Update to Technical Note on

Results of WP8300 and WP8500

14 August, 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

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INTRODUCTION

The present document is a follow-up of the technical note delivered to ESA on July 2, 2001 entitled “Results of WP8300 and WP8500”. After the delivery of that technical note (referred as “***TNor*** document” from now on) some further actions were identified in order to better exploit the result of the activities carried out within WPs 8300, 8400, and 8500. In the present document the ***TNor*** document is assumed as known so that we only describe the rationale of the new activities and their outcome.

WP8300

As it has been stressed in ***TNor*** document, WP8300 was a 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.

After completion of the retrievals the reference profiles were made available, that is the profiles used by the Reference Forward Model (RFM) to produce the simulated observations. In presence of this new information it is meaningful to compare the reference profiles with the profiles that have been retrieved and their uncertainties. For this purpose the set of figures from 1 to 28 associated to this “update” report the above mentioned comparisons for all retrievals operated on the four atmospheric scenarios. In these plots the horizontal bars represent the *total* error associated with the retrieved quantity; this error was also reported (as % value) in tables from 2 to 13 of ***TNor*** document.

In order to interpret the new figures we recall that, in simulating the analyzed observations, 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 that should be taken into account by the quantifiers associated to the occupation matrices. In the reported figures, the occurrence of situations in which the reference value does not lay within the error bar of the retrieved value, indicates the underestimate of one or more of the error quantifiers and/or the unexpected correlation between different error sources.

