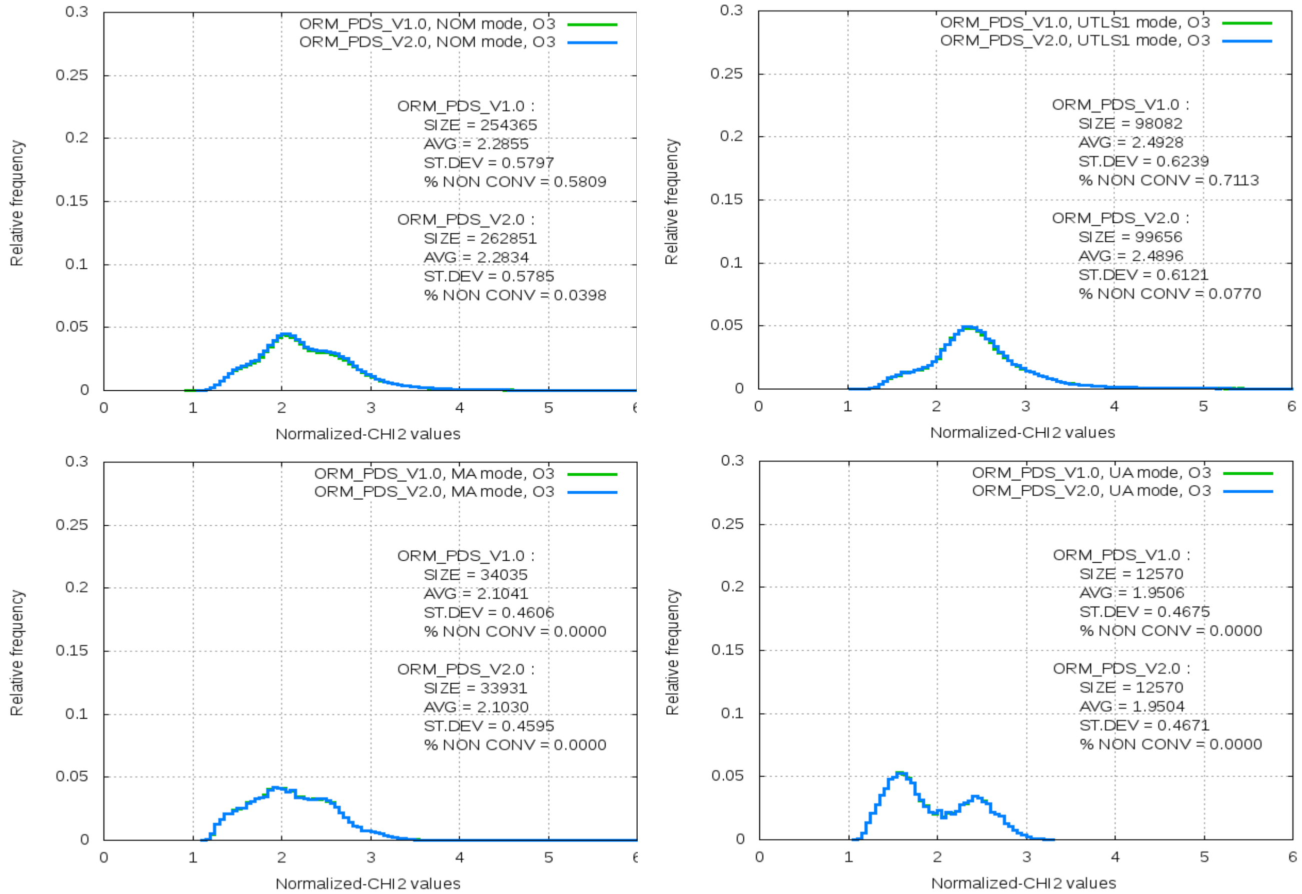
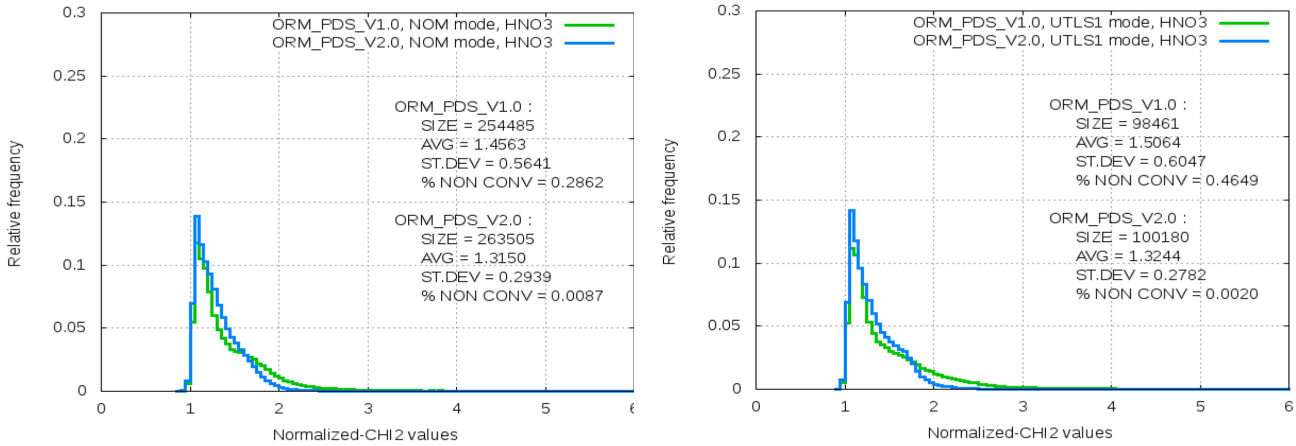


Figure 3: Same as Figure 1 but relating to O3 retrievals.



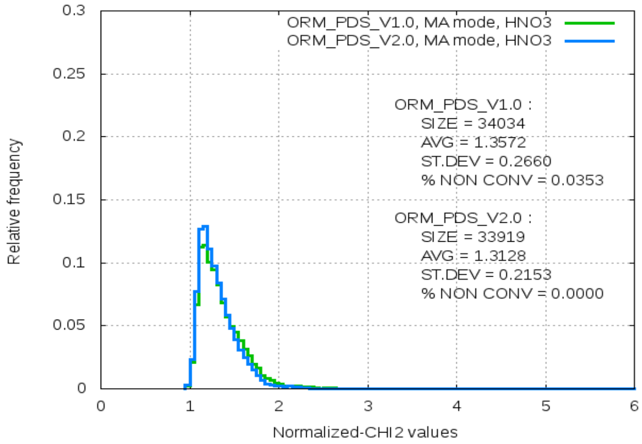


Figure 4: Same as Figure 1 but relating to HNO3 retrievals. Note that in this case the CHI2N distributions for ORM_PDS_V1.0 and V2.0 are slightly different (the green curve is now visible). Note also that HNO3 is not retrieved from UA measurements (the bottom right plot is missing).

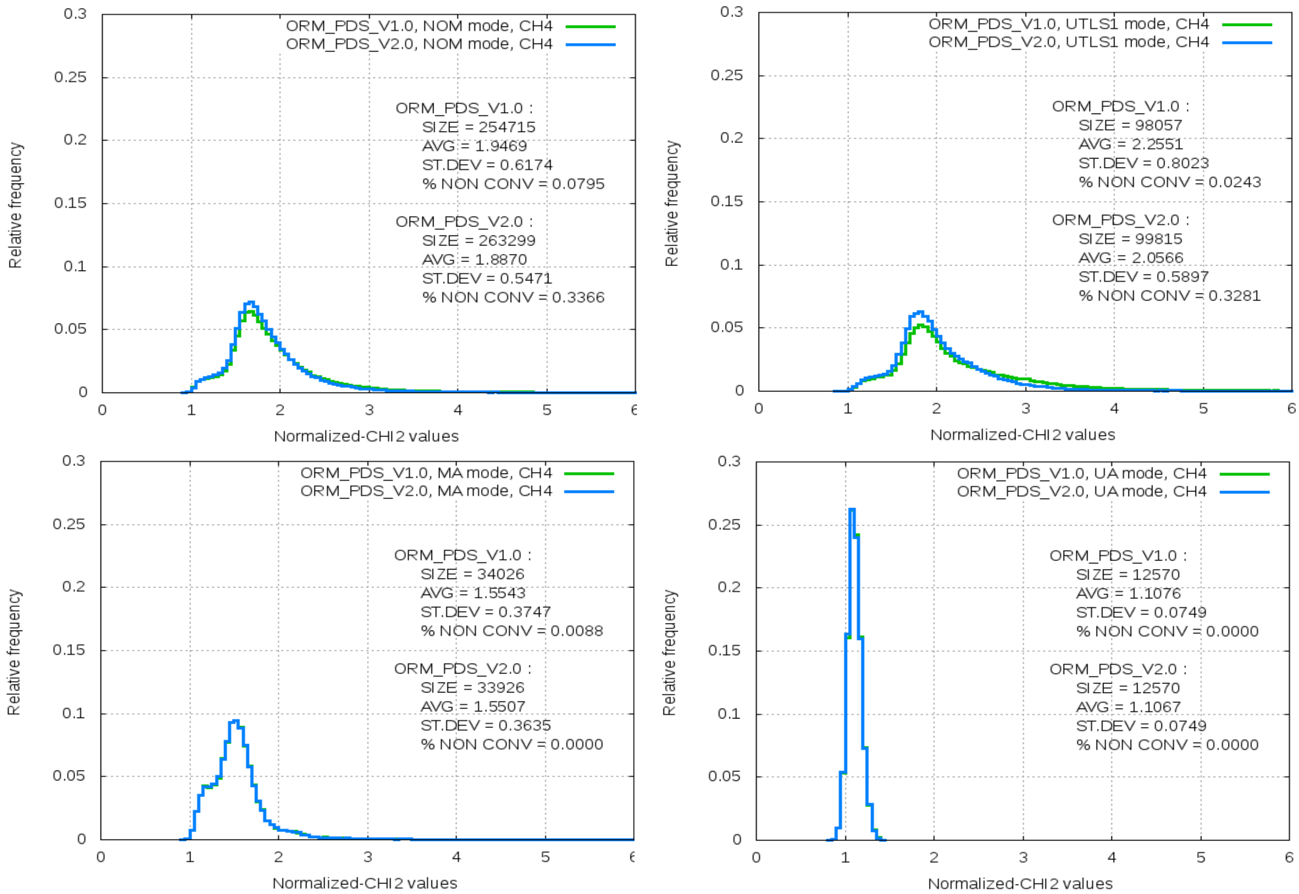


Figure 5: Same as Figure 1 but relating to CH4 retrievals.

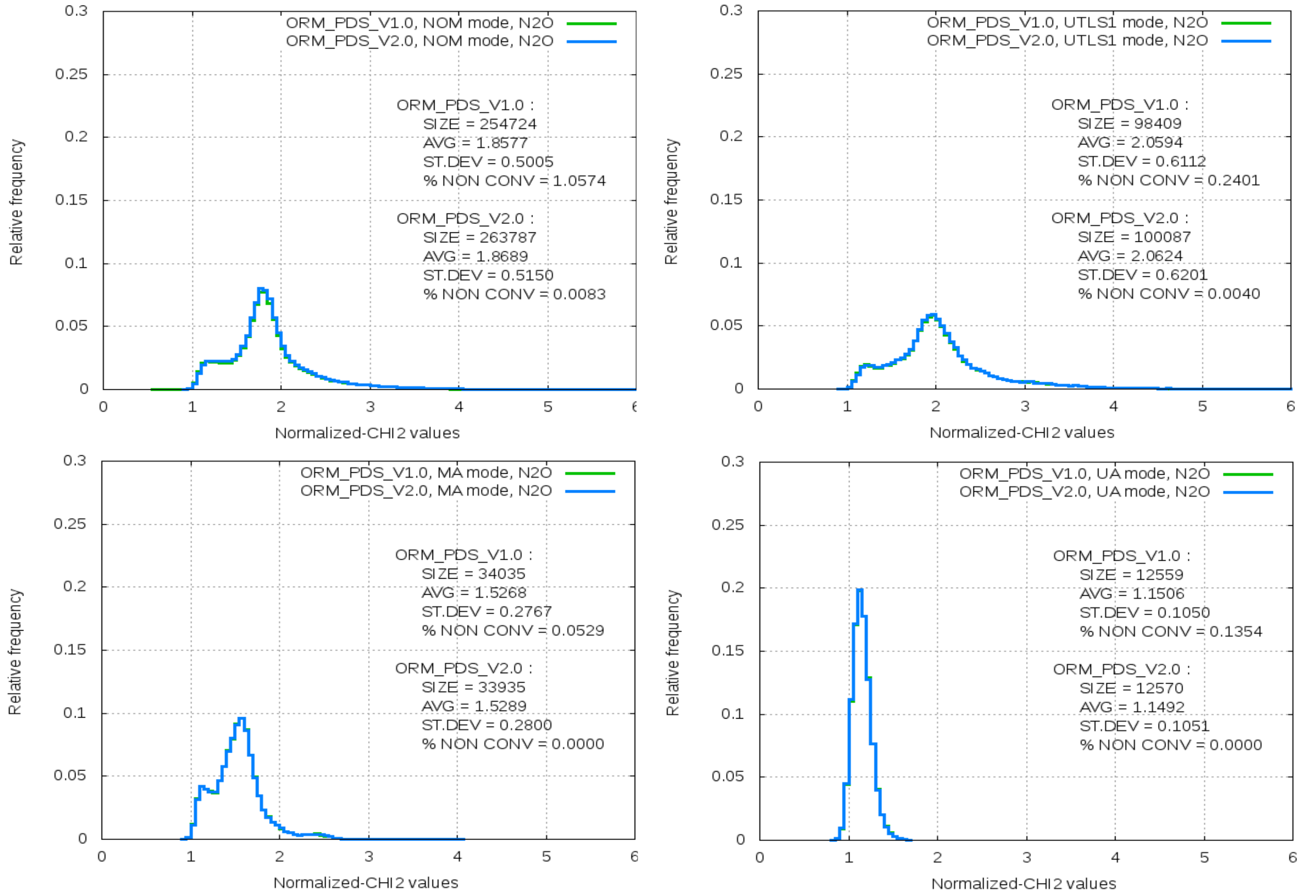


Figure 6: Same as Figure 1 but relating to N2O retrievals.

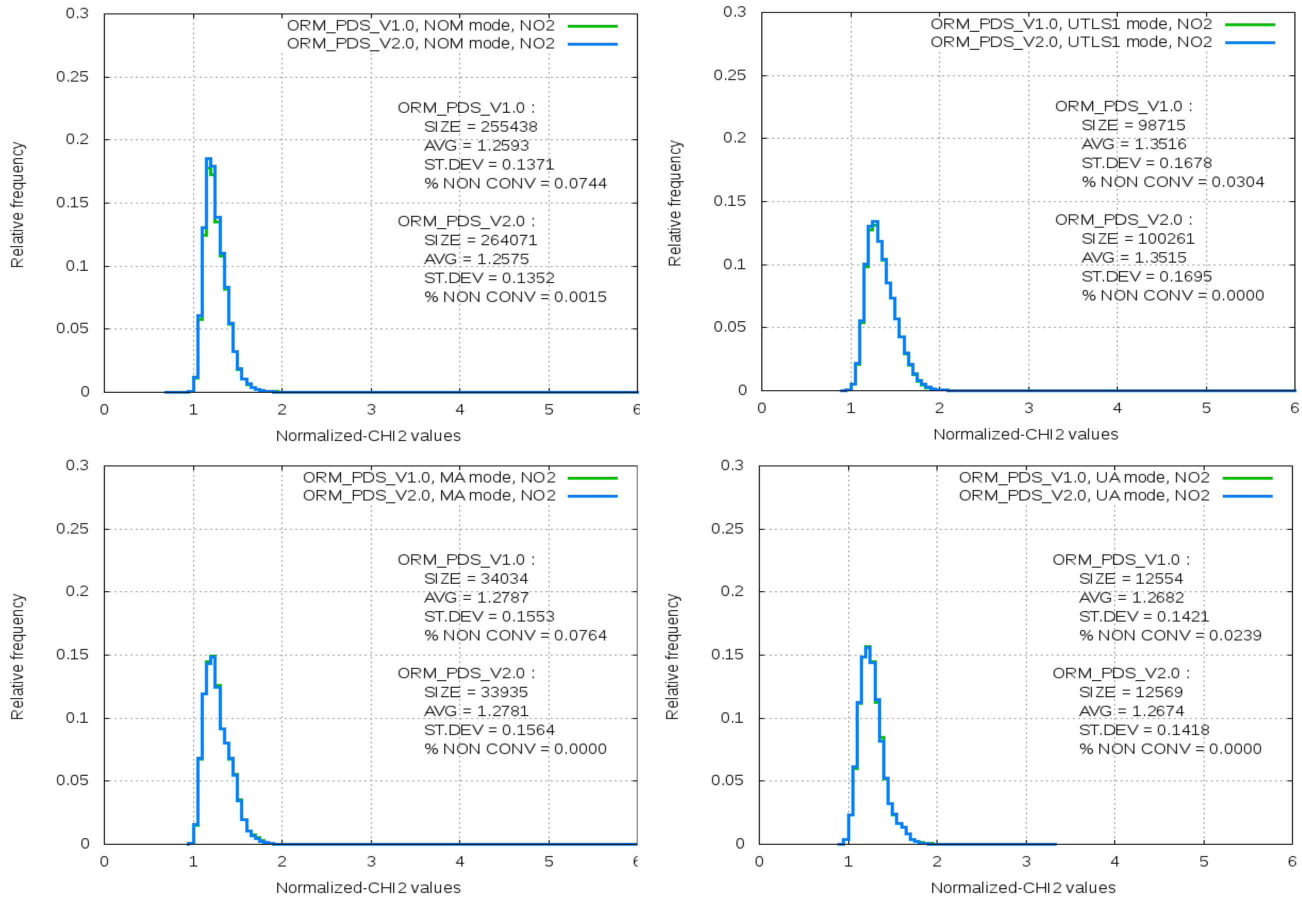


Figure 7: Same as Figure 1 but relating to NO2 retrievals.

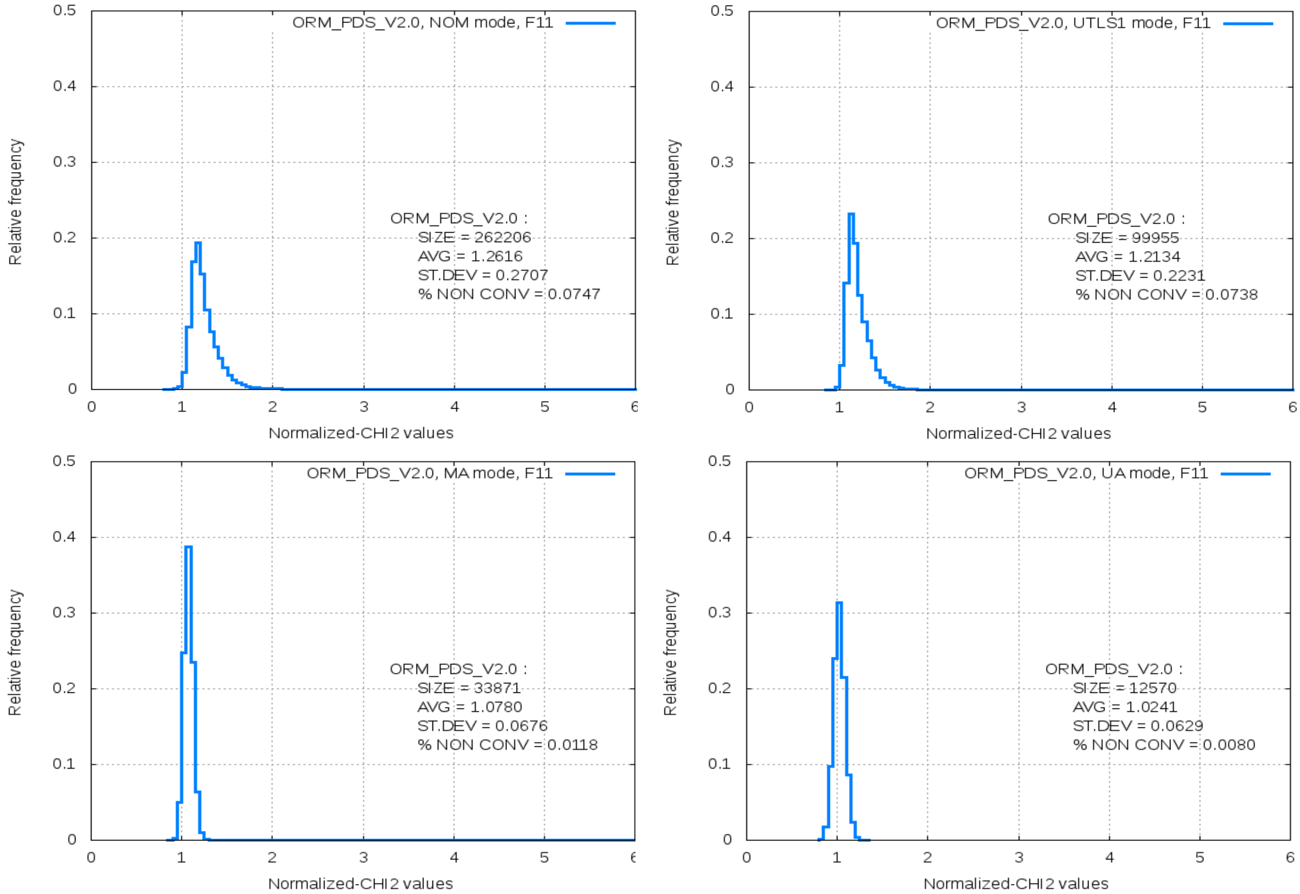


Figure 8: Same as Figure 1 but relating to F11. F11 is retrieved only in ORM_PDS_V2.0.

