REC Analysis of MIPAS data
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Abstract

This document describes the 'Residuals and Error Correlation' (REC) analysis of ESA's MIPAS L2 products from August 2002 until the end of February 2003. The analysis consists of a statistical correlation between the monthly average of residual spectra (i.e., MIPAS measurements − forward model) extracted from the NRT L2 data and spectra characterising various sources of error such as contaminant species and instrumental artefacts.

The main change in the processing during this period, which occurred on November 13th, led to a improvement (i.e., reduction) in most residual signatures. However, there still appear to be problems associated with the pT, HNO_3, H_2O and NO_2 retrievals, as well as with some of the climatological profiles assumed for contaminant species.

Contents

1 Introduction

1.1 REC Analysis

The Residuals and Error Correlation (REC) analysis is a statistical fit of predetermined error spectra to the observed residuals, defined as (observed − forward model) spectra. The error spectra are defined as (perturbed − nominal) spectra where the perturbations represent a change in some forward model or instrumental parameter. In all cases, the nominal and perturbed spectra are defined for mid-latitude day-time conditions.

If $\mathbf{y}$ represents a set of residual spectra (m measurements in total), and $\mathbf{x}$ represents the set of fit coefficients for error spectra from n different parameters, $\mathbf{y}$ is modelled as

$$\mathbf{y} = \mathbf{K}\mathbf{x} + \delta\mathbf{y} \tag{1}$$

where $\mathbf{K}$ is a $m \times n$ matrix, each column containing the equivalent m spectral points from the error spectra of one particular error source, and $\delta\mathbf{y}$ is the (apodised) NESR, covariance $\mathbf{S}_y$, reduced in accordance with the number of spectra averaged. The coefficients of $\mathbf{x}$ are defined so that $+1$ is equivalent to a $+1\sigma$ perturbation in the error source.

In practice, the residual and error spectra for each microwindow are adjusted to have zero mean value. There is an option to fit the residual values at only the 'unmasked' spectral points but here the full microwindow spectra are used in order to establish the maximum signal for the error sources rather than just the signal in the measurements used for the retrievals.

The simplest method of determining the coefficients $\mathbf{x}$ is to perform a 'least squares fit' for each error component independently

$$x_i = \left(\mathbf{k}_i^T \mathbf{S}_y^{-1} \mathbf{k}_i\right)^{-1} \mathbf{k}_i^T \mathbf{y} \tag{2}$$

where $\mathbf{k}_i$ is the column of matrix $\mathbf{K}$ for error source i. This is applied to each microwindow/tangent altitude independently but can only be used for error spectra with a distinct signatures in *all* residuals, i.e., the 0th, 1st and 2nd derivative signatures.

For other error sources which may only have signatures at particular altitudes or spectral ranges an optimal estimation approach is used

$$\mathbf{x} = \mathbf{a} + \mathbf{S}_a \mathbf{K}^T \left(\mathbf{S}_y + \mathbf{K}\mathbf{S}_a\mathbf{K}^T\right)^{-1} (\mathbf{y} - \mathbf{K}\mathbf{a}) \tag{3}$$

where $\mathbf{a}$ is a vector of *a priori* estimates for each fit coefficients (0 in most cases, 1 for approximations in the forward model expected to result in a known bias, §6). $\mathbf{S}_a$ is the *a priori* covariance. Since columns of $\mathbf{K}$ are defined as 1σ perturbed spectra, $\mathbf{S}_a$ is simply the identity matrix $\mathbf{I}$.

1.2 Averaging Residuals

ESA L2 data have been collected routinely by ftp since August (earlier data have also been collected but shows large anomalies so have not been included in this report). The most general case is to average residuals for each microwindow at each nominal altitude but further subdivisions have been employed. Note that within the L2 data itself the residuals represent such an average over successive scans. There are five domains over which residuals have either been averaged or divided

1. Time — monthly averages. Note that 'October' includes November data prior to Nov 13th.
2. Latitude — 6 'MIPAS' bands bounded by 90S, 65S, 20S, Equator, 20N, 65N, 90N
3. Altitude — nominal sweep tangent height (12–68 km for operational retrievals)
4. Wavenumber — i.e., position of microwindow within MIPAS coverage
5. Solar Zenith Angle — i.e., whether atmosphere is illuminated by the sun or not

A subset of domains has been selected appropriate to each error source.

Time

The main subdivision adopted throughout this report is in time: residuals from the ESA L2 processing are averaged for each month and analysed separately, in principle allowing any slowly varying trends to be identified as well as step-changes in the processing (notably the pitch adjustment and spectral calibration changes which occurred on Nov 13th).

Latitude

Within each month, residuals for 6 latitude bands have been averaged separately. This is actually an averaging of residuals separately for each occupation matrix: occupation matrices 001 to 006 are all so-called 'nominal' occupation matrices with numbers which only serve to distinguish the different latitude bands. Note that the results presented for distinct latitude bands therefore only include residuals from the nominal OMs. The latitude subdivision has been applied to all except the spectral derivative signatures (§7), which are not observed to have any significant latitudinal dependence compared to the spectral and altitude domains.

Altitude

Residuals are averaged separately for each microwindow/sweep altitude but there is a choice as to whether to perform the REC analysis for each altitude separately, allowing a profile of error fit coefficients to be established, or to combine all altitudes and retrieve a single fit coefficient representing a perturbation of the entire vertical profile. Where altitude divisions have been employed an average over all latitudes is used.

Wavenumber

In most cases, spectral signatures are expected to be fully correlated with wavelength (e.g., if a contaminant is overestimated in one region of the spectrum it should be overestimated in all regions) so fitting over all wavenumbers (i.e., microwindows) is an advantage in discriminating between signatures of different species.

However, in the case of the spectral derivatives the least squares fit has been applied to each microwindow (and tangent height) separately in order to detect any spectral trend with wavenumber (or altitude).

Solar Zenith Angle

Certain species are expected to be affected by photochemical or non-LTE effects. Where these are expected to be significant these have been overplotted on the other plots. This has also been done for the REC analyses of the key-species in order to check the magnitude of such effects.

1.3 Caveats

The REC analysis is a convenient tool but there are a number of problems associated with such an statistical approach.

1. it is assumed that *all* significant errors are adequately represented by the error spectra considered.

2. it is assumed that the contaminant profiles only differ from the Initial Guess data by a simple perturbation 'shape'. In most cases the residual fit in the latitude plots will be influence largely by the low altitude values irrespective of what happens at higher altitude.

3. that the residuals from each error component are sufficiently distinct that they are not aliassed. This is less true for weak signatures with broad spectral structures, such as associated with the absorption cross-section of heavy molecules.

2 Explanation of Plots

2.1 Nominal Microwindows

For the optimal estimation REC analyses, each page starts with a plot of the spectral/altitude coverage of the nominal microwindows (originally selected in January, 2002) and their labels. The horizontal grey lines are the MIPAS measurement/retrieval altitudes from 12–68 km. Note that since there are no nominal microwindows in the D-band (1820–2410 cm^{-1}) this is not included. However, note that some non-nominal occupation matrices do include D-band microwindows.

2.2 Error Spectrum

Under the plot of nominal microwindows is a plot of the 1σ error spectrum for 12 km tangent height, also excluding the D-band. For scaling purposes, the MIPAS NESR 'requirements' are also overplotted as dashed lines (actual NESR values are up to a factor 2 smaller).

2.3 REC Analysis - Latitude

A plot of the fitted coefficient in units of 1σ for each latitude band. Different colours/symbols represent different months, offset slightly in the y-direction for clarity. The solid vertical line indicates 0 mean fit and dashed lines at $\pm 1\sigma$. Positive values imply that the observations contain a larger concentration than the assumed/retrieved profile. For species with an expected diurnal variation the residuals for 'day'/'night' profiles (according to solar zenith angle) are plotted separately as open/solid symbols and dashed/solid lines.

2.4 Variability

Assumed vertical profiles and uncertainties for each species. The solid black line is the mid-latitude day-time profile and the dashed lines are the $\pm 1\sigma$ perturbed profiles. The numbers on the right axis at 5, 15, ... 45km represent the 1σ value expressed as a percentage of the mid-latitude daytime profile at those altitudes. Different colours represent other atmospheric conditions: blue is mid-latitude nighttime (only plotted if different from the day-time), red is polar summer, green is polar winter and yellow is day-time equatorial. The shaded area represents the range of values included in the MIPAS Initial Guess dataset. Where there is no shaded area the IG data just consists of a single profile for all latitudes/seasons.

2.5 REC Analysis - Altitude

A plot of the fitted coefficient for REC analyses performed for each altitude independently (averaging over all microwindows/latitudes). The actual fit is in terms of 1σ climatological SD as with the latitude plot, however this is scaled by the day-time profile value at each altitude to convert to more convenient units (% for pressure, ppmv or ppbv for other species). For the volume mixing ratios, overplotted are the $\pm 1\sigma$ differences as dashed lines, and two pairs of dotted lines representing $\pm 10\%$ and $\pm 100\%$ of the mid-lat daytime profile value. The horizontal grey lines are the MIPAS measurement/retrieval altitudes from 12–68 km. In effect, this is a linear retrieval correction to the assumed profile. Positive values imply that the observations contain a larger concentration than the assumed/retrieved profile.

2.6 Target Species - Additional plots

For the target species the latitude and altitude analyses are repeated analysing the residuals in target species 'other' microwindows separately. In addition, there are latitude and altitude analyses separating residuals from 'day' and 'night' (according to solar zenith angle) retrievals.

3 Target Species

The retrieval adjusts the profile of the target species so that the residual signature is eliminated (at least in the 'unmasked' points). Consequently there should be no significant signature compared with the climatological variability or at a level representing more than a few percent.

However, the retrieval only acts to reduce the target species residuals in the particular microwindows chosen for the retrieval, so the absence of any residual signature in the other microwindows acts as an independent check.

The retrieval sequence may also be significant: pT, H_2O, O_3, HNO_3, CH_4, N_2O and NO_2. When the L2 retrievals are working continously, the assumed profile for each target species will either be the retrieved profile from earlier within the same scan or from the previous scan, but essentially it will be the retrieved profile most of the time. However, when the retrieval is fragmented (as appears to be the usual case with the L2 data analysed here), the assumed profiles for target species later in the sequence are more likely to reflect the IG climatology (e.g., the H_2O retrievals will more often use O_3 profiles from the IG data than the previous scan).

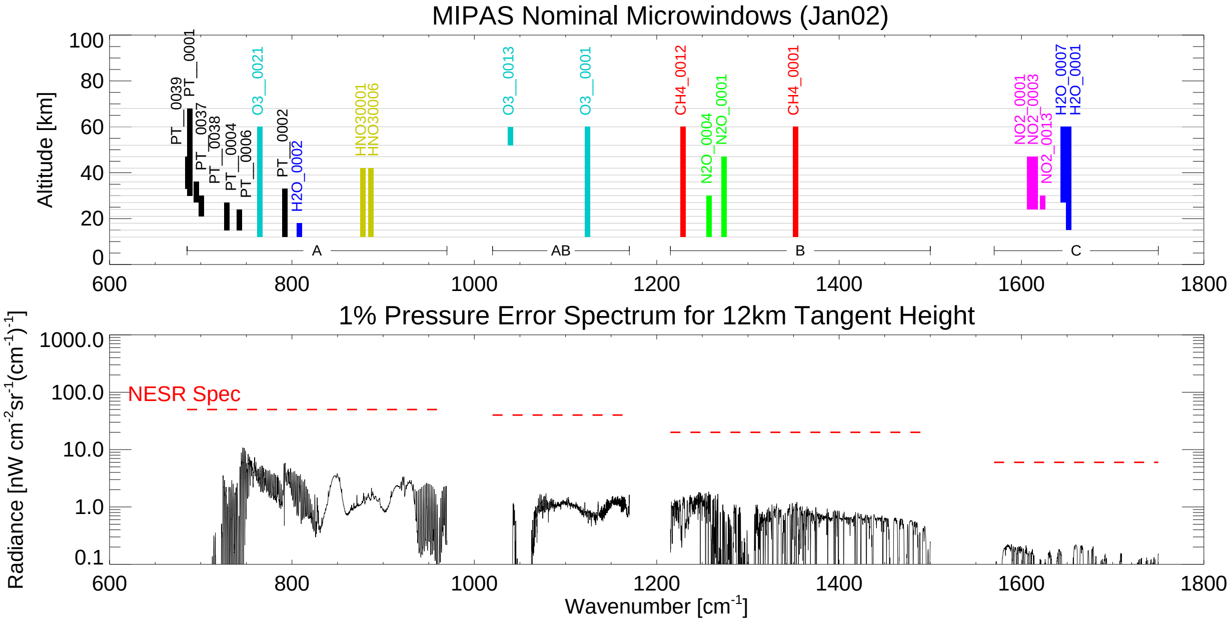
3.1 Problem Areas

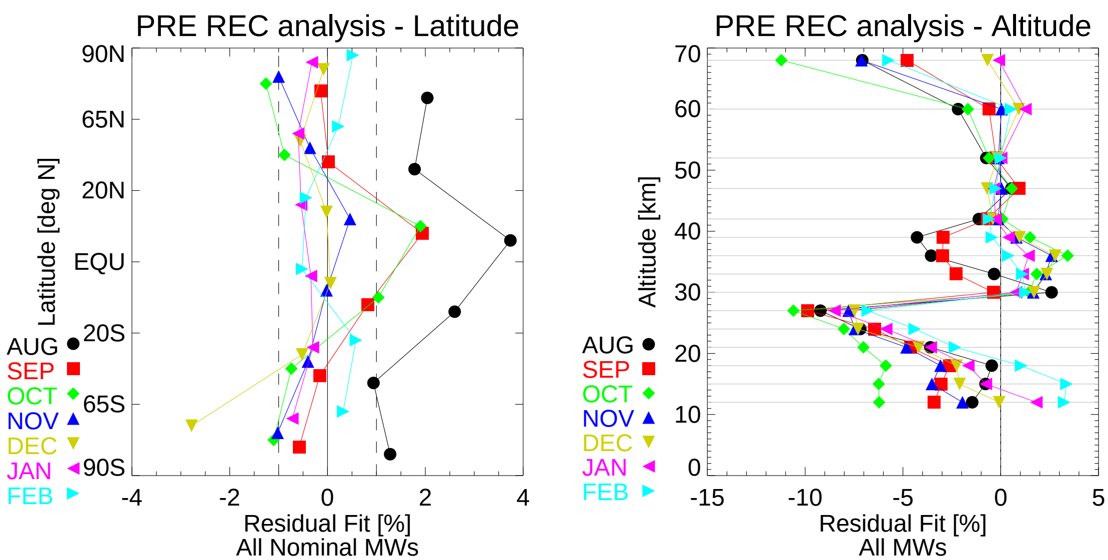
Large residuals in target microwindows might indicate problems with retrieval convergence or (at high altitudes) influence of the upper atmospheric column.

Large/different residual signatures in other microwindows could result from inconsistent spectroscopic data. Note, however, that residual spectra from 'other' microwindows can be from altitudes above the top retrieval level of the target species, in which case the residual may indicate deviations of the IG data from the true atmosphere rather than the target species.

Diurnal variations in residual spectra might indicate non-LTE effects or incorrectly retrieved diurnal variations in the target species.

3.2 Pressure





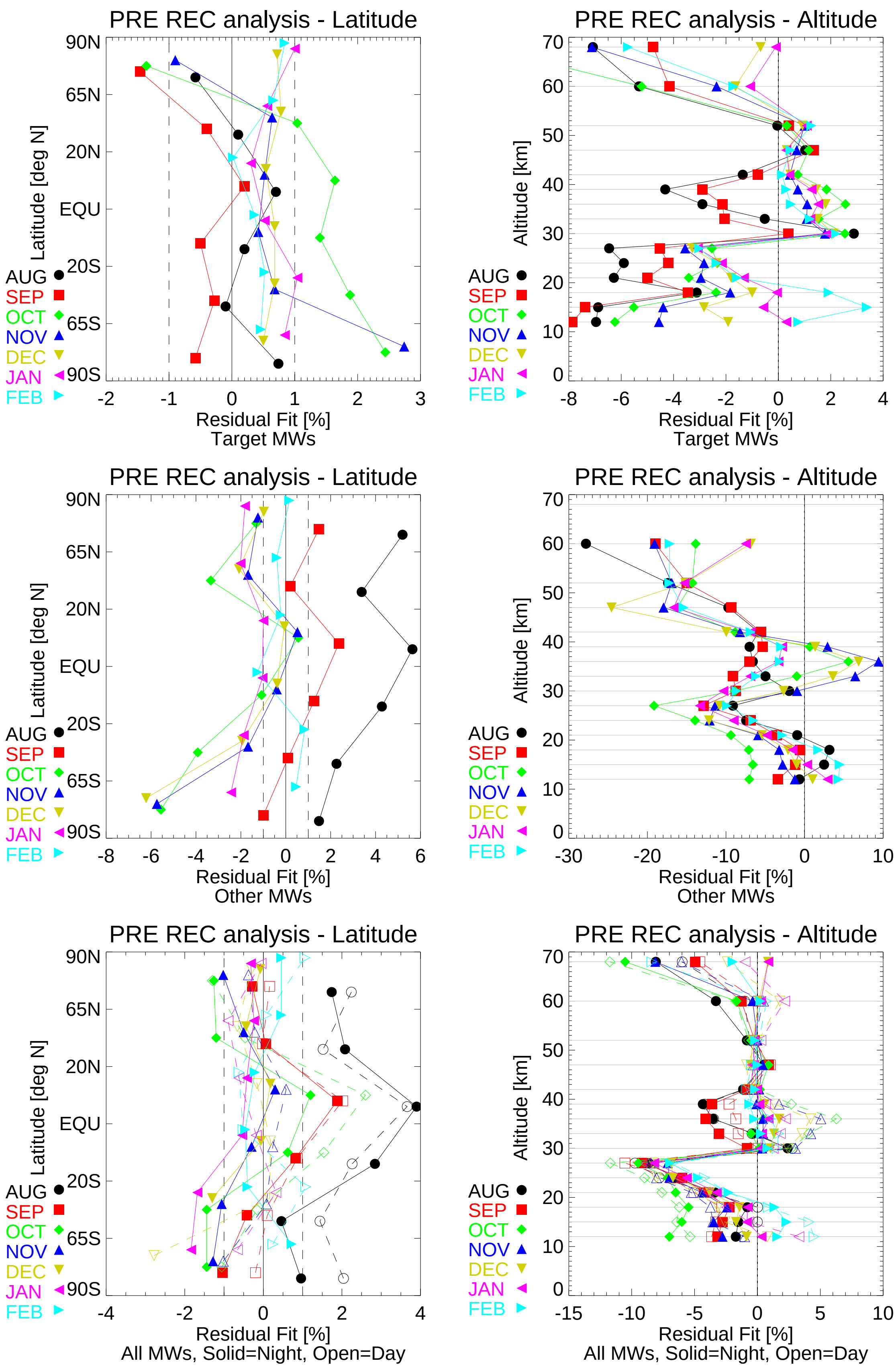
Comments

The Latitude plot indicates pressure was underestimated by 1–4% in August, with a larger underestimate at the equator, and that this error reduced in Sep/Oct, but from Nov 13th was within ±1%. However there appears to be a significant variation with altitude. At lower altitudes there is an *overestimate* reaching 10% at 27 km but reducing sharply to within 1 or 2% at higher altitudes, with a possible 5–10% overestimate at 68 km. Apart from the 30–40 km altitude range there appears to be no significant difference in residual pressure as a function of altitude after Nov 13th.

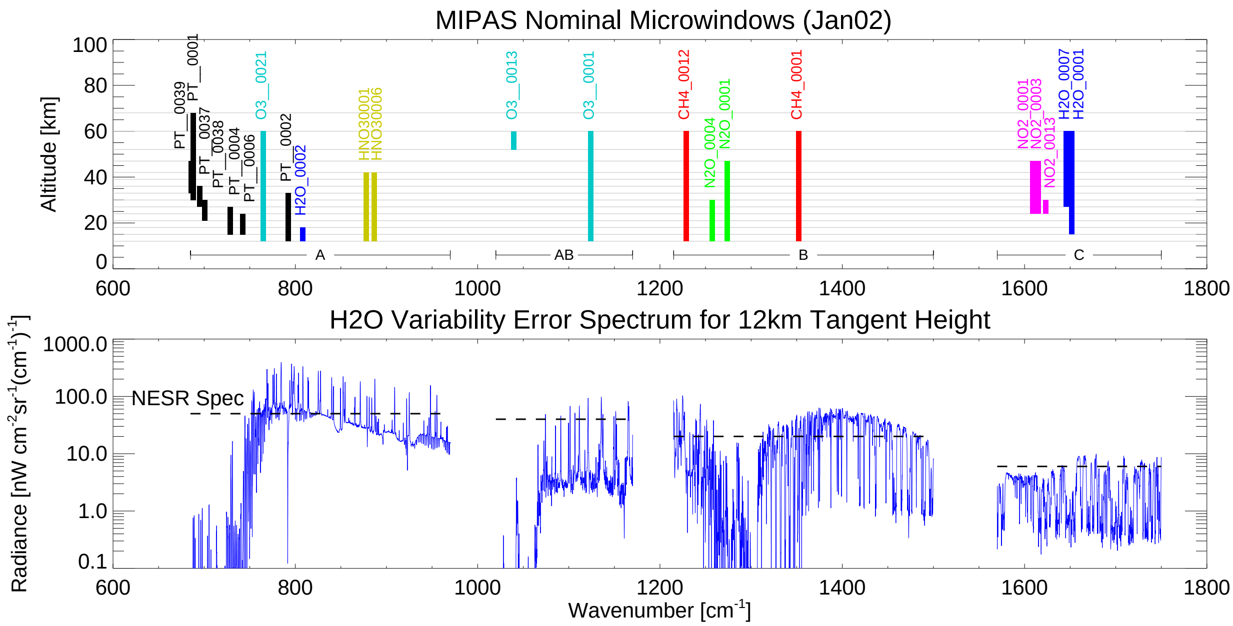
Note that at low altitudes the pressure residual is correlated with the ‘spread’ signature (§7.5) (+ve pressure equating to +ve spread) while at high altitudes it correlates with the ‘gain’ signature (§7.3).