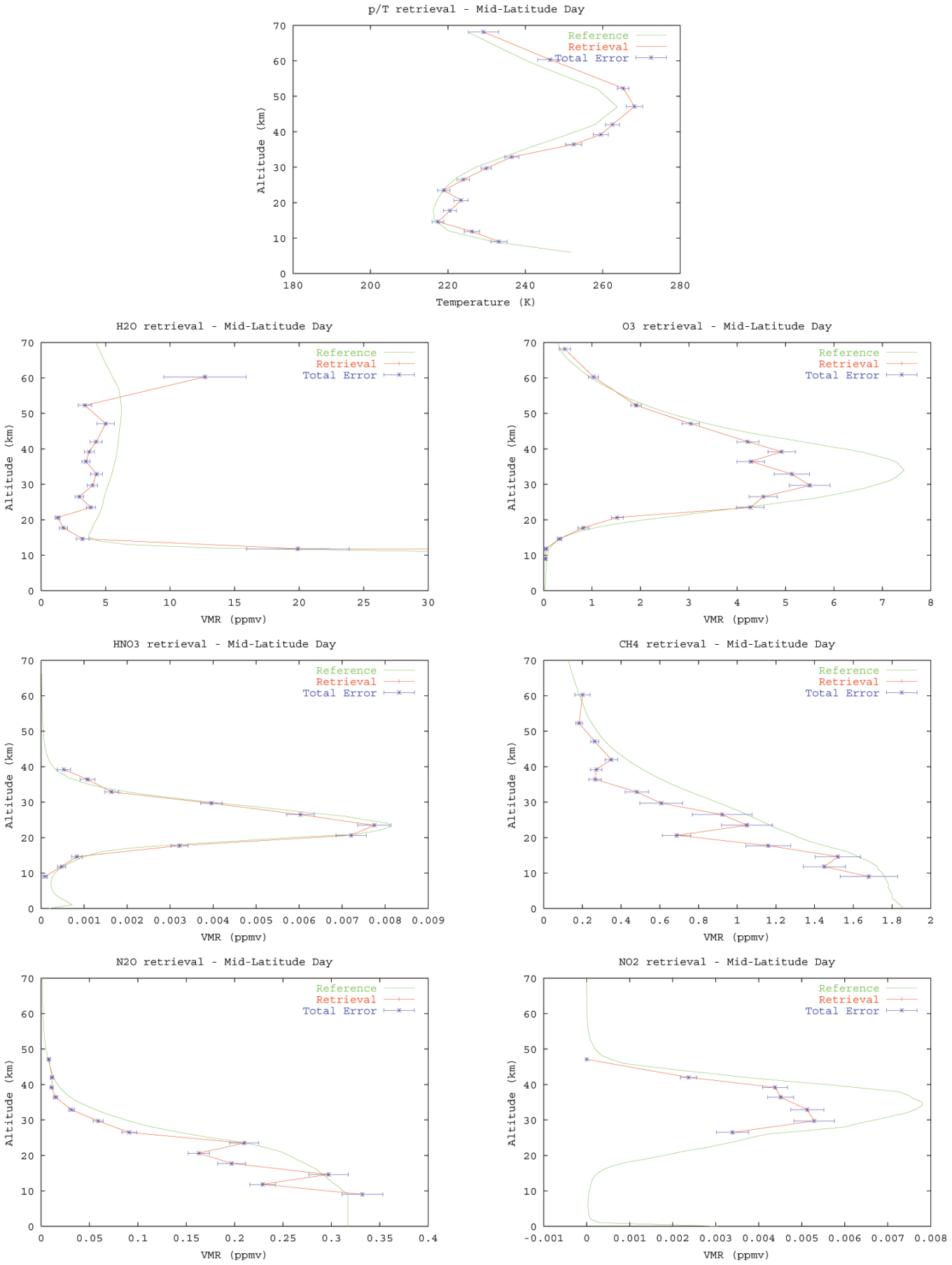


Figure from 1 to 7: plots that report the reference profile (green curve) and the retrieved quantities (red curve), together with their total errors (blue lines), for the Day scenario.