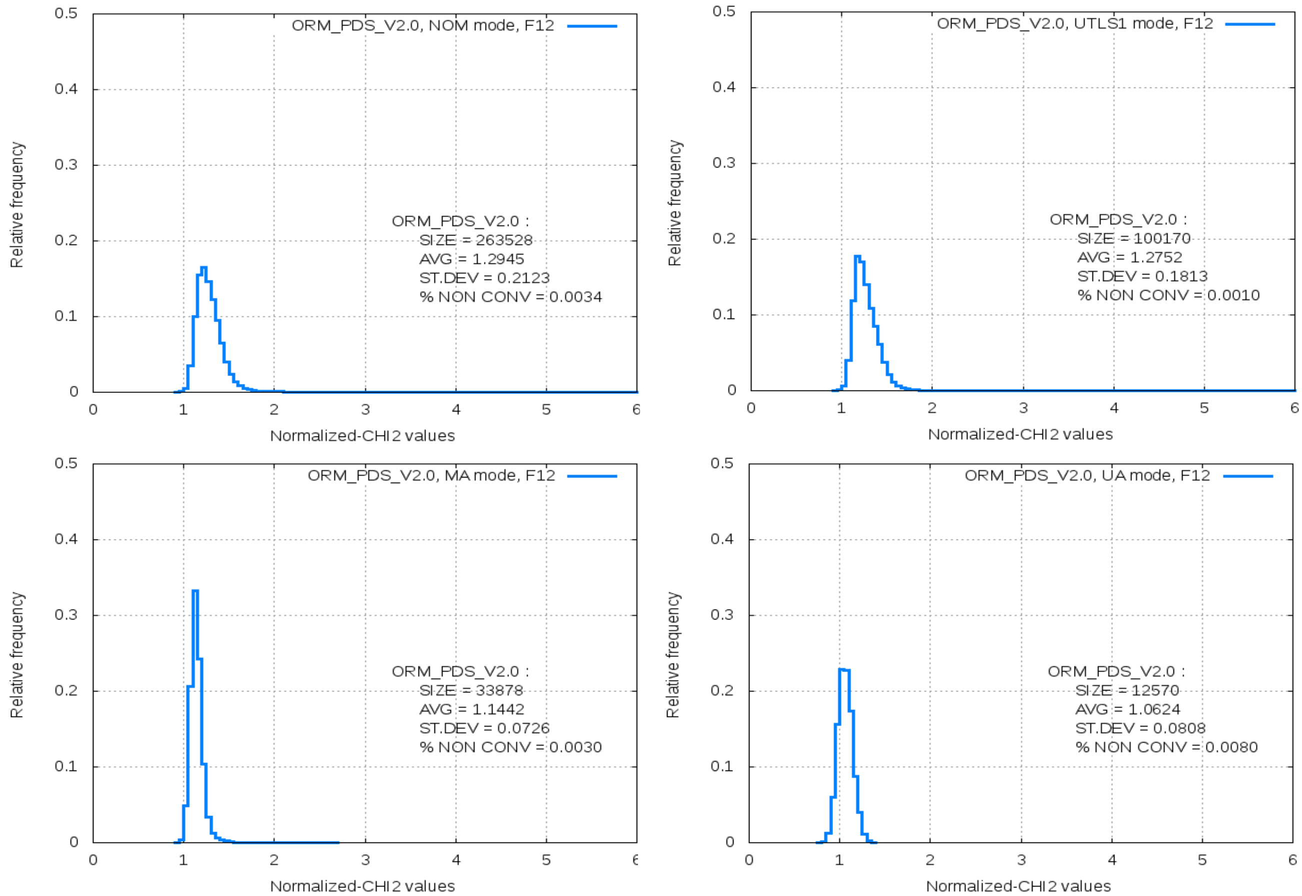


Figure 9: Same as Figure 1 but relating to F12. F12 is retrieved only in ORM_PDS_V2.0.

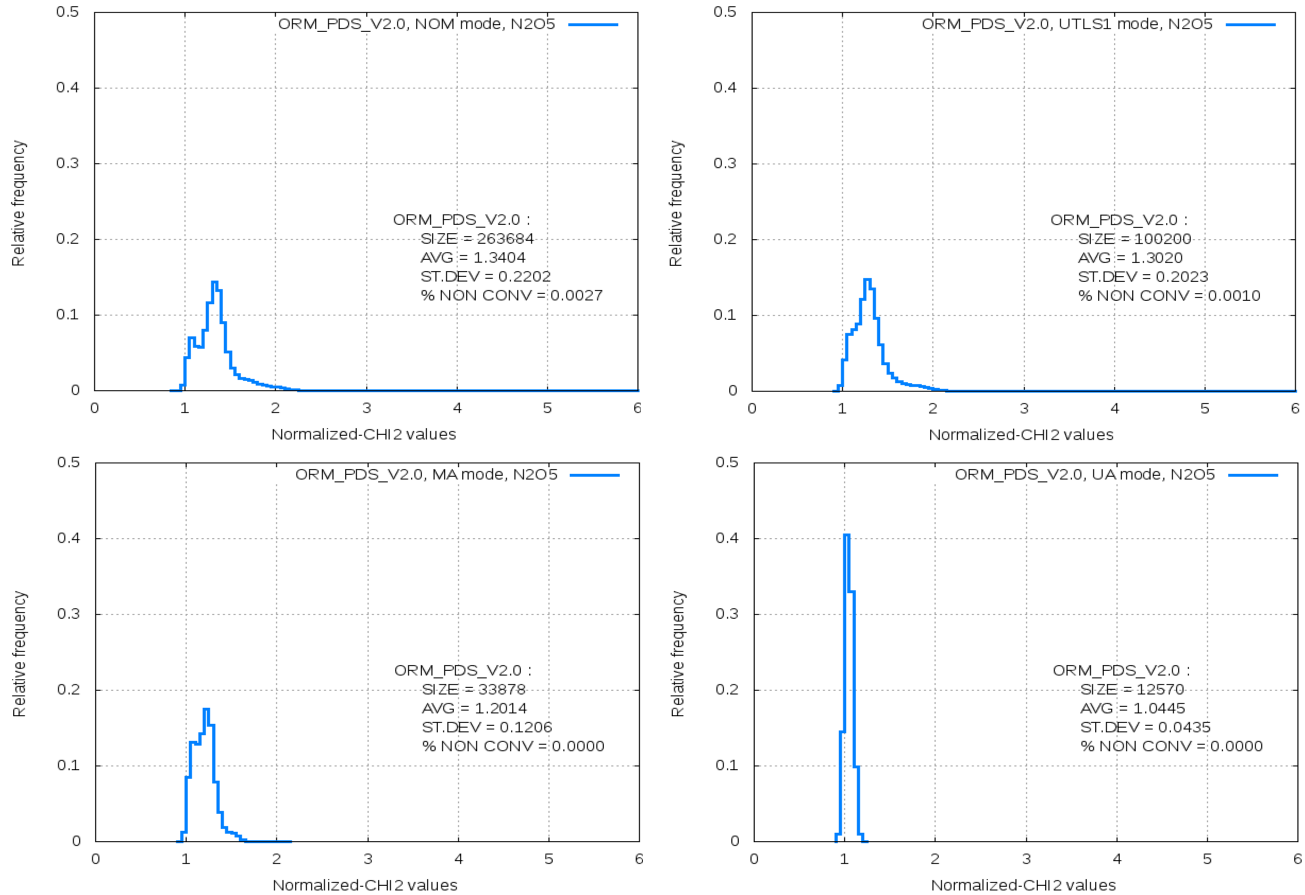
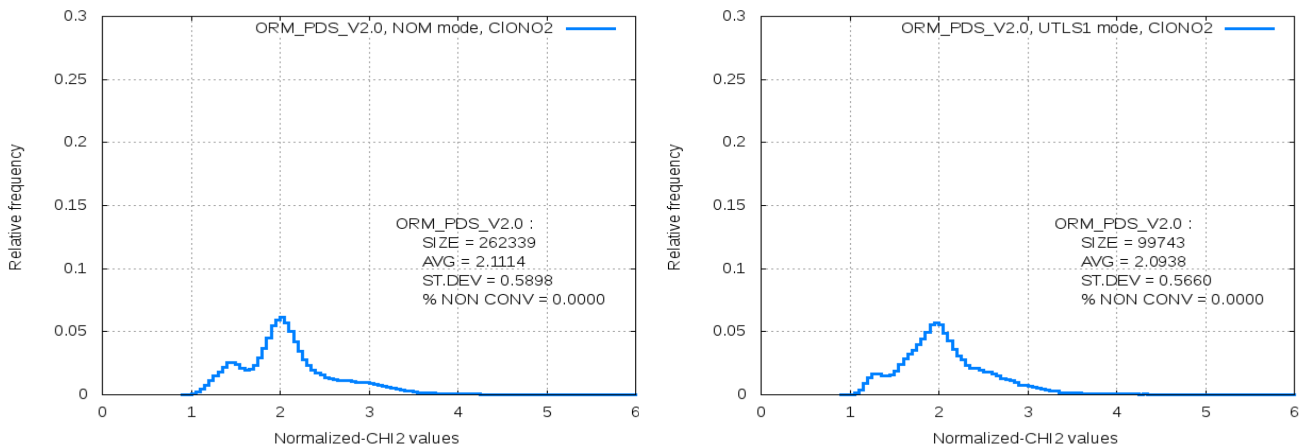


Figure 10: Same as Figure 1 but relating to N2O5. N2O5 is retrieved only in ORM_PDS_V2.0.



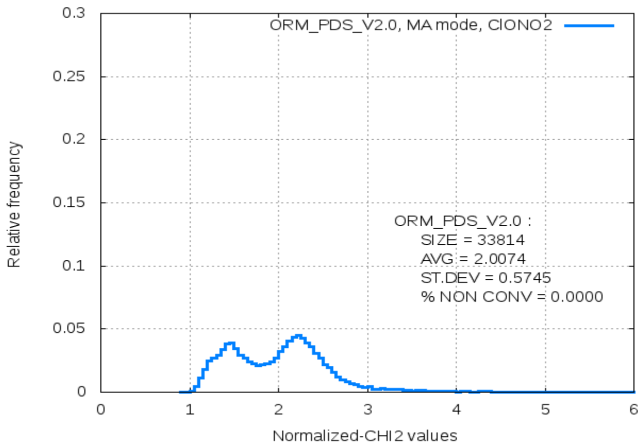


Figure 11: Same as Figure 1 but relating to ClONO2 retrievals. Note that ClONO2 is retrieved only in Version 2 of the ORM_PDS and not from the UA measurements (the bottom right plot is missing).

To ease the discussion of the results, in Table 1 we report both the vertical scan range for the various MIPAS measurement modes as well as the vertical retrieval range used for the various targets of the retrieval. Note that:

- As mentioned earlier, both HNO3 and ClONO2 are not retrieved from UA measurements because of the too small overlap between the retrieval and the measurement ranges.
- At the time of the ORM_PDS retrievals the OMs for UTLS1, MA and UA modes were available only for the main MIPAS targets. The OMs required for the ORM_PDS_V2.0 retrievals of the additional species (F11, F12, N2O5 and ClONO2) from UTLS1, MA and UA modes were generated manually, by extending the corresponding OMs calculated by Oxford University for the NOM mode.
- At the time of the ORM_PDS processing, the Oxford-supplied OMs for the UA retrievals of the main targets incidentally contained a mistake: the retrievals were starting from 45 km instead of 42 km that is the lowest measured altitude in the UA mode. This error was then incidentally transferred to the UA OMs generated manually for the additional species. These mistakes will be corrected in the OMs that will be used for the IPF V6.0 processing.

Measurement mode	Vertical range of measurements (km)
NOM	6 – 70 (FLOATING)
UTLS1	5.5 – 49 (FLOATING)
MA	18 – 102 (FIXED)
UA	42 – 172 (FIXED)

Target parameter of the retrieval	Vertical retrieval range (km) in the various measurement modes			
	NOM	UTLS1	MA	UA
pT	6 – 70	5.5-49	18-69	45-69
H2O	6 – 70	5.5-49	18-69	45-69
O3	6 – 70	5.5-49	18-69	45-69
HNO3	9 – 43	8.5-49	18-42	
CH4	6 – 70	5.5-49	18-69	45-69
N2O	6 – 58	5.5-49	18-57	45-63
NO2	25 – 70	25-49	24-69	45-69
F11	6 – 34	5.5 – 49	18 – 69	45 – 69
F12	6 – 40	5.5 – 49	18 – 69	45 – 69
N2O5	15 – 46	14.5–49	18 – 69	45 – 69
ClONO2	13.5-43	13-49	18-51	

Table 1: vertical range of the MIPAS measurement modes (left) and vertical ranges used for the retrieval of the various targets (right).

In Table 2 we report some additional quantifiers useful to evaluate the performance of the ORM_PDS retrievals. For each retrieval target (first column) and measurement mode (second column) we report for both V1.0 and V2.0 retrievals: the total number of retrieved profiles (NTOT_PROF, 3rd and 4th columns), the percentage of these profiles for which the retrieval terminates with convergence not fulfilled (%_NON_CNV, 5th and 6th columns), the number of retrievals terminating with CHI2N > 7.0 (considered outliers, N_CHI2N > 7.0, in the 7th and 8th columns), the average number of total (macro + micro) iterations (AVG_TOT_ITER, in the 9th and 10th columns) and the average CHI2N achieved (AVG_CHI2N in the 11th and 12th columns). The values of both AVG_CHI2 and %_NON_CNV reported in Table 2 coincide with the values reported in the plots key of Figures 1 to 10. The green / red cells of Table 2 highlight the situations in which V2.0 retrievals provide better / worse performance compared to V1.0.
Note that:

- if a retrieval terminates due to "too many Marquardt iterations" no output profile is generated, therefore this retrieval is not counted among the NTOT_PROF.
- If a pT retrieval terminates with final CHI2N > 5.0 then the ORM_PDS_V2.0 does not proceed with the subsequent VMR retrievals from the same scan. This explains why e.g. for the V2.0 VMR profiles from MA measurements NTOT_PROF is significantly less than that for V1.0. Of course this is not an indication of bad functioning of V2.0 retrievals, it means only that pT retrievals with CHI2N > 5.0 are not discarded in the V1.0 processing.

Target	Mode	NTOT_PROF		%_NON_CNV		N_CHI2N > 7.0		AVG_TOT_ITER		AVG_CHI2N	
		V1.0	V2.0	V1.0	V2.0	V1.0	V2.0	V1.0	V2.0	V1.0	V2.0
pT	NOM	265878	265902	3.9217	0.0086	225	452	3.823	3.309	2.0192	2.0216
	UTLS1	101191	101092	2.4409	0.0049	312	340	3.089	2.811	2.0844	2.0947
	MA	34071	34071	0.1057	0.0029	35	21	1.572	1.526	2.1476	2.1491
	UA	12570	12570	0.0000	0.0000	0	0	1.246	1.246	2.0423	2.0421
H2O	NOM	255445	264324	0.1852	0.0057	60	31	2.797	2.378	1.2859	1.2842
	UTLS1	98721	100294	0.2168	0.0090	28	9	2.673	2.290	1.3269	1.3234
	MA	34035	33947	0.0029	0.0000	0	0	1.051	1.039	1.2262	1.2264
	UA	12570	12570	0.0000	0.0000	0	0	1.035	1.029	1.1451	1.1451
O3	NOM	254796	263508	0.5809	0.0398	431	657	4.028	3.482	2.2855	2.2834
	UTLS1	98416	99983	0.7113	0.0770	334	327	3.965	3.472	2.4928	2.4896
	MA	34035	33935	0.0000	0.0000	0	4	1.102	1.081	2.1041	2.1030
	UA	12570	12570	0.0000	0.0000	0	0	1.045	1.042	1.9506	1.9504
HNO3	NOM	255378	264042	0.2862	0.0087	893	537	3.557	2.386	1.4563	1.3150
	UTLS1	98721	100267	0.4649	0.0020	260	87	3.631	2.086	1.5064	1.3244
	MA	34034	33934	0.0353	0.0000	0	15	1.925	1.208	1.3572	1.3128
CH4	NOM	255437	264101	0.0795	0.3366	722	802	2.957	3.437	1.9469	1.8870
	UTLS1	98715	100265	0.0243	0.3281	658	450	1.769	3.249	2.2551	2.0566
	MA	34035	33935	0.0088	0.0000	9	9	1.524	1.444	1.5543	1.5507
	UA	12570	12570	0.0000	0.0000	0	0	1.078	1.068	1.1076	1.1067
N2O	NOM	255435	264076	1.0574	0.0083	711	289	3.986	3.082	1.8577	1.8689
	UTLS1	98712	100261	0.2401	0.0040	303	174	3.110	2.741	2.0594	2.0624
	MA	34035	33935	0.0529	0.0000	0	0	1.657	1.423	1.5268	1.5289
	UA	12559	12570	0.1354	0.0000	0	0	1.332	1.116	1.1506	1.1492
NO2	NOM	255440	264077	0.0744	0.0015	2	6	1.4625	1.125	1.2593	1.2575
	UTLS1	98715	100261	0.0304	0.0000	0	0	1.126	1.079	1.3516	1.3515
	MA	34034	33935	0.0764	0.0000	0	0	1.274	1.168	1.2787	1.2781
	UA	12554	12569	0.0239	0.0000	0	0	1.129	1.054	1.2682	1.2674
F11	NOM		263702		0.0747		1496		3.118		1.2616
	UTLS1		100204		0.0738		249		3.163		1.2134
	MA		33878		0.0118		7		1.978		1.0780
	UA		12570		0.0080		0		1.440		1.0241
F12	NOM		263703		0.0034		175		2.474		1.2945
	UTLS1		100204		0.0010		34		2.696		1.2752
	MA		33878		0.0030		0		3.049		1.1442
	UA		12570		0.0000		0		2.625		1.0624
N2O5	NOM		263706		0.0027		22		2.458		1.3404
	UTLS1		100204		0.0010		4		2.679		1.3020
	MA		33878		0.0000		0		3.382		1.2014
	UA		12570		0.0000		0		1.405		1.0445
ClONO2	NOM		263703		0.0000		1364		3.381		2.1114
	UTLS1		100203		0.0000		460		3.500		2.0938
	MA		33878		0.0000		64		3.905		2.0074

Table 2: some additional quantifiers useful to evaluate the performance of the ORM_PDS retrieval. See the text for the description of the quantities reported in the various columns of this Table.

The “double-peak” shape of some of the CHI2N histograms of Fig.s 1 – 11 suggests that there could be a sort of “bi-stability” of the retrievals corresponding to the day-night cycle of the measurements. To investigate this possibility we include hereafter in Fig.s from 12 to 22 the cross-correlation plots of CHI2N versus the Solar Zenith Angle (SZA) calculated at the tangent point of the mid-sweep used in each retrieval. The data refer to the ORM_PDS_V2.0 retrievals. Since the statistical distributions of CHI2N for V1.0 and V2.0 retrievals are very similar (see Fig.s 1 – 11), also the cross-correlation plots of CHI2N versus SZA change negligibly from V1.0 to V2.0. For this reason here we are not showing the cross-correlation plots relating to V1.0 retrievals. As usual, in each of these figures the four plots refer to the four measurement modes processed: NOM (top-left), UTLS1 (top-right), MA (bottom-left), UA (bottom-right).

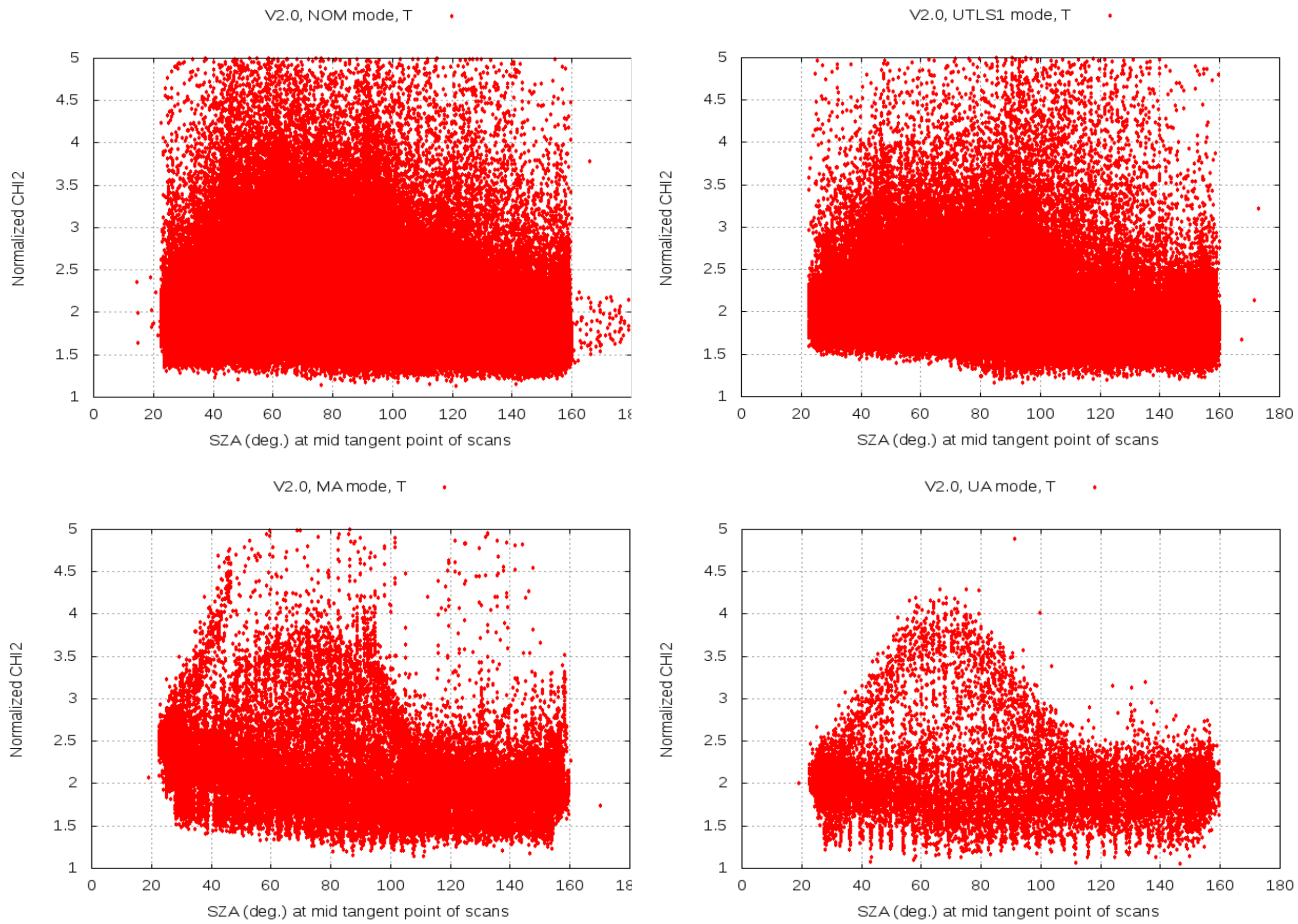


Figure 12: Plots of CHI2N versus SZA in the case of ORM_PDS_V2.0 retrievals of pT. The four plots refer to the four measurement modes processed: NOM (top-left), UTLS1 (top-right), MA (bottom-left), UA (bottom-right).