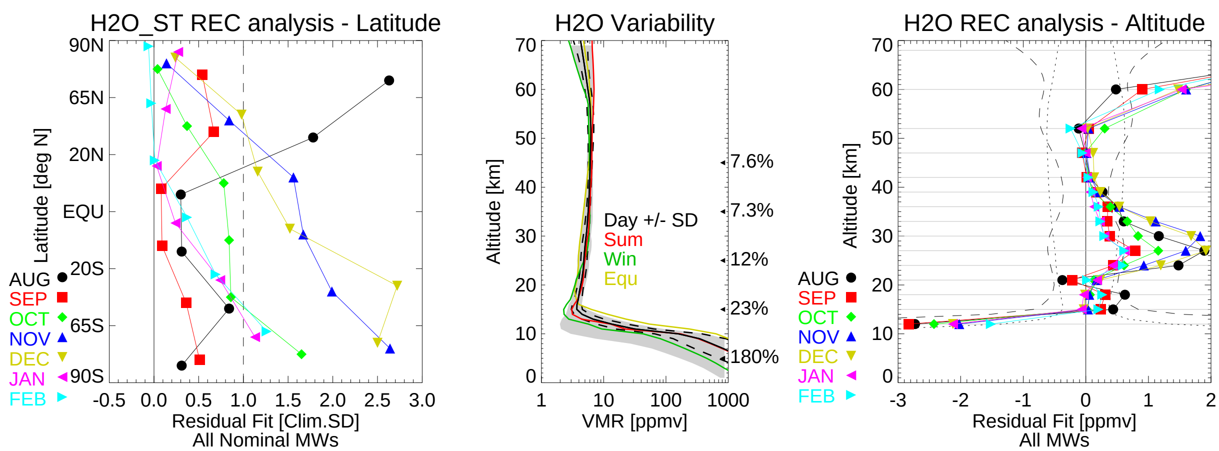
Recommendations

Investigate source of large residual signature peaking at 27 km.


PRE REC analysis - Latitude
Latitude [deg N]
90N
65N
20N
EQU
20S
65S
90S
AUG
SEP
OCT
NOV
DEC
JAN
FEB
Residual Fit [%]
Target MWs
PRE REC analysis - Altitude
Altitude [km]
Residual Fit [%]
Target MWs
PRE REC analysis - Latitude
Residual Fit [%]
Other MWs
PRE REC analysis - Altitude
Residual Fit [%]
Other MWs
PRE REC analysis - Latitude
Residual Fit [%]
All MWs, Solid=Night, Open=Day
PRE REC analysis - Altitude
Residual Fit [%]
All MWs, Solid=Night, Open=Day

3.3 H_2O



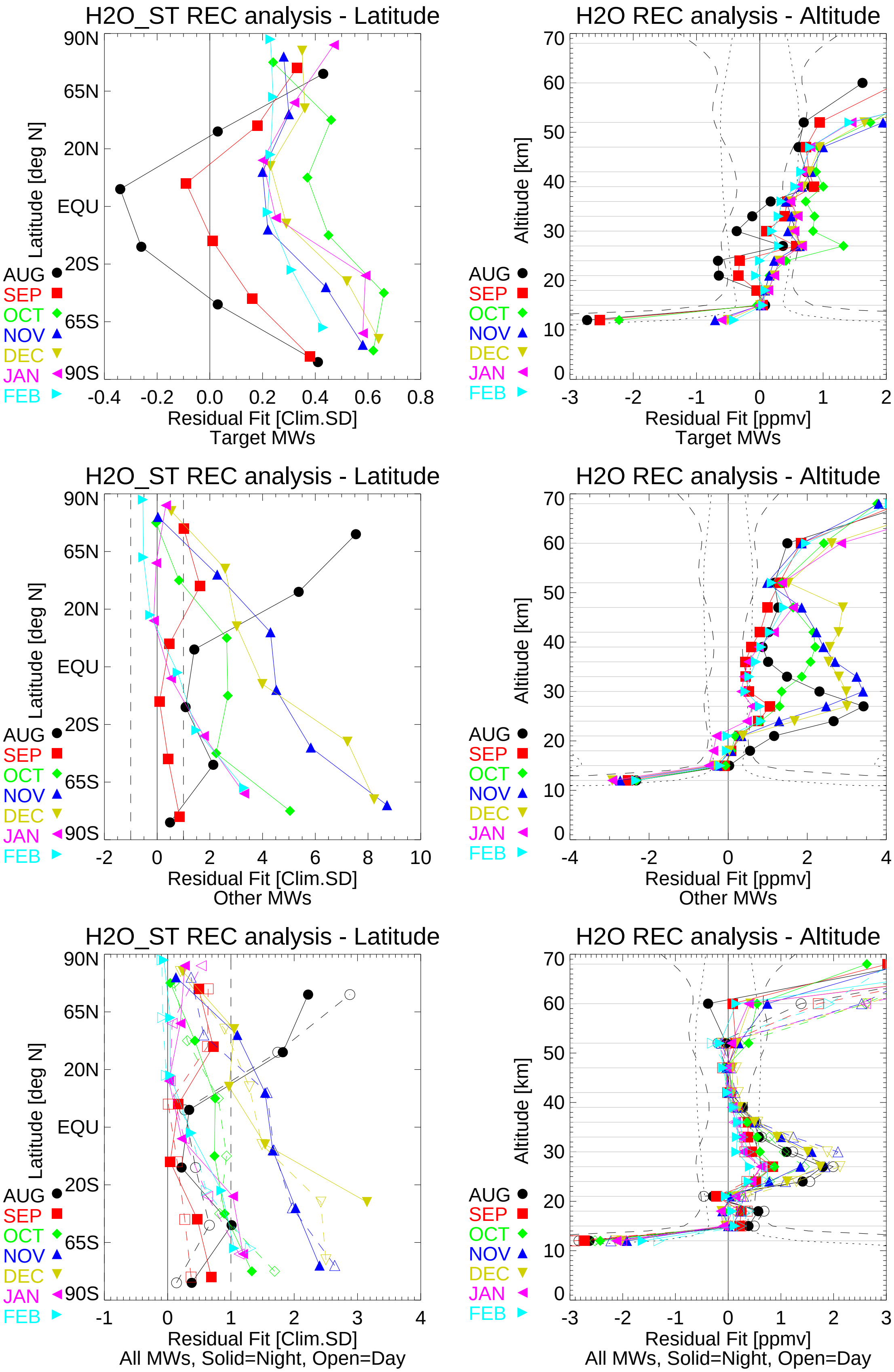


Comments

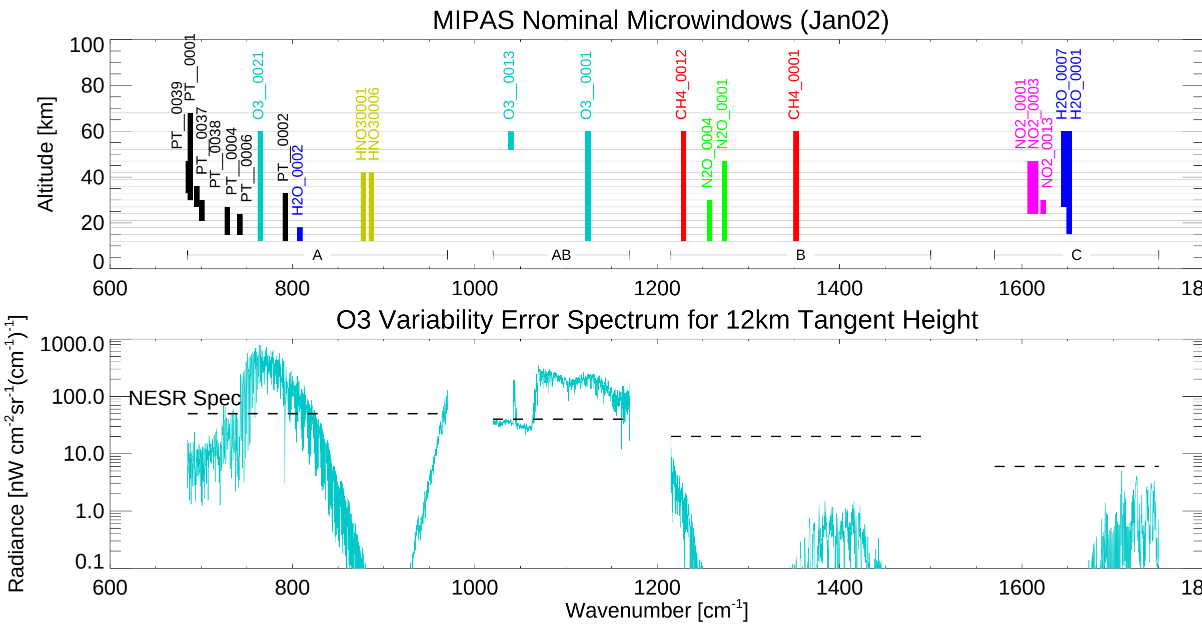
The latitude fit excludes 12 km (tropospheric) tangent height so mostly stratospheric component, August shows a large underestimate in the northern hemisphere while for Nov/Dec it is the southern hemisphere, which appears to be associated with the 3ppmv underestimate at 27km indicated in the non-target microwindows for these months. Apart from this, both target and non-target microwindows show an underestimate which increases with altitude from zero at 15 km to 2 ppmv at 60 km, but note that this trend disappears between 30–52km when all microwindows are analysed together, perhaps due to an inconsistent spectral signature. An apparent 3ppmv overestimate at 12 km reduced after Nov 13th to less than 1ppmv in the target microwindows but remains in the non-target microwindows. A significant diurnal signature (day-time enhanced by 20–30%) is apparent only at 60 km.

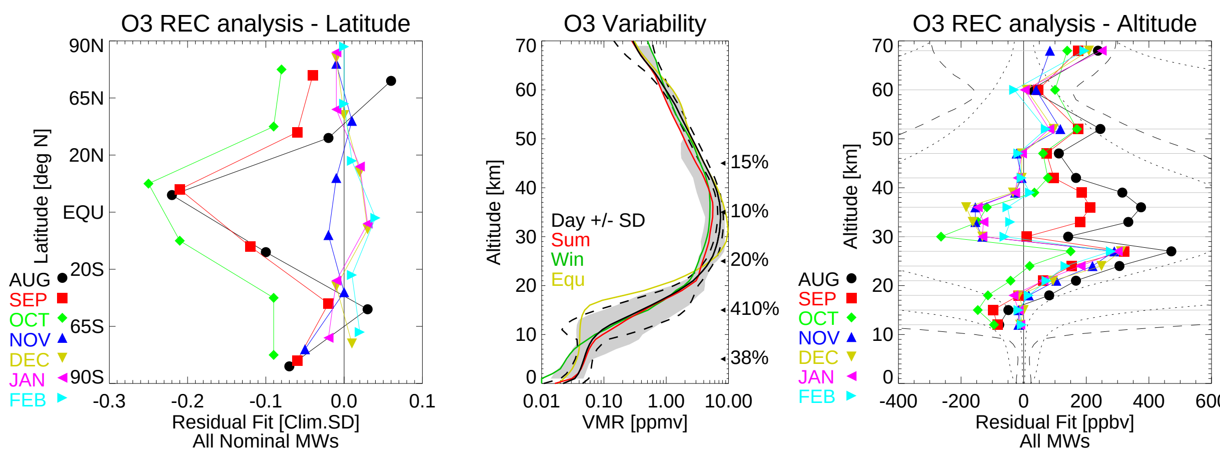
Recommendations

Investigate trend with altitude, spectral signatures in target and non-target microwindows, and cause of anomalous Aug, Nov, Dec residuals.


H2O_ST REC analysis - Latitude
H2O REC analysis - Altitude
Latitude [deg N]
Altitude [km]
90N
65N
20N
EQU
20S
65S
90S
AUG
SEP
OCT
NOV
DEC
JAN
FEB
Residual Fit [Clim.SD]
Target MWs
Residual Fit [ppmv]
Target MWs
Residual Fit [Clim.SD]
Other MWs
Residual Fit [ppmv]
Other MWs
Residual Fit [Clim.SD]
All MWs, Solid=Night, Open=Day
Residual Fit [ppmv]
All MWs, Solid=Night, Open=Day

3.4 O_3



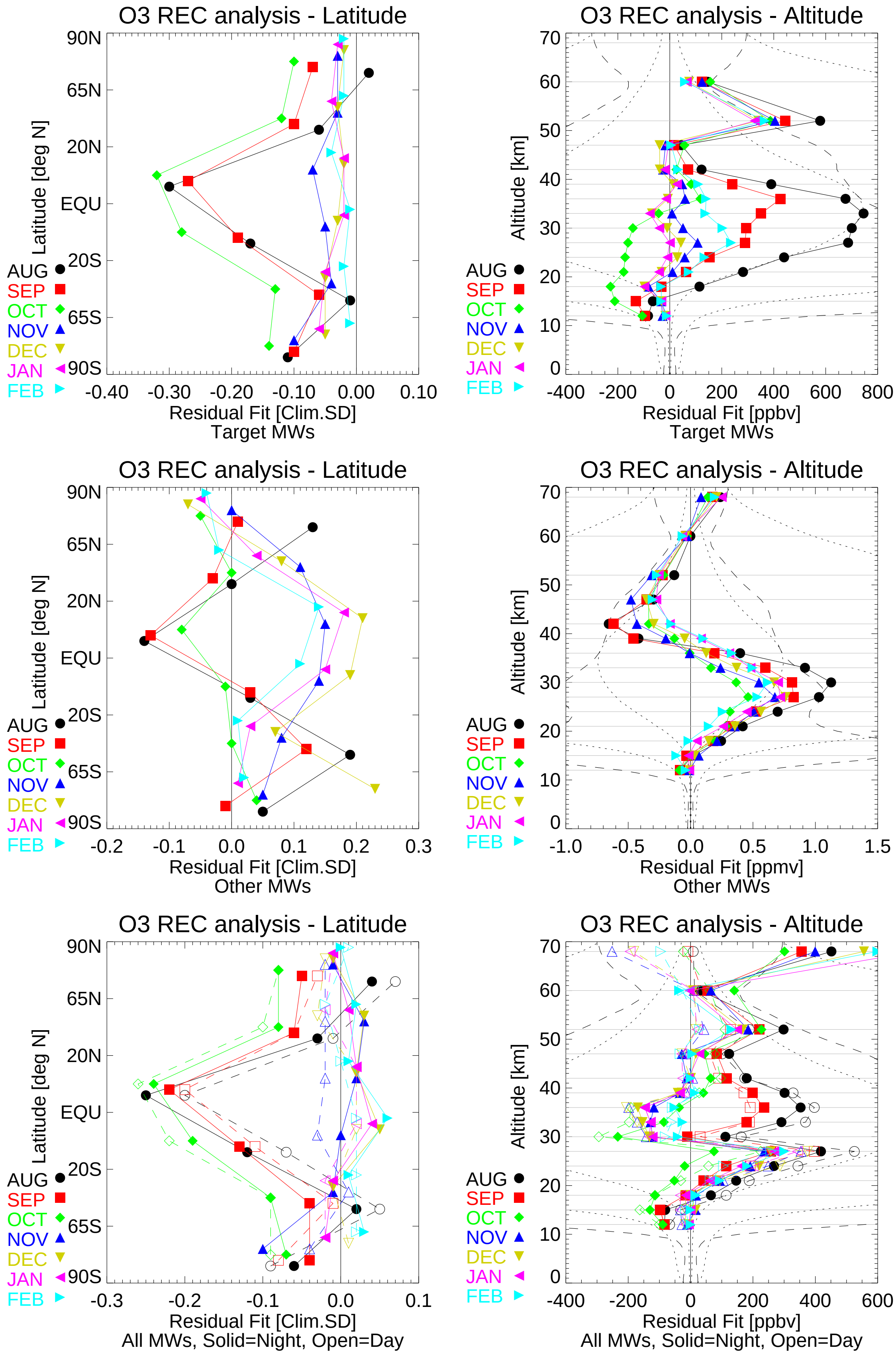


Comments

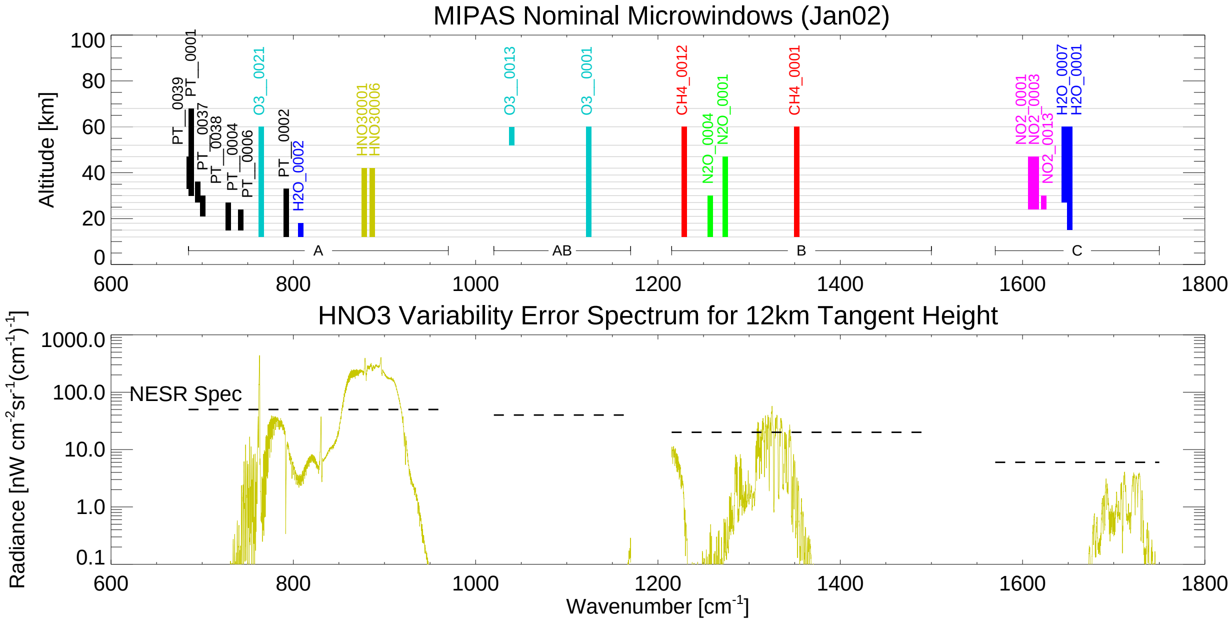
O_3 residuals significantly improved after Nov 13th. The non-target microwindows suggest an overall underestimate at mid-latitudes, 0.5 ppmv underestimate at 30 km and 0.5 ppmv overestimate at 42km, but since most of these are in pT microwindows (earlier in retrieval sequence) this may indicate a bias in the IG climatology. Within the O3 microwindows themselves the residuals are generally small (after Nov 13th) except at 52km where there may be an underestimate of 0.5ppmv. A diurnal variation of about ±0.3 ppmv is evident at 70 km (above the top retrieval level).

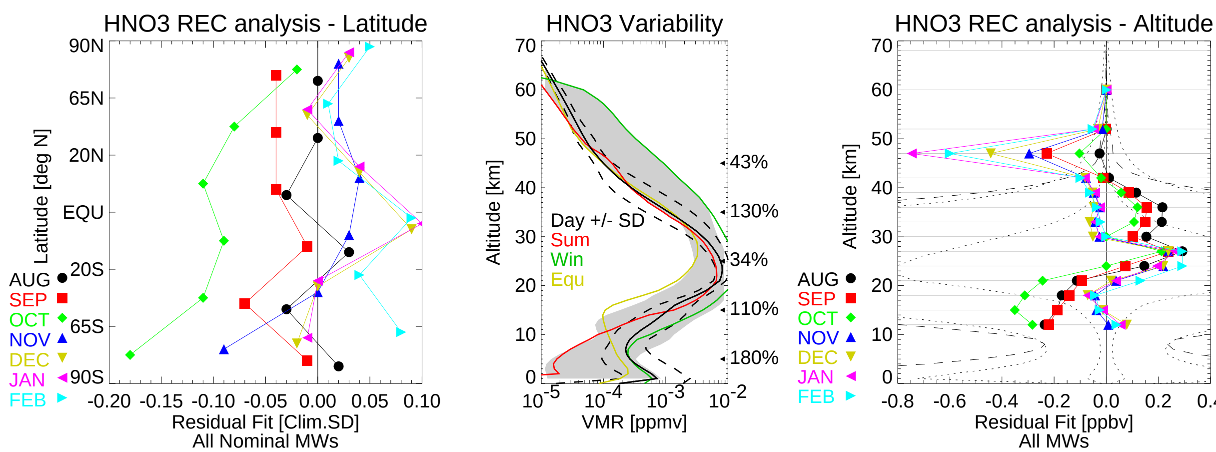
Recommendations

Check if vertical and latitude structure indicated by non-target microwindows is from the IG profile or from the retrieval.