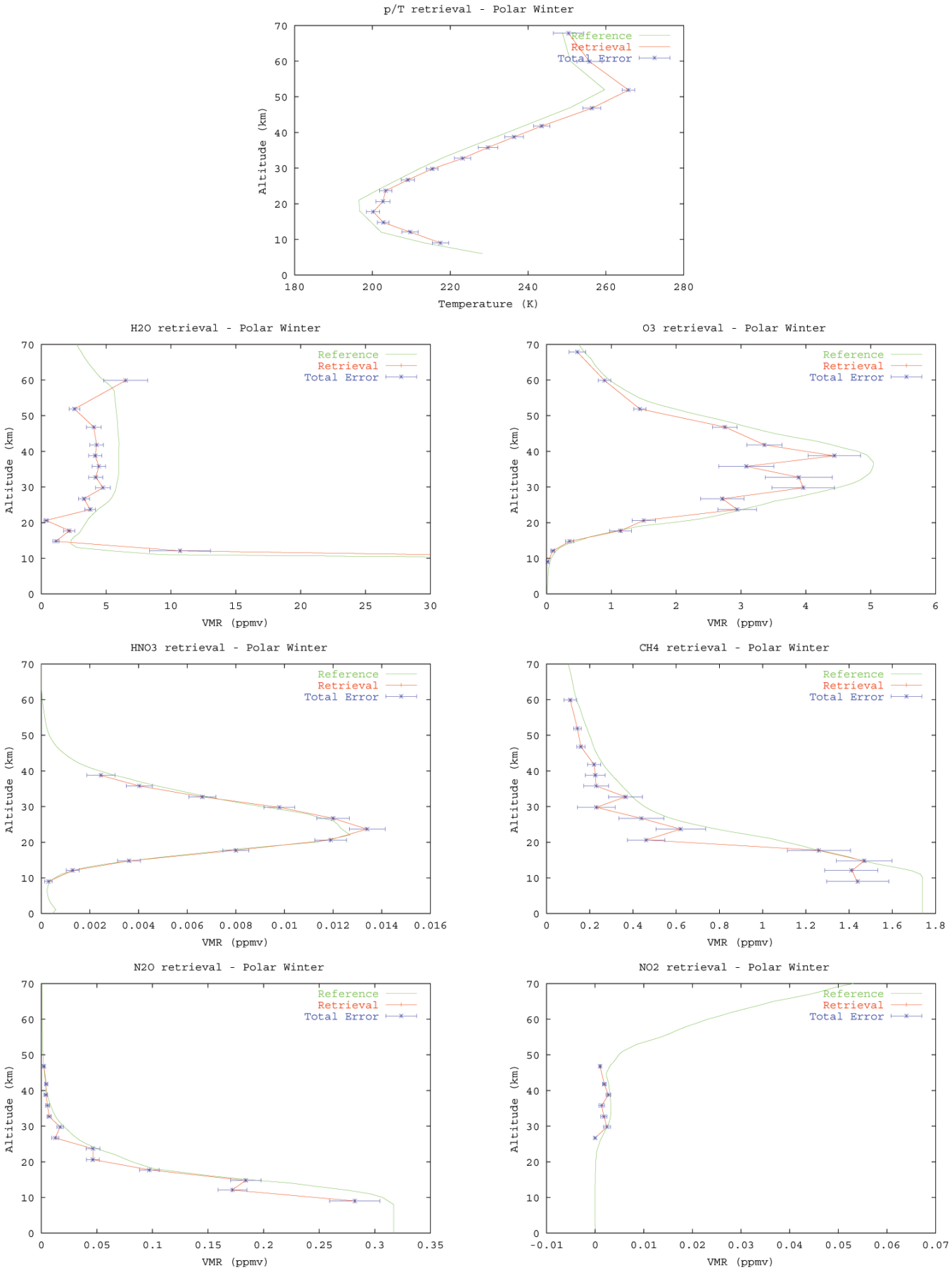


Figure from 8 to 14: plots that report the reference profile (green curve) and the retrieved quantities (red curve), together with their total errors (blue lines), for the Winter scenario.