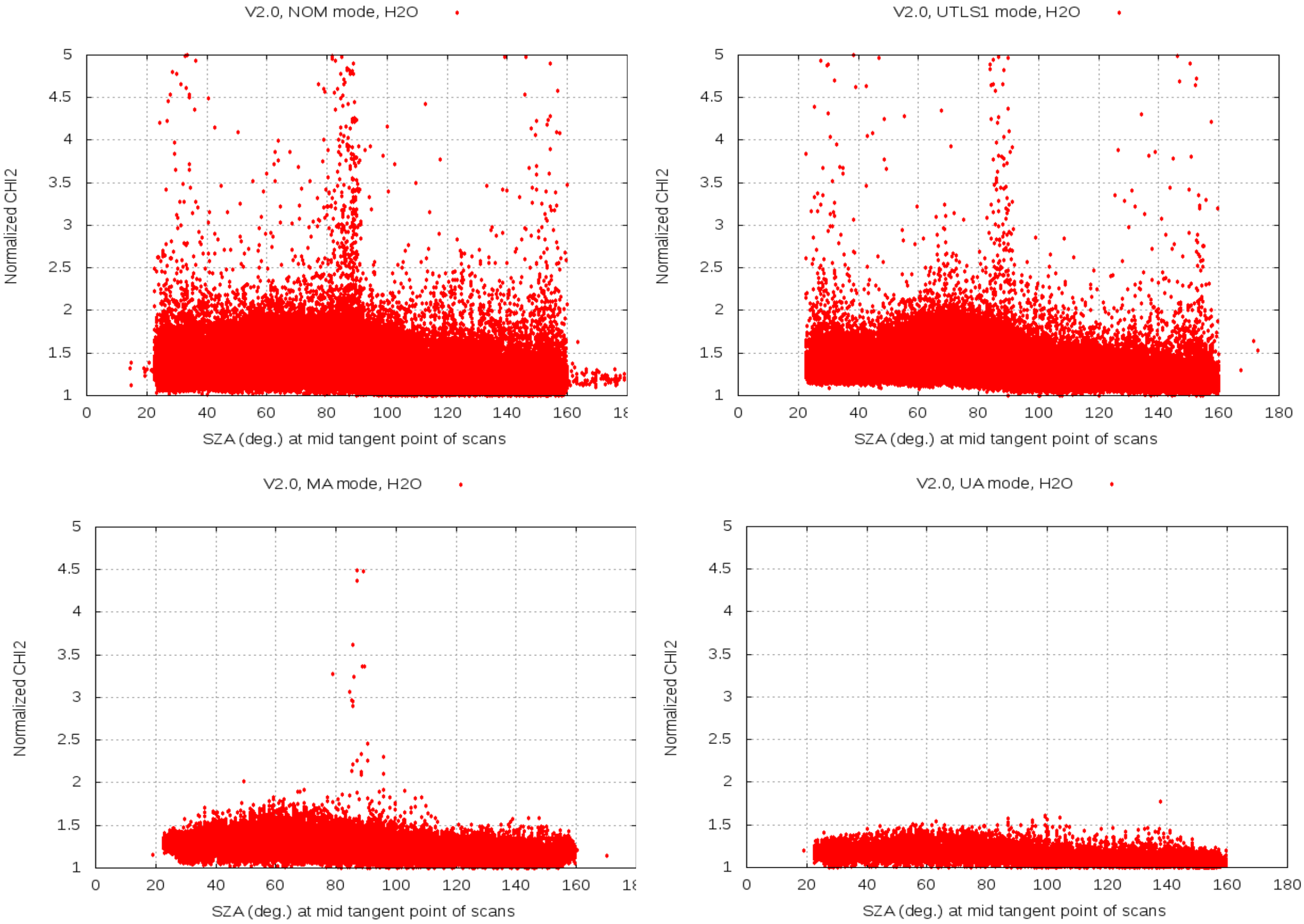


Figure 13: Same as Figure 12 but for ORM_PDS_V2.0 retrievals of H2O.

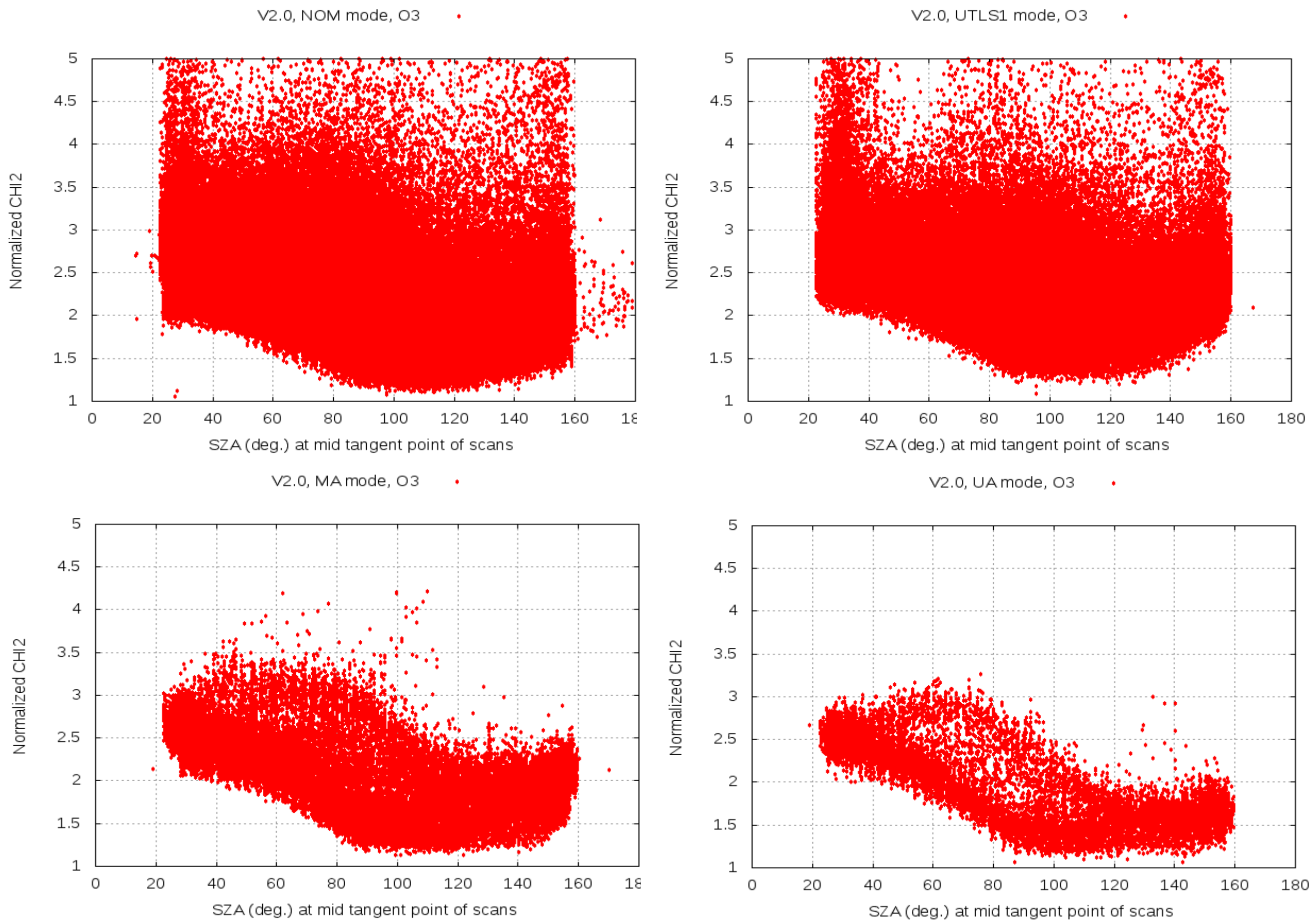


Figure 14: Same as Figure 12 but for ORM_PDS_V2.0 retrievals of O3.

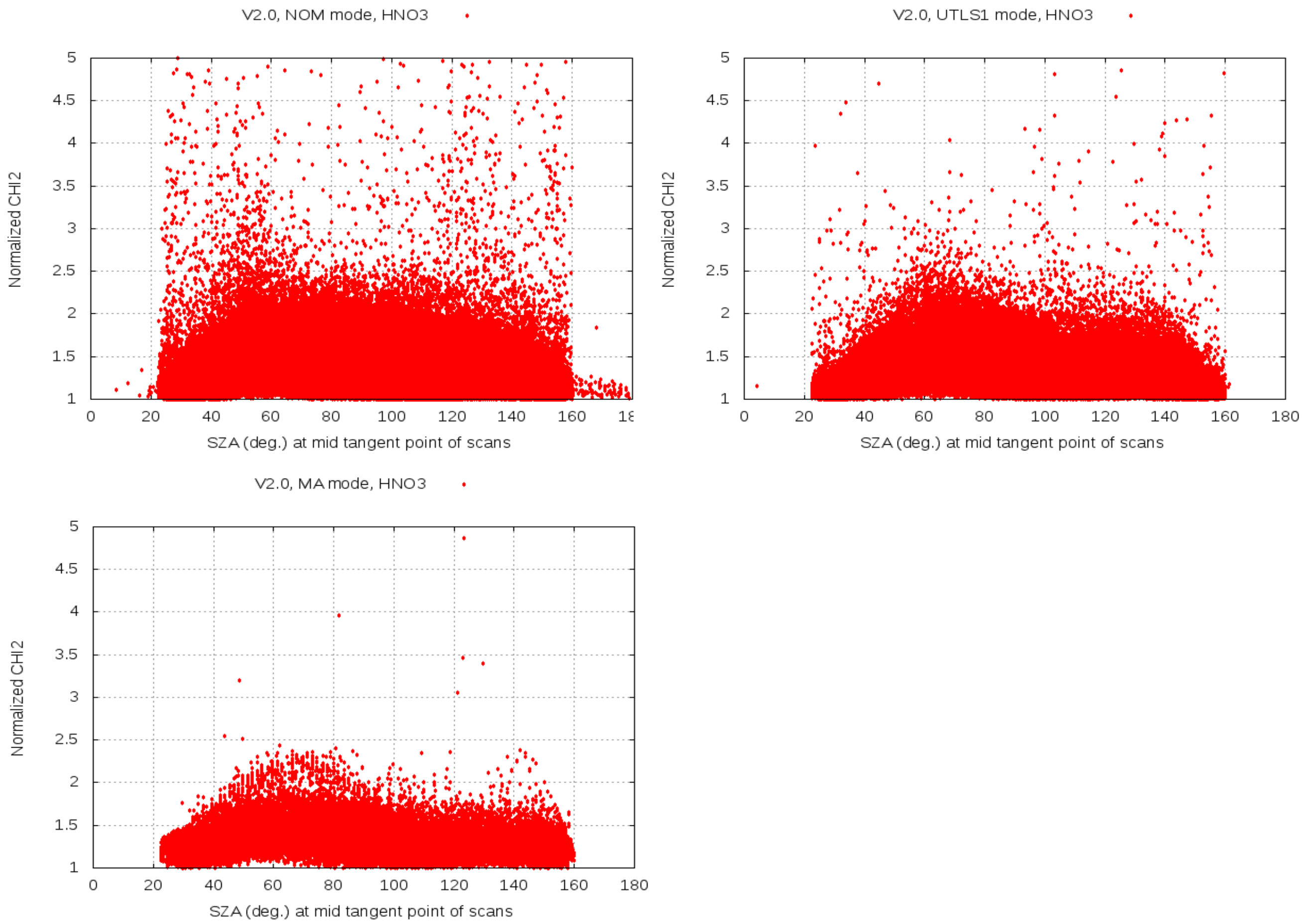


Figure 15: Same as Figure 12 but for ORM_PDS_V2.0 retrievals of HNO3. Remind that HNO3 is not retrieved from UA measurements (the bottom right plot is missing).

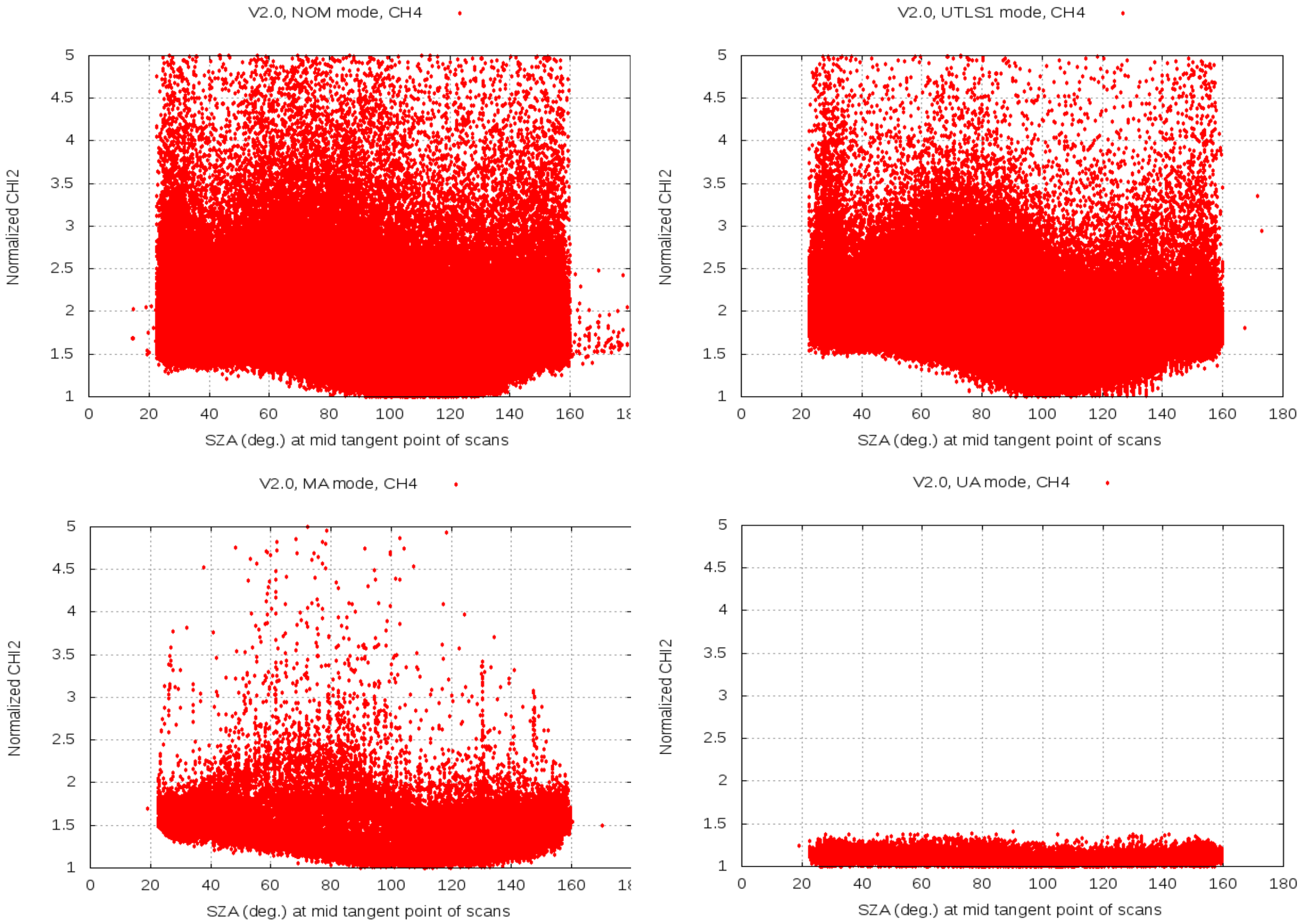


Figure 16: Same as Figure 12 but for ORM_PDS_V2.0 retrievals of CH4.

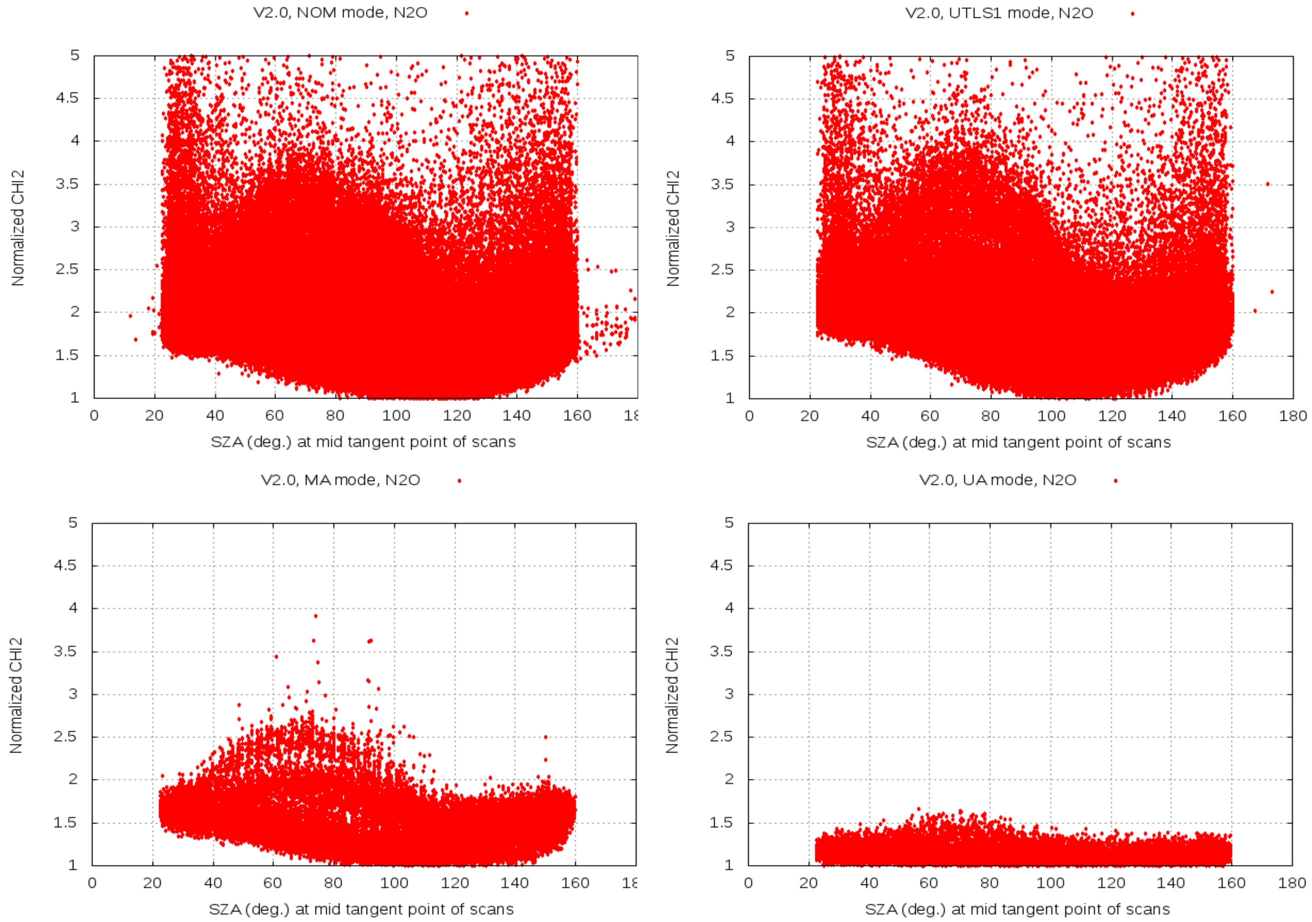


Figure 17: Same as Figure 12 but for ORM_PDS_V2.0 retrievals of N2O.

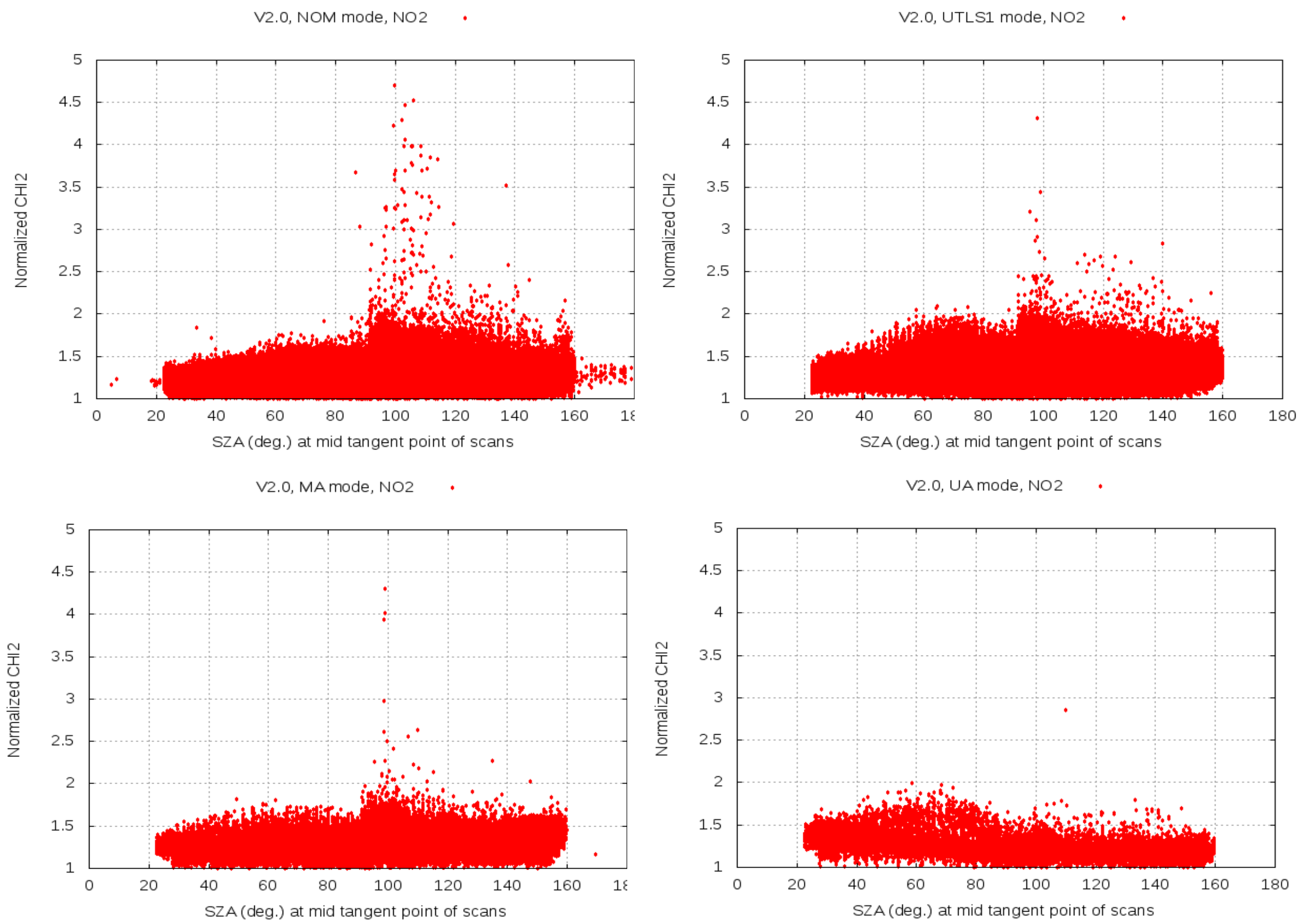


Figure 18: Same as Figure 12 but for ORM_PDS_V2.0 retrievals of NO2.