O3 REC analysis - Latitude
Latitude [deg N]
90N
65N
20N
EQU
20S
65S
90S
AUG
SEP
OCT
NOV
DEC
JAN
FEB
-0.40 -0.30 -0.20 -0.10 0.00 0.10
Residual Fit [Clim.SD]
Target MWs
O3 REC analysis - Altitude
Altitude [km]
70 60 50 40 30 20 10 0
-400 -200 0 200 400 600 800
Residual Fit [ppbv]
Target MWs
O3 REC analysis - Latitude
-0.2 -0.1 0.0 0.1 0.2 0.3
Residual Fit [Clim.SD]
Other MWs
O3 REC analysis - Altitude
-1.0 -0.5 0.0 0.5 1.0 1.5
Residual Fit [ppmv]
Other MWs
O3 REC analysis - Latitude
-0.3 -0.2 -0.1 0.0 0.1
Residual Fit [Clim.SD]
All MWs, Solid=Night, Open=Day
O3 REC analysis - Altitude
-400 -200 0 200 400 600
Residual Fit [ppbv]
All MWs, Solid=Night, Open=Day

3.5 HNO_3





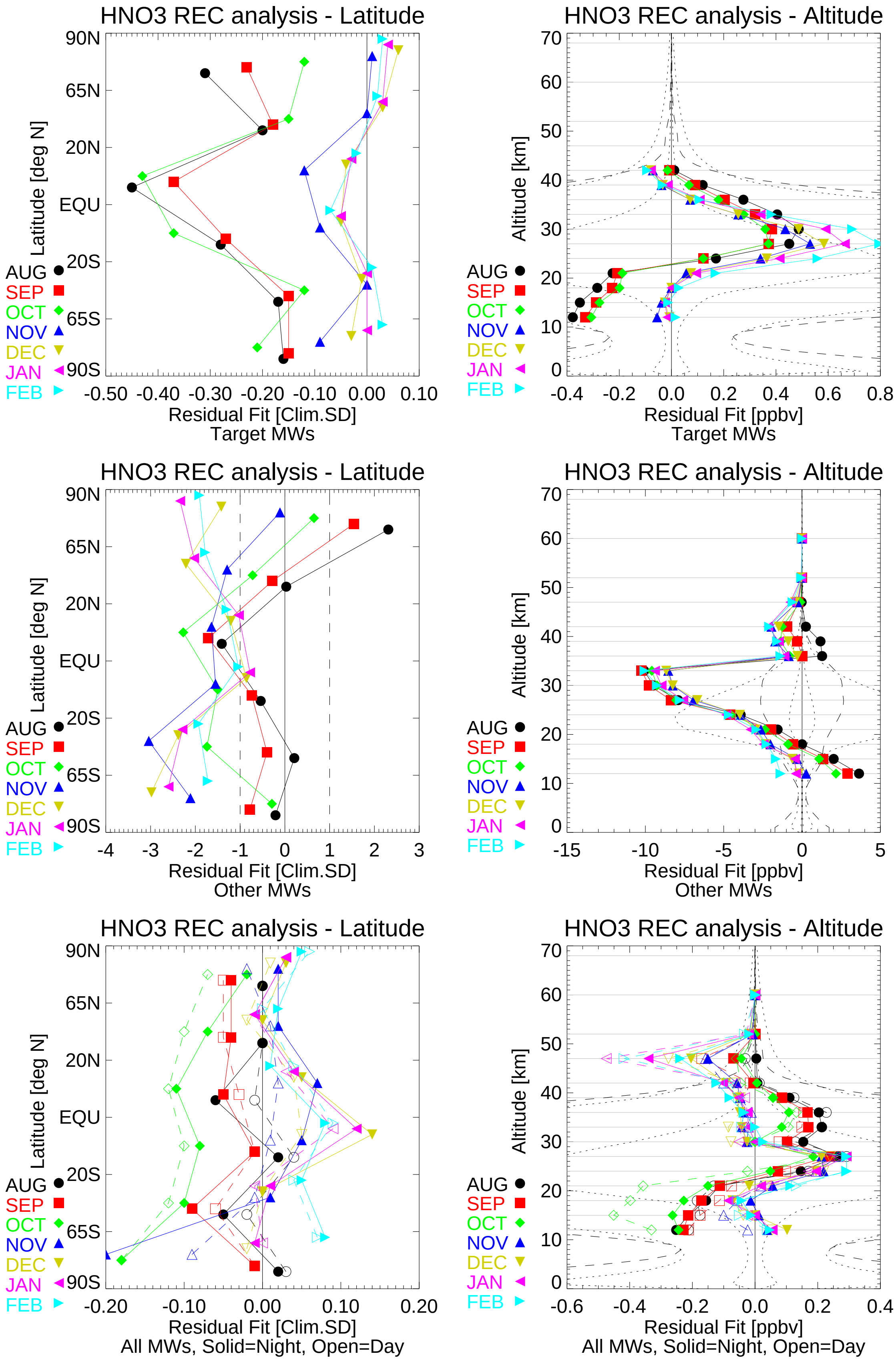
Comments

The HNO_3 residuals show very different signatures in the target and non-target microwindows. In the target microwindows the latitude plot indicates a significant reduction in residuals after Nov 13th, although with a slight overestimate at low latitudes. The altitude plot also suggests an underestimate of reaching 0.5 ppbv at 27 km (∼10% of the mixing ratio).

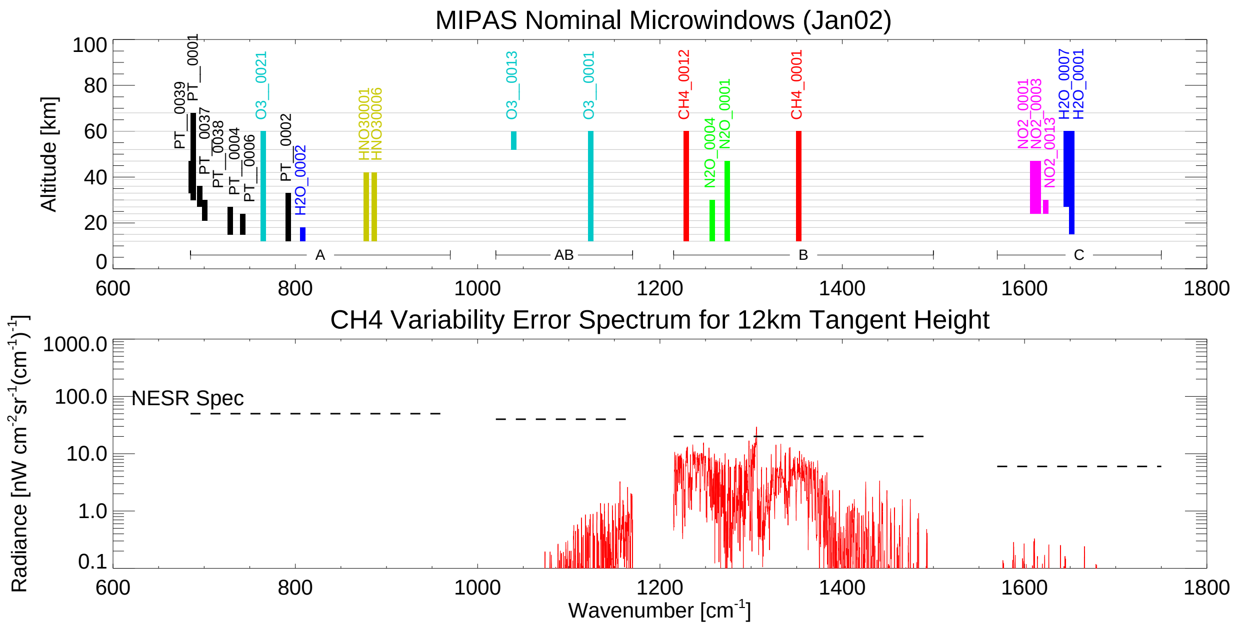
However the non-target microwindows show a general overestimate of HNO_3 at all latitudes, peaking at 10ppbv at 33 km. This may be explained by known errors in HNO_3 spectroscopy (v2 of MIPAS spectroscopic database), e.g., if the linestrengths in the HNO_3 microwindows are too weak.

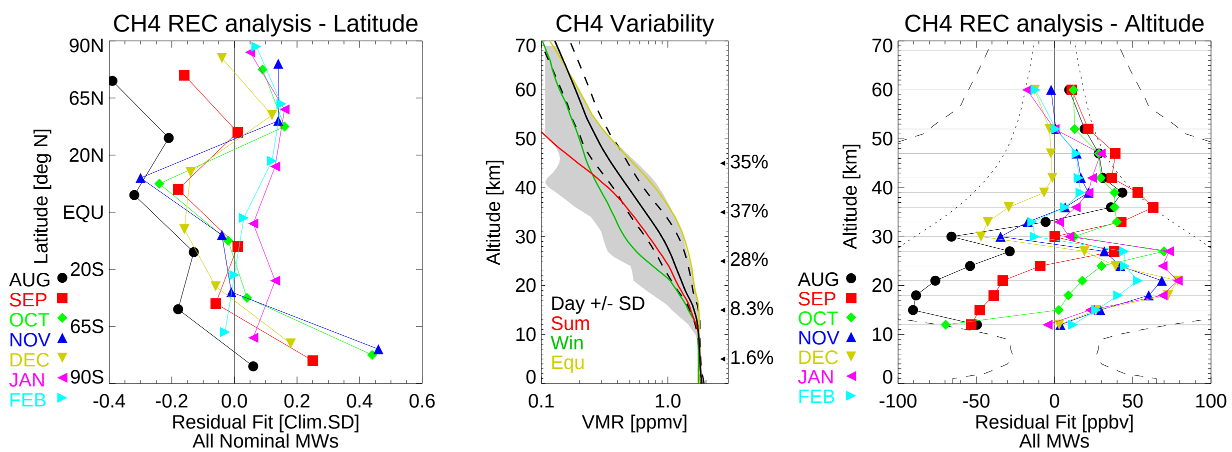
Recommendations

Check if this is corrected with delivery of new HNO_3 LUT data (based on v3.1 of MIPAS spectroscopic database)


HNO3 REC analysis - Latitude
HNO3 REC analysis - Altitude
Latitude [deg N]
90N
65N
20N
EQU
20S
65S
90S
Altitude [km]
70
60
50
40
30
20
10
0
AUG
SEP
OCT
NOV
DEC
JAN
FEB
-0.50 -0.40 -0.30 -0.20 -0.10 0.00 0.10
Residual Fit [Clim.SD]
Target MWs
-0.4 -0.2 0.0 0.2 0.4 0.6 0.8
Residual Fit [ppbv]
Target MWs
-4 -3 -2 -1 0 1 2 3
Residual Fit [Clim.SD]
Other MWs
-15 -10 -5 0 5
Residual Fit [ppbv]
Other MWs
-0.20 -0.10 0.00 0.10 0.20
Residual Fit [Clim.SD]
All MWs, Solid=Night, Open=Day
-0.6 -0.4 -0.2 0.0 0.2 0.4
Residual Fit [ppbv]
All MWs, Solid=Night, Open=Day

3.6 CH_4





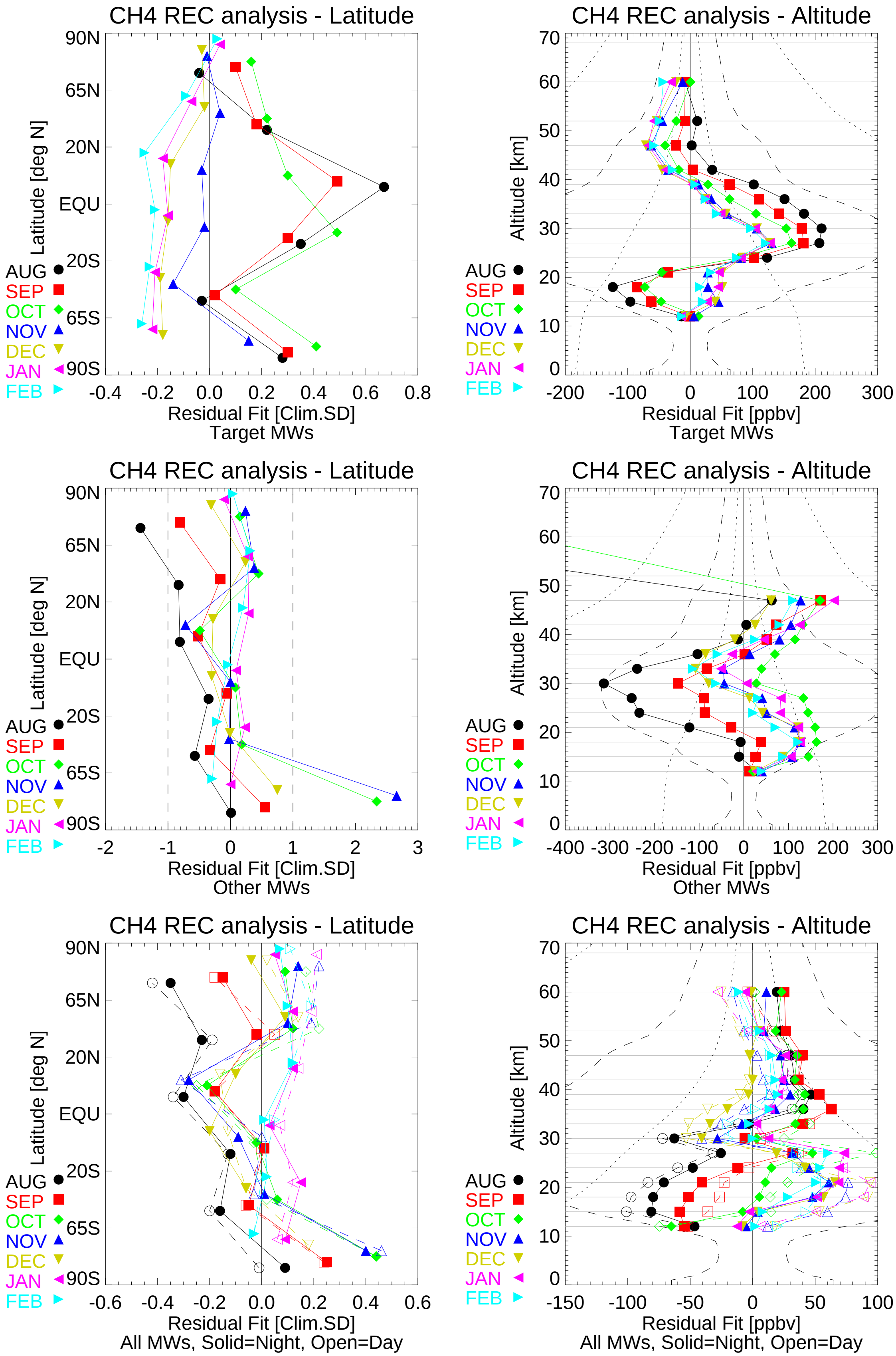
Comments

Residual signatures at low latitudes and low altitudes in target microwindows were reduced significantly after Nov 13th but there remains some underestimate of atmospheric CH_4 reaching 0.1 ppmv (∼10%) at 27 km, and overestimate of 0.05ppmv (∼20%) at 47 km. The non-target microwindows (mostly N_2O) give a different altitude signature, −0.1ppmv at 18 km, +0.1ppmv at 33 km, −0.1ppmv at 47 km.

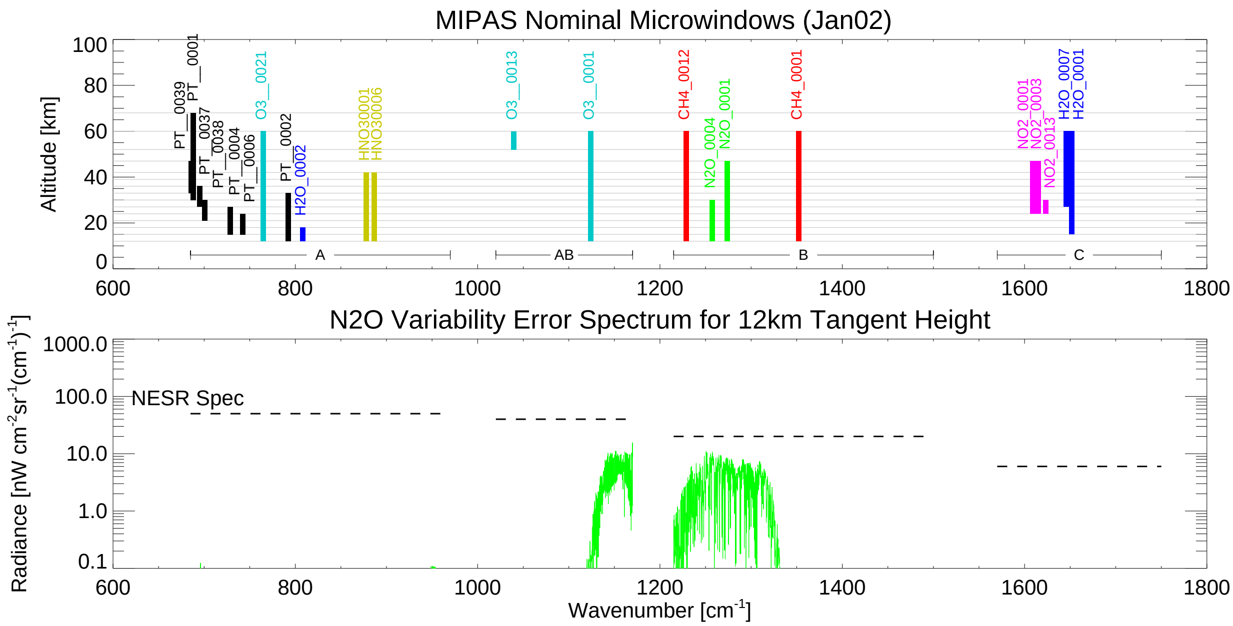
Nevertheless, the residuals are well within climatological 1-σ variability, which, for methane is rather small.

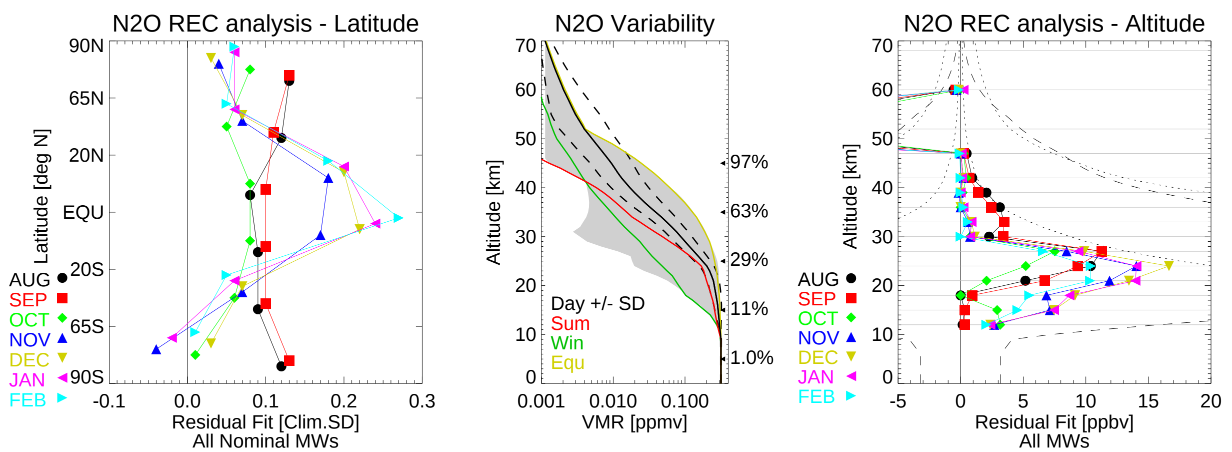
Recommendations

Check convergence.


CH4 REC analysis - Latitude
Latitude [deg N]
Residual Fit [Clim.SD]
Target MWs
CH4 REC analysis - Altitude
Altitude [km]
Residual Fit [ppbv]
Target MWs
CH4 REC analysis - Latitude
Residual Fit [Clim.SD]
Other MWs
CH4 REC analysis - Altitude
Residual Fit [ppbv]
Other MWs
CH4 REC analysis - Latitude
Residual Fit [Clim.SD]
All MWs, Solid=Night, Open=Day
CH4 REC analysis - Altitude
Residual Fit [ppbv]
All MWs, Solid=Night, Open=Day
AUG
SEP
OCT
NOV
DEC
JAN
FEB

3.7 N_2O



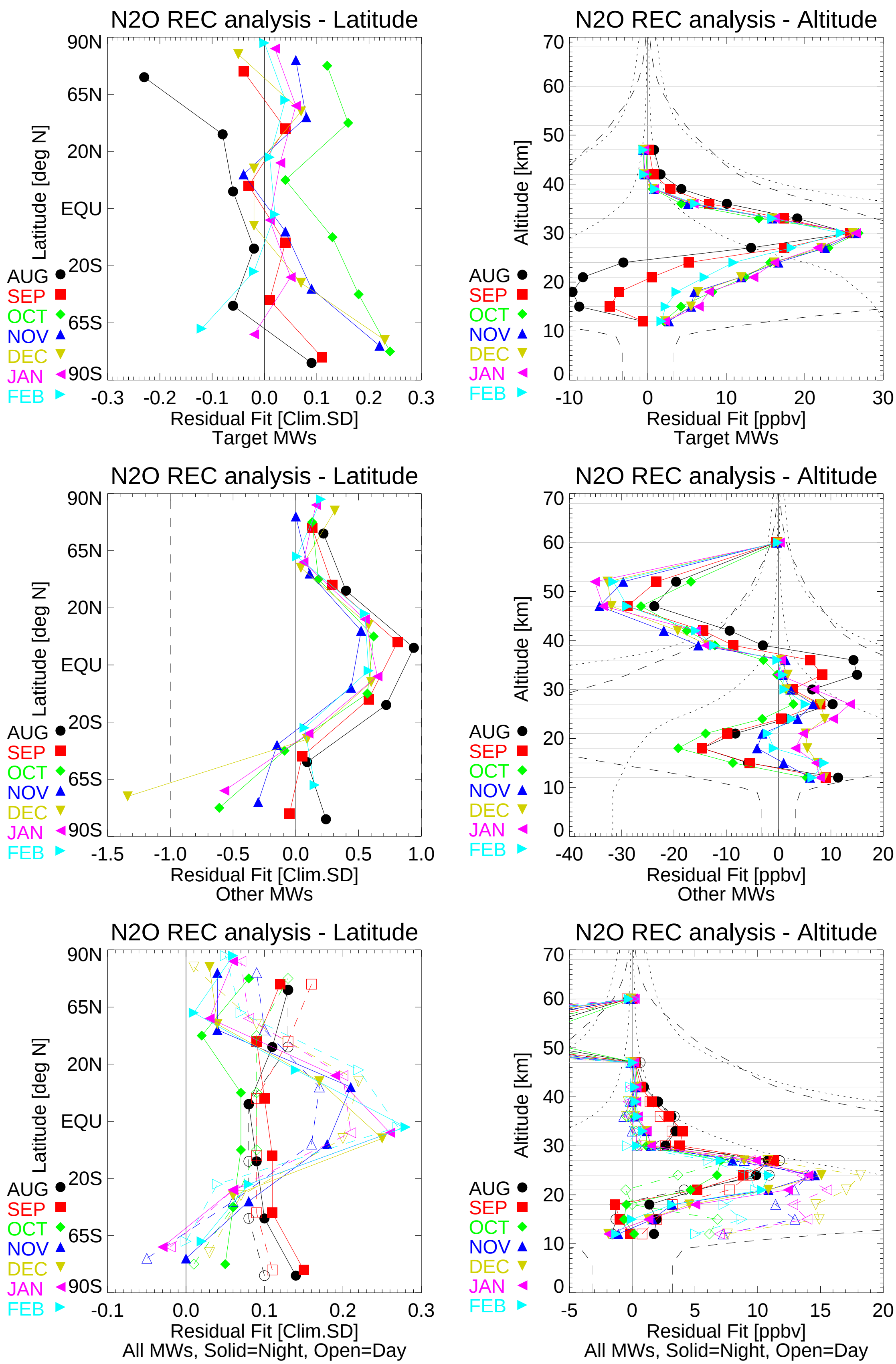


Comments

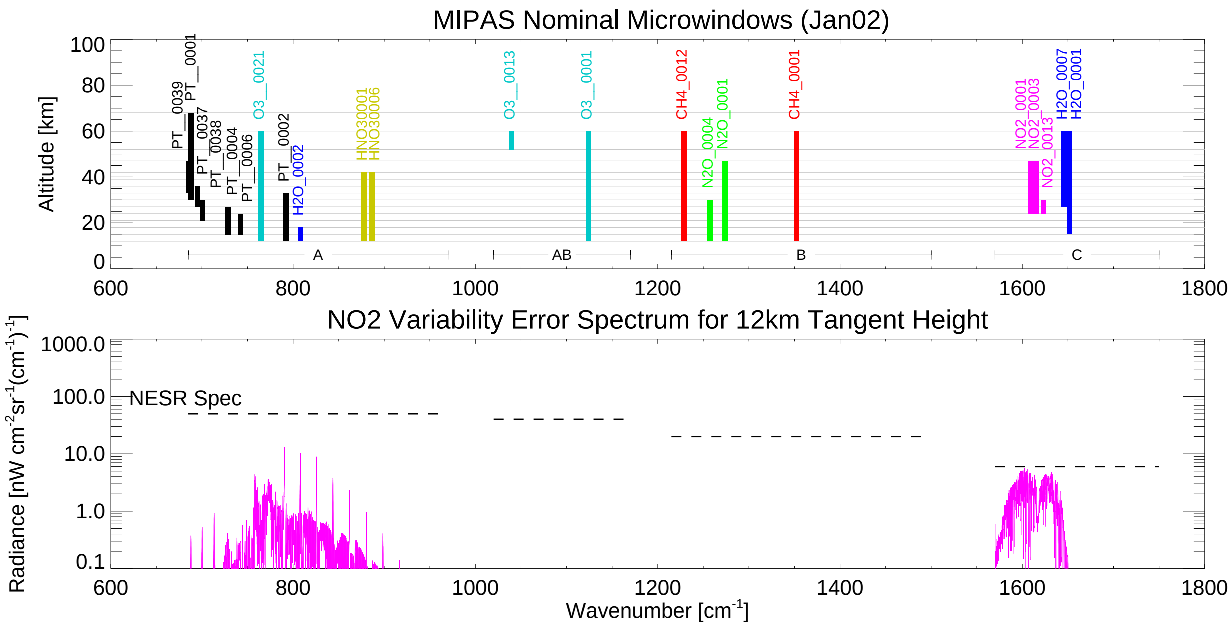
N_2O residuals in non-target microwindows indicate underestimated profiles at low latitudes. Target microwindows show an underestimate reaching 25 ppbv at 30 km (~30%) but non-target microwindows imply less than 10 ppbv up to 30 km. Above that the non-target microwindows indicate an overestimate reaching 30ppbv at 50 km (ie several orders of magnitude) but this is probably spurious.