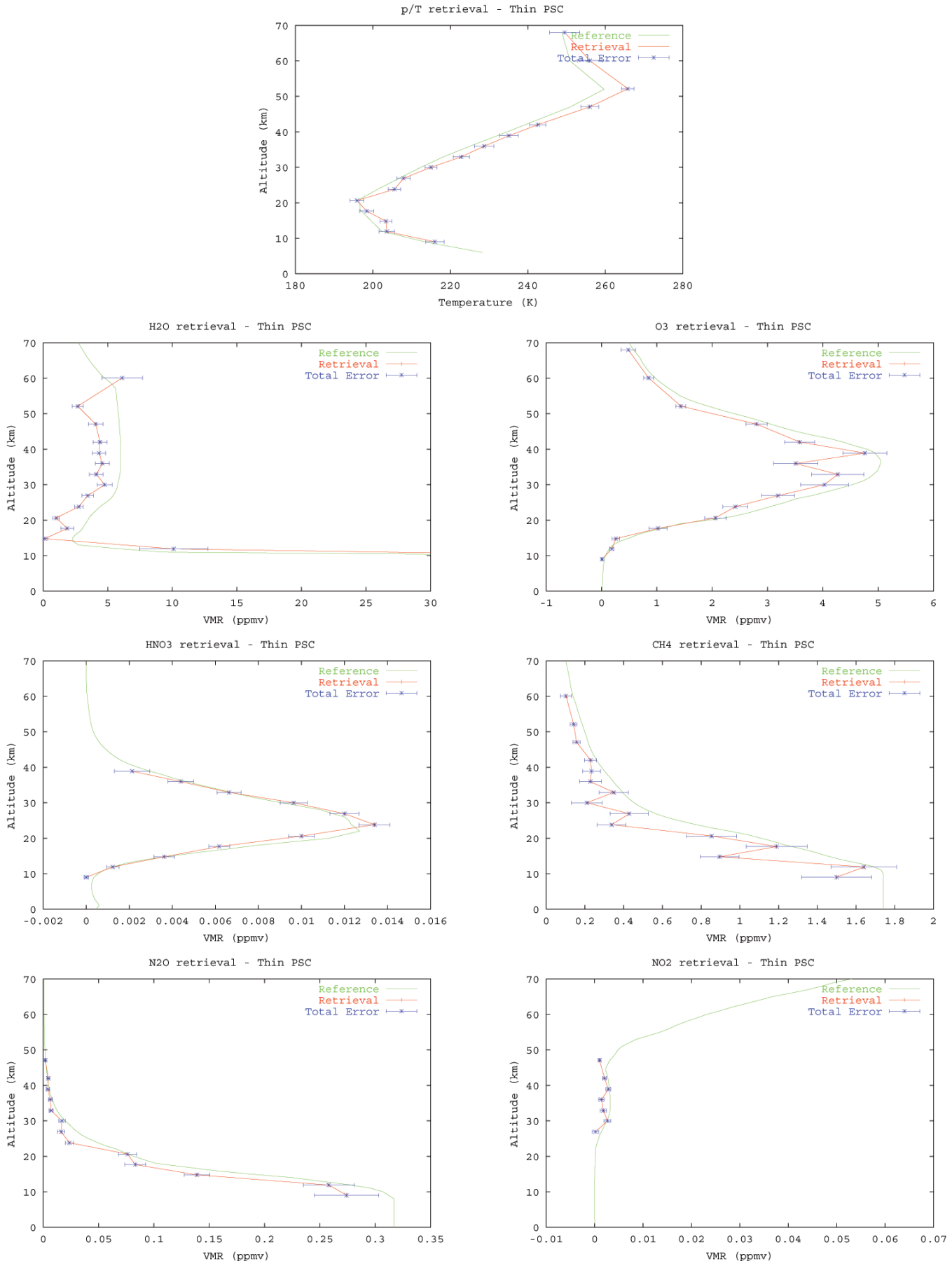


Figure from 15 to 21: plots that report the reference profile (green curve) and the retrieved quantities (red curve), together with their total errors (blue lines), for the PSC1 scenario.