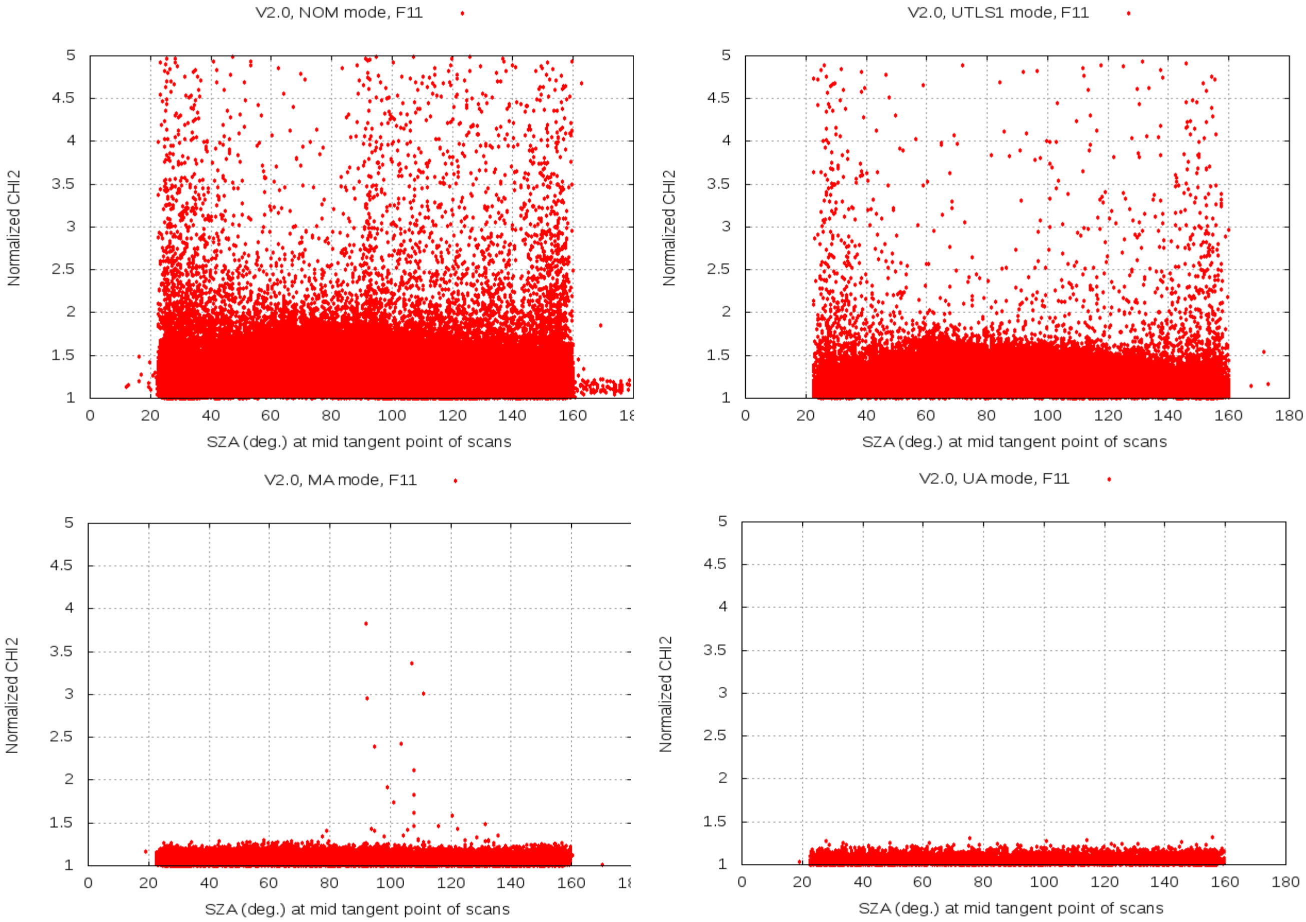


Figure 19: Same as Figure 12 but for ORM_PDS_V2.0 retrievals of F11.

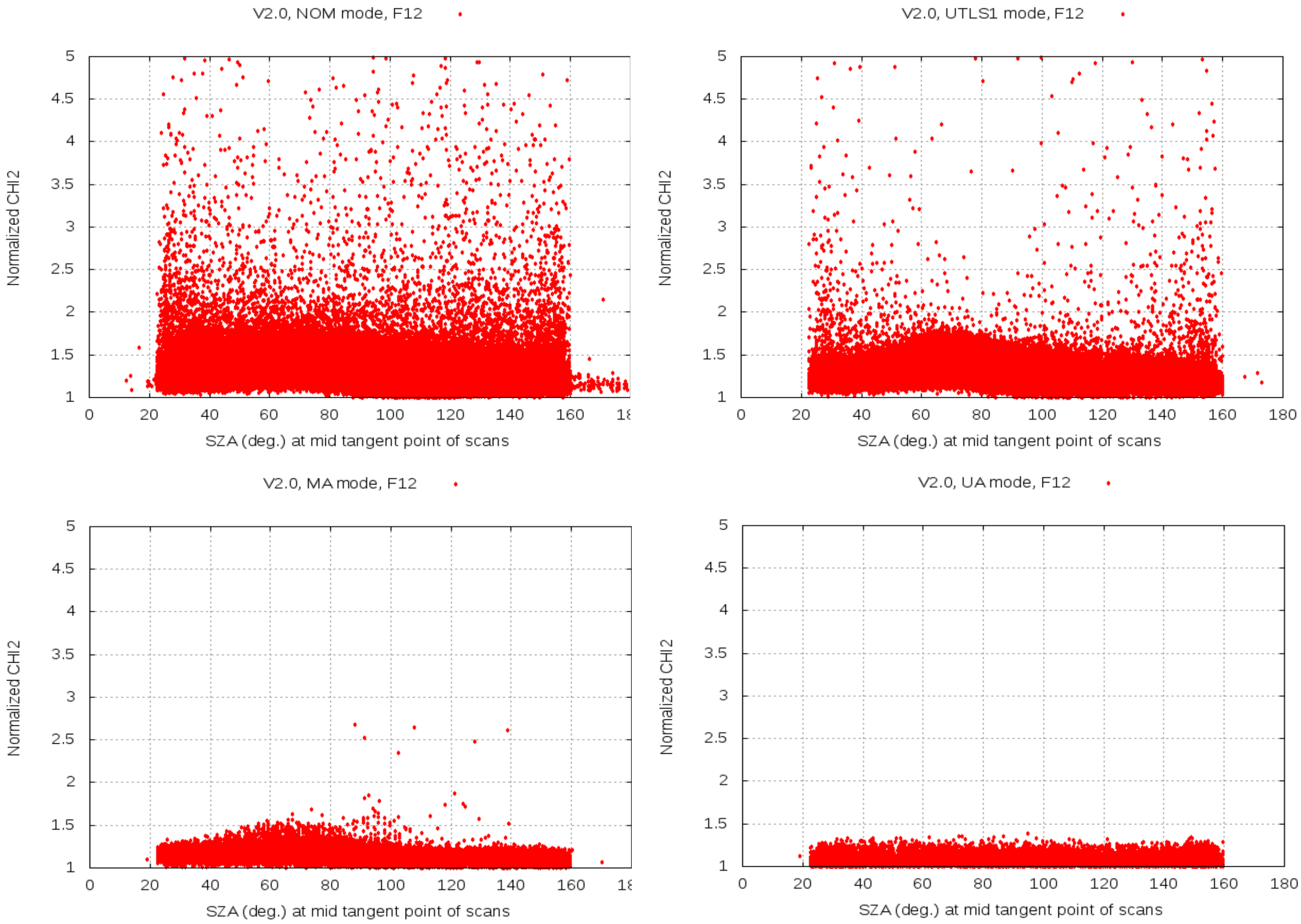


Figure 20: Same as Figure 12 but for ORM_PDS_V2.0 retrievals of F12.

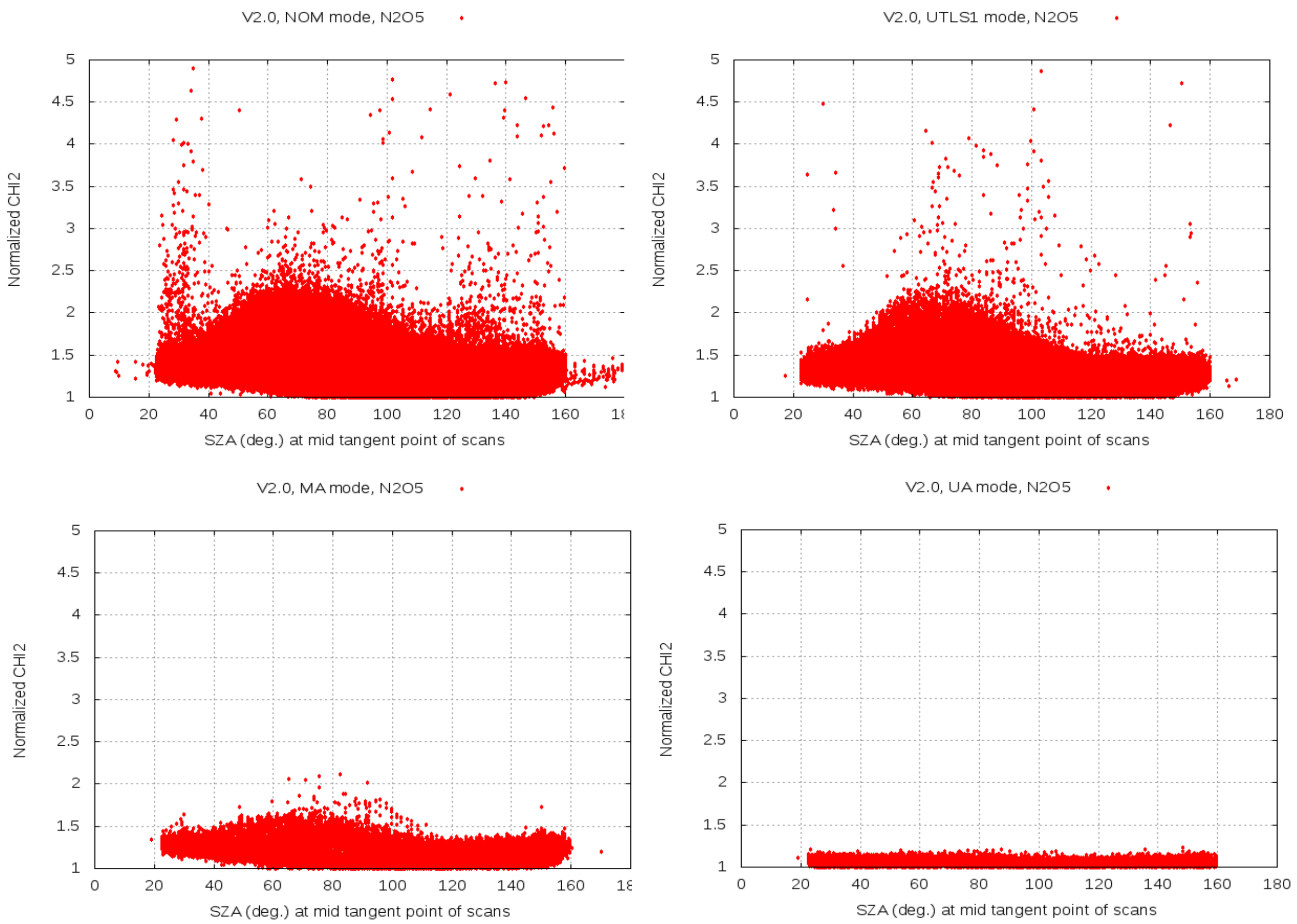


Figure 21: Same as Figure 12 but for ORM_PDS_V2.0 retrievals of N2O5.

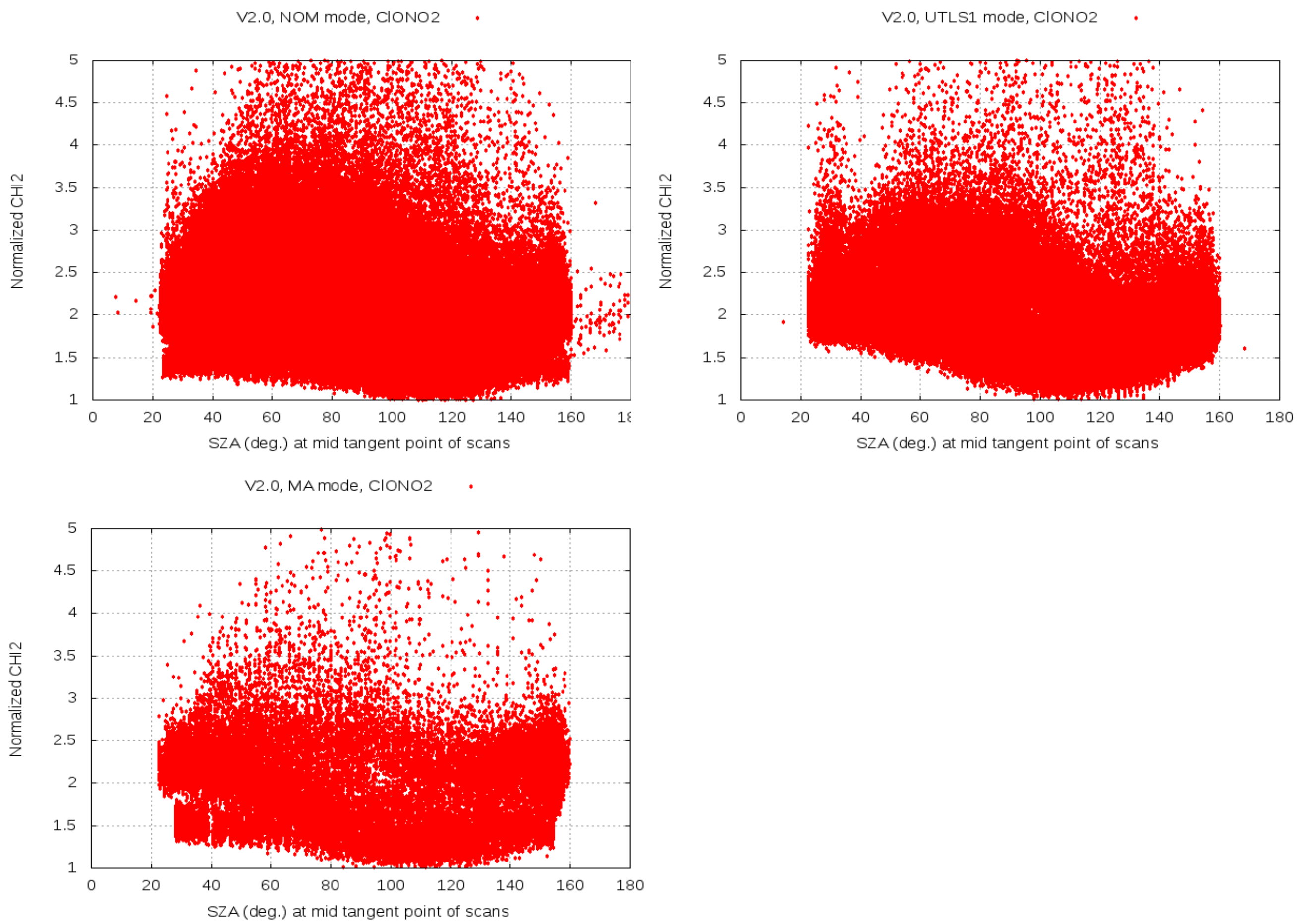


Figure 22: Same as Figure 12 but for ORM_PDS_V2.0 retrievals of ClONO2. Remind that ClONO2 is not retrieved from UA measurements (the bottom right plot is missing).

6.1.1 Considerations on the differences between results from ORM_PDS_V1.0 and V2.0 retrievals

From Figures 1 to 11 it is clear that the statistical distributions of CHI2N from ORM_PDS_V1.0 and V2.0 retrievals are mostly coincident. The only exceptions are HNO3 and CH4 in NOM and UTLS1 modes. In these cases the CHI2N distributions obtained from ORM_PDS_V2.0 retrievals are significantly narrower and shifted to lower values compared to the corresponding distributions obtained from ORM_PDS_V1.0 (see also the cells relating to HNO3 and CH4 in columns 11 and 12 of Table 2). This achievement could be due to removal or reduction of a systematic error component due to the interference of the additional species retrieved in V2.0 (F11, F12, N2O5 and ClONO2). The reduction of this interference error is not so evident in the MA or UA modes analysis, therefore the interference seems localized mainly at altitudes below 18 km.

Apart from these specific cases, the CHI2N distributions obtained from V1.0 and V2.0 retrievals are very similar from the point of view of both average value and standard deviation. This means that the new convergence criteria permit to achieve a final CHI2N very close to that achieved with the old criteria (compare columns 11 and 12 of Table 2 and check Fig.s 1 – 11). Furthermore, we see that the new criteria as well as the correction of the bug in the Levenberg-MArquardt loop of pT retrieval, reduce significantly both the number of non converging inversions (compare columns 5 and 6 of Table 2) and the number of iterations required to reach convergence (compare columns 9 and 10 of Table 2). The CH4 retrieval from NOM and UTLS1 modes seems an exception to these results. In this case the smaller CHI2N obtained in V2.0 retrievals seems achieved at the expenses of a larger number of iterations. In addition, in this case the fraction of non-converging retrievals is larger in V2.0 retrievals. It seems that the possibly reduced error due to the interference from the additional

species retrieved by the ORM_PDS_V2.0 makes the CHI2N minimum more difficult to reach. The validation activities should verify if in these cases the smaller CHI2N achieved in V2.0 really corresponds to CH4 profiles in better agreement with validation measurements.
Columns 7 and 8 of Table 2 (N_CHI2N>7) report the number of outliers obtained in V1.0 and V2.0 retrievals respectively. In this document we call “outlier” a retrieval terminating with CHI2N > 7.0. We see that the number of outliers in V2.0 retrievals is not always smaller than in V1.0. This result, may arise from several causes. First, in all cases but pT and HNO3, NTOT_PROF is significantly larger in V2.0 retrievals compared to V1.0. This means that some retrievals that in V1.0 terminate due to an excess of micro-iterations (and therefore are not counted in NTOT_PROF), in V2.0 are converging but with a large value of CHI2N (CHI2N > 7.0). In case of pT (NOM and UTLS1) and HNO3 (MA), the larger number of outliers could be due both to the new convergence criteria and to the non-optimal quality of the additional species retrieved by the ORM_PDS_V2.0.

6.1.2 Considerations applicable to both ORM_PDS_V1.0 and V2.0 retrievals.

The comparison of the CHI2N statistical distributions obtained from the different measurement modes provides information regarding the quality of the fit in various altitude ranges. In fact, compared to the NOM mode, in the UTLS1 mode the measurements from 50 to 70 km height are missing. This means that in case of fitting problems localized at high altitudes, the CHI2N distribution from the UTLS1 mode should be narrower and shifted towards lower CHI2N values, compared to the distribution from the NOM mode. Conversely, compared to NOM, the MA and UA retrievals miss the lower altitude measurements. In particular, measurements from the 6 – 16.5 km range are missing in the MA mode and measurements from the 6 – 42 km range are missing in the UA mode. This means that in case of fitting problems localized at low altitudes (e.g. in case of badly modeled interferences) the CHI2N distribution should progressively get narrower and shifted towards lower values when moving from NOM to MA and finally to UA retrievals.
The presence of a double peak in the CHI2N distribution suggests that the distribution itself may originate from the superposition of two different distributions shifted from each other. This can occur for example if the residuals of the fit have a day-night dependence. The possible day-night dependence of the residuals must be checked by inspecting the cross-correlation plots of CHI2N versus SZA.

On the light of these guidelines we note that:

- pT retrievals: the CHI2N distributions obtained in the four different observation modes (Fig. 1) are similar, there is no evidence of fitting problems concentrated in a particular altitude range. There is no evidence of a day-night dependence of the residuals (see also Fig. 12).
- H2O retrievals: the CHI2N distribution (Fig. 2) gets narrower and shifted to lower values when moving from NOM to MA and UA modes. Moreover UTLS1 performs worse than NOM. All these elements confirm the known difficulties associated with the H2O fitting in the UTLS region and particularly below the tropopause. There is no evidence of a day-night dependence of the residuals (see Fig. 13).
- O3 retrievals: the obtained CHI2N distributions (Fig. 3) are quite broad. Furthermore we clearly see a double peak in the distribution obtained from UA retrievals. Even if less evident, this double peak exists also in the NOM, UTLS1 and MA distributions. This originates from a day / night dependence of CHI2N (i.e. of the residuals). Figure 14 shows the cross-correlation plots of CHI2N from the O3 ORM_PDS_V2.0 retrievals versus SZA at the tangent point of the mid-sweep of the limb scan processed. From Fig. 14 we can see that the minimum achievable CHI2N depends on the SZA for all the measurement modes processed. Considering the altitude coverage of the O3 retrievals in the various measurement modes (see Table 1) we conclude that this dependence is significant also at altitudes below 49 km (that is the top altitude retrieved in the UTLS1 mode). In past investigations this problem was found to be due to inadequate modeling of

some CO2 lines affected by Non-Local Thermodynamic Equilibrium (NLTE). The question of whether this modeling deficiency affects also the values of the retrieved ozone is still open.