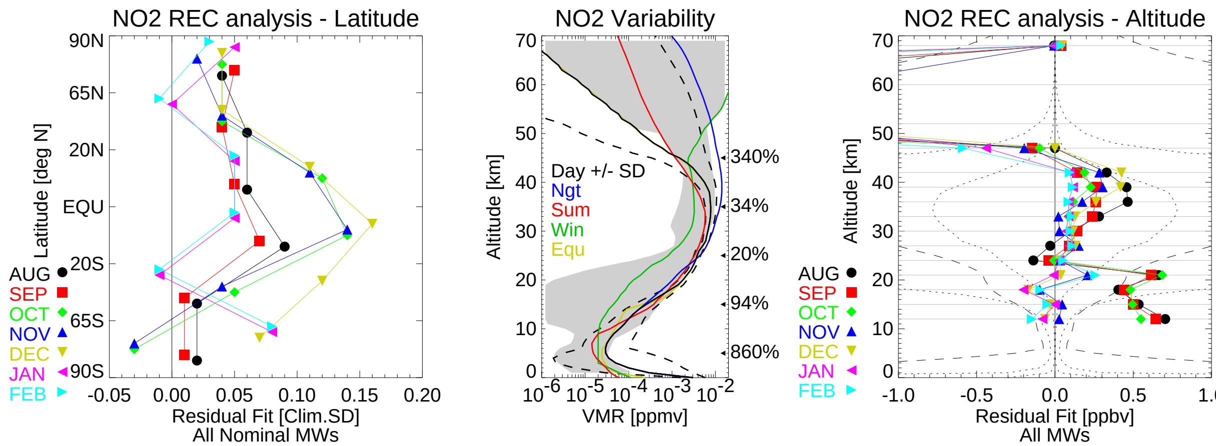
Recommendations

Check N_2O climatology for bias with respect to retrievals.


N2O REC analysis - Latitude
Latitude [deg N]
90N
65N
20N
EQU
20S
65S
90S
AUG
SEP
OCT
NOV
DEC
JAN
FEB
-0.3 -0.2 -0.1 0.0 0.1 0.2 0.3
Residual Fit [Clim.SD]
Target MWs
N2O REC analysis - Altitude
Altitude [km]
70 60 50 40 30 20 10 0
AUG
SEP
OCT
NOV
DEC
JAN
FEB
-10 0 10 20 30
Residual Fit [ppbv]
Target MWs
N2O REC analysis - Latitude
Latitude [deg N]
90N
65N
20N
EQU
20S
65S
90S
AUG
SEP
OCT
NOV
DEC
JAN
FEB
-1.5 -1.0 -0.5 0.0 0.5 1.0
Residual Fit [Clim.SD]
Other MWs
N2O REC analysis - Altitude
Altitude [km]
70 60 50 40 30 20 10 0
AUG
SEP
OCT
NOV
DEC
JAN
FEB
-40 -30 -20 -10 0 10 20
Residual Fit [ppbv]
Other MWs
N2O REC analysis - Latitude
Latitude [deg N]
90N
65N
20N
EQU
20S
65S
90S
AUG
SEP
OCT
NOV
DEC
JAN
FEB
-0.1 0.0 0.1 0.2 0.3
Residual Fit [Clim.SD]
All MWs, Solid=Night, Open=Day
N2O REC analysis - Altitude
Altitude [km]
70 60 50 40 30 20 10 0
AUG
SEP
OCT
NOV
DEC
JAN
FEB
-5 0 5 10 15 20
Residual Fit [ppbv]
All MWs, Solid=Night, Open=Day

3.8 NO_2





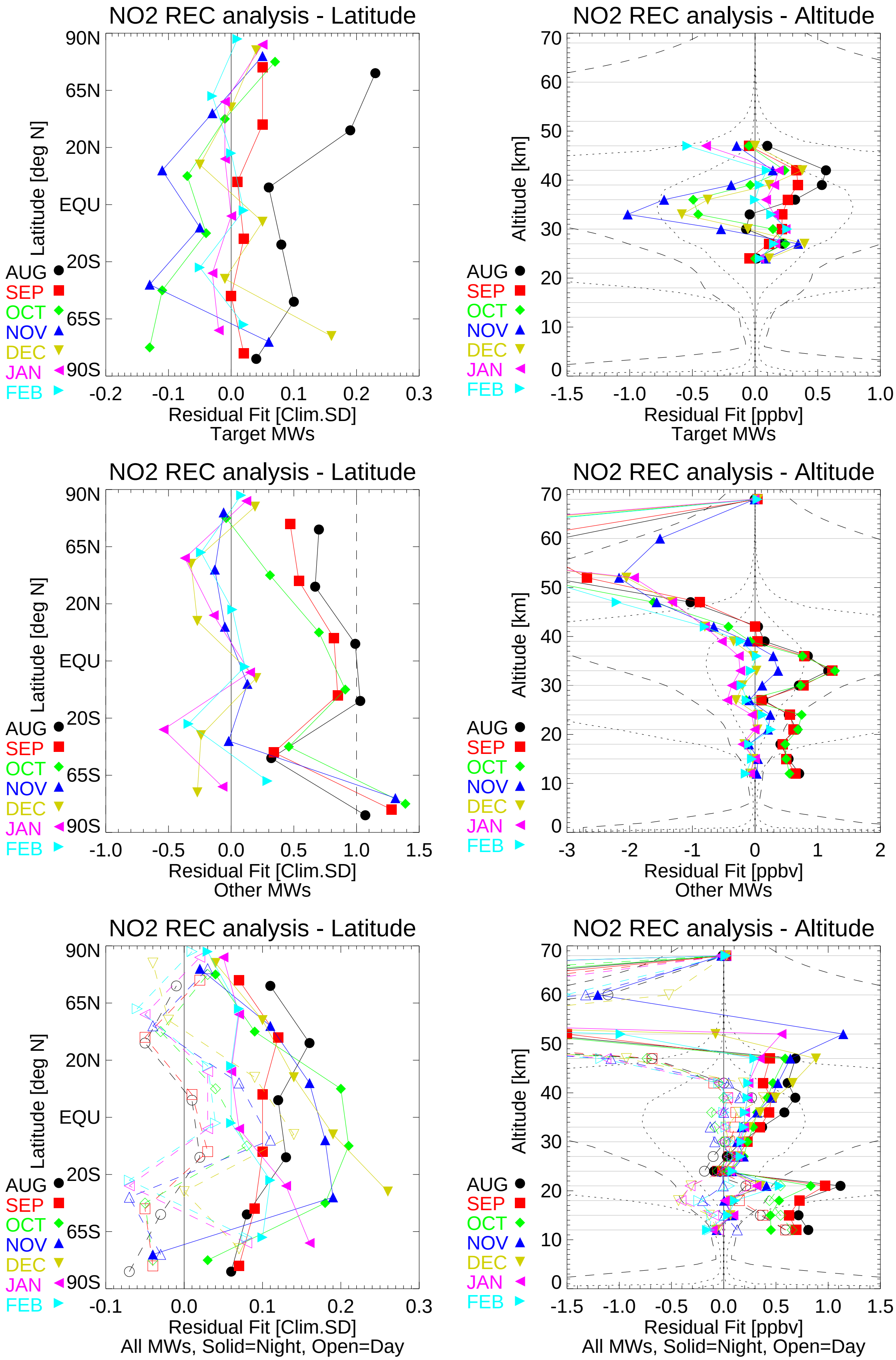
Comments

The residuals in the non-target microwindows reduced significantly after Nov 13th but there was little effect in the target microwindows. There is a persistent large -ve residual from 47 km and above (indicating overestimate) and, prior to Nov 13th, a large +ve residual below 21 km. Note, however, that NO_2 is only retrieved from 24–42 km so these reflect the climatological NO_2 in other microwindows. In the target microwindows themselves the residual is generally within ±10 ppbv, equivalent to less that 10% of the VMR.

NO_2 has a significant diurnal variability but this appears to be reasonably well eliminated within the retrieval range. The climatology has no diurnal variation so that outside the retrieval range the residuals show the expected atmospheric variation of enhanced nighttime concentrations NO_2 (solid symbols more +ve than open symbols).

Recommendations

Check NO_2 high altitude climatology.


NO2 REC analysis - Latitude
90N
65N
20N
EQU
20S
65S
90S
Latitude [deg N]
AUG
SEP
OCT
NOV
DEC
JAN
FEB
-0.2
-0.1
0.0
0.1
0.2
0.3
Residual Fit [Clim.SD]
Target MWs
NO2 REC analysis - Altitude
70
60
50
40
30
20
10
0
Altitude [km]
AUG
SEP
OCT
NOV
DEC
JAN
FEB
-1.5
-1.0
-0.5
0.0
0.5
1.0
Residual Fit [ppbv]
Target MWs
NO2 REC analysis - Latitude
90N
65N
20N
EQU
20S
65S
90S
Latitude [deg N]
AUG
SEP
OCT
NOV
DEC
JAN
FEB
-1.0
-0.5
0.0
0.5
1.0
1.5
Residual Fit [Clim.SD]
Other MWs
NO2 REC analysis - Altitude
70
60
50
40
30
20
10
0
Altitude [km]
AUG
SEP
OCT
NOV
DEC
JAN
FEB
-3
-2
-1
0
1
2
Residual Fit [ppbv]
Other MWs
NO2 REC analysis - Latitude
90N
65N
20N
EQU
20S
65S
90S
Latitude [deg N]
AUG
SEP
OCT
NOV
DEC
JAN
FEB
-0.1
0.0
0.1
0.2
0.3
Residual Fit [Clim.SD]
All MWs, Solid=Night, Open=Day
NO2 REC analysis - Altitude
70
60
50
40
30
20
10
0
Altitude [km]
AUG
SEP
OCT
NOV
DEC
JAN
FEB
-1.5
-1.0
-0.5
0.0
0.5
1.0
1.5
Residual Fit [ppbv]
All MWs, Solid=Night, Open=Day

4 Contaminant Species - Variable profiles

4.1 Description

Contaminant gases in each microwindow which are not one of the retrieved species are modelled using profiles derived from 'Initial Guess' (climatology) data. For some species different profiles are stored for each season and each latitude band. The spread of IG profiles is indicated by the shaded region in the variability plot.

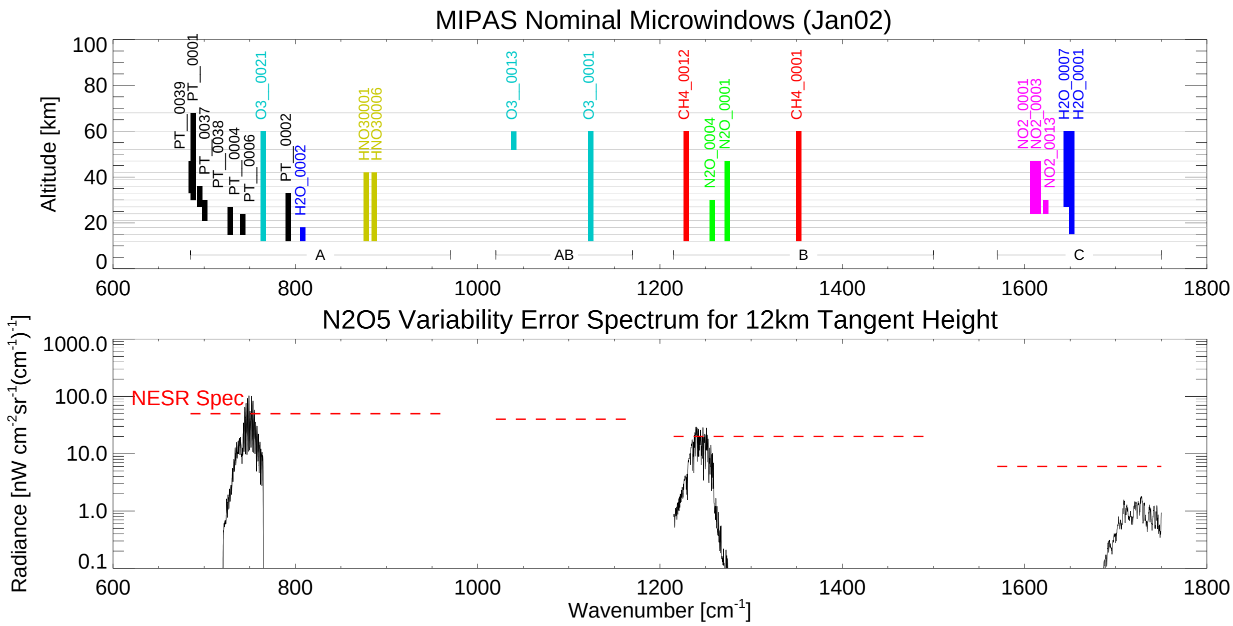
The absorbers in this section are listed in order of decreasing 'confidence' in the REC analysis.

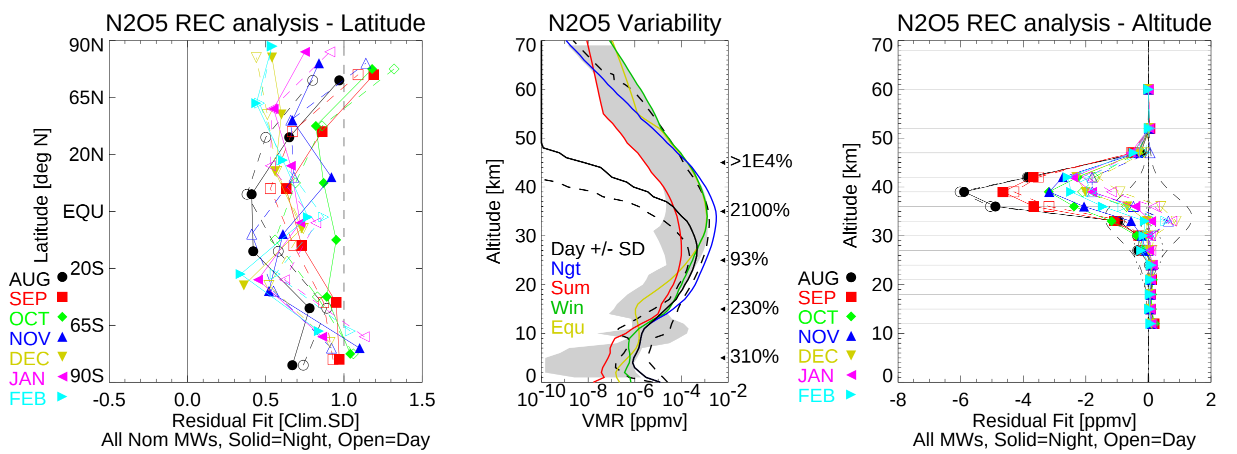
4.2 Problem Areas

The REC analysis identifies any discrepancy between the IG data and the atmospheric variations of these species, i.e., whether the climatology is appropriate.

Note that the IG data is changed every three months (1st Sep, 1st Dec, 1st Mar, 1st Jun) so some discontinuities may be apparent at these times. Also, the initial guess data represents a diurnal mean, so for species with any expected diurnal variation day and night averages have been plotted separately.

4.3 N_2O_5





Comments

N_2O_5 has a strong signature in several A and B band microwindows, but it is modelled by a relatively smooth absorption cross-section so the REC analysis may not be reliable.

The latitude plot suggests that N_2O_5 is generally underestimated, but within the climatological variability.

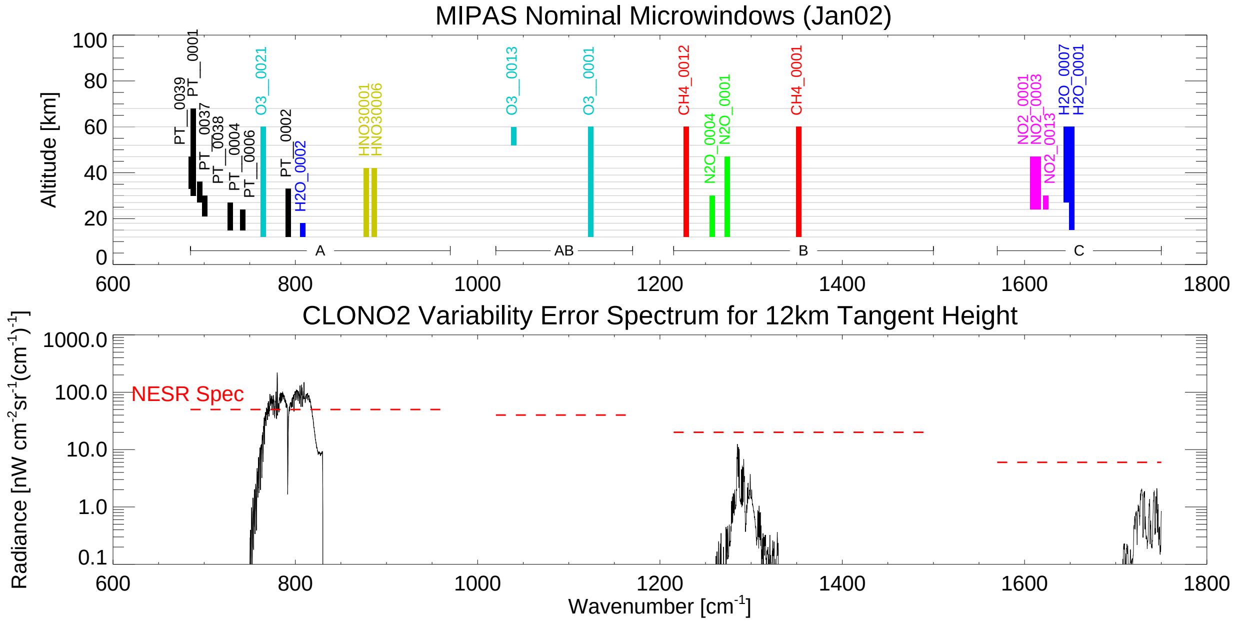
N_2O_5 varies diurnally, being formed during the night and destroyed during the day, yet no clear difference is apparent in the day/night residuals. N_2O_5 photochemistry has a timescale $\sim$ hours (*cf.* $\sim$ minutes for NO_2) it may be the case that the MIPAS 'night-time' observations (10pm local time) have similar concentrations to the 'day-time' observations (10am local time).

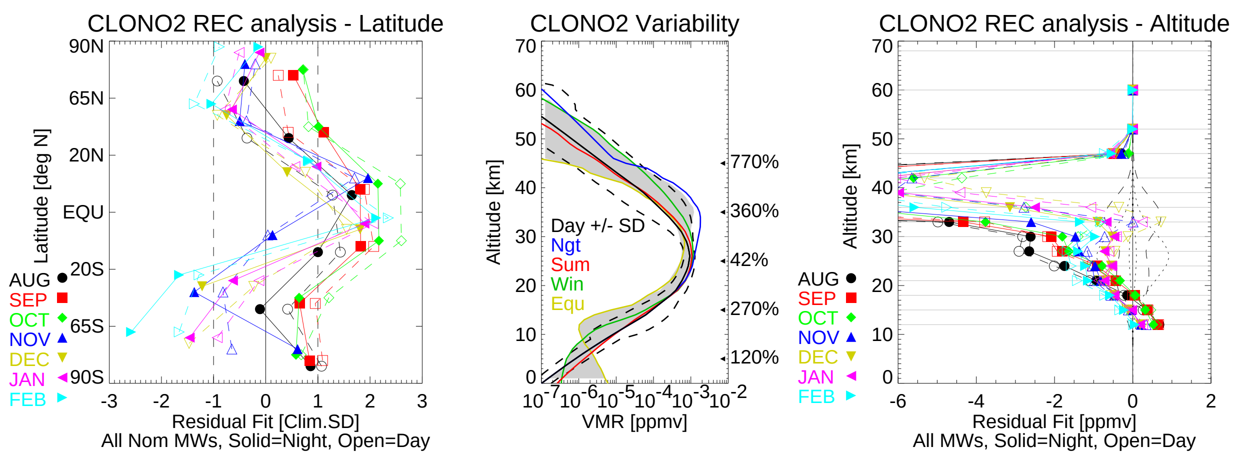
Whether night or day, it appears that the IG profiles are biased negative with respect to the real atmosphere by $\sim$10s of %. The negative peak at 40 km in the altitude plot is probably a spurious fit to some other spectral feature in the residuals.