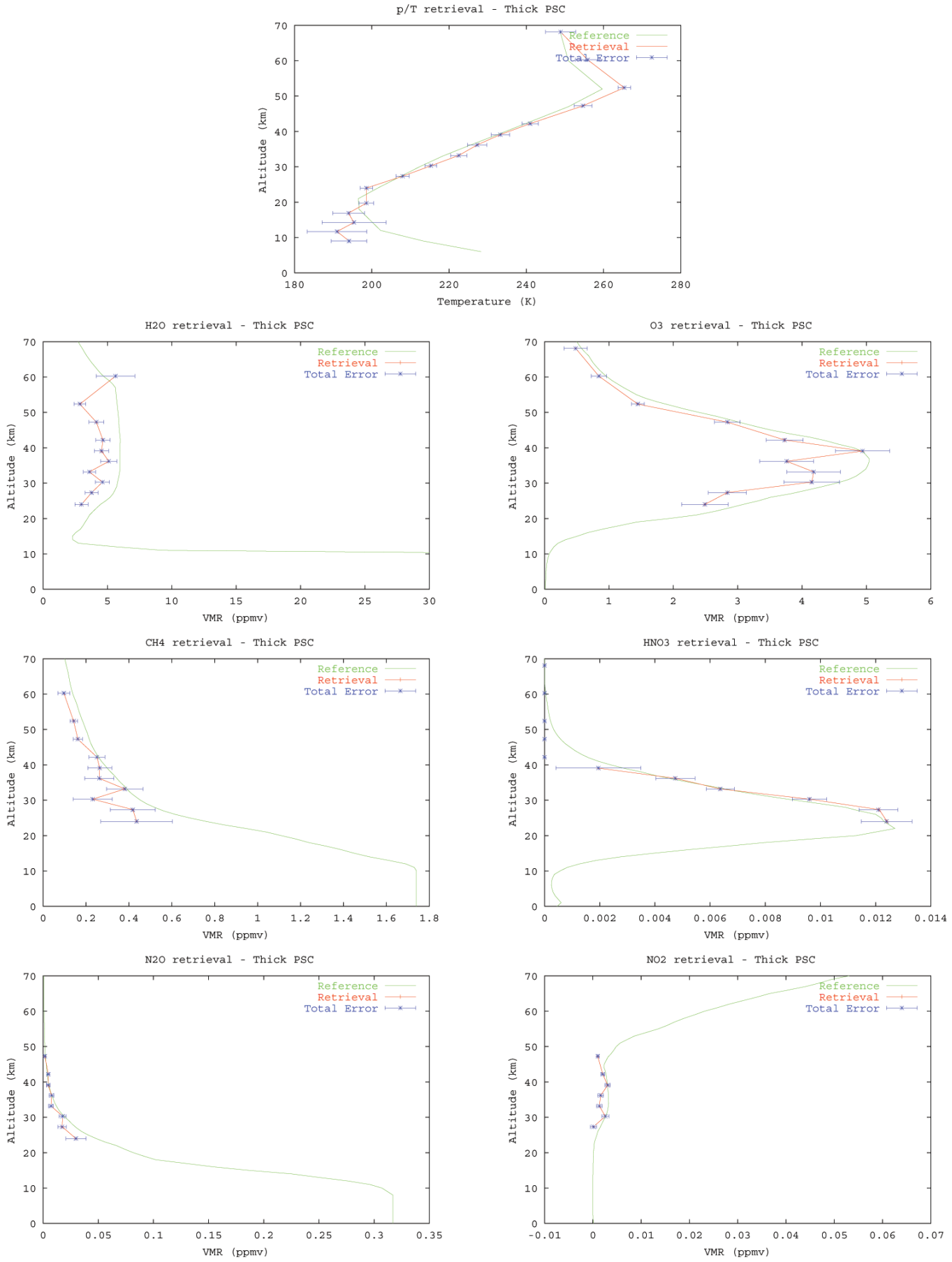


Figure from 22 to 28: plots that report the reference profile (green curve) and the retrieved quantities (red curve), together with their total errors (blue lines), for the PSC2 scenario.

WP8500

We recall that in this WP observations covering a full orbit (75 limb-scanning sequences) were simulated and analyzed with ORM. The profiles retrieved from each limb-scanning sequence were used as initial guess for the target quantities in the analysis of the following sequence. The IG2 profile-database was used to quantify the contaminant species and to provide the initial guess for the target quantities in the analysis of the first sequence of the orbit.

The problem was encountered of a lack of convergence in *p*,T and water retrievals when the altitude of tropopause in the initial guess atmosphere significantly differs from the altitude of tropopause in the atmosphere that generates the observations. The lack of convergence derives from the large difference between water (and temperature) profiles below the highest of the two tropopauses. In the tests carried out within WP8500 it was verified that, along the orbit, the occurrence of this problem depends on the distribution of spectral noise. However the problem showed up most frequently in the first limb-scanning sequence when IG2 profiles are used as initial guess for the target species.

In ***TNor*** document it was shown that a successful strategy to overcome the lack of convergence is to re-iterate the *p*,T and water retrievals using as initial guess the profiles derived in the previous (unsuccessful) retrievals. However this strategy was not considered applicable to the level-2 processor (because it requires code modifications) and two sequential tests were proposed in order to identify a solution that can be implemented through input files. These tests are:

1. Start the analyzed orbit with a limb-scanning sequence located at arctic latitude (Kiruna latitude was identified as reference) instead of the mid latitude previously used in the WP8500 tests. This test is aimed to start the retrievals where the tropopause altitude is expected to be more stable.

2. Eliminate from the retrieval observations and parameters that correspond to the two lowest tangent altitudes (9 and 12 km). This test is aimed to identify a safe retrieval scenario in which only stratospheric observations are analyzed.

Test 1

As input to WPs 8400 and 8500 ESA provided the geo-location of the tangent points of all the observation geometries along one orbit starting around mid latitude in the southern hemisphere (see Fig. 44 of ***TNor*** document). Data from this input were rearranged in order to obtain an orbit starting at Kiruna latitude. Figure 29 shows the geo-location of the mid point for each sequence of this new orbit.

Since the occurrence of the lack-of-convergence problem depends on the distribution of spectral noise the simulated-retrieval scheme was repeated 5 times on the new orbit. In no case we had lack of convergence in correspondence of the

starting limb-scanning sequence. Nevertheless the problem still showed up for sequences around the antarctic vortex.