- HNO3 retrievals: see also comments made in Sect. 6.1.1. Here the CHI2N distribution seems independent from both the measurement mode and the SZA (see Fig.s 4 and 15).
- CH4 and N2O retrievals: see also comments made in Sect. 6.1.1 regarding CH4. There seem to be some fitting problems localized below 45 km. The CHI2N statistical distribution relating to UA is significantly narrower compared to those obtained from the other measurement modes (see Fig.s 5 and 6). In addition, for these species the shape of the CHI2N distributions obtained for the NOM, UTLS1 and MA measurements suggests the presence of two peaks and hence a dependence of CHI2N on the SZA. This hypothesis is confirmed by the plots of Figures 16 and 17. This dependence, however, is localized at altitudes below 45 km, it is not noticeable in the UA retrievals.
- NO2 retrievals: in this case the CHI2N distribution from UTLS1 measurements (see Fig. 7) is slightly broader and shifted to higher values compared to the distributions obtained from the other measurement modes. Since in the UTLS1 measurements the sweeps with tangent height from 50 to 70 km are missing, most likely in this case the retrieval has not enough freedom to account for the relatively large NO2 amounts at high-altitude during night-time. Possibly this problem will disappear when diurnally varying Initial Guess (IG) profiles will be used. We remind that the ORM_PDS retrievals use as IG either the last retrieved profile in the orbit or a climatological profile extracted from the IG2 database [RD1] (NO2 day profile). The CHI2N distributions in this case do not show double peaks, therefore the day / night dependence of CHI2N can be excluded. This conclusion is also confirmed by the cross-correlation plots reported in Fig. 18.
- F11 and F12 retrievals. The CHI2N distributions obtained from MA and UA measurements (see Fig.s 8 and 9) are significantly narrower and shifted to lower values compared to the distributions obtained from NOM and UTLS1 modes. This suggests a less than perfect fitting at altitudes below 18 km, i.e. the lowest altitude of the MA mode. The CHI2N distribution from the UA mode shows also that significant number of retrievals terminates with CHI2N < 1, suggesting that the measurement noise could be overestimated at these altitudes. No day / night dependence of CHI2N is visible (see also Fig.s 19 and 20).
- N2O5 retrievals. The CHI2N distributions (Fig. 10) obtained from MA and UA measurements are significantly narrower and shifted to lower values compared to the distributions from the NOM and UTLS1 modes (fitting difficulties below 18 km). The double peak structure of the distributions from NOM, UTLS1 and MA modes suggests a dependence of CHI2N on the SZA. The plots of Figure 21 show that for NOM, UTSL1 and MA modes the minimum achievable CHI2N changes from 1 to 1.2 as the SZA changes from 60 to 20 degrees. The sensitivity on the SZA is limited to altitudes below 45 km, it is not present in the distribution from the UA measurements.
- ClONO2 retrievals. The CHI2N distributions (Fig. 11) obtained from NOM, UTLS1 and MA measurements are similar to each other and quite broad. The double peak structure of the distributions reveals that CHI2N depends on the SZA. This dependence is confirmed by the plots of Figure 22. The minimum CHI2N achievable changes from 1 to approximately 1.3 as the SZA changes from 100 to 20 degrees. We remind that ClONO2 is not retrieved from the UA measurements.

6.2 Analysis of tangent height corrections

A preliminary inspection of the ESA summary reports mentioned in Sect. 5.3 highlighted that the tangent height corrections (THCs) derived by the ORM_PDS processors are by far larger than those obtained from the IPF processor when FR MIPAS measurements are analyzed. The large THCs were first observed in the ORM_PDS (both V1.0 and V2.0) retrievals from the MA measurements of 12 January 2005. Figure 23 shows the THCs obtained from the mentioned measurements, for selected sweeps with nominal tangent altitudes of 69, 66, 63, 51, 42 and 24 km (see the plot's legend). To ease the graphical representation, these THCs are shifted by 70, 69, 68, 67, 66 and 65 km respectively. The horizontal axis of the plot in Fig. 23 reports the so called "orbital coordinate" of the tangent points of sweeps. The orbital coordinate is a polar angle that, together with the altitude, can be used to identify a tangent point on the orbit plane. The origin of this coordinate is taken at the equator, therefore in the interval from 0 to 90 degrees it coincides with latitude (North), if the orbit is assumed exactly polar. In Fig. 23 we can see THCs as large as 1 km. Such a large values are not expected on the basis on the MIPAS pointing performance, recently improved also with updates in the Level 1b algorithm.

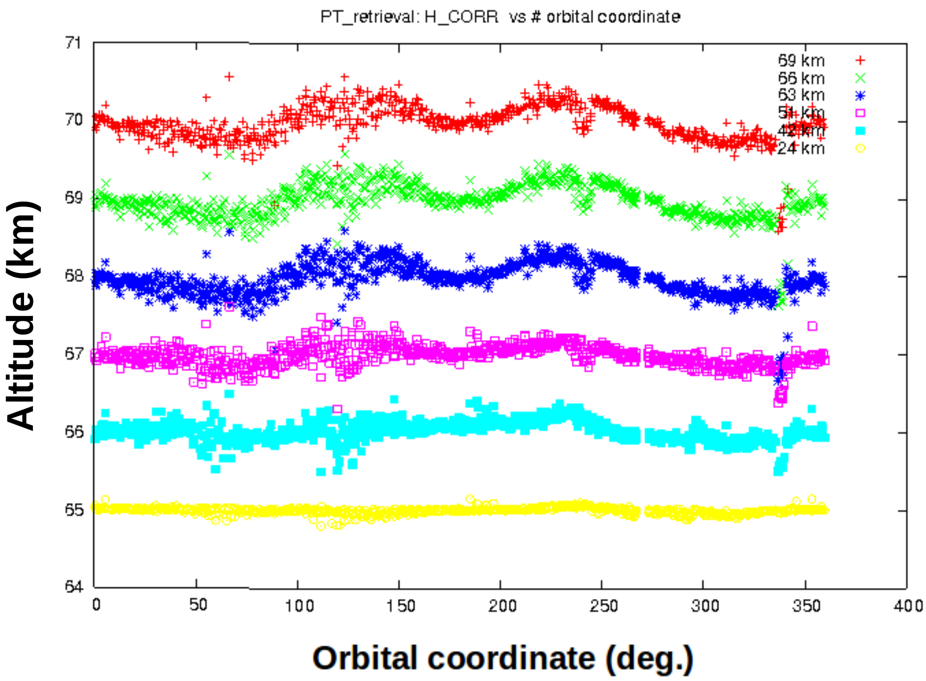


Figure 23: Tangent height corrections obtained from ORM_PDS_V2.0 retrievals for the MA orbits of 12 January 2005. The values are vertically shifted to improve the readability of the plot.

These large THCs retrieved by the ORM_PDS pushed us to think that these could originate from a pT retrieval strongly affected by the water vapor interference error. For this reason we attempted the following test (Test 1): for each limb scan, we repeated for three times the pT and H2O retrievals, each retrieval using as IG or assumed profiles the Temperature and H2O profiles last retrieved from the same scan. In case of strong mutual correlation between T and H2O, this approach should sequentially minimize the effect of the spectral interferences and therefore should provide more realistic (smaller) THCs. The THCs obtained from this test are very reasonable from point of view of the a-priori estimated MIPAS pointing performance, they are shown in Figure 24. Such a strong interference of H2O in pT Mws, however, is not fully justified from the spectroscopic point of view. Therefore we attempted the following additional test (Test 2): for each scan we repeated for three times only the pT retrieval, each time the retrieval starting from the H2O profile retrieved from the previous scan (the standard ORM_PDS approach) and the last retrieved T profile from the same scan. The THCs obtained in this case mostly coincide with those retrieved in test 1, they are shown in Figure 25.

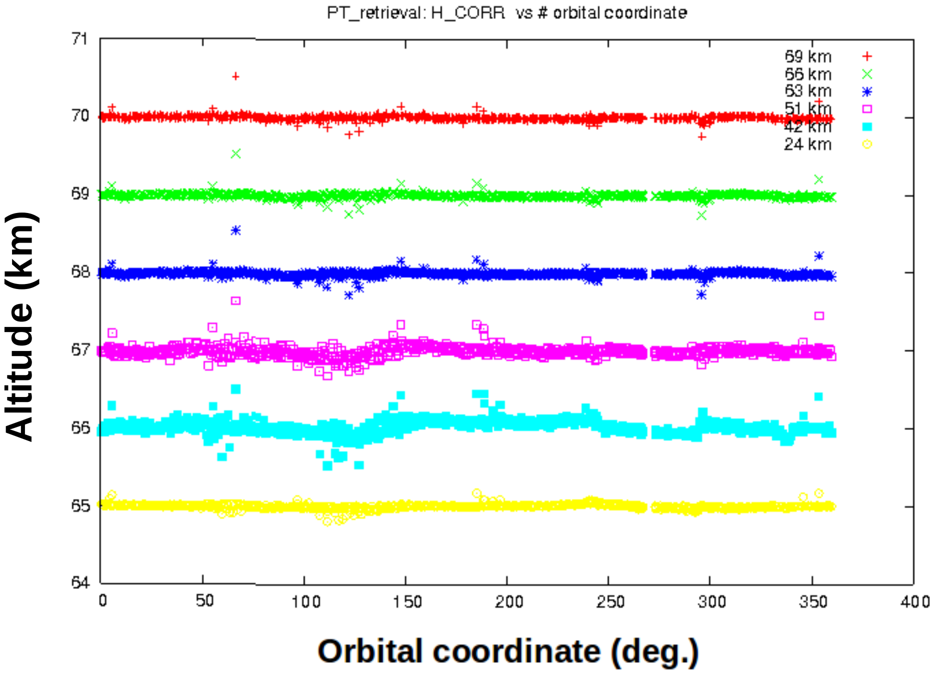


Figure 24: Tangent height corrections obtained from test 1 with the ORM_PDS_V2.0: pT and H2O retrievals repeated for 3 times in each scan. Retrievals are from the MA orbits of 12 January 2005. The values are vertically shifted to improve the readability of the plot.

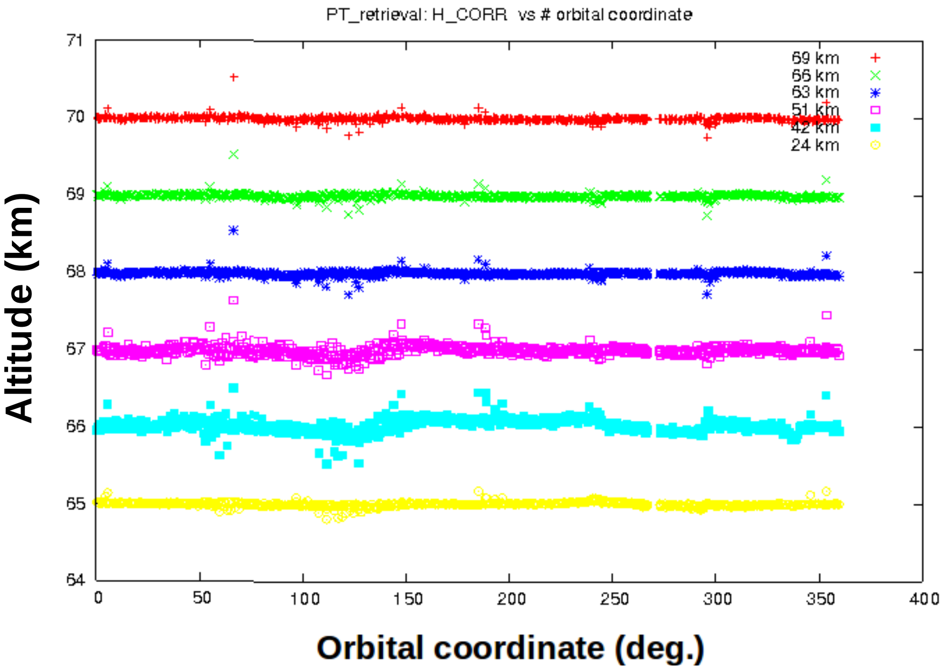


Figure 25: Tangent height corrections obtained from test 2 with the ORM_PDS_V2.0: pT retrieval is repeated for 3 times in each scan. Retrievals are from the MA orbits of 12 January 2005. The values are vertically shifted to improve the readability of the plot.

In summary, tests 1 and 2 show that the large THCs found in the ORM_PDS retrievals are not due to the spectral interference of H_2O in pT MWs. In addition, the results of test 2 show that the THCs resulting from ORM_PDS retrievals depend on "how good" is the IG Temperature profile of pT retrieval. In test 2 the third pT retrieval from a given scan starts from the engineering tangent altitudes provided in the L1b products and from an IG Temperature profile (represented in pressure grid) previously retrieved from the same scan, i.e. a Temperature profile already compatible with the given observations. The behavior of pT retrieval is illustrated in Fig. 26 in the case of a limb scan consisting of only two sweeps.

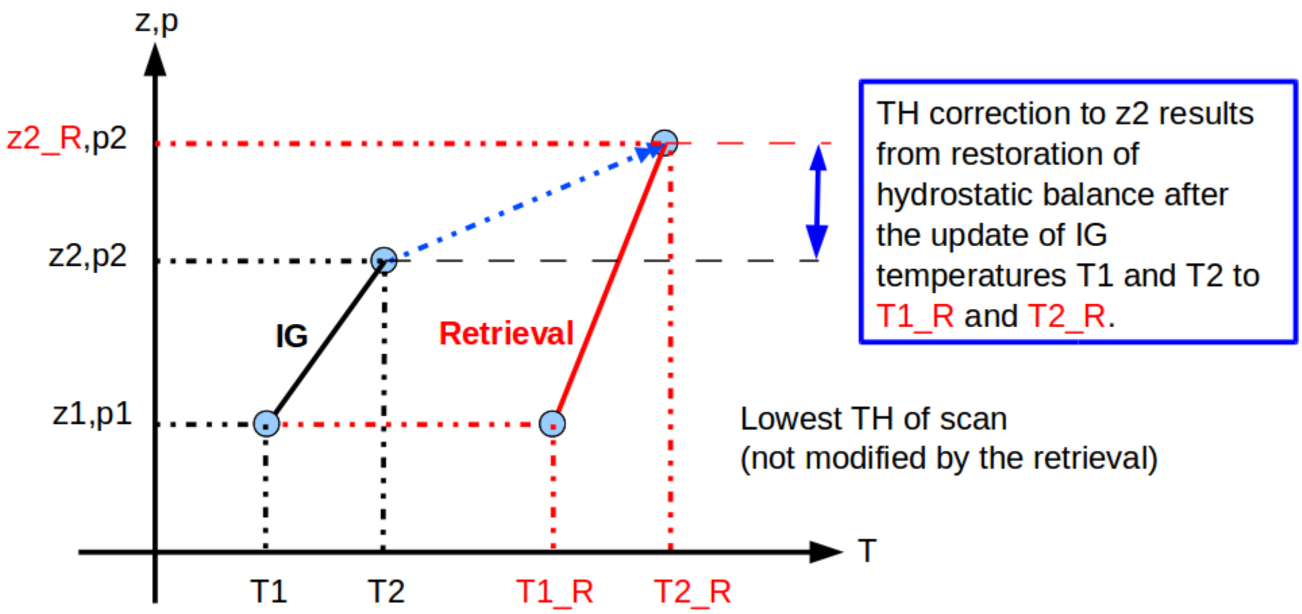


Figure 26: Illustration of the functioning of pT retrieval in the ORM_PDS.

In this figure the black elements refer to the initial status of the retrieval, while the red elements refer to an hypothetic final situation at the end of the retrieval. The retrieval uses the measurements from two sweeps with tangent points at IG altitudes z1 and z2 (the engineering values), pressures p1 and p2, temperatures T1 and T2. Assume that p1 and p2 have already optimal values, i.e. already perfectly compatible with the given observations, the real values of pressure at the tangent points. Assume also the real value of temperature to be greater than the initial guesses T1 and T2. The inversion algorithm will not change p1 and p2, while it will increase T1 and T2 to the new (retrieved) values T1_R and T2_R. After this update of temperature, the algorithm will then restore the hydrostatic balance by adjusting the altitude z2 to the new (retrieved) value z2_R. The altitude z1 will not be changed by the algorithm because it is the tangent height of the lowermost sweep included in the inversion and is assumed a known quantity. In conclusion, the algorithm ends up with the tangent height correction z2_R – z2 even if both z1 and z2 are correct. The correction depends on the difference between the retrieved and initial guess temperature.

We conclude that the reason why the ORM_PDS retrieves THCs larger than those of the IPF processor is in the selection of the initial guess temperature. While the IPF processor exploits the rather accurate ECMWF temperature estimates, the ORM_ABC uses simply the temperature retrieved from the previous scan, if available, or, in alternative, the climatological estimate included in the IG2 database. As a consequence, the THCs retrieved by the ORM are not accurate as they rely on the accuracy of the IG temperature and of the altitude scale associated to it. This limitation of the ORM approach confirms that the output profiles should always be represented on the grid of the retrieved pressures.

6.3 Consistency between the OR and FR datasets

Due to the changed spectral resolution, the retrievals from OR measurements use different MWs compared to the retrievals from FR measurements. The MWs selected for processing the OR measurements are significantly different compared to those used to process the FR measurements. To give an idea of the differences, in Table 3 we show the total percentage of spectral overlap between FR and OR MWs.

PT	5.4%
H_2O	16.9%
O_3	11.4%
HNO_3	12.8%
CH_4	9.0%
N_2O	31.7%
NO_2	25.5%

Table 3: Total percentage of spectral overlap between FR and OR MWs.

Different MWs imply different systematic errors in the retrieved profiles, therefore systematic differences (or a bias) may exist between the FR and OR datasets. For use of MIPAS L2 products in scientific applications this bias must be carefully characterized.

With the aim of characterizing this bias, we selected 472 FR orbits of NOM measurements (approximately one month of measurements) and processed them up to Level 2 with the ORM_PDS, using two different approaches. The first approach (a) consists in the usual processing of the FR measurements with the HR MWs. The second approach (b) consists in first degrading the FR spectra to the OR and then apply the standard processing setup used for the OR measurements. The average of the differences between profiles resulting from (a) and (b) characterizes the systematic mismatch (or bias) between the FR and OR datasets, due to using different MWs. Figures from 27 to 34 show these average differences for all the MIPAS key targets. Averages are computed over the whole dataset, for each altitude, without any binning in latitude bands. All the figures but Fig. 28 (relating to temperature) consist of two panels. The left panels report the absolute differences while the right panels report the percentage differences. As a term of reference, each plot shows also the average random (noise) error for both the HR and OR retrievals and the systematic error relating to the HR retrievals, as calculated by University of Oxford [RD9].

The systematic differences between HR and OR retrieved pressures and temperatures are not negligible. For this reason, for the calculation of the differences between OR and HR retrieved VMR profiles, each VMR profile point from the HR retrieval was scaled to match the air density of the corresponding OR profile point.

The observed systematic differences between OR and HR profiles are not negligible, however they are consistent with the predicted HR systematic error. As a qualitative summary of this analysis, we find the following systematic behavior of the differences between OR and HR measurements (differences OR - HR): positive bias of H2O above 55 km and around the tropopause region, positive bias in O3 around 40 km and below 10 km, negative bias of CH4 and N2O below 20 km. On the basis of the results of the validation activities, the results of the test presented here will help to improve the MW selection for future MIPAS data reprocessing.

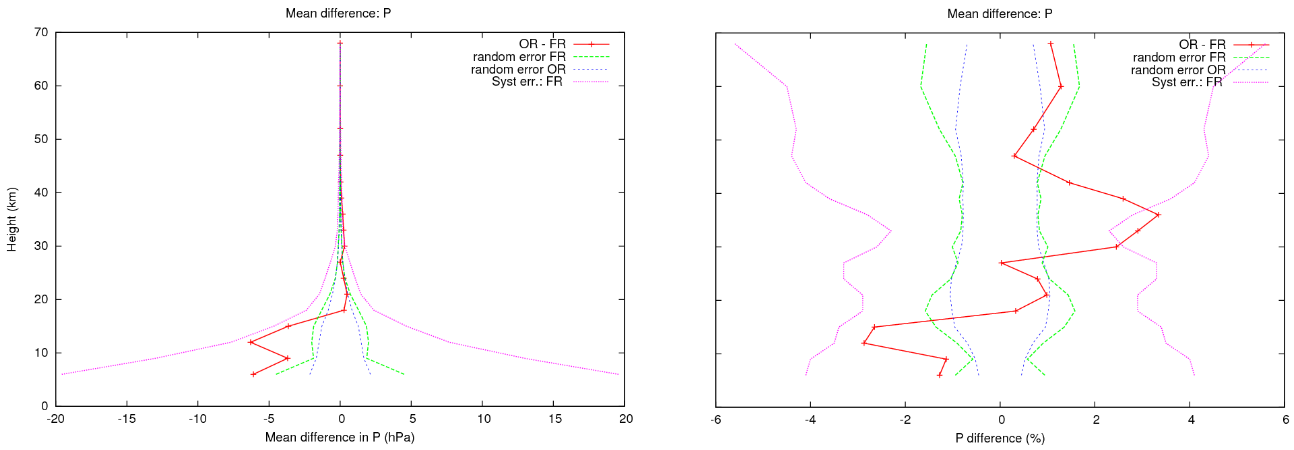


Figure 27: Absolute (left) and percentage (right) average differences between tangent pressures retrieved using OR and FR MWs. Retrievals performed from the same set of HR measured spectra.

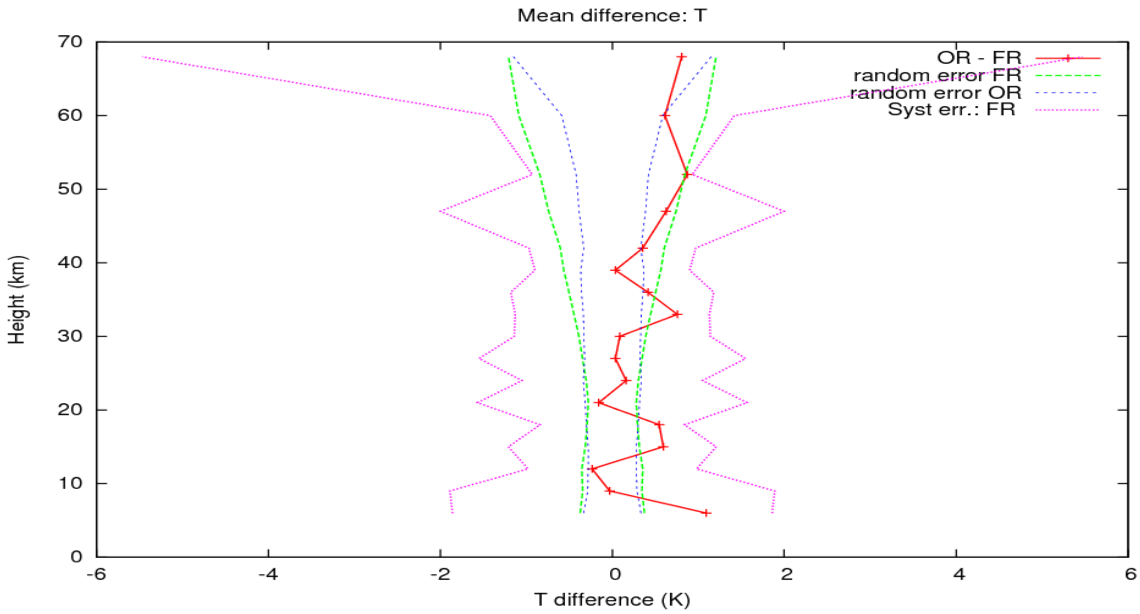


Figure 28: Average differences between temperatures retrieved using OR and FR MWs. Retrievals performed from the same set of HR measured spectra.