Recommendations

Investigate residual signature causing peak at 40km.

4.4 $ClONO_2$





Comments

$ClONO_2$ has a strong signature in several A and B band microwindows, but it is modelled by a relatively smooth absorption cross-section so the REC analysis may not be reliable.

The latitude plot suggests that $ClONO_2$ is generally underestimated, but within the climatological variability.

$ClONO_2$ has a slow diurnal variability similar to N_2O_5 and the latitude residuals exhibit similar features. The IG profiles appear to underestimate $ClONO_2$ at the equator and overestimate at the poles, particularly the summer pole.

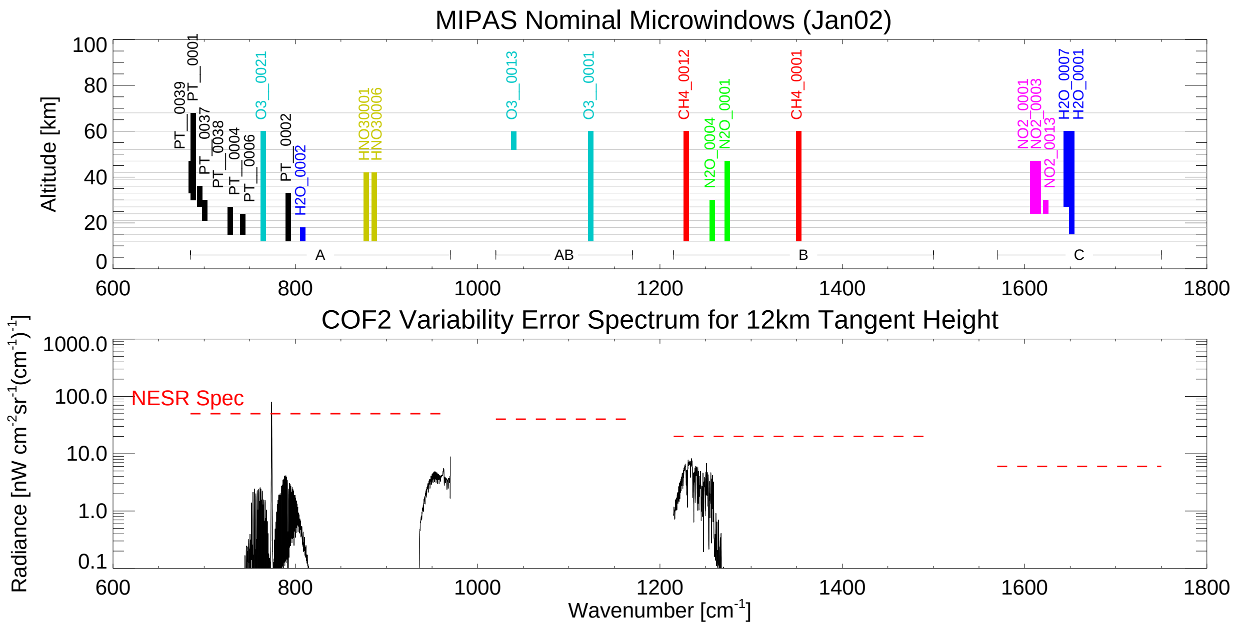
The altitude plot shows a large peak at 40 km corresponding to an overestimate of atmospheric $ClONO_2$ by several ppmv, which is too large to be reasonable (as with N_2O_5). This suggests that the fit is affected by some other feature in the residual spectrum, so other conclusions should be regarded with suspicion.

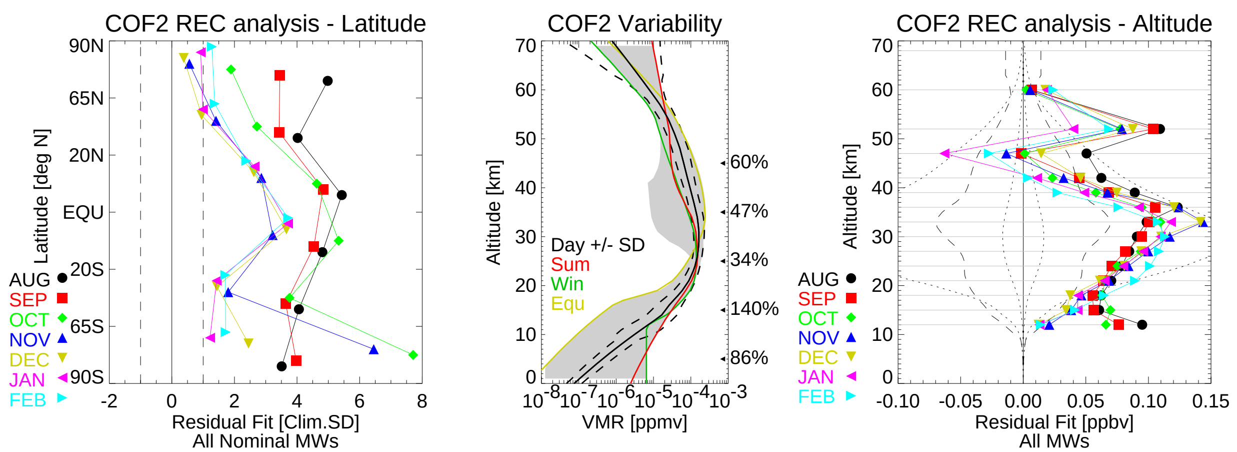
At low altitude the atmospheric $ClONO_2$ may be overestimated.

Recommendations

Investigate residual signature causing peak at 40km.

4.5 COF_2





Comments

COF_2 has a sharp peak in the A-band but this does not coincide with the nominal microwindows so most of the signature is likely to come from the B-band. It is modelled with line data and has features in several microwindows so REC analyses should be reasonably reliable.

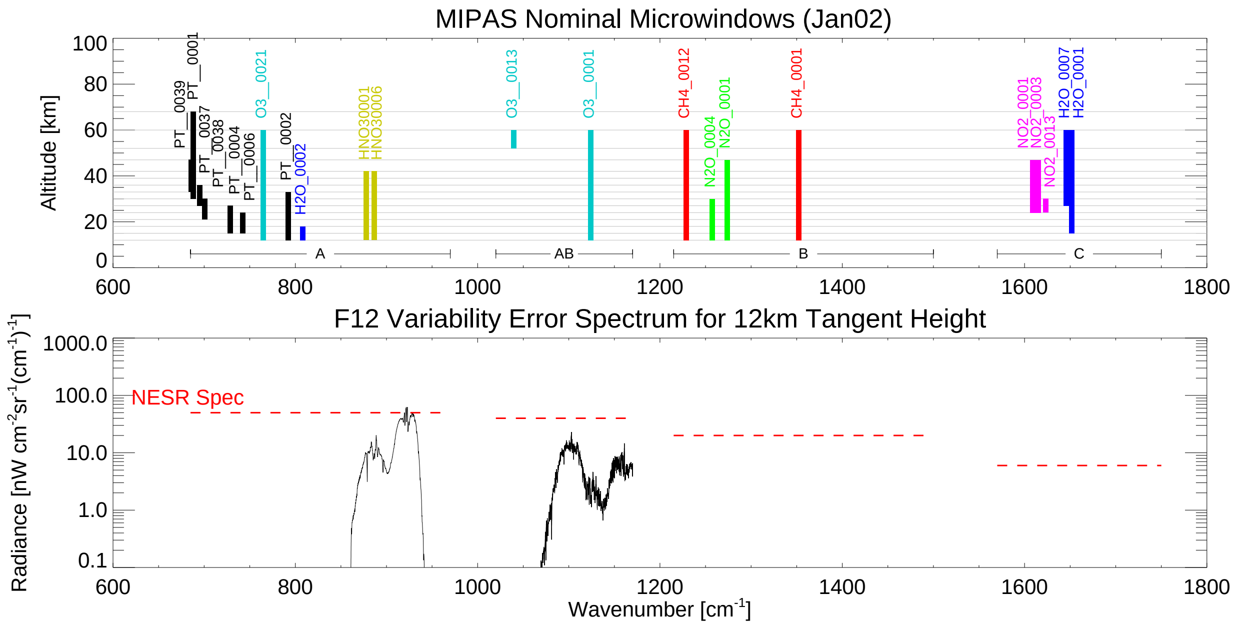
The latitude plot shows a significant improvement after Nov 13th after which there remains a general underestimate, mostly at low latitudes. However, the COF_2 appears to be underestimated by an amount beyond expected climatological variability.

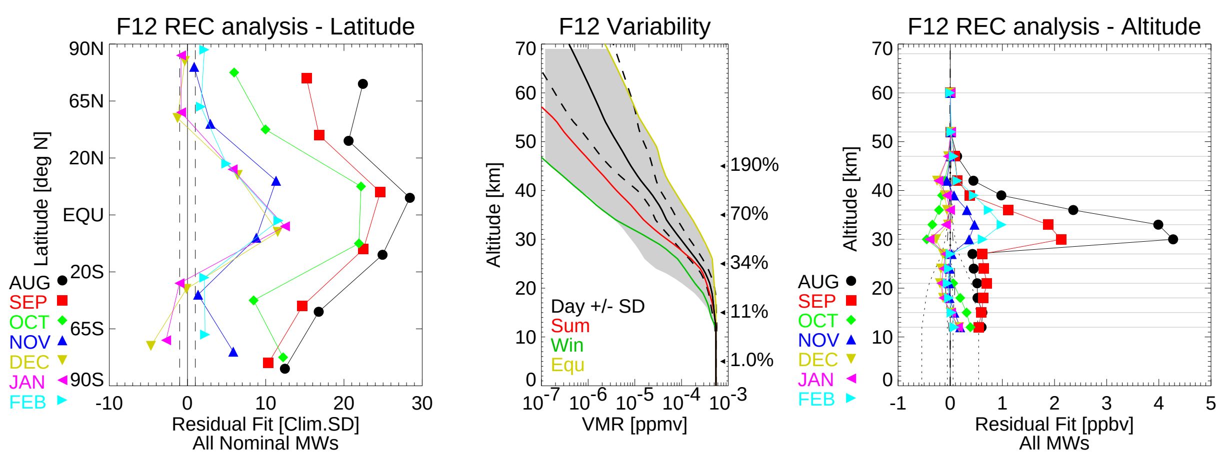
The altitude plot suggests that the true profile is of the order of 75% larger than the IG up to 40 km, peaking at 0.1 ppbv at 33 km. The profiles coincide at 47 km but the IG may also underestimate the true profile by 0.1 ppbv at 52 km.

Recommendations

Increase COF_2 climatological profiles.

4.6 CFC-12 (CF_2Cl_2)





Comments

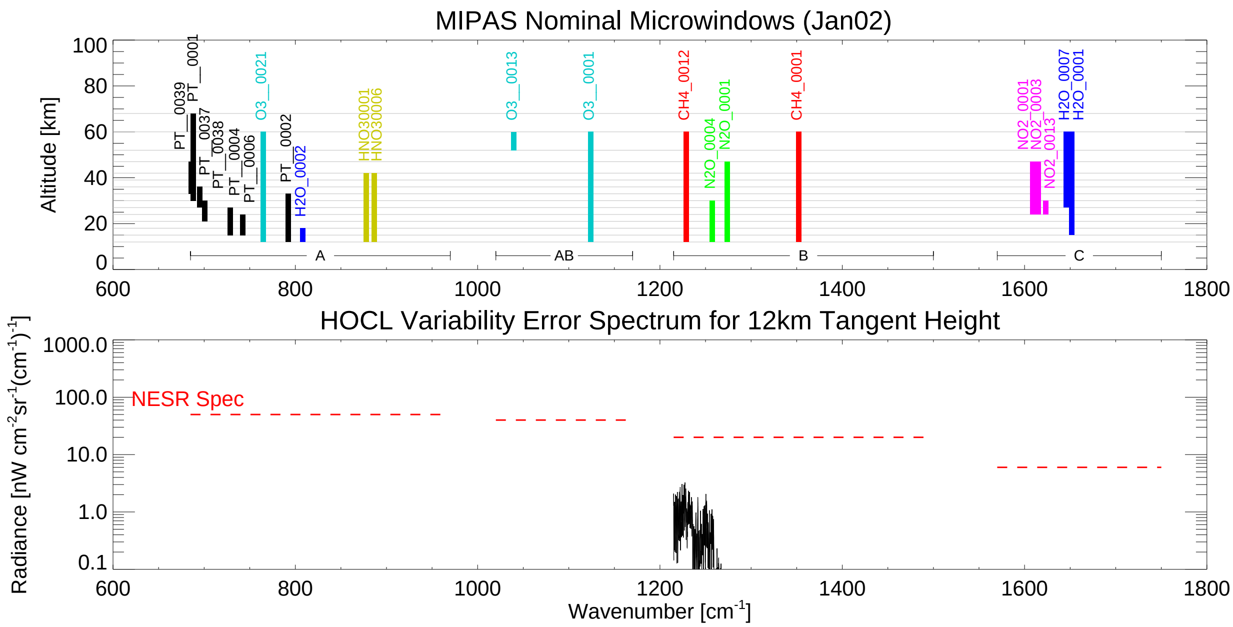
CFC-12 is a cross-section molecule with only weak signatures in the operational microwindows, mostly the HNO_3 microwindows but also some O_3 microwindows, so REC results should be treated with caution.

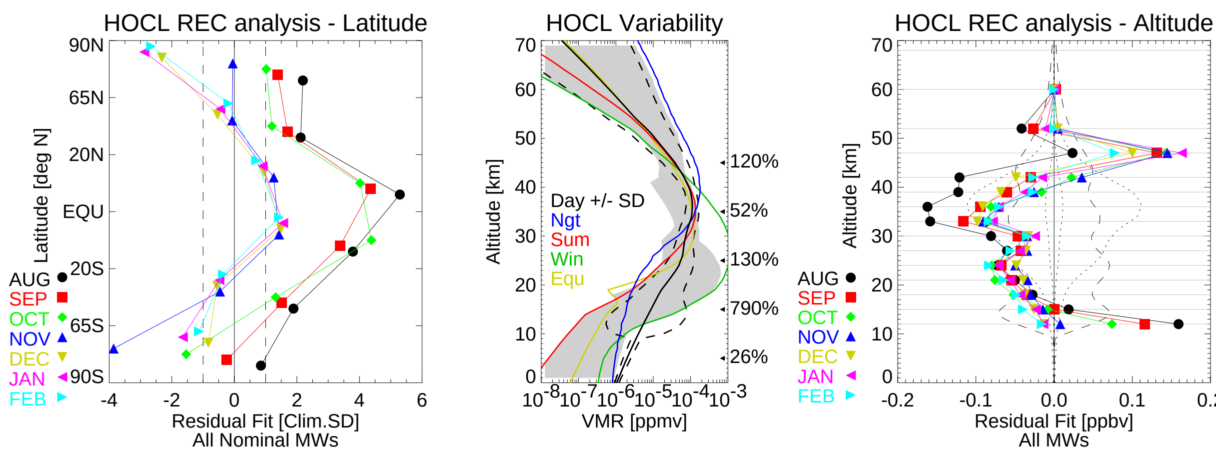
The latitude plot indicates that the fit improved after Nov 13th, but still underestimates at low latitudes, possibly by a factor 2. Since CFC-12 is a passive tracer with a long lifetime, it's climatological variability is assumed to be rather small. The altitude plot suggests an underestimate of the order of 0.1 ppbv (10–20%) below 20km. The peaks at higher altitude may represent differences between the true profile and the point at which the IG profiles no longer maintain the tropospheric concentrations, but the differences are not consistent from month to month.

Recommendations

Check climatology at low altitude and low latitude.

4.7 HOCl





Comments

HOCl is a line molecule with a weak signature in the B-band nominal microwindows.

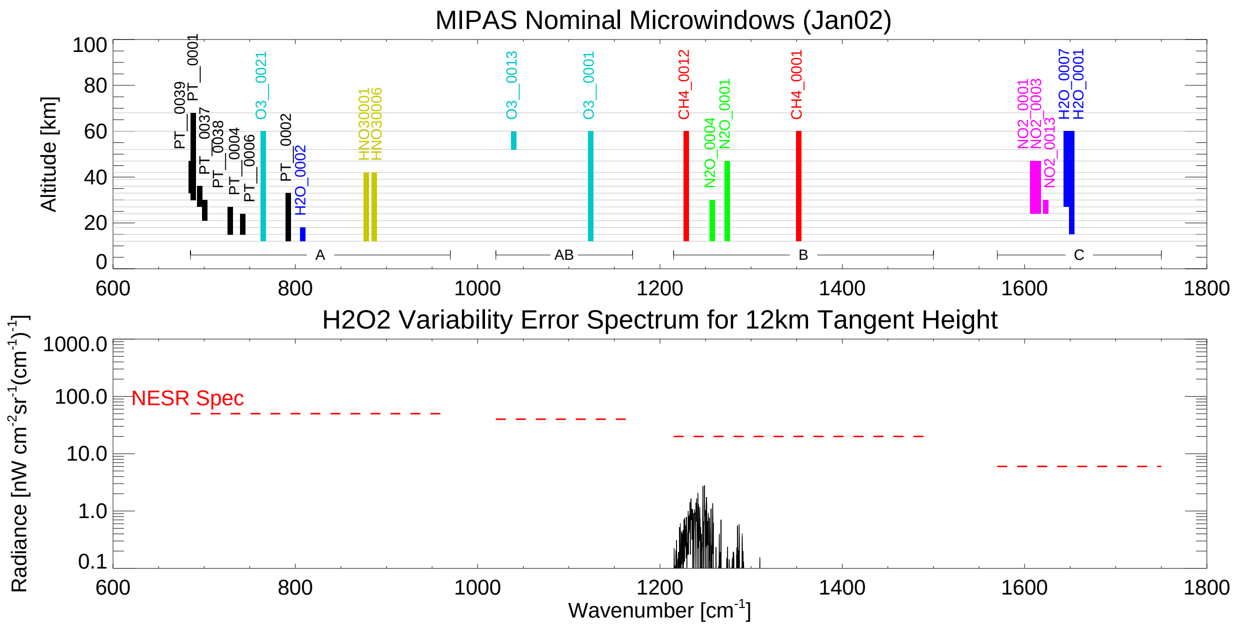
The latitude plot shows a significant reduction in the residual signature after Nov 13th, subsequently showing that the IG underestimates the true profile at low latitudes and overestimates at high latitudes.

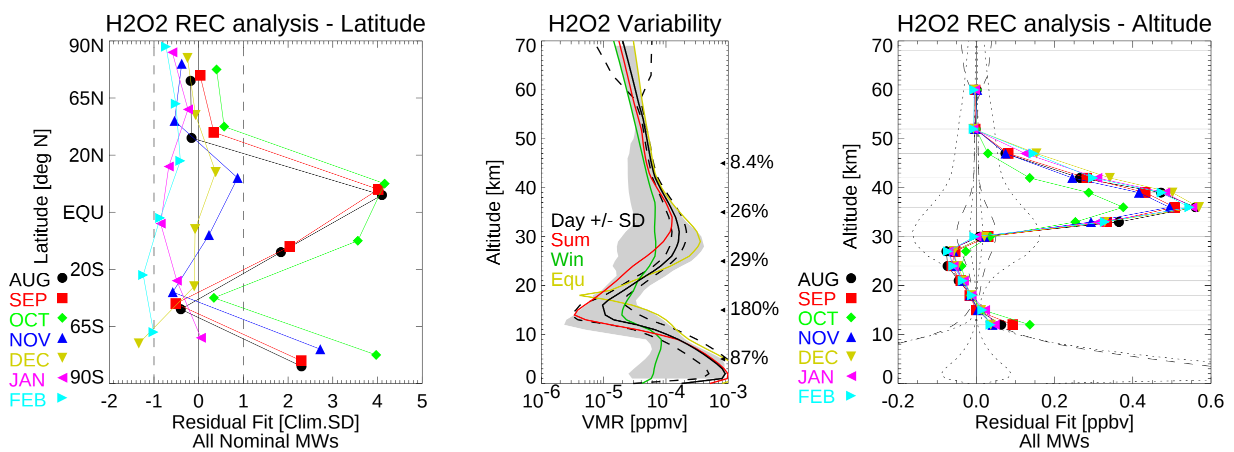
The altitude plot shows mostly an overestimate of the order of 100%, meaning that the HOCl features in the residuals are approximately the same strength as the assumed HOCl emission features but negative. Therefore the true profile may be an order of magnitude lower than the assumed profile.

Recommendations

Check if climatology should be reduced by an order of magnitude.

4.8 H_2O_2





Comments

H_2O_2 is a line molecule with a weak signature in the B-band nominal microwindows.