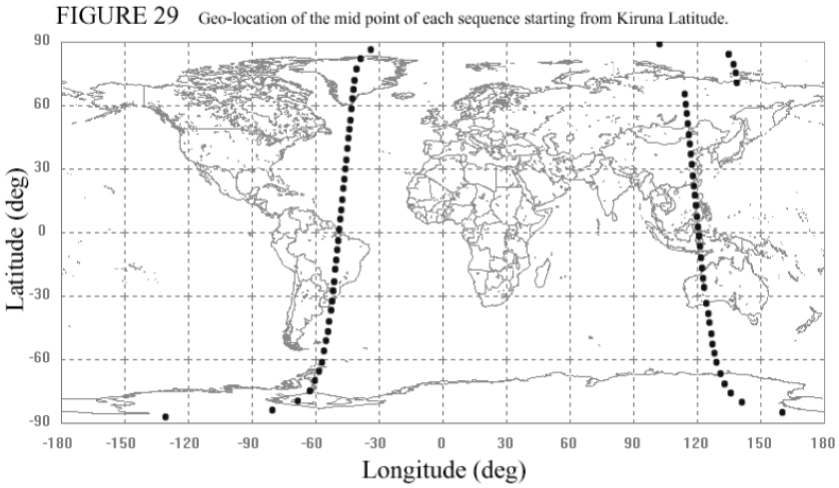


Figure 29: Geo-location of the mid point of each limb-scanning sequence starting from Kiruna latitude.

Test 2

The new orbit was also used for test 2. The simulated-retrieval scheme was repeated eliminating observations and parameters that sequentially correspond to 9, 12 and 15 km tangent altitudes. In no case we got a full orbit without the occurrence of the lack-of-convergence problem for sequences around the antarctic vortex.

Further test

Once verified the failure of test 2 we made several additional tests in order to identify a solution that can be implemented in the level-2 processor through input files. The rationale for these tests was that, once solved the problem for the starting sequence,

- the lack of convergence occurs in correspondence of a marked horizontal discontinuity in the atmospheric fields,
- along the orbit the discontinuities are a few and well separated between themselves.

The objective is therefore to force the retrieval system not to reach the maximum number of allowed iterations by regarding as satisfied the convergence criteria even in presence of the “poor” retrieval that occurs when crossing the horizontal discontinuity. If this happens the retrieved profiles are “poor” but they will be fed as initial guess to the next sequence acting as the result of a first *p*,T and water iteration for that sequence. Since the occurrence of horizontal discontinuities is not known in advance, the adopted strategy was to look for less stringent convergence criteria that, however, are still acceptable for all sequences of the orbit. The

convergence criteria determined for the PSC2 atmospheric scenario (see WP8300 of ***TNor*** document) were considered for this purpose for *p*,T and water retrievals. After a few tests these criteria were refined so that a new set was determined that is satisfactory for both the PSC2 atmospheric scenario of WP8300 and the full orbit retrievals provided that, in the second case, observations and parameters that correspond to 9 km tangent altitude are excluded from the retrievals. We summarize in the following table all the convergence criteria that have been adopted for all target quantities:

	rconvc(1)	rconvc(2)	rconvc(3)
***p*,T**	0.1	0.015	0.5

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

	rconvc(1)	rconvc(2)
H_2O	0.01	0.01
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

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

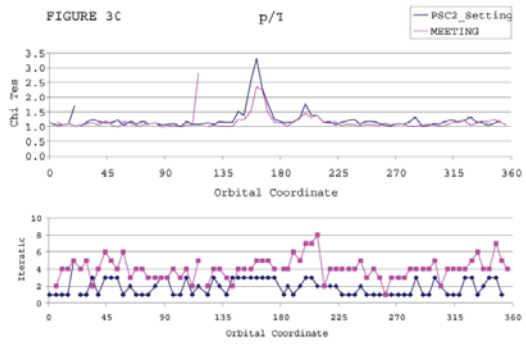
With these retrieval conditions no lack of convergence occurred after retrieval simulations operated with 6 different spectral-noise distributions. In figures from 30 to 36 the blue drawings refer to these retrieval conditions and report (for all target quantities) the χ-test value at convergence and the number of iterations for each limb-scanning sequence. In the figures the red drawings refer to the previous retrieval conditions and represent the same quantities as already reported in Figs. from 52 to 58 of ***TNor*** document. In order to make comparable the results obtained with the two retrieval conditions, the "orbital coordinate" is reported on the *x*-axis instead of the "sequence number" as in the figures of ***TNor*** document. The inspection of the new figures shows that the worsening of χ-test values is not dramatic while (as expected) the number of required iterations is generally lower with the new retrieval conditions. However, in this comparison, it must not be forgotten that the 9 km tangent altitude has been eliminated in the new retrieval conditions.