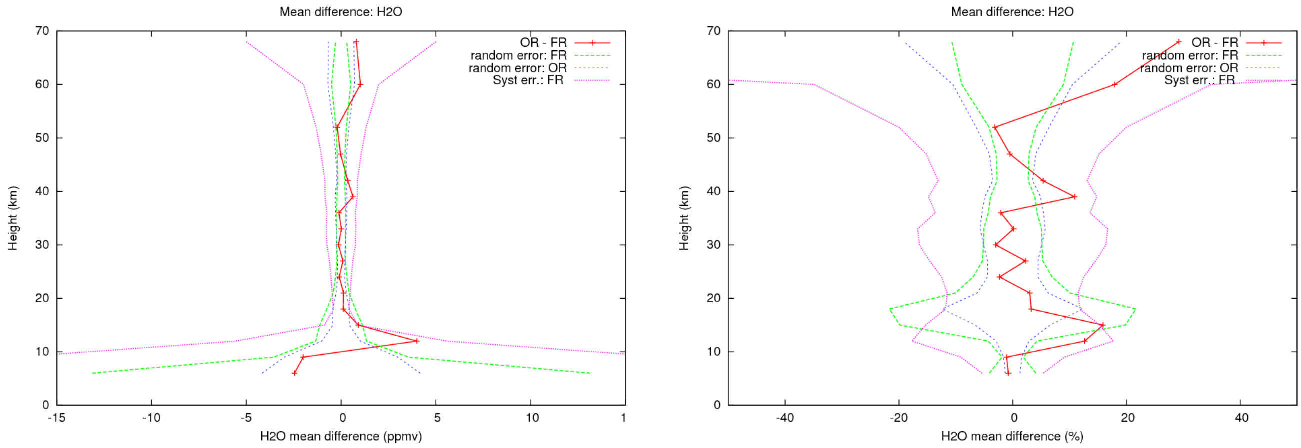


Figure 29: Absolute (left) and percentage (right) average differences between H2O VMR retrieved using OR and FR MWs. The retrievals were performed from the same set of HR measured spectra.

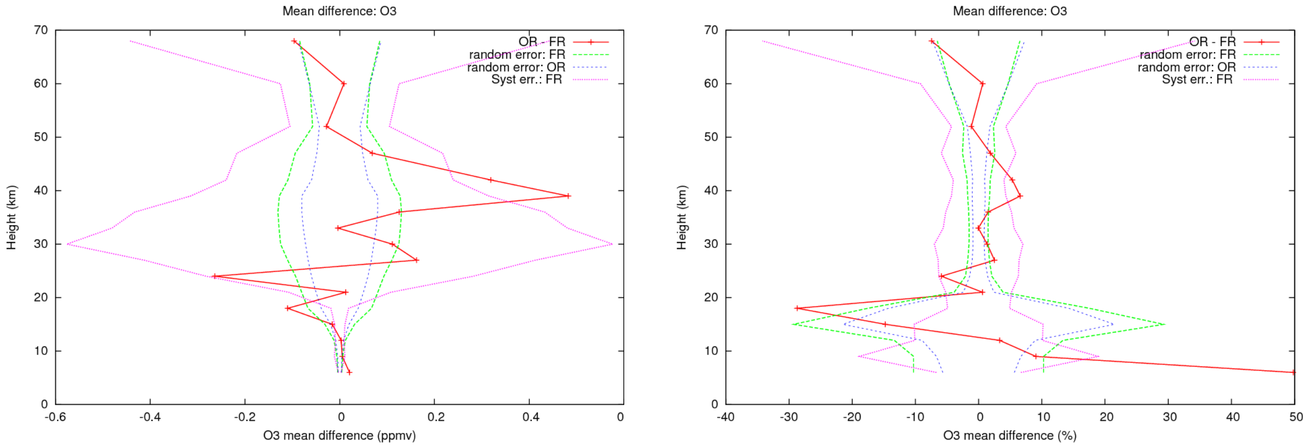


Figure 30: Absolute (left) and percentage (right) average differences between O3 VMR retrieved using OR and FR MWs. The retrievals were performed from the same set of HR measured spectra.

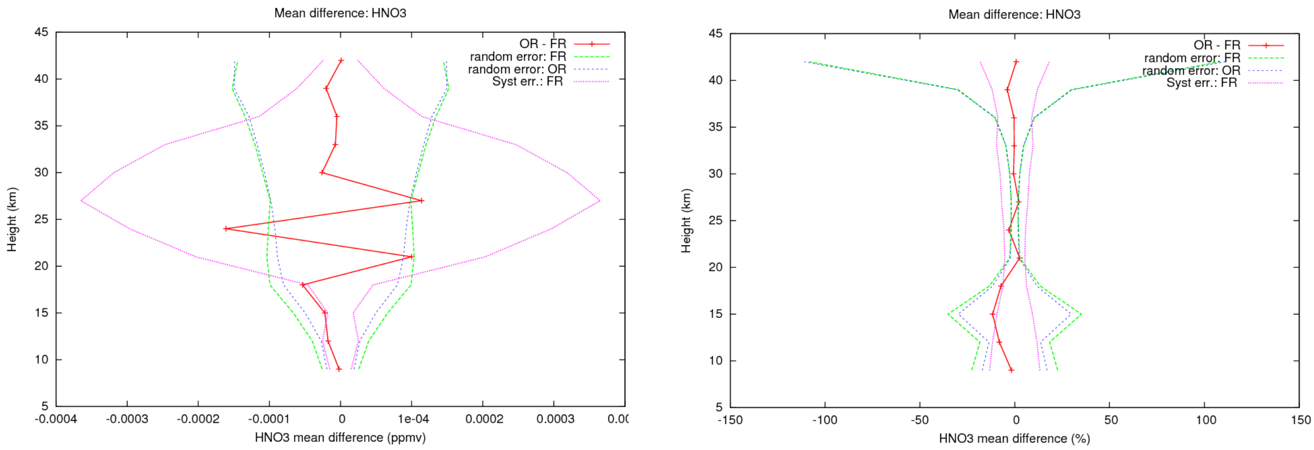


Figure 31: Absolute (left) and percentage (right) average differences between HNO3 VMR retrieved using OR and FR MWs. The retrievals were performed from the same set of HR measured spectra.

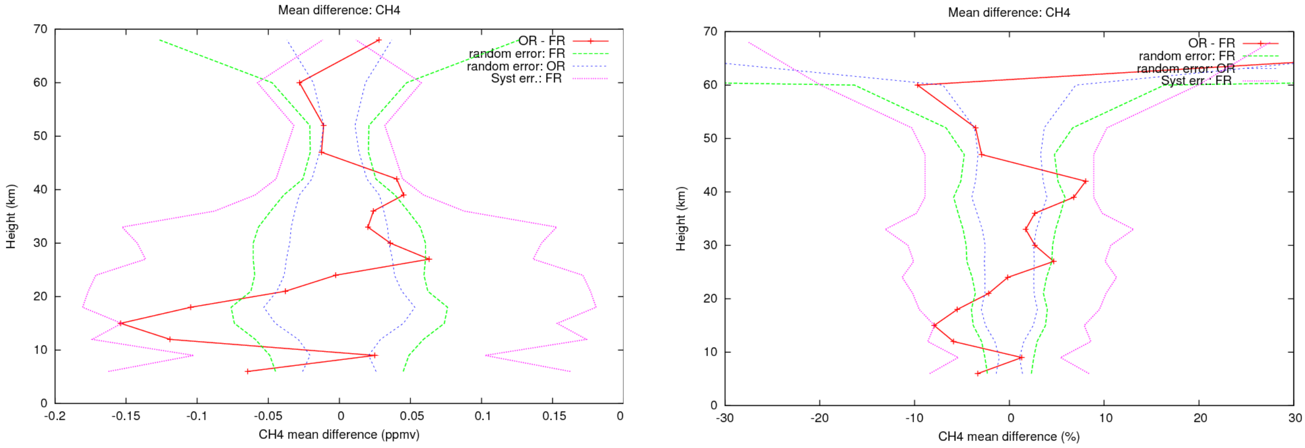


Figure 32: Absolute (left) and percentage (right) average differences between CH4 VMR retrieved using OR and FR MWs. The retrievals were performed from the same set of HR measured spectra.

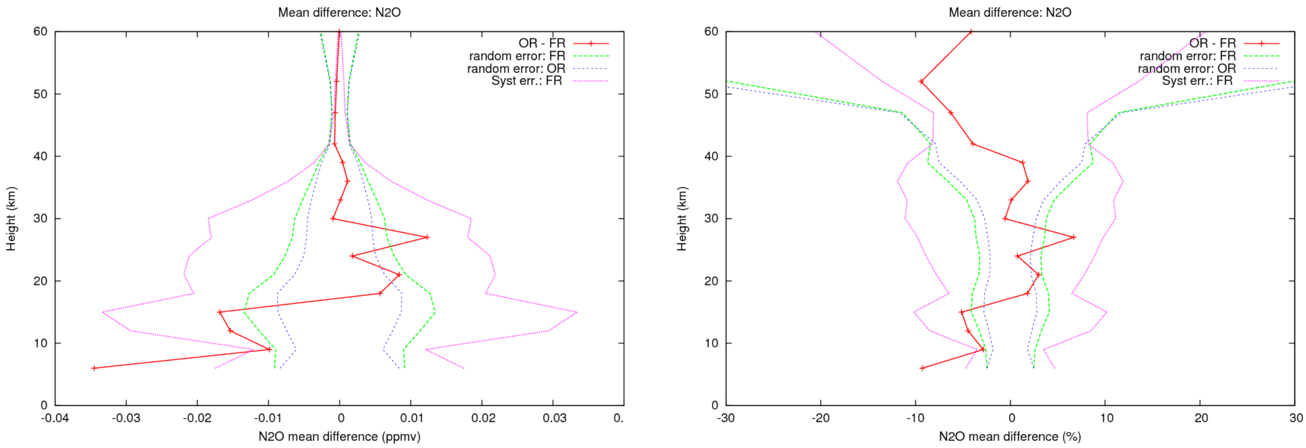


Figure 33: Absolute (left) and percentage (right) average differences between N2O VMR retrieved using OR and FR MWs. The retrievals were performed from the same set of HR measured spectra.

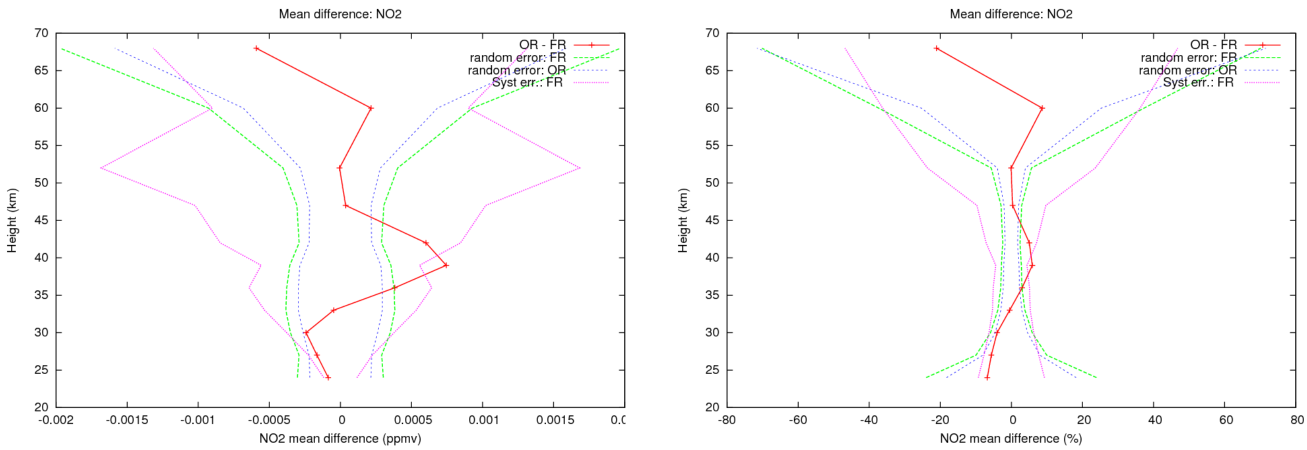


Figure 34: Absolute (left) and percentage (right) average differences between NO2 VMR retrieved using OR and FR MWs. The retrievals were performed from the same set of HR measured spectra.

In order to further characterize the FR / OR systematic differences possibly induced by the different MWs used, we processed with the ORM_PDS_V2.0 also the FR reprocessed L1b (V.5.0.1) orbits available on the ESA server at the end of June 2010. The L2 profiles generated in this analysis were then used together with the OR validation dataset to evaluate the time series of monthly averages of the various MIPAS targets. In Figures from 35 to 48 we show some time series of monthly averages of the retrieved targets. The time series relating to the main targets are extended also to the FR measurements, while the additional species (F11, F12, N_2O_5 and $ClONO_2$) are limited to the OR validation dataset. Whenever a diurnal variation is expected we show separately the time series relating to averages of night-time and day-time measurements.

From Fig.s 35 to 48 we can draw the following qualitative conclusions:

- Temperature: there is no evidence of a significant systematic difference between FR and OR Temperature retrievals.
- H_2O: for pressures smaller than 0.5 hPa the FR H_2O is smaller than the corresponding OR value. The OR value seems more realistic. The "tape recorder" effect is also visible.
- O_3 and HNO_3: no large systematic differences between FR and OR are visible.
- CH_4 and N_2O: for pressures greater than 50 hPa the OR measurements provide lower values compared to the FR measurements. Since the validation of FR CH_4 and N_2O indicated an overestimate of these quantities in this altitude range, figures 39 and 40 suggest the OR measurements in this case should better agree with correlative measurements.
- NO_2: the diurnal cycle is well visible. There might be differences between FR and OR measurements but they are embedded in the atmospheric variability, no final conclusion can be drawn in this case.
- F11 and F12: the atmospheric distributions are reasonable.
- N_2O_5 and $ClONO_2$: the diurnal cycle is visible. The atmospheric distributions are reasonable.

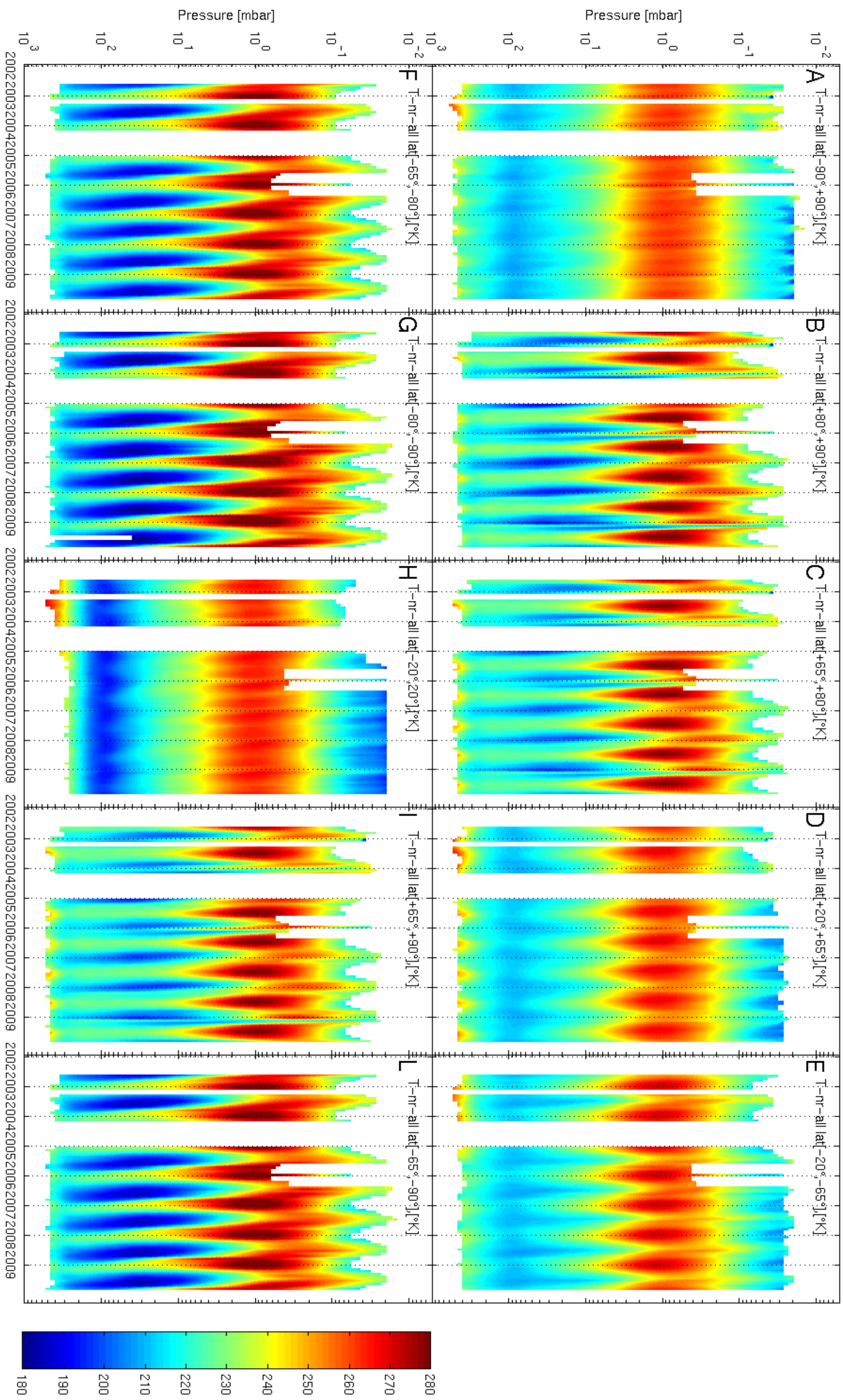


Figure 35: Time series of monthly averaged Temperature (color scale, in K) as a function of pressure. Averages are shown for various latitude bands as indicated in the plots key. In this case averages include both day and night measurements.

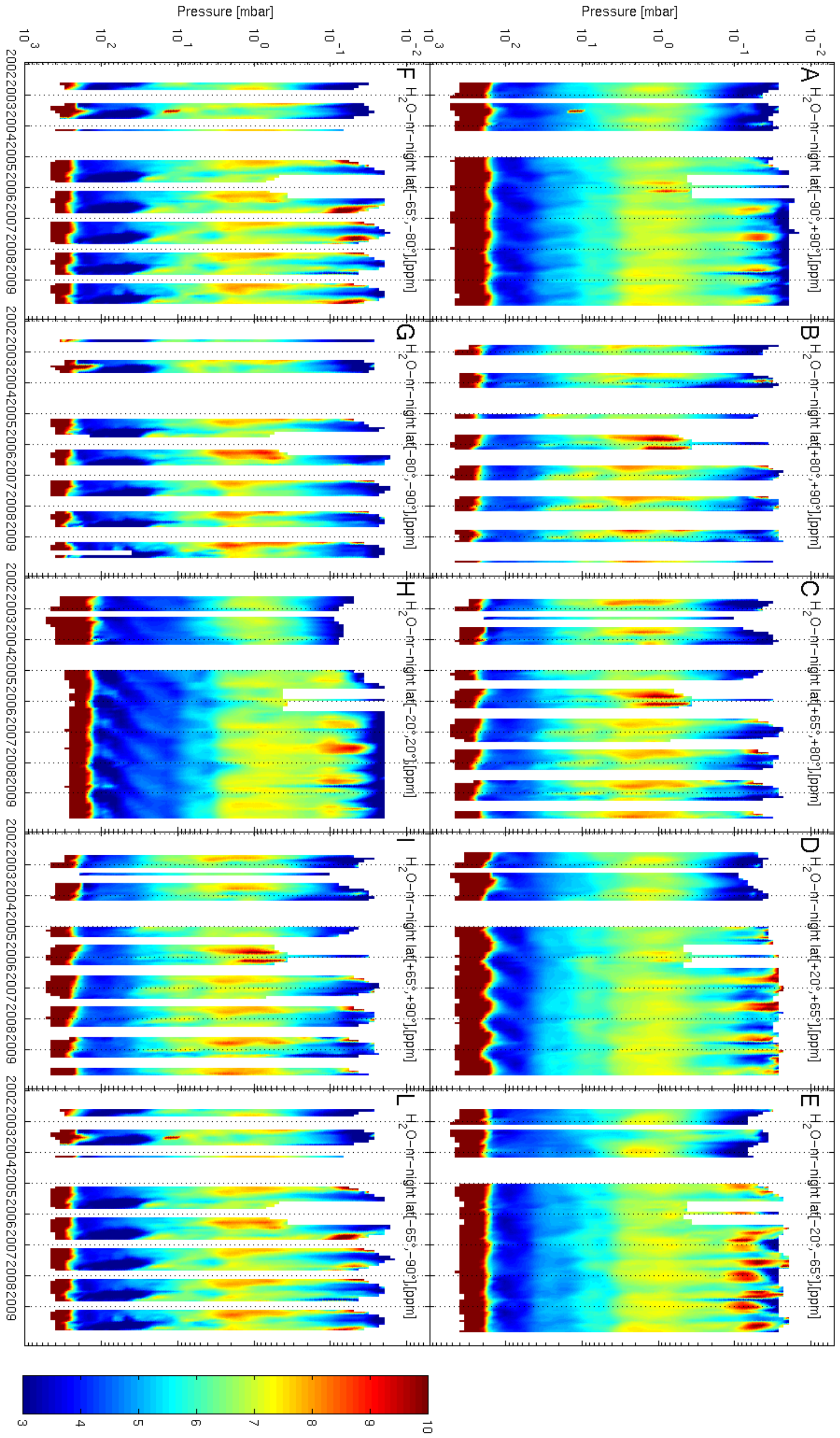


Figure 36: Time series of monthly averaged H2O VMR (color scale, in ppmv) as a function of pressure. Averages are shown for various latitude bands as indicated in the plots key. In this case averages include <u>only night-time measurements</u>.