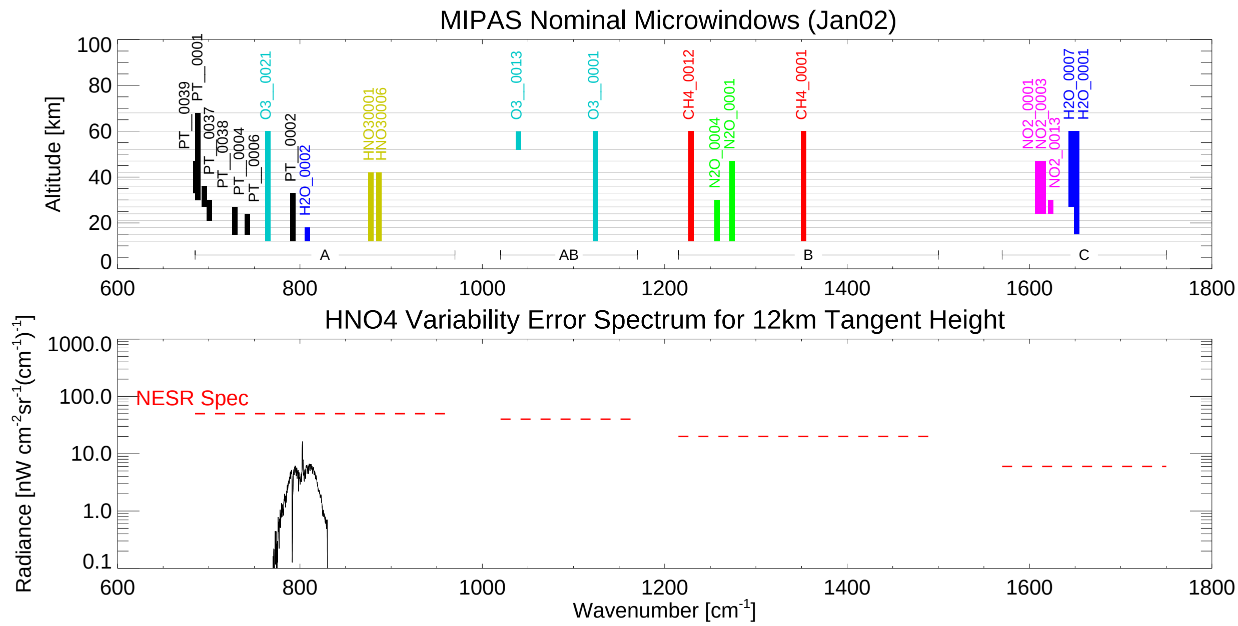
The latitude plot indicates a significant improvement after Nov 13th, and subequent fits generally lie within the climatological SD.

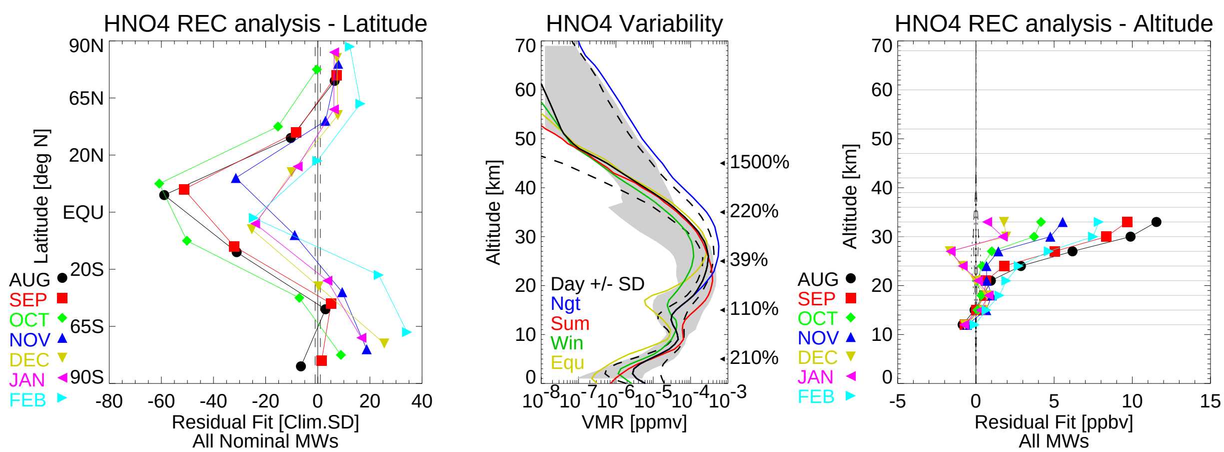
The altitude plot shows consistent results for all months: that the IG underestimates the atmospheric concentration by 0.05 ppbv at 12 km, overestimates by 0.05 ppbv at 27 km, and then significantly underestimates the high altitude peak at 36 km by 0.5 pppv (the IG peak being lower and smaller).

Recommendations

Investigate high altitude peak in climatology.

4.9 HNO_4





Comments

HNO_4 is a cross-sectional molecule with a signature in pT and H_2O microwindows in the A-band.

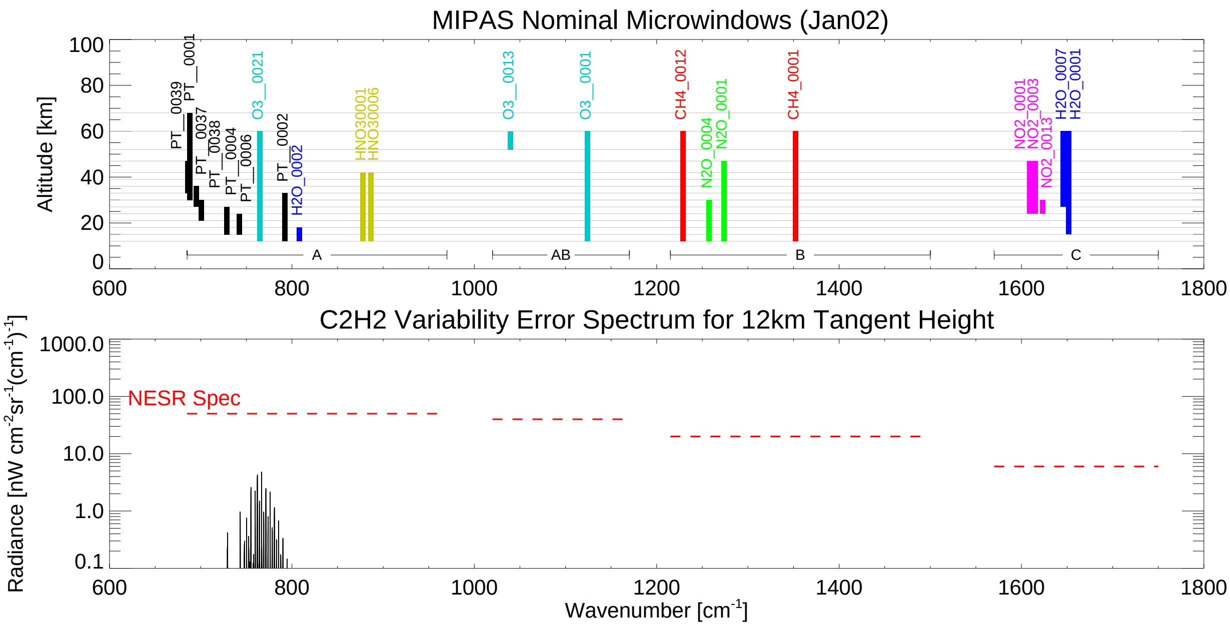
The latitude plot shows a reduction in residual signatures after Nov 13th, after which the IG overestimates the true atmosphere at low latitudes and underestimates at high latitudes by an amount significantly larger than the climatological SD.

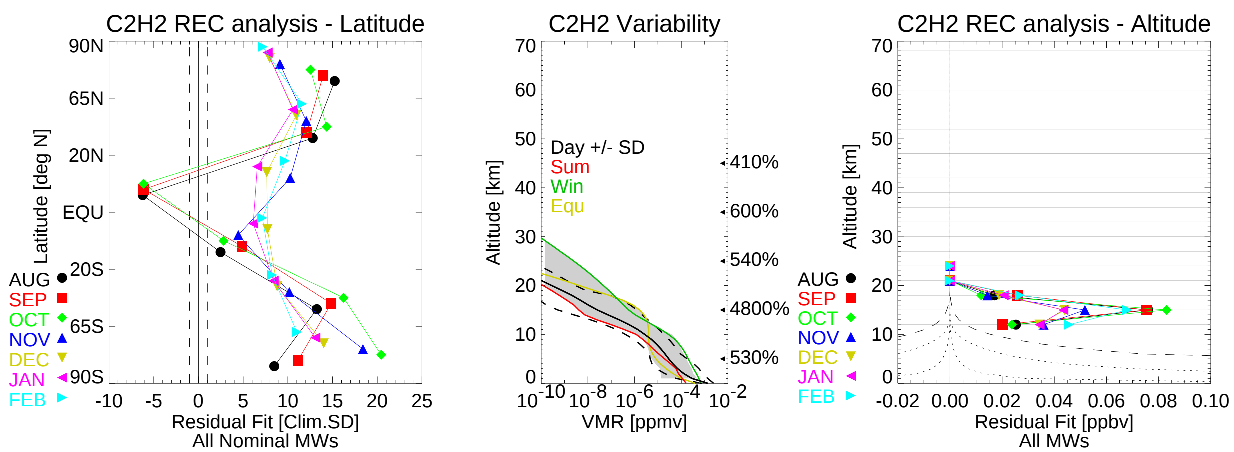
The altitude plot indicates an overestimate of 0.1 ppbv at 12 km and an underestimate of 0.1 ppbv at 21 km, with no systematic trend and probably spurious values at higher altitudes.

Recommendations

Increase climatological uncertainty by an order of magnitude.

4.10 C_2H_2





Comments

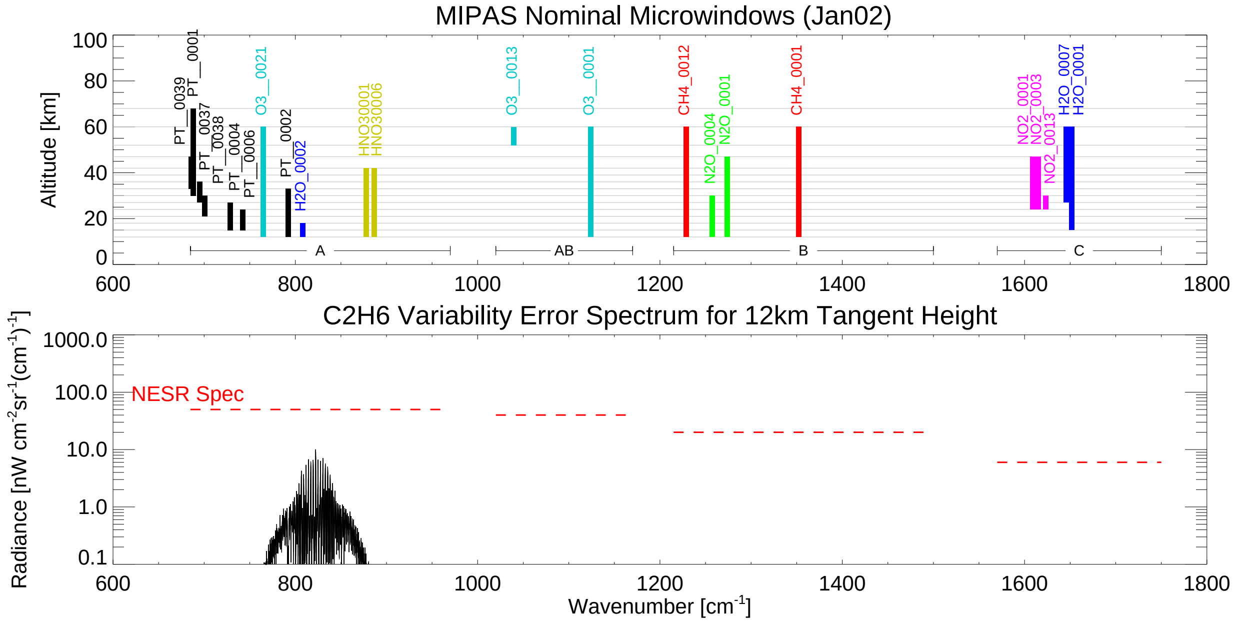
C_2H_2 is a line molecule with weak absorption features in the A-band microwindows.

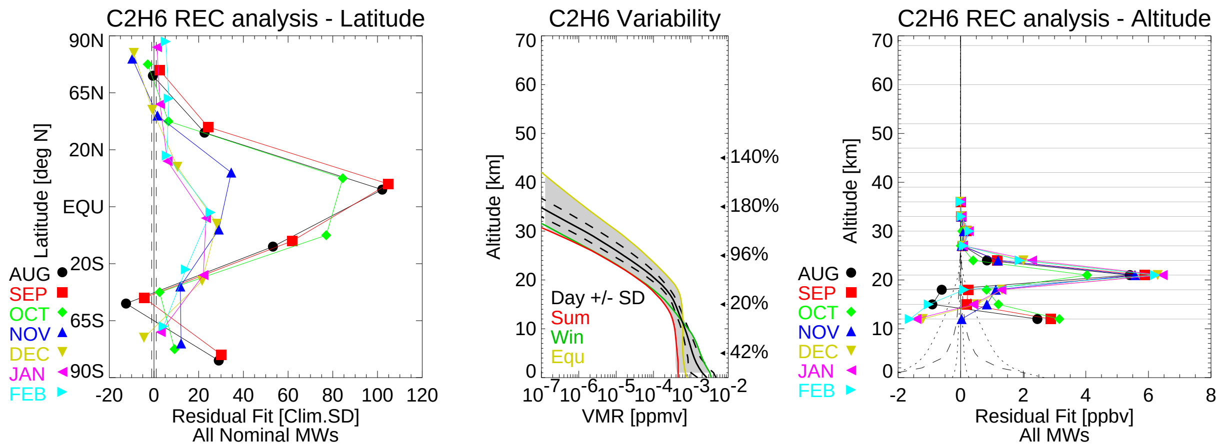
The residuals indicate a significantly larger concentration of C_2H_2 than assumed in the climatology, possibly slightly more at higher latitudes but always well above the climatological variability. Most of this enhancement seems to be at 15 km, a value 0.05ppbv suggesting that the climatological profile may fall off too rapidly with altitude.

Recommendations

Check climatological profile shape.

4.11 C_2H_6





Comments

C_2H_6 is a line molecule with a broad but weak absorption feature spanning several A-band microwindows.

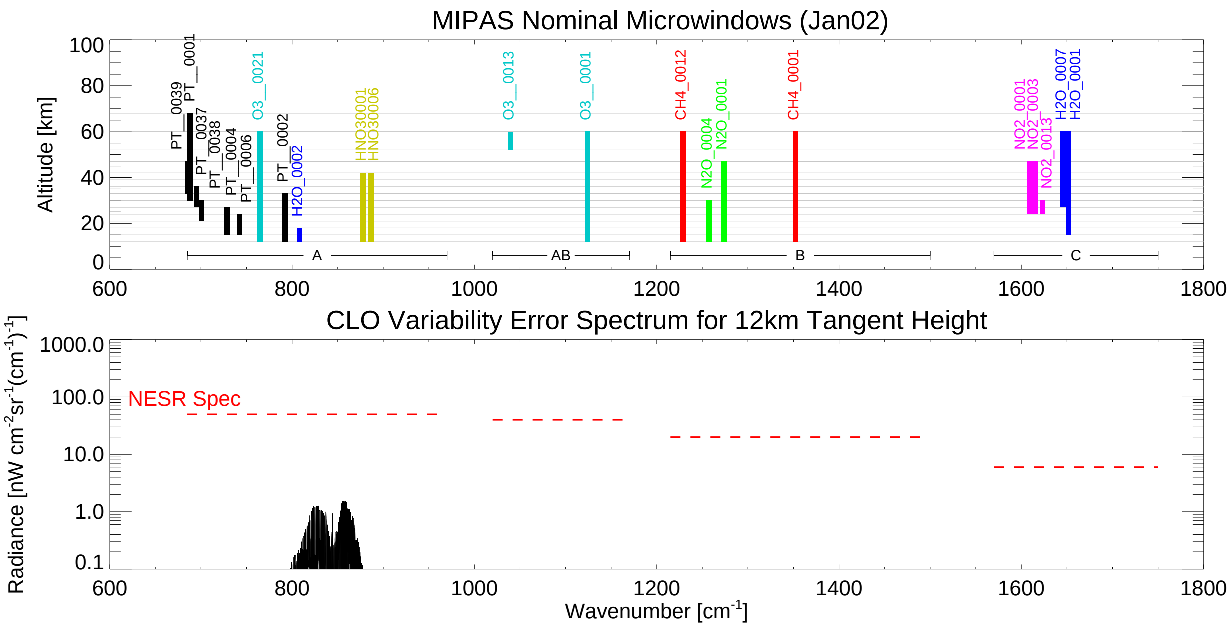
The latitude plot shows significant improvement after Nov 13th but with a remaining tendency to underestimate the atmospheric concentration, particularly at low latitudes, but an amount significantly larger than the climatological variability.

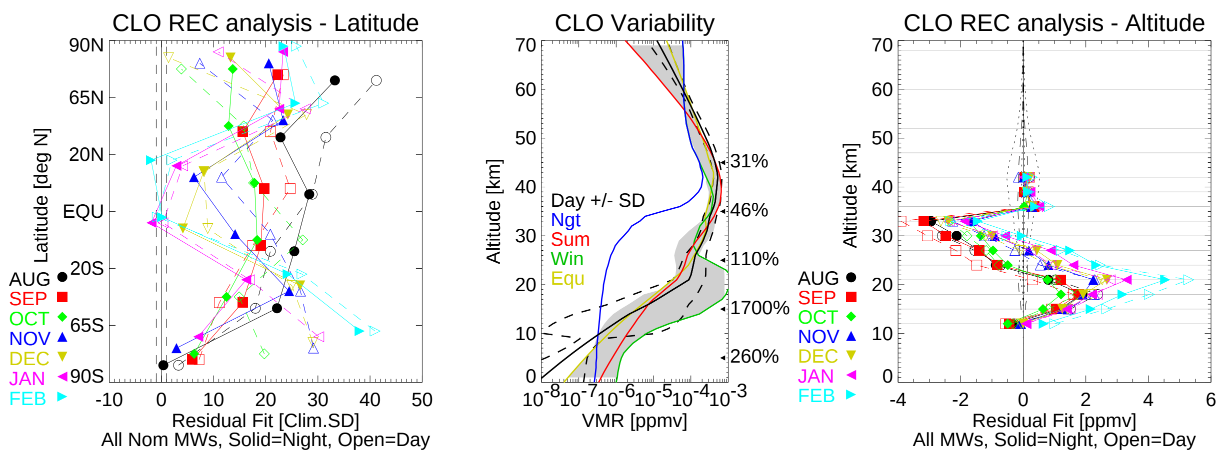
The altitude plot suggests (after Nov 13th) that the true profile may be overestimated by 2 ppbv at 12km, but underestimated by 6 ppbv at 21 km. The 21 km feature may indicate that the IG profiles start to decrease rapidly at too low an altitude.

Recommendations

Check climatology and variability.

4.12 ClO





Comments

ClO is a line molecule with weak absorption features in the A-band and an expected large enhancement in the polar winter. Although expected to show some diurnal variability (enhanced during the day-time through conversion from $ClONO_2$) the signal is not clear.

The latitude plot shows an underestimate of atmospheric ClO except at low latitudes. From the altitude plot, the main features are an undrestimate of 2 ppmv at 21 km, and an overestimate of 2 ppmv at 33 km, but since these are orders of magnitude larger than the expected ClO concentration they are probably spurious.

Recommendations

Investigate residual signature.

5 Contaminant Species - Fixed Profiles

5.1 Description

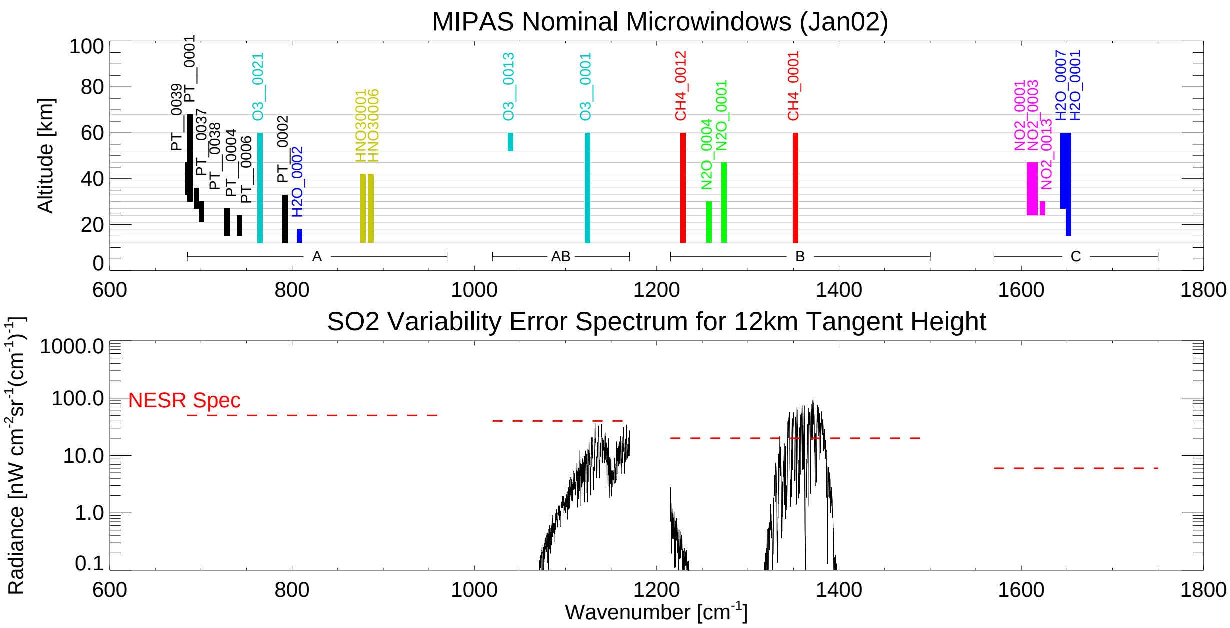
These are profiles which are assumed fixed in the retrieval and for which there is only a single climatological profile in the 'Initial Guess' (IG) data.