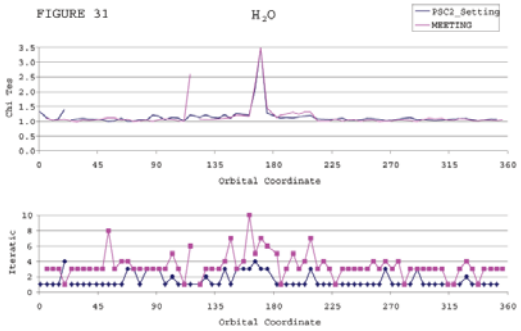
In ***TNor*** document three-dimensional maps were included for each target quantity reporting, as a function of both orbital coordinate and altitude, the distribution of ESD and of retrieved - reference (|Retr-Ref|) values. With the new orbit, starting at Kiruna latitude, and with the new retrieval conditions, the distribution of the above quantities is (of course) changed. The updated maps are

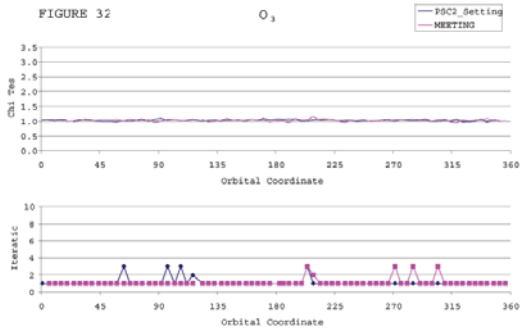
available, however we chose not to include them to this “update” because what they show is a slight overall decay of the quality of the retrievals, that can also be appreciated in figures from 30 to 36. Instead we include figures from 37 to 44 that report maps representing the distribution of the quantity ***D*** defined as:

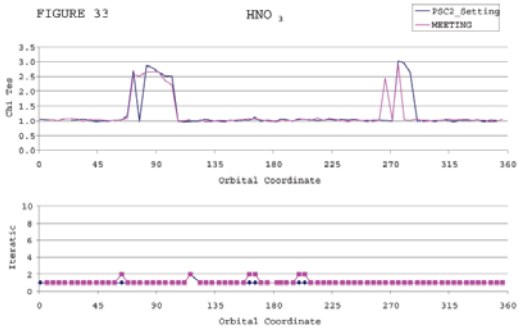
$$D = |Retr-Ref|/(Total)$$

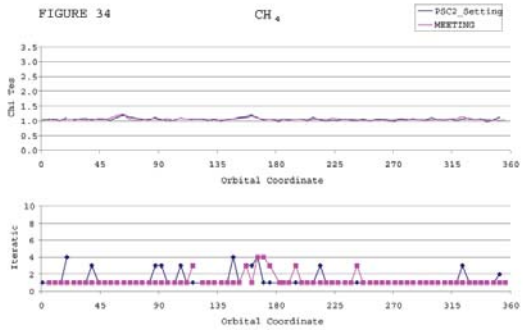
in which ***Total*** is the total error as defined at point 4 of Sect. 2.1 of ***TNor*** document (page 6) and plotted in figures from 10 to 17 of that document. The aim of these maps is to compare the predicted accuracy of the retrievals (represented by ***Total***) with the actual errors. The new maps indicate an overestimate of the accuracy whenever ***D*** exceeds the unity.

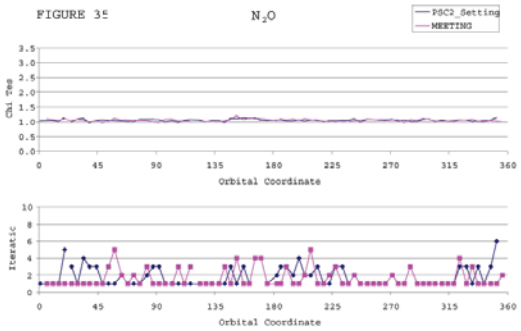












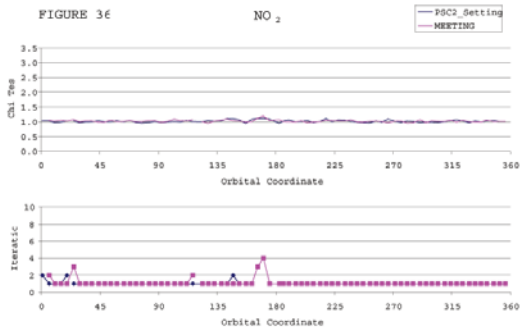


Figure from 30 to 36: plot reporting the χ-test value at convergence and number of iterations for each limb-scanning sequence obtained with the two retrieval conditions.