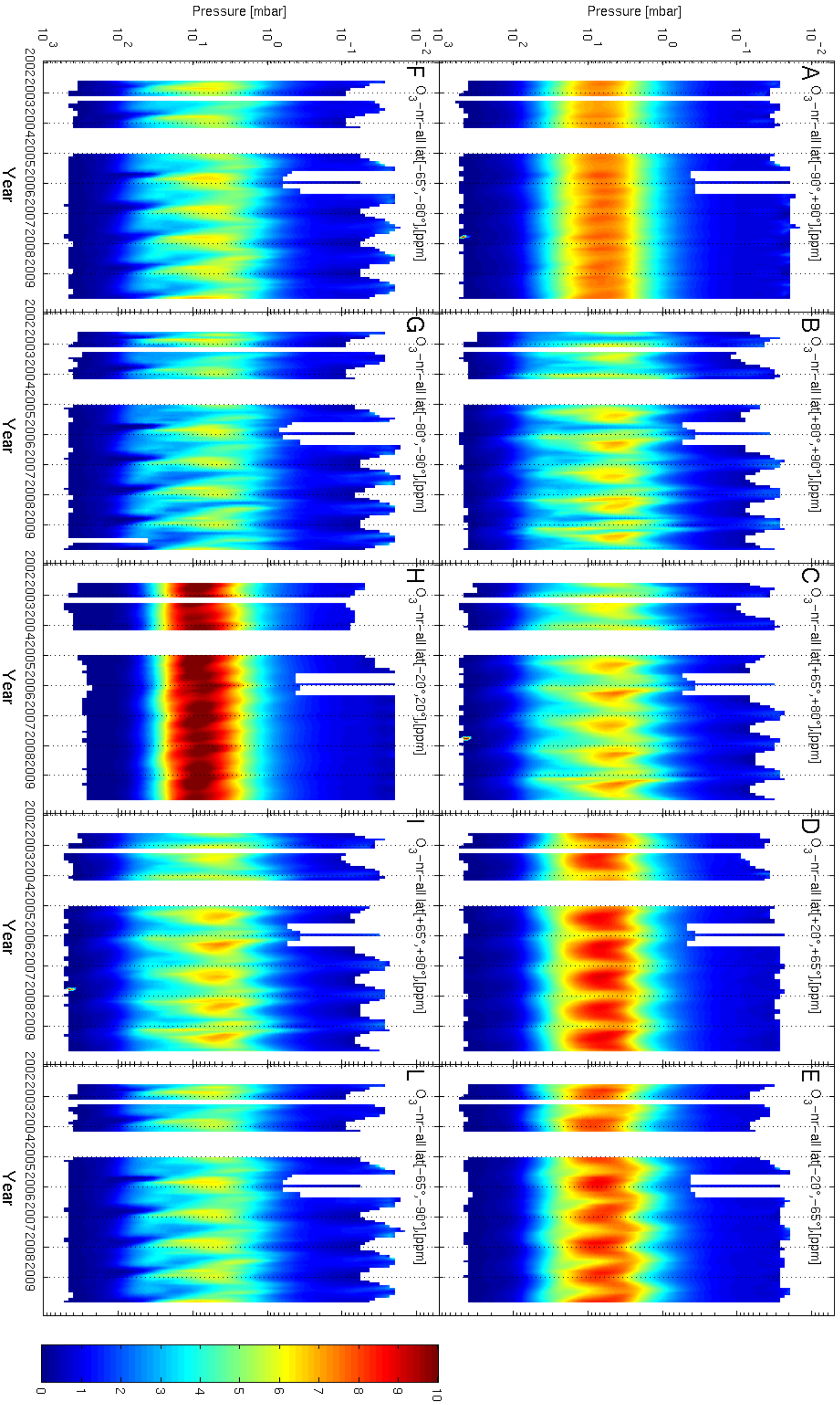


Figure 37: Time series of monthly averaged O3 VMR (color scale, in ppmv) as a function of pressure. Averages are shown for various latitude bands as indicated in the plots key. In this case averages include <u>both day and night measurements</u>.

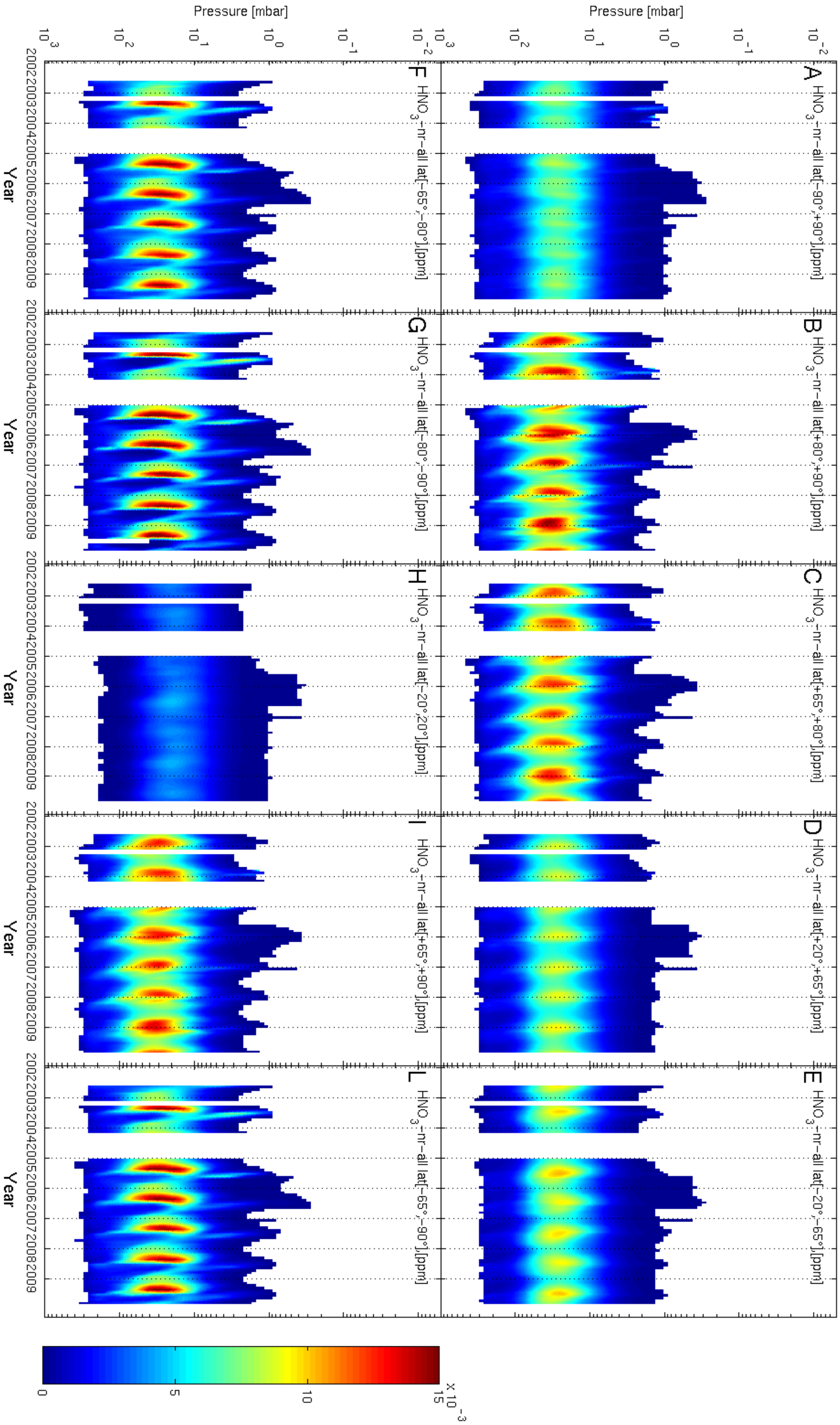


Figure 38: Time series of monthly averaged HNO3 VMR (color scale, in ppmv) as a function of pressure. Averages are shown for various latitude bands as indicated in the plots key. In this case averages include <u>both day and night measurements</u>.

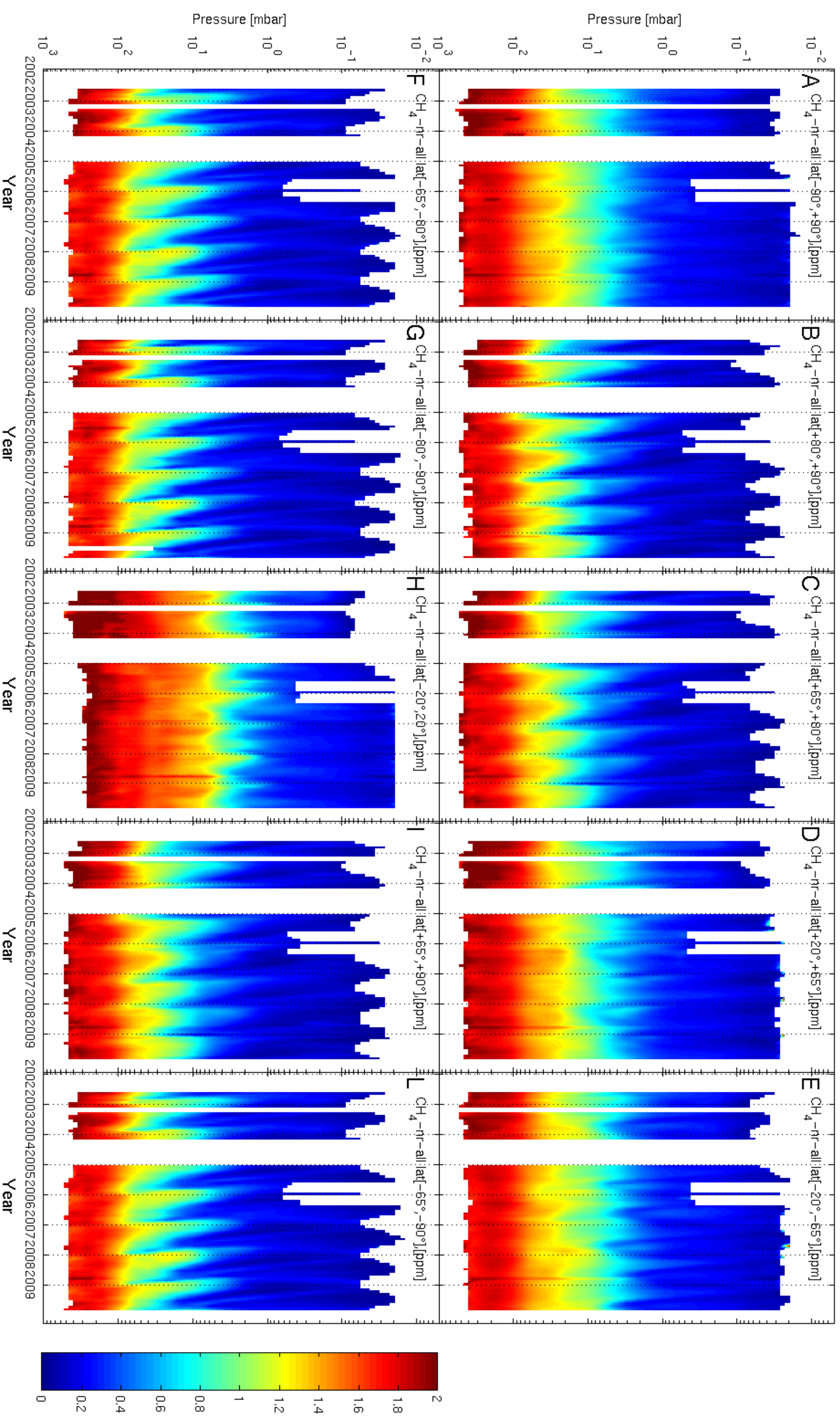


Figure 39: Time series of monthly averaged CH4 VMR (color scale, in ppmv) as a function of pressure. Averages are shown for various latitude bands as indicated in the plots key. In this case averages include both day and night measurements.

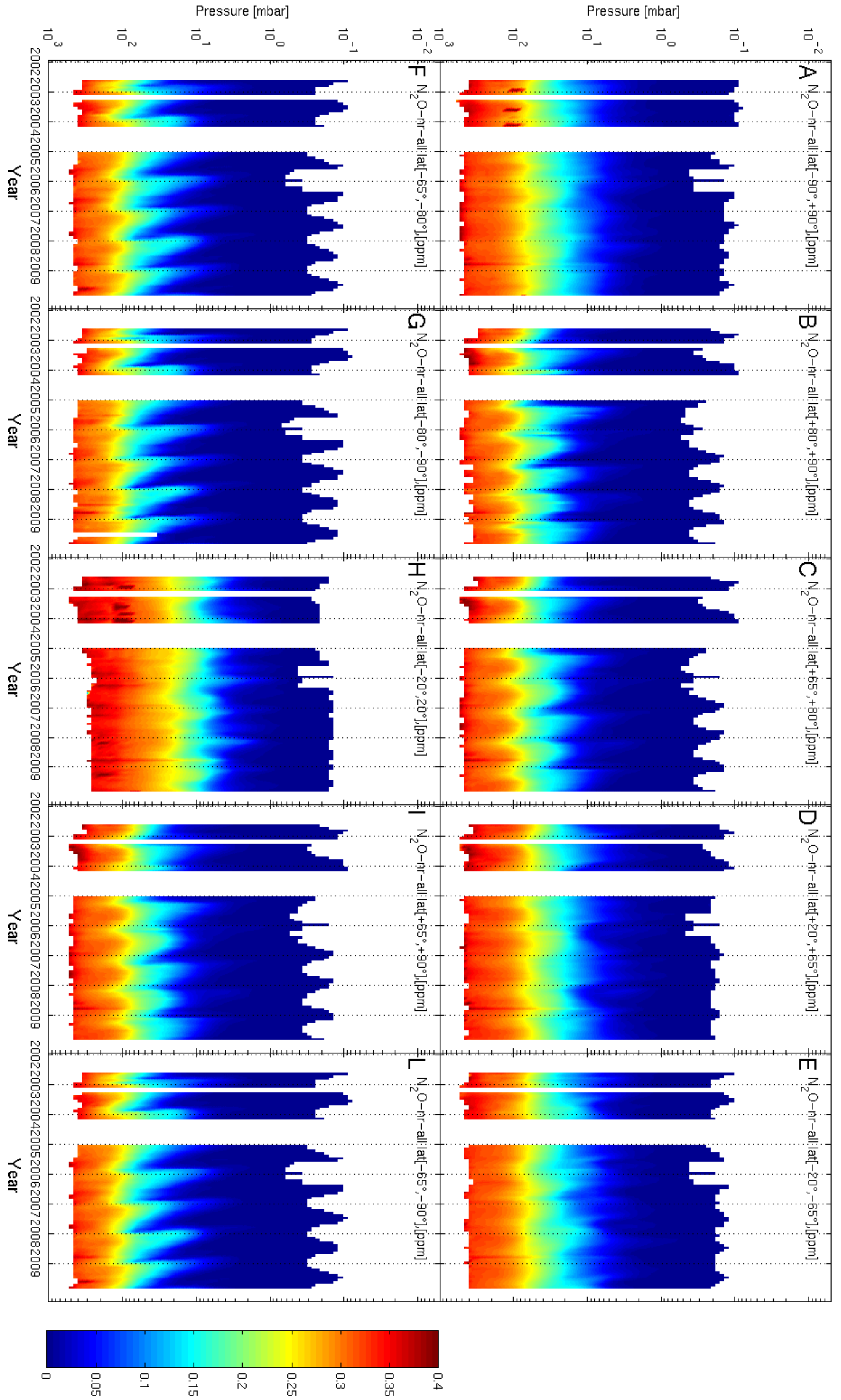


Figure 40: Time series of monthly averaged N2O VMR (color scale, in ppmv) as a function of pressure. Averages are shown for various latitude bands as indicated in the plots key. In this case averages include <u>both day and night measurements</u>.

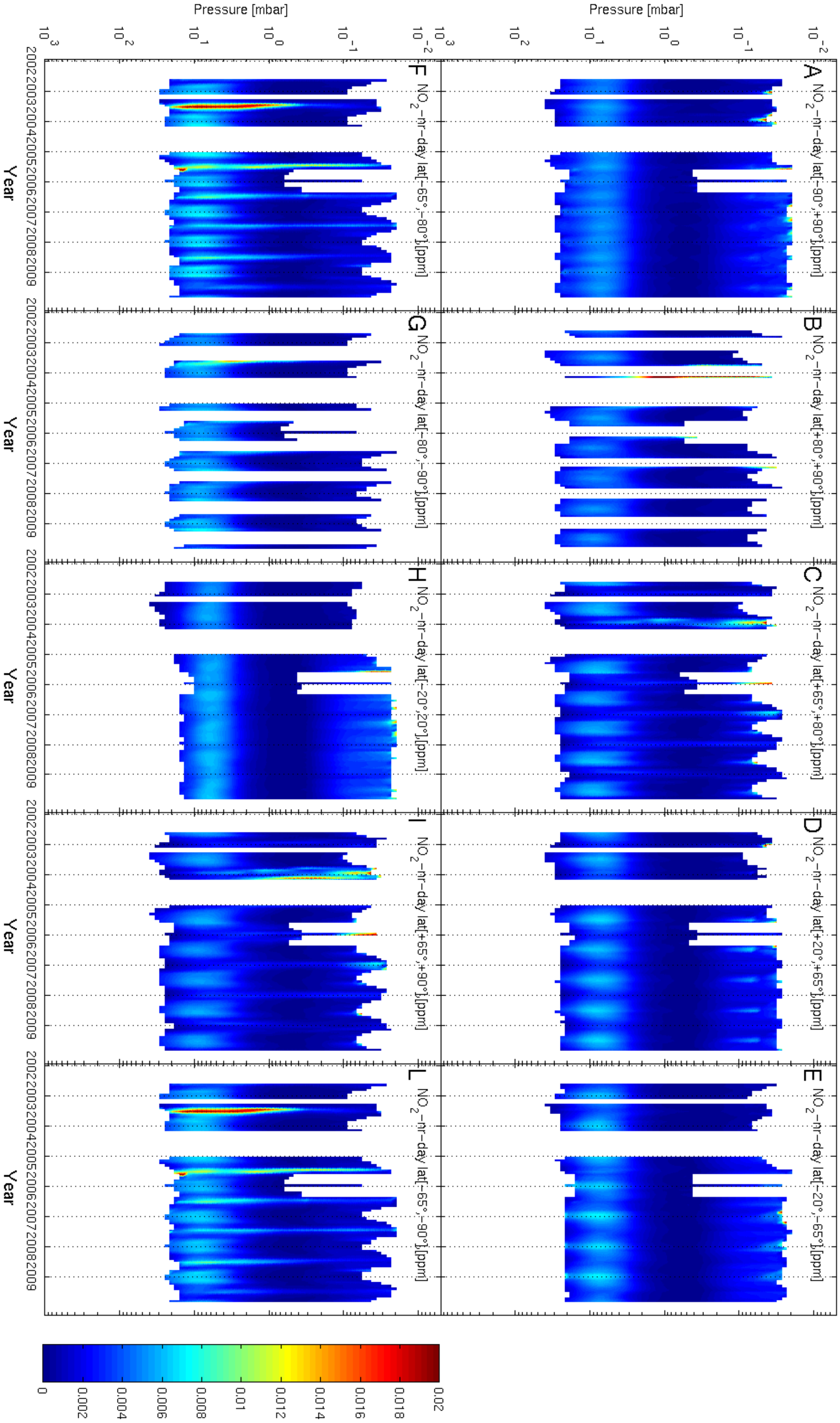


Figure 41: Time series of monthly averaged NO2 VMR (color scale, in ppmv) as a function of pressure. Averages are shown for various latitude bands as indicated in the plots key. In this case averages include <u>only day-time measurements</u>.

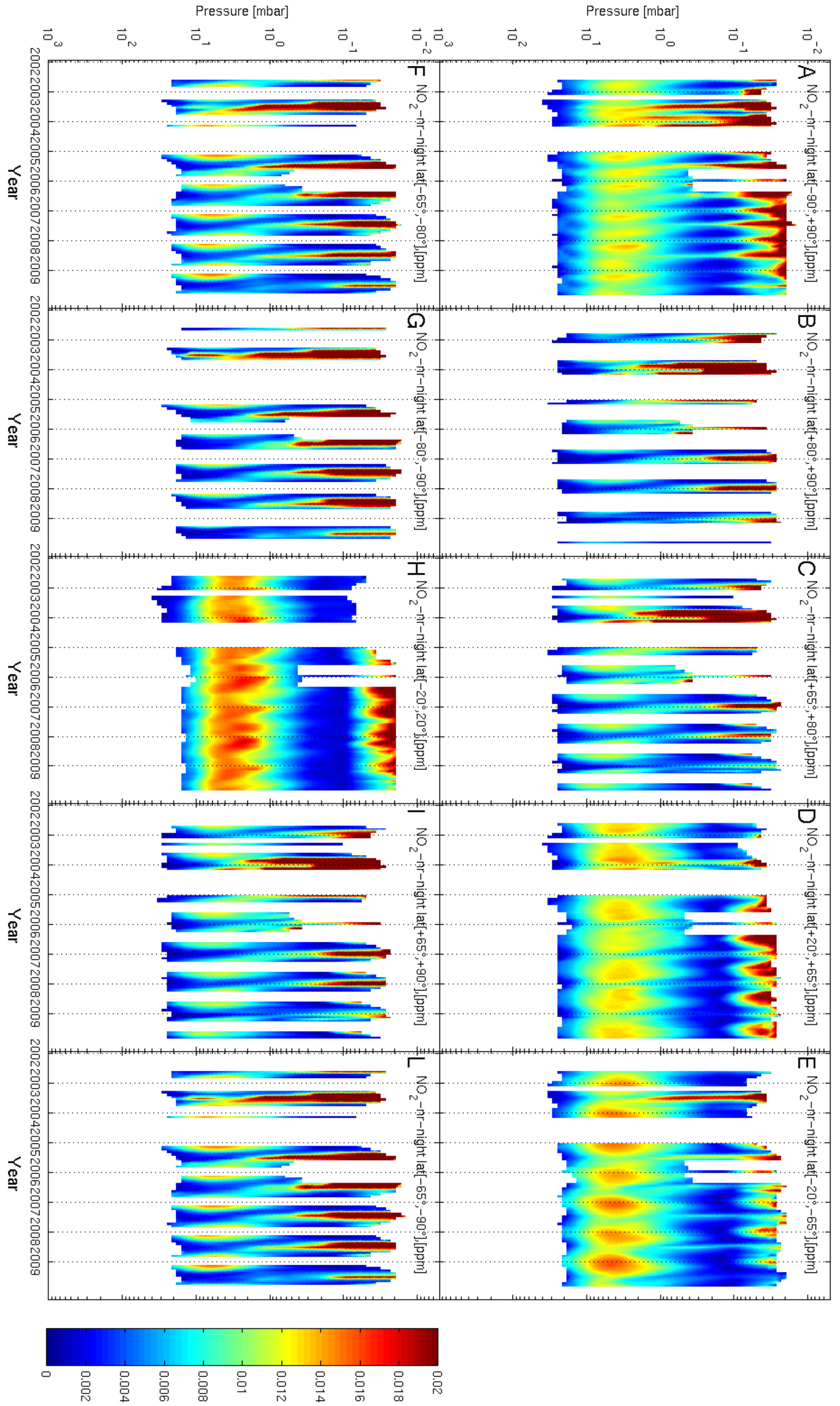


Figure 42: Time series of monthly averaged NO2 VMR (color scale, in ppmv) as a function of pressure. Averages are shown for various latitude bands as indicated in the plots key. In this case averages include <u>only night-time measurements</u>.