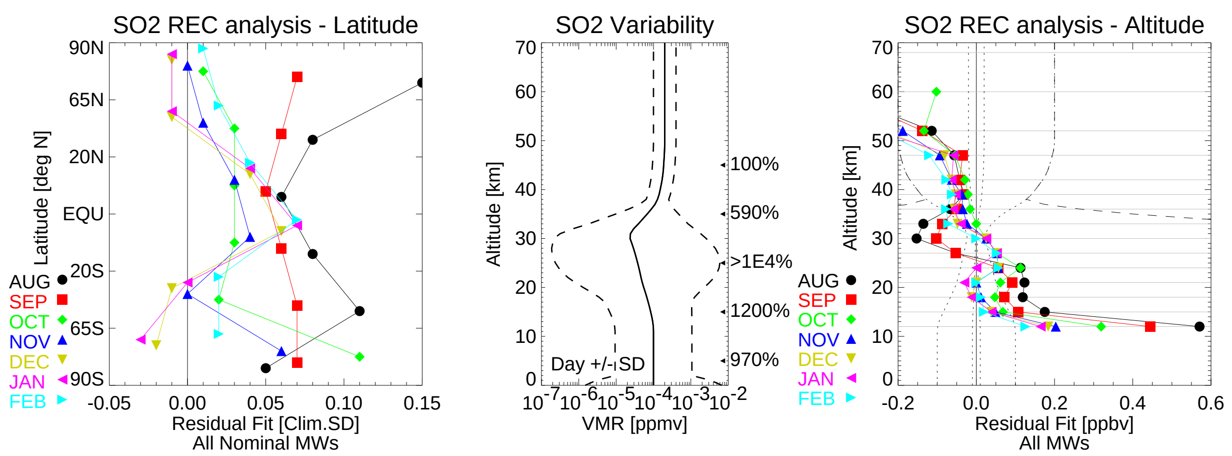
Tropospheric source gases (usually those with profiles which decrease with altitude) are expected to give positive residuals at the equator where stratospheric concentrations are enhanced, and negative residuals at the poles, especially the winter pole.

5.2 Problem Areas

The REC analysis identifies any discrepancy between the IG data and the climatology, i.e. whether the climatological uncertainty assigned to these species adequately reflects the seasonal, latitudinal and, in some cases, diurnal variability of the true atmosphere. Problems are indicated if the residuals lie significantly outside the dashed lines representing the assumed 1σ uncertainty.

5.3 SO_2





Comments

SO_2 is a line molecule with strong absorption features in the AB and B bands.

The REC analysis indicates SO_2 variability much smaller than assumed by the climatological variability. This is due to the climatological variability allowing for volcanic activity whereas there have been no significant eruptions affecting stratospheric SO_2 recently.

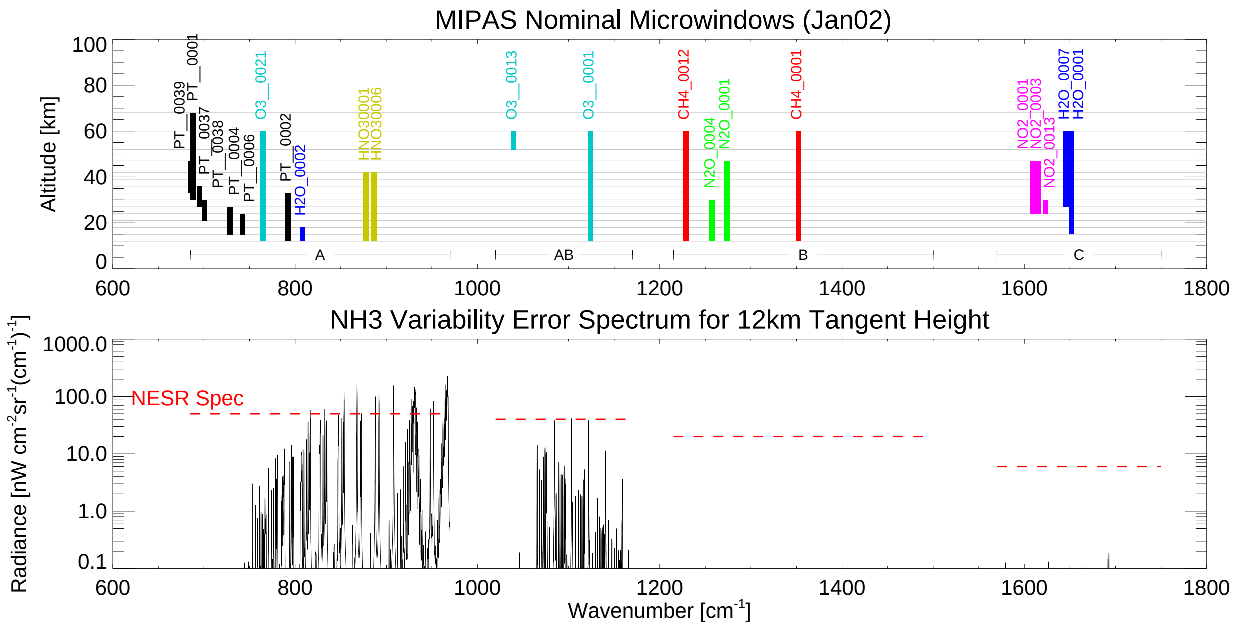
Since Nov 13th the latitude plot shows underestimated SO_2 at the equator, as expected for a tropospheric source, but approximately correct at high latitudes.

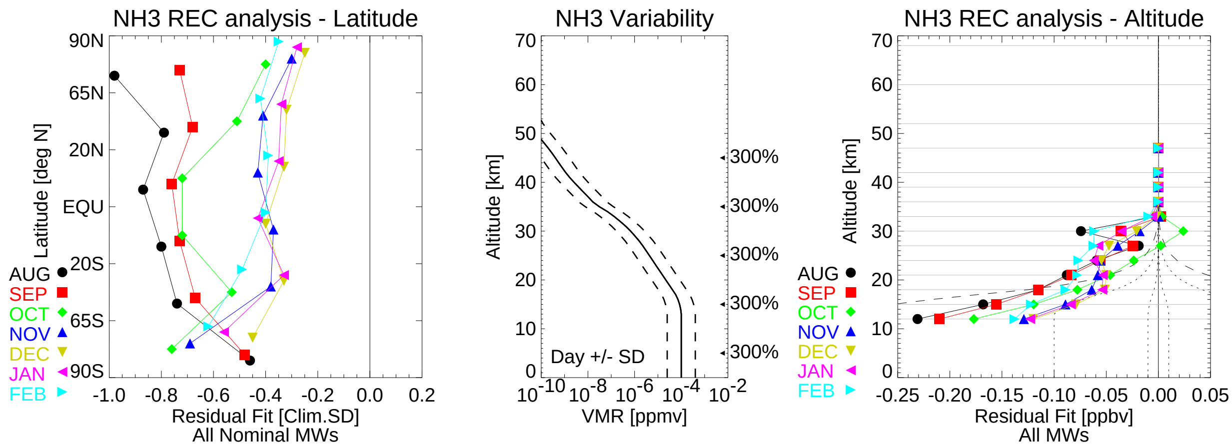
The altitude plot shows fairly consistent results from Nov 13th onwards: 0.2 ppbv underestimate at 12km, approximately correct from 12–21 km, 0.1 ppbv underestimate at 24–27 km, then 0.1 ppbv overestimate from 36 km and above.

Recommendations

Reduce climatological variability by a factor 10 since this is currently a significant component of the error budget for CH_4.

5.4 NH_3





Comments

NH_3 is a line molecule with widespread absorption features throughout the A and AB bands.

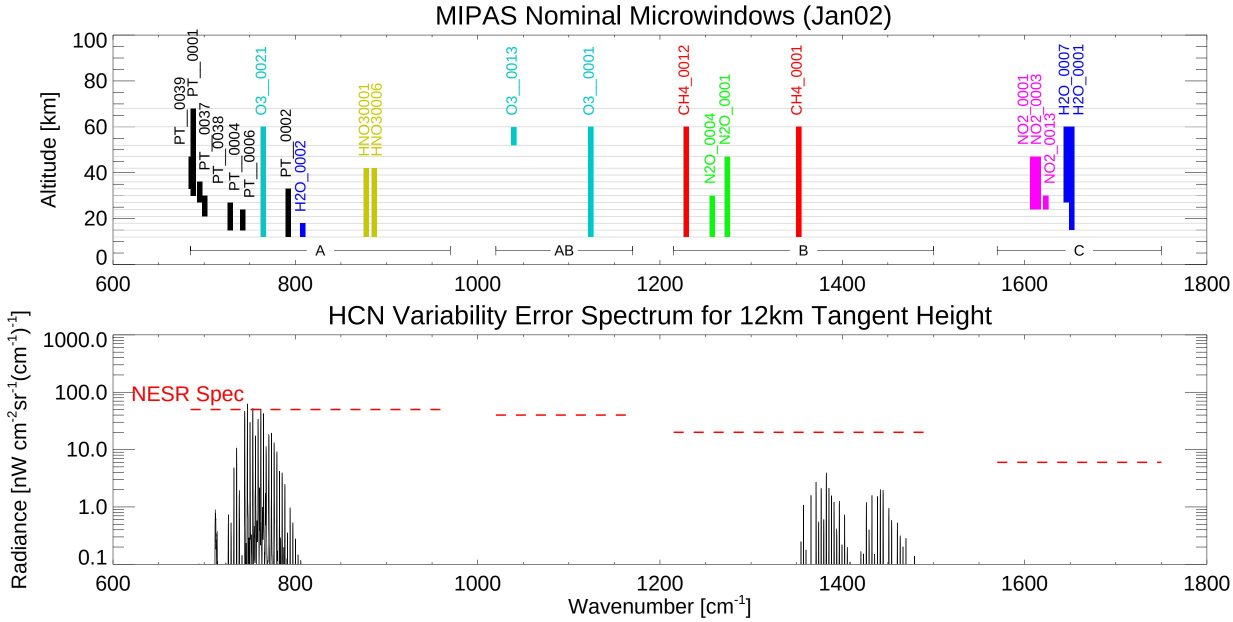
The latitude plot shows that the fitted NH_3 residual signature reduced by a factor 2 after Nov 13th but the remaining months show a consistent overestimate of the atmospheric concentration, especially towards the south pole.

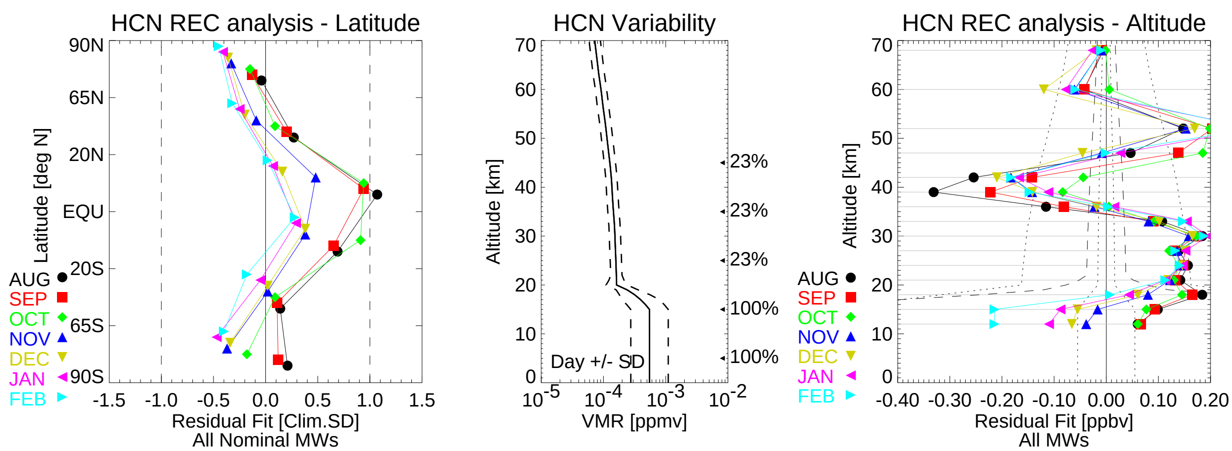
The altitude plot shows residuals which are of the order of the size of the NH_3 contribution, suggesting that the profile is uniformly overestimated by possibly an order of magnitude.

Recommendations

Check if NH_3 climatology should be reduced by an order of magnitude.

5.5 HCN





Comments

HCN is a line molecule with a strong signature in the A-band.

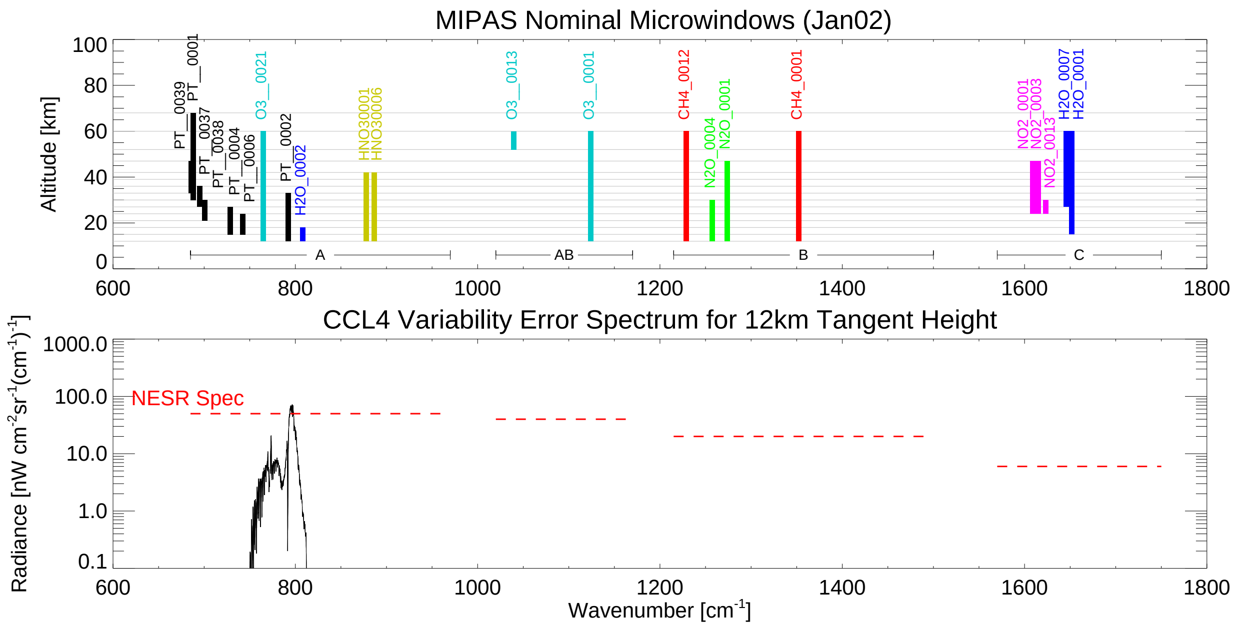
The latitude plot indicates a reduction in residuals after Nov 13th, with a slight overestimate at high latitudes and underestimate at the equator although well within the climatological variability.

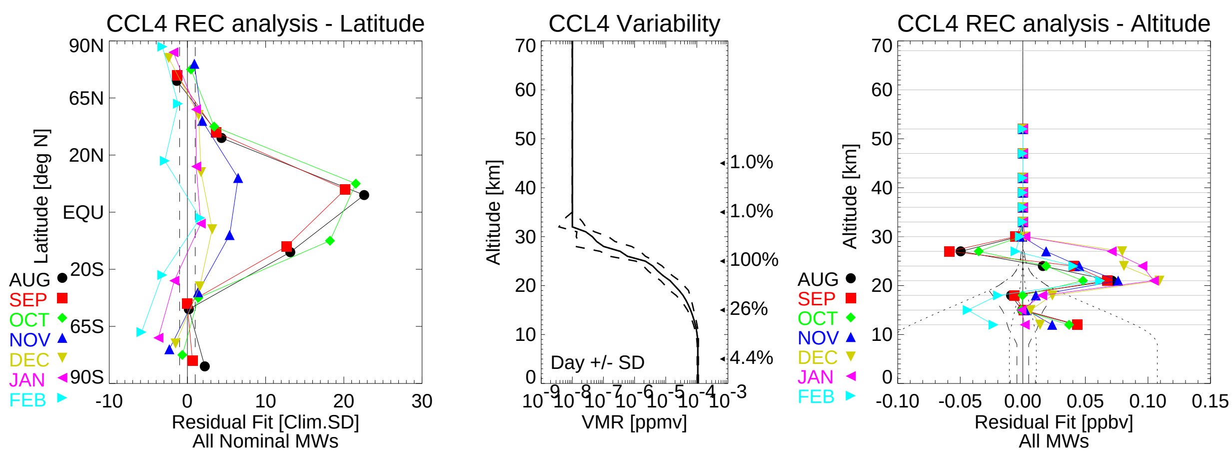
The altitude plot shows an underestimate of 0.2 ppbv at 30 km but an overestimate of 0.2 ppbv at 39 km. The climatological profile reduces sharply above 15 km but the altitude plot suggests that the profile remains constant to 30 km before falling off more sharply. The apparent secondary maximum at 50km is probably spurious.

Recommendations

Investigate HCN profile structure and increase climatological uncertainty for stratosphere.

5.6 CCl_4





Comments

CCl_4 is a cross-section molecule but with a fairly strong signature in the A-band.

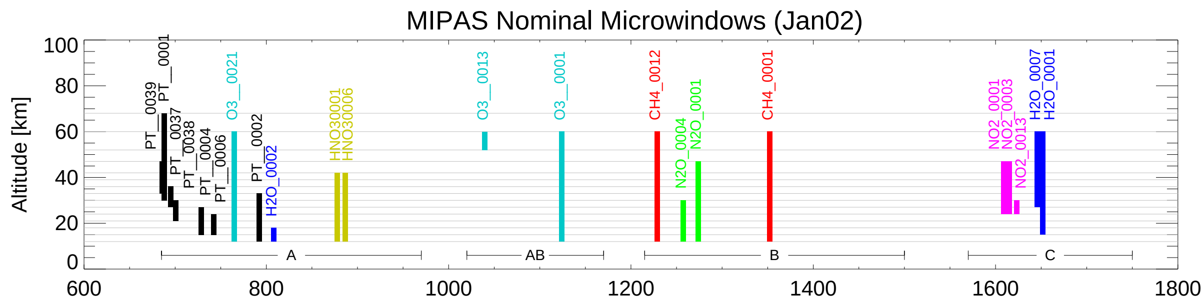
The latitude plot shows a significant reduction in residuals after Nov 13th and subsequently a slight underestimate at low latitudes and overestimate at high latitudes as expected for a tropospheric source gas characterised by a single profile. However the variation is larger than the assumed climatological SD.

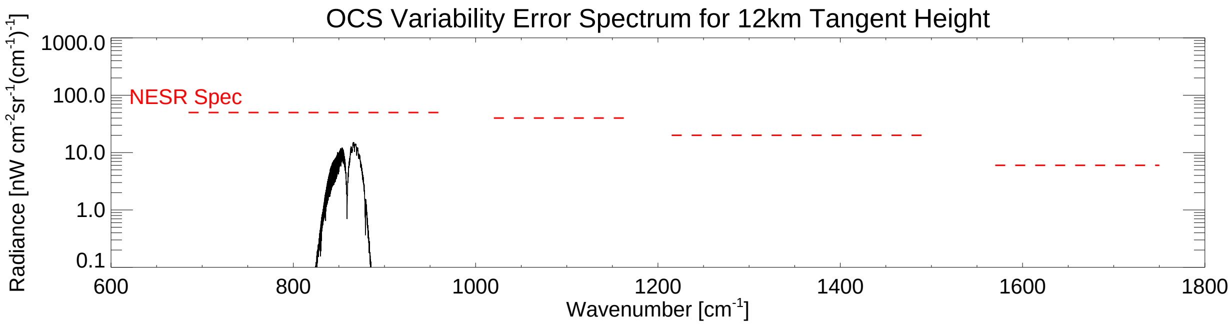
The altitude plot shows an underestimate of the atmospheric profile by 0.05–0.1 ppbv at 21 km which may indicate that the assumed IG profile falls off too rapidly with altitude above 18km.

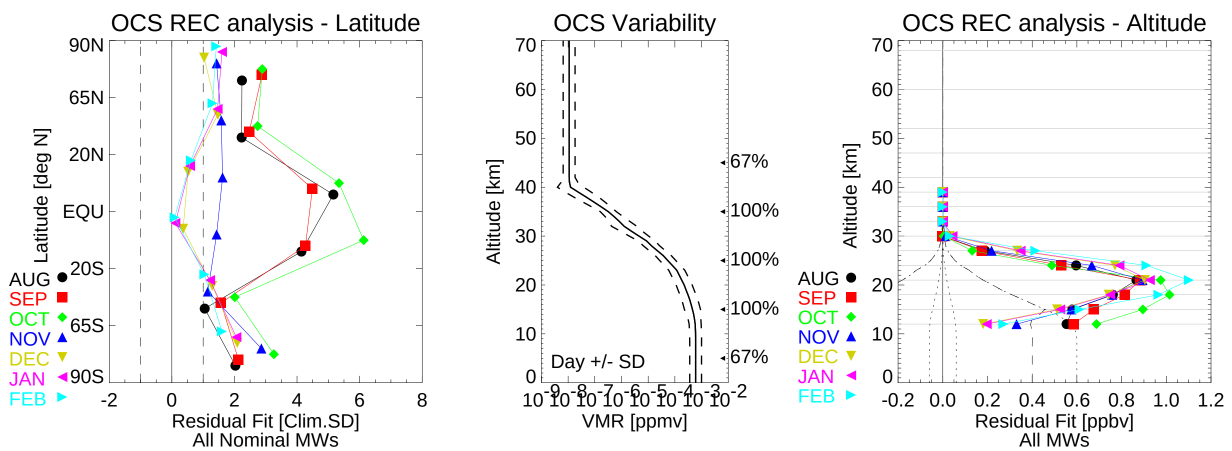
Recommendations

Investigate CCl_4 profile, increase error bars associated with CCl_4 variability.

5.7 OCS







Comments

OCS is a line molecule with only a weak signature in the HNO_3 microwindows.

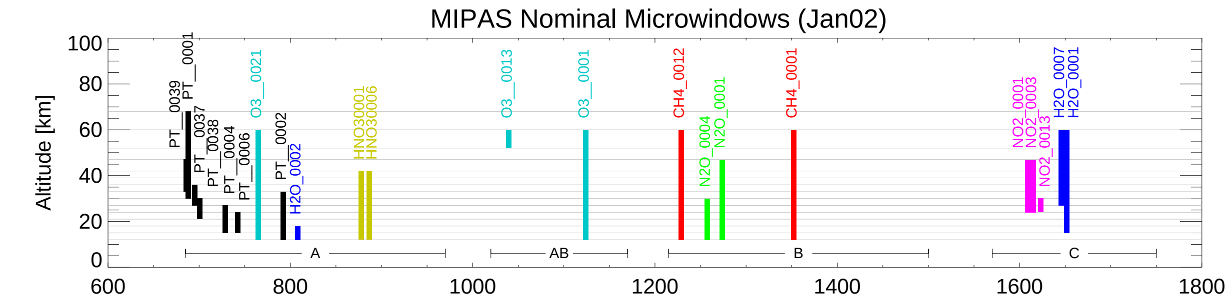
The latitude plot shows that the residuals reduced significantly after Nov 13th to a level approximately 1 SD (=factor 2) above the expected value at high latitudes but correct at low latitudes, which is surprising for a tropospheric source gas.

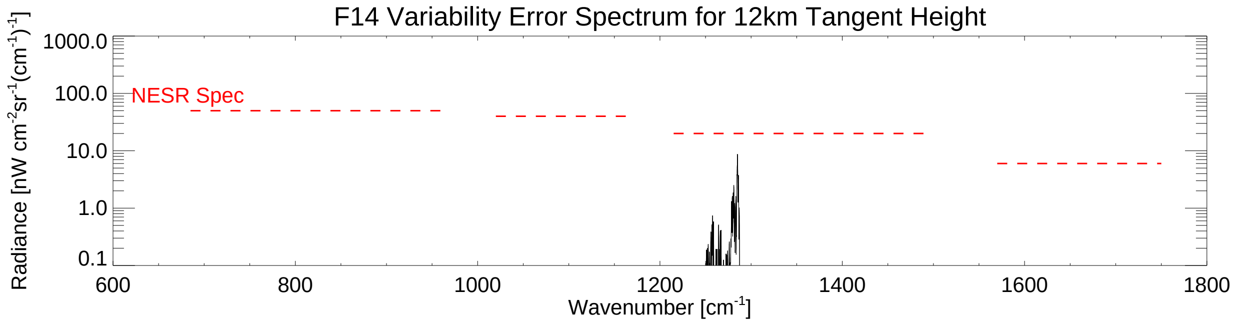
The altitude plot suggests an underestimate of 0.5 ppbv at 12 km reaching 1 ppbv at 20 km, characteristic of an IG profile which decreases too rapidly with altitude in the stratosphere.

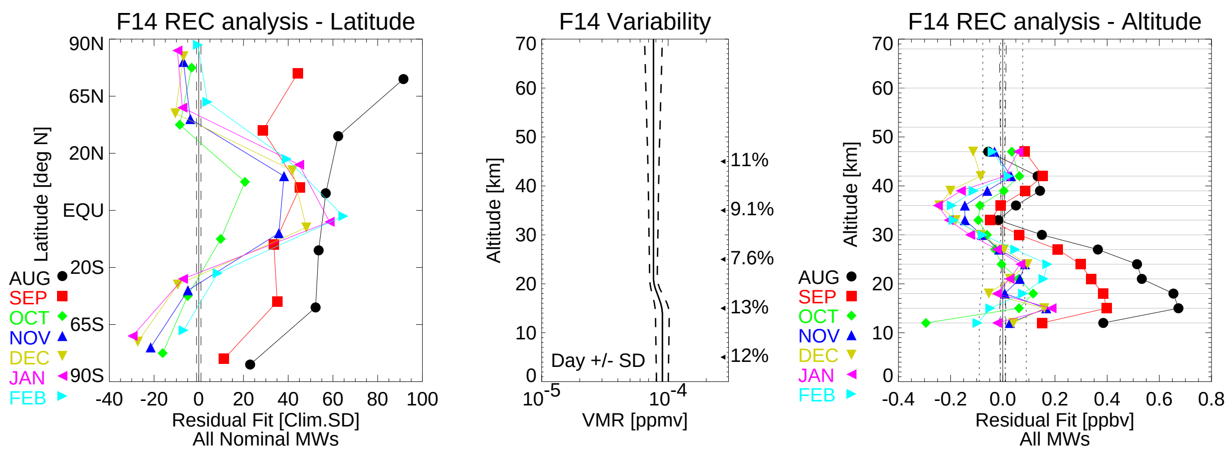
Recommendations

Investigate shape of OCS profile.

5.8 CFC-14 (CF_4)







Comments

CFC-14 is a cross-sectional molecule with weak features in the B-band so that the REC analysis is expected to be less reliable.

The latitude plot shows that, from Nov 13th, there is a consistent underestimate at low latitudes as expected for a tropospheric source gas. The altitude plot shows an underestimate of the order of 0.1 ppbv (∼assumed mixing ratio) below 24 km, and a possible overestimate at higher altitudes peaking at 0.2 ppbv at 36 km. All variations are much larger than the assumed climatological variability but this may reflect the poor REC fit.

Recommendations

Investigate CFC-14 climatology.

6 Forward Model Approximations

6.1 Description

Various approximations are made in the forward model which can be characterised as error spectra by taking the difference between calculations with and without the particular approximation. These error spectra are expected to correlate with features in the residual spectra with a mean fit value of +1.

6.2 Problem Areas

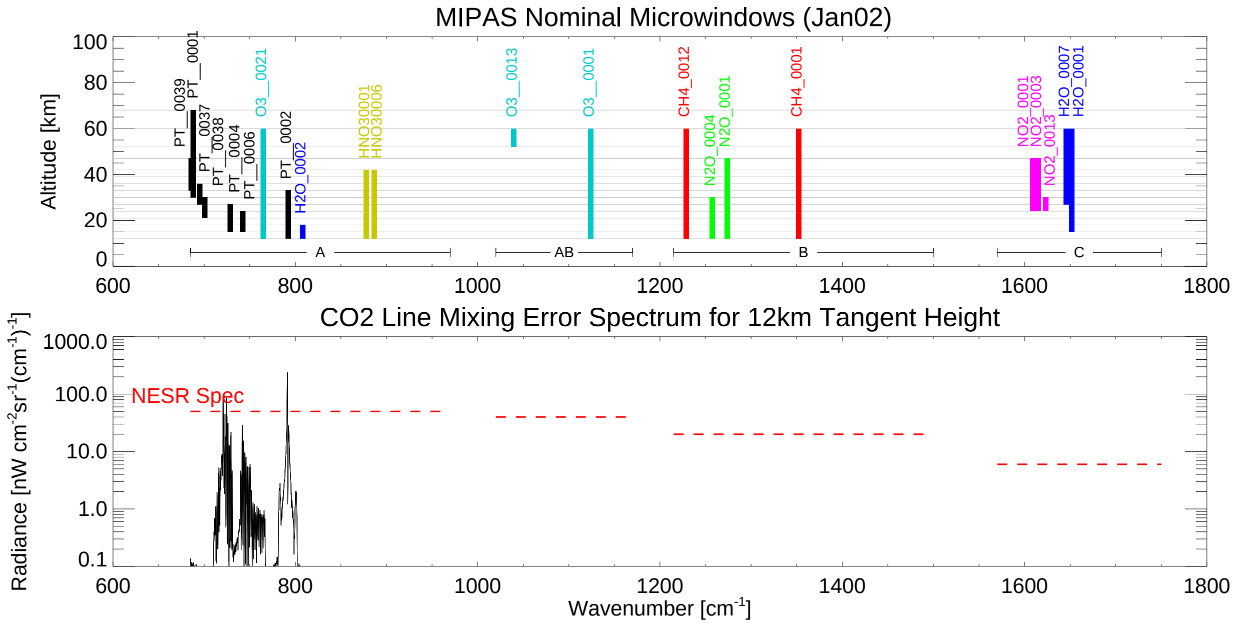
CO_2 line-mixing is quantum effect where the net emission from strong, densely-packed energy levels is not a simple summation of the contribution of each line. This affects only the strongest parts of the CO_2 band.

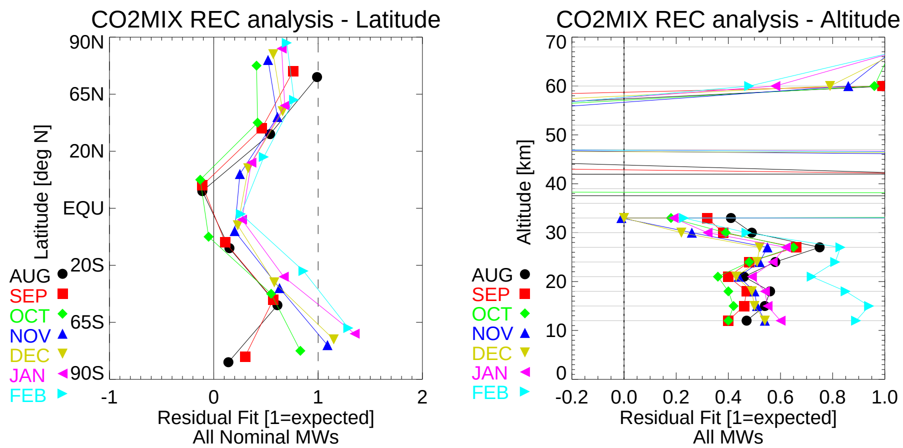
Non-LTE effects occur when the emission source function is no longer the Planck function characterised by the local kinetic temperature. Such effects usually occur at high altitudes and during day-time, so may also show up as a diurnal variation in residuals of the retrieved species at high altitudes.

Microwindows have been selected to avoid, or mask out, spectral regions where such effects lead to a significant source of retrieval error. Therefore the presence of such a signal is not in itself a problem, but a fit value significantly different from 1 suggests the models used to estimate such effects may be significantly in error.

A further forward model error is the impact of horizontal gradients — the forward model assumes a horizontally homogeneous atmosphere. Microwindow selection also includes this as an error source but since the average gradient, and therefore gradient error, is zero no characteristic signature is expected in a long-term average of residuals.

6.3 CO_2 Line Mixing





Comments

CO_2 line-mixing affects only the stronger CO_2 lines in the A and D bands, so is only expected to affect the pT microwindows.

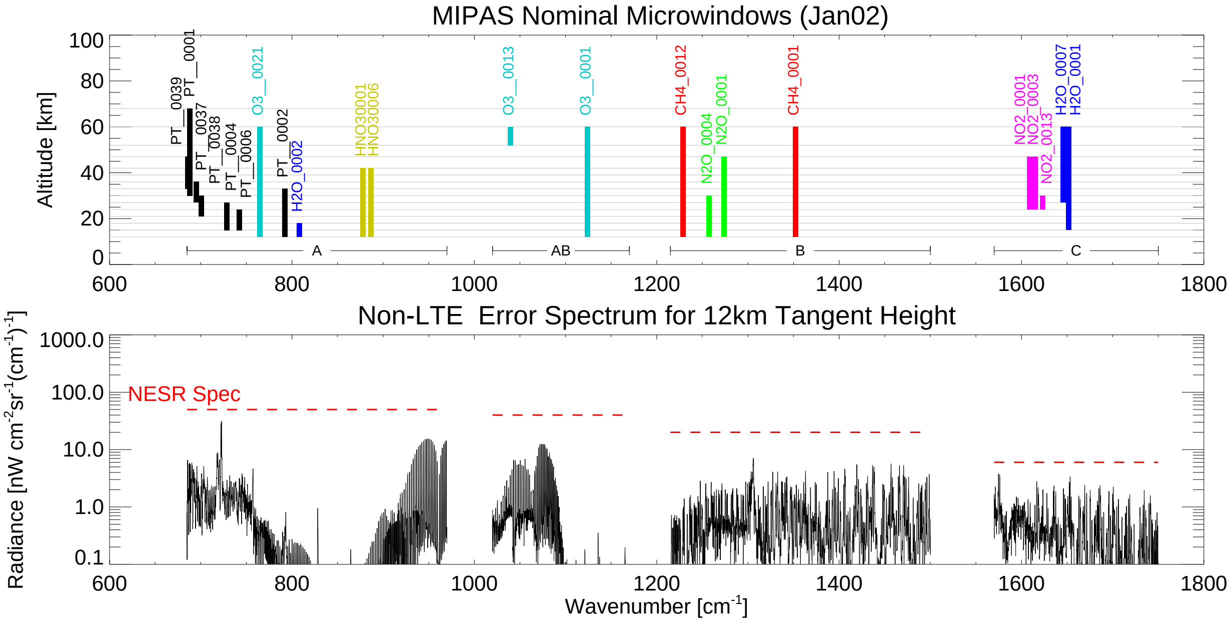
The line-mixing signature approaches its expected value of 1 at high latitudes but is much reduced at the equator. There was a slight increase at all latitudes following Nov 13th.

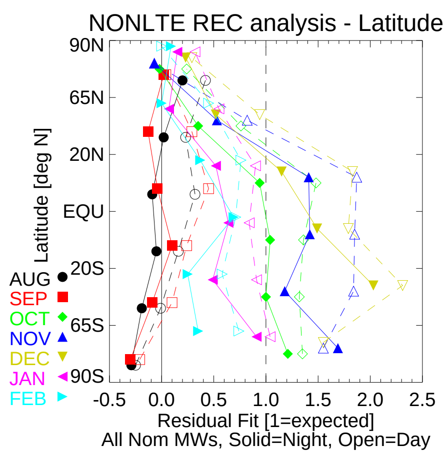
In the altitude plot the fitted value seems to remain around 0.5 up to 30 km but close to 1.0 for February. Above that it becomes 'noisy' (but consistent from month to month) until approaching its *a priori* constraint of 1 at 60 km and 68 km. Since CO_2 line-mixing is associated with high pressures the signal is expected to fall off rapidly with altitude and it may be that the signal becomes aliassed with some other spectral feature in the residuals at higher altitudes.

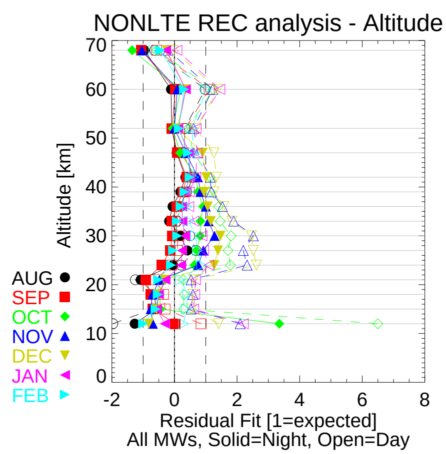
Recommendations

Investigate latitudinal variation and February altitude signature.

6.4 Non-LTE







Comments

Non-LTE effects occur in all microwindows to some extent, but are expected to be (relatively) more significant at high altitudes. SThe non-LTE error spectra fitted are those associated with mid-latitude day-time conditions, nighttime signatures are expected to be much smaller and polar summer signatures larger.

The latitude plot shows day-time signatures enhanced with respect to night-time, but generally of the order of 50% the expected magnitude, and an enhancement in both day and nighttime signatures at southern latitudes.

The altitude plot shows less distinct day-night differences at low altitudes but a clearer separation at 50km and above where magnitude broadly agrees with prediction.

Recommendations

Detailed investigation required to investigate effects in each microwindow.

7 Spectral Derivatives

7.1 Description

Unlike most of the previously considered errors which all have spectrally localised signatures associated with particular molecules, various sources of error can result in residual spectra which are proportional to 0th, 1st or 2nd derivatives of the complete observed spectra.

Since there is a strong signature at all altitudes for all microwindows, these analyses have been performed for each microwindow/tangent altitude individually using a least squares fit (§1.1).

7.2 Problem Areas

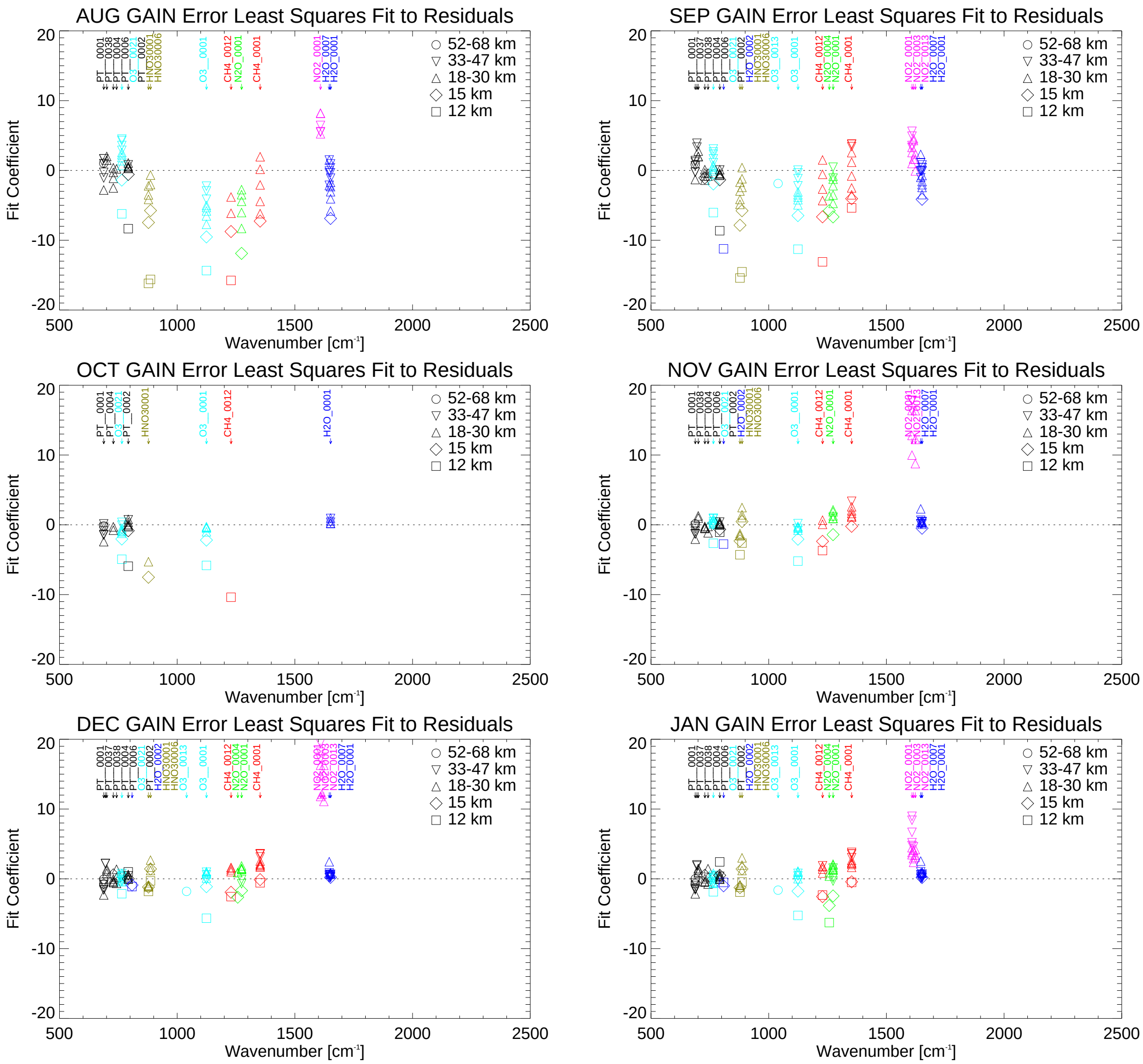
These analyses spectra are primarily intended to detect instrumental errors.

Radiometric gain inconsistencies will appear as residuals proportional to the original spectrum ('gain' - 0th derivative), spectroscopic calibration errors (including Doppler shifts) will result in modelled spectra shifted with respect to atmospheric spectra ('shift' - 1st derivative) and instrument line shape errors will result in modelled lines with different convolved widths to atmospheric spectra ('spread' - 2nd derivative).

Spectroscopic errors in line strength, line position (including pressure shift) and line width will appear as 0th, 1st and 2nd derivative spectra respectively. However, since these derivatives are fitted for all the lines within a single microwindow rather than individual lines they may not necessarily show up in this analysis.

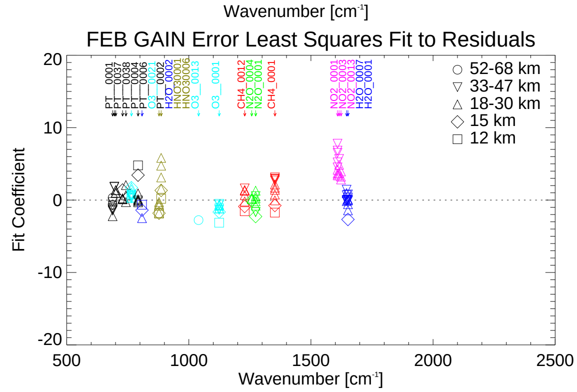
Temperature errors may appear as a 0th derivative spectra, pressure errors (although analysed separately in §3.2) may appear as 2nd derivative spectra at low altitude (where the effects of pressure broadening can be seen at MIPAS resolution) or 0th derivative spectra at high altitude where pressure errors simply translate as errors in the number of molecules in the tangent path.

7.3 Gain (0th Derivative)



Comments

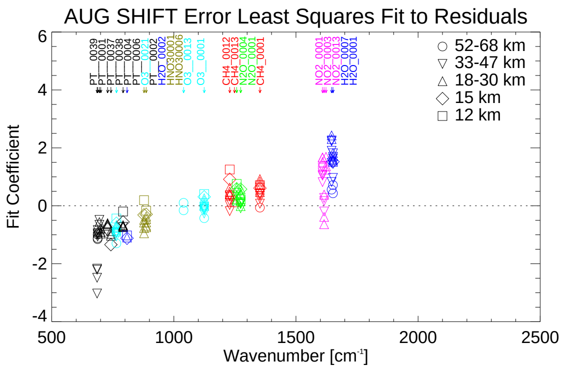
Fit coefficient +1 corresponds to a residual signature which is 1% of the nominal spectrum, e.g., if the radiometric gain is underestimated by 1% (assumed uncertainty is ±2%). While the fit is best at the wavelength extremes (corresponding to the pT and H_2O microwindows) there is a negative dip between, corresponding to 10% in the Aug–Sep data and still a few % in the subsequent data. Also, for all microwindows, the fit is more negative for lower altitudes. This might suggest that the retrievals are overestimating concentrations at low altitudes in these microwindows and possibly underestimating high altitudes. The fit in the NO_2 microwindow is persistently high.

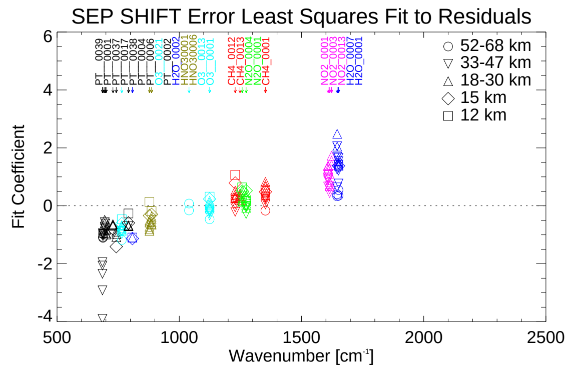