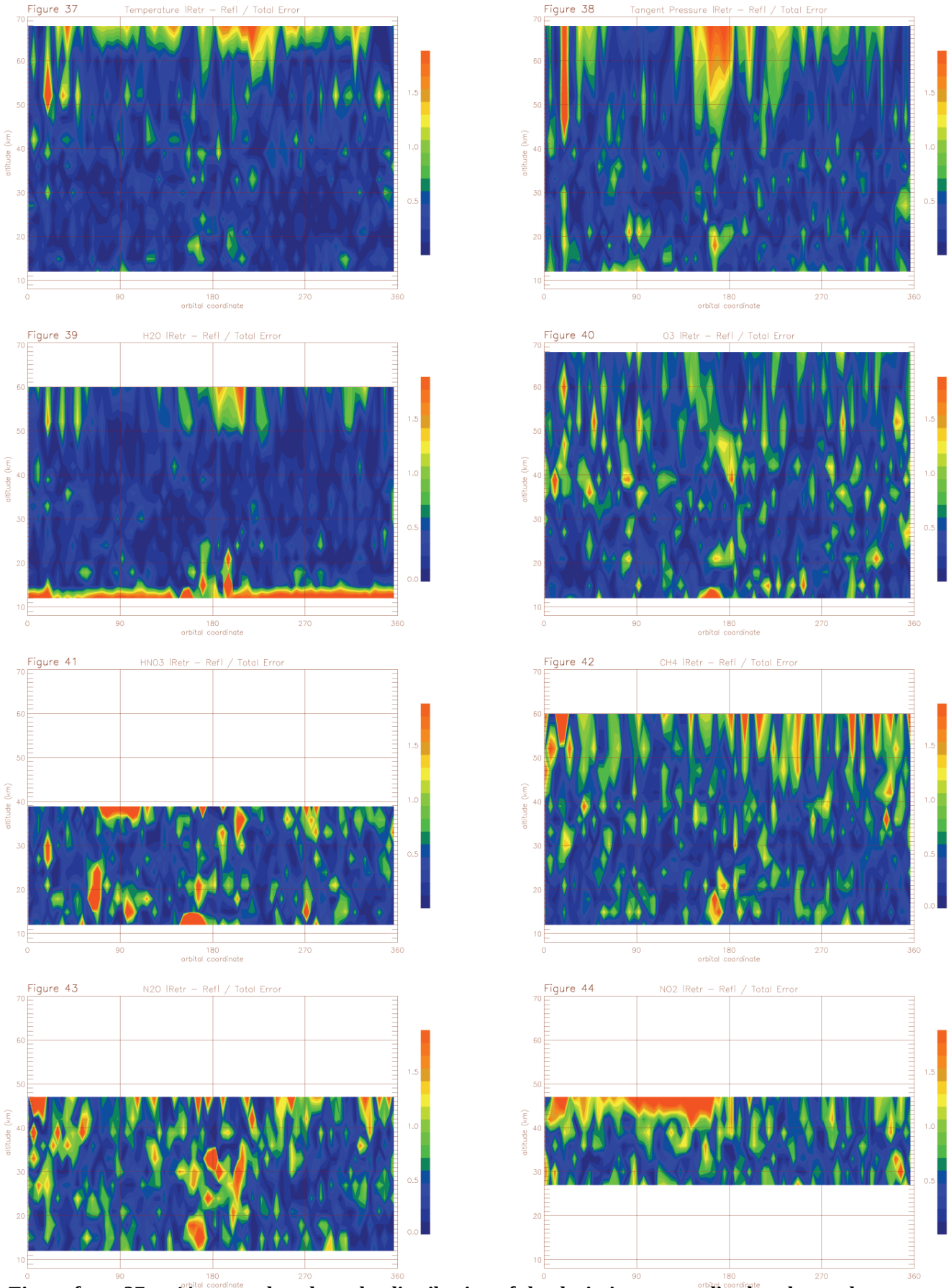


Figure from 37 to 44: maps that show the distribution of the deviations normalized to the total errors of the retrieved quantity.