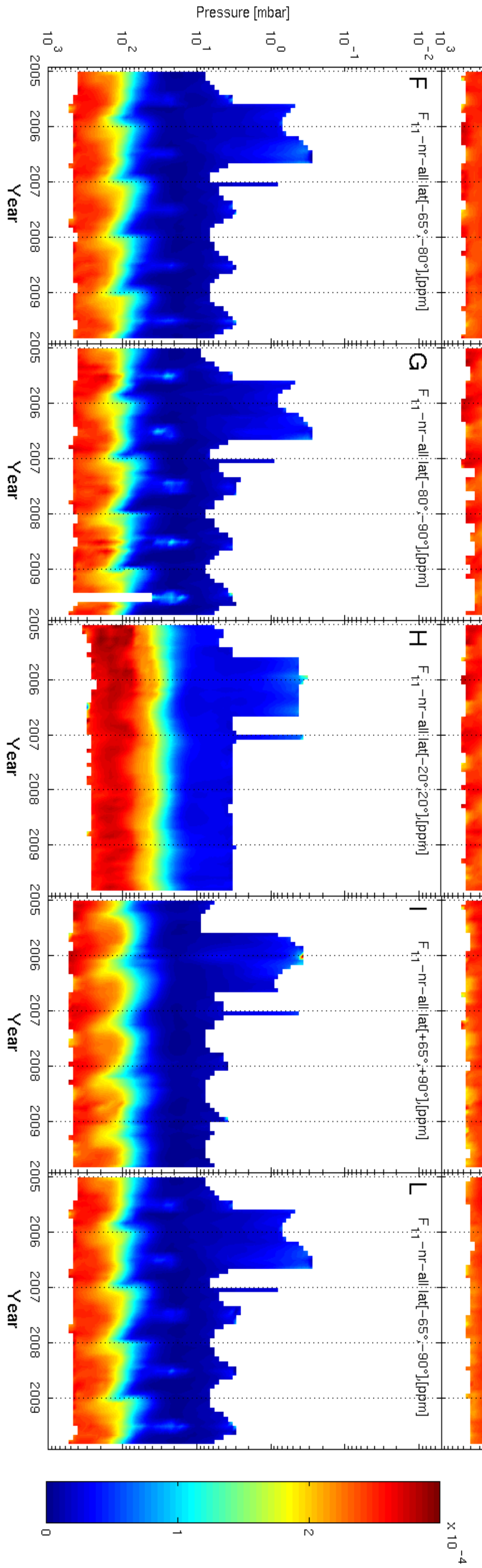


Figure 43: Time series of monthly averaged F11 VMR (color scale, in ppmv) as a function of pressure. Averages are shown for various latitude bands as indicated in the plots key. In this case averages include <u>both day and night-time measurements</u>.

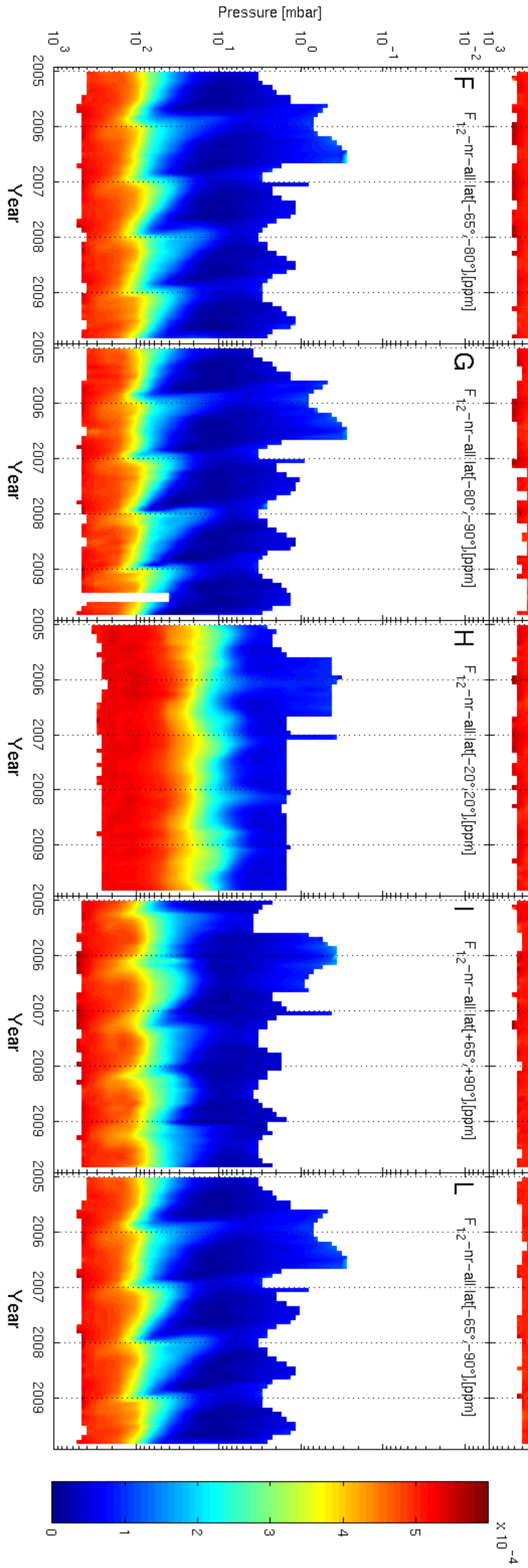


Figure 44: Time series of monthly averaged F12 VMR (color scale, in ppmv) as a function of pressure. Averages are shown for various latitude bands as indicated in the plots key. In this case averages include <u>both day and night-time measurements</u>.

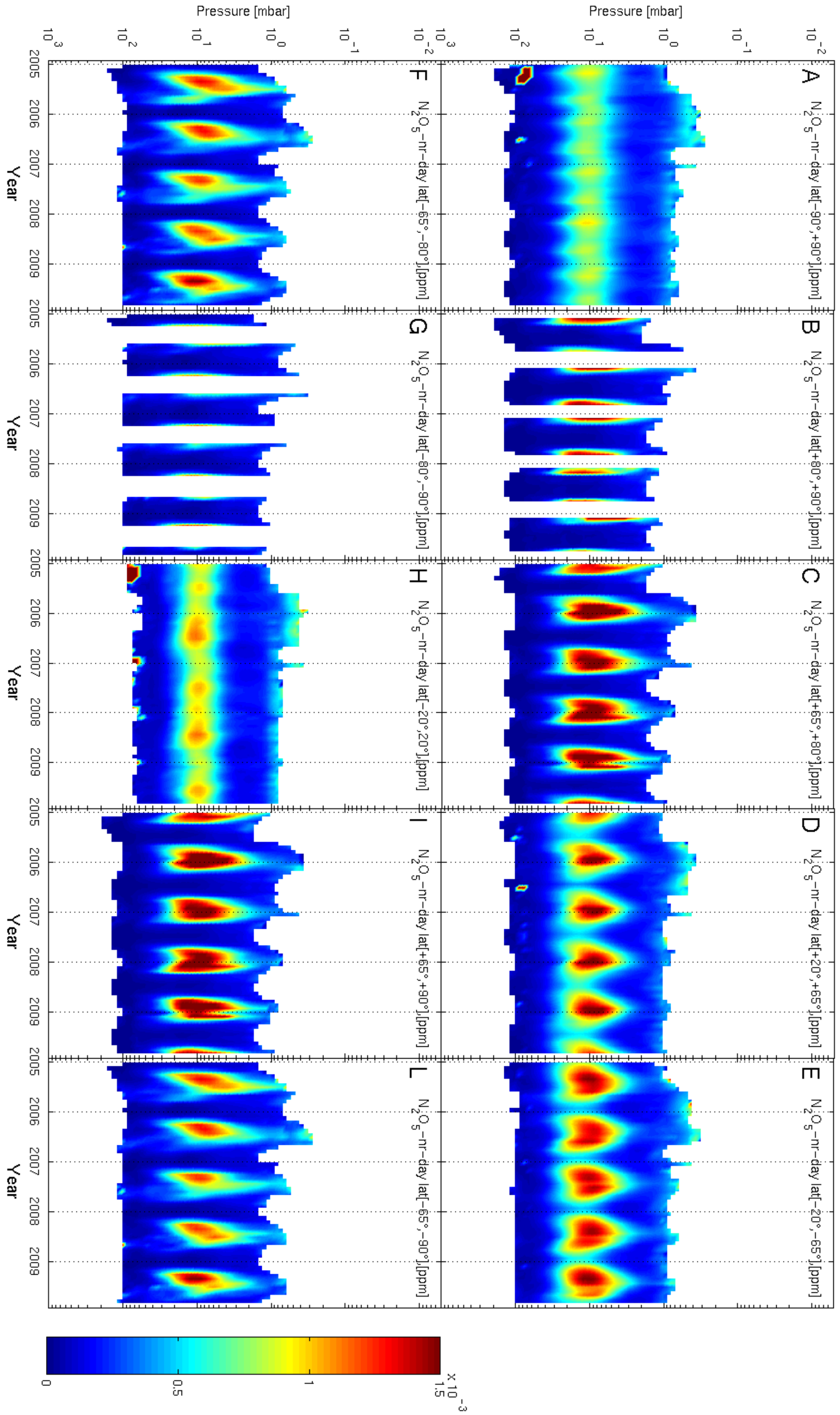


Figure 45: Time series of monthly averaged N2O5 VMR (color scale, in ppmv) as a function of pressure. Averages are shown for various latitude bands as indicated in the plots key. In this case averages include <u>only day-time measurements</u>.

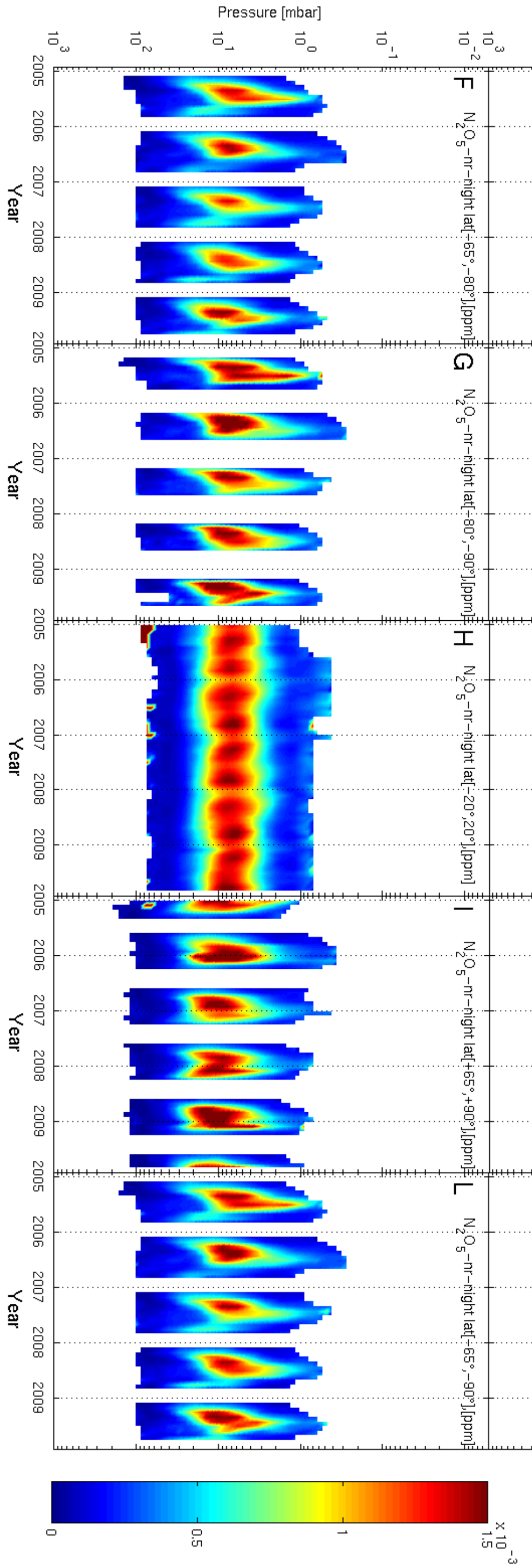


Figure 46: Time series of monthly averaged N2O5 VMR (color scale, in ppmv) as a function of pressure. Averages are shown for various latitude bands as indicated in the plots key. In this case averages include <u>only night-time measurements</u>.

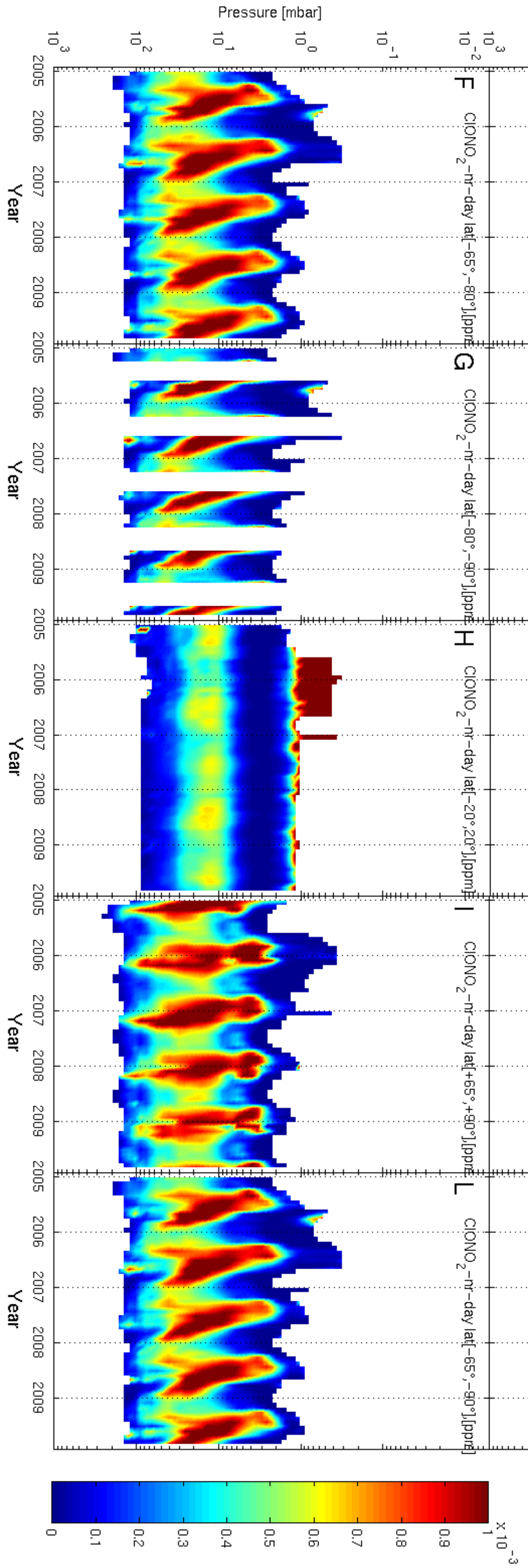


Figure 47: Time series of monthly averaged ClONO2 VMR (color scale, in ppmv) as a function of pressure. Averages are shown for various latitude bands as indicated in the plots key. In this case averages include <u>only day-time measurements</u>.

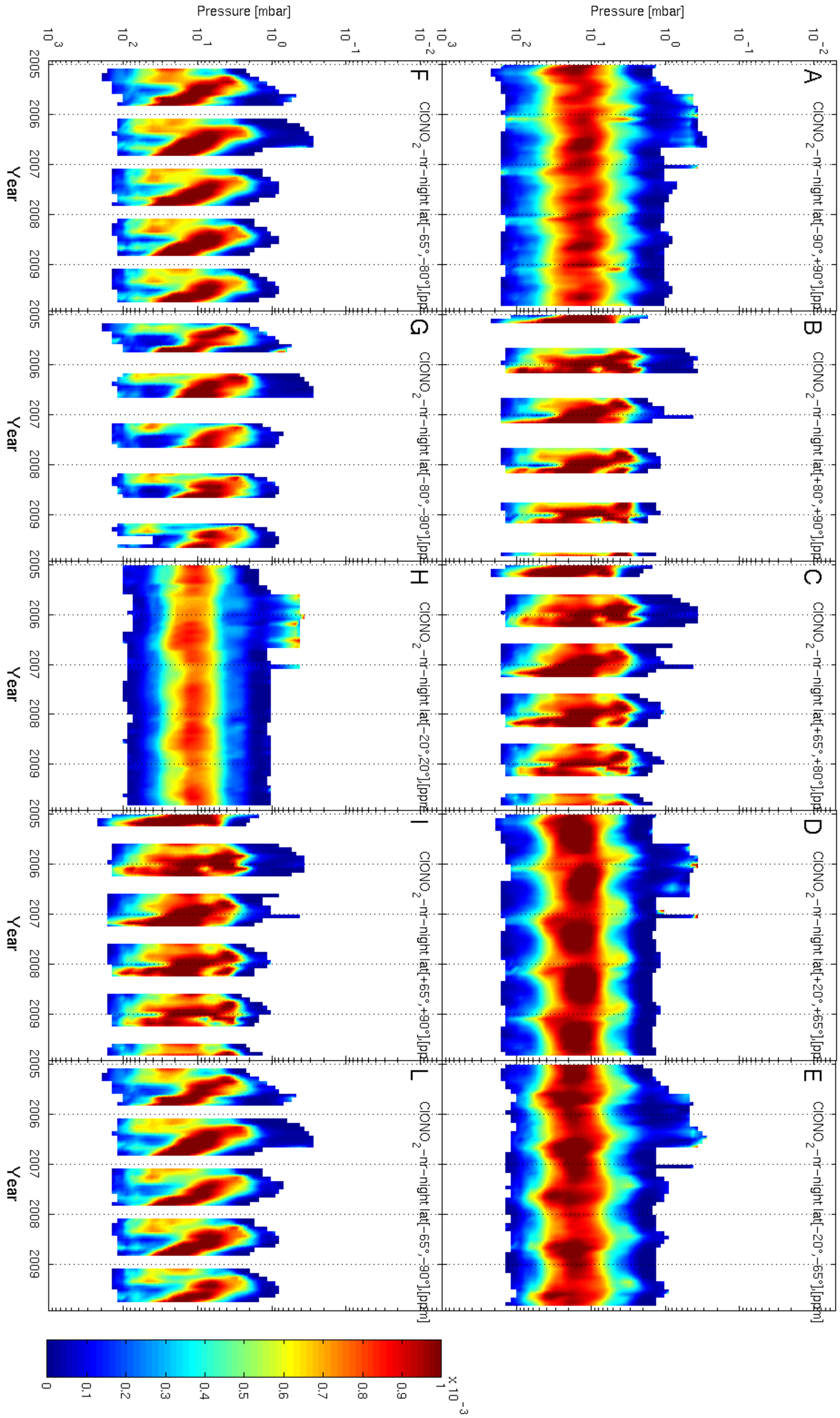


Figure 48: Time series of monthly averaged ClONO2 VMR (color scale, in ppmv) as a function of pressure. Averages are shown for various latitude bands as indicated in the plots key. In this case averages include only night-time measurements.

7 Summary

The ORM_PDS is the scientific baseline for the ESA Level 2 on-line processor (IPF) for MIPAS. In particular, the ORM_PDS_V1.0 is aligned with the current version of the IPF (IPF V. 5.0.5), while the ORM_PDS_V2.0 is aligned with the coming release of the IPF (IPF V.6.0). Both the versions of the ORM_PDS were used to process to L2 a set of approximately 4500 MIPAS orbits acquired in the time frame from January 2005 to November 2009 in the OR configuration.

In this report we show the results of the preliminary analysis of the performance and the quality of the ORM_PDS products. The main findings can be summarized as follows:

- The analysis of the final chi-square (CHI2N) reached in the inversions shows that the retrieval of some species, namely O3, CH4, N2O, N2O5 and ClONO2 is sensitive to the solar zenith angle (SZA) at the tangent point of the mid-sweep of the scan. The minimum value achieved by CHI2N increases as the SZA becomes smaller than 95 deg. i.e. as soon as the sun rises from the local horizon at the tangent point of the mid-sweep of the scan. Further investigations are necessary to understand the origin of the problem (non-LTE ?) and to quantify the related error impacting the retrieved profiles (i.e. does the large final CHI2N mean also large systematic error on the retrieved VMR ?)
- Systematic differences between FR and OR products. For some retrieval targets (namely H2O, CH4 and N2O) we found evidence of systematic differences between FR and OR products. Considering the results of the FR validation activities, we argue that the OR products should be of better quality (compared to the FR), meaning that the OR products seem more realistic and should better agree with correlative measurements.
- The tangent height corrections calculated by the ORM_PDS depend on the initial guess temperature profile used, therefore they are not reliable. Compared to the ORM_PDS, the IPF processor contains an additional algorithm for correction of the tangent heights. This algorithm is based on the retrieved tangent pressures and temperatures and uses the altitude scale provided by ECMWF data. For this reason the final tangent height corrections provided by the routine IPF processing are considered more reliable compared to those provided by the ORM_PDS.
- Comparison ORM_PDS_V1.0 versus V2.0:
  - ✔ The new convergence criteria used by the ORM_PDS_V2.0 permit to achieve, on average, the same value of the final CHI2N. At the same time the new criteria reduce significantly both the number of iterations required to reach convergence and the number of non-converging retrievals.
  - ✔ The retrieval of the additional species (F11, F12, N2O5, ClONO2) in the ORM_PDS_V2.0 reduces the error due to interference of these species in the spectral intervals used for the inversion of the other MIPAS targets. This error reduction is clearly visible only in the cases of HNO3 and CH4, below 18 km. The final CHI2N achieved by the ORM_PDS_V2.0 for these species in NOM and UTLS1 modes is smaller than that achieved in V1.0 retrievals. For CH4, however, the smaller CHI2N is achieved with a larger number of iterations. For the IPF V.6.0 operations we should make sure that possible oscillating and / or unphysical profiles of the additional species retrieved are not used as assumed or initial guess profiles in the retrieval of the main targets.
  - ✔ The ORM_PDS_V2.0 provides, as an additional output, also the so called “measurement space solution” (MSS). The MSS results are freely distributed by IFAC-CNR for science development purposes (see Sect. 5.2 and RD7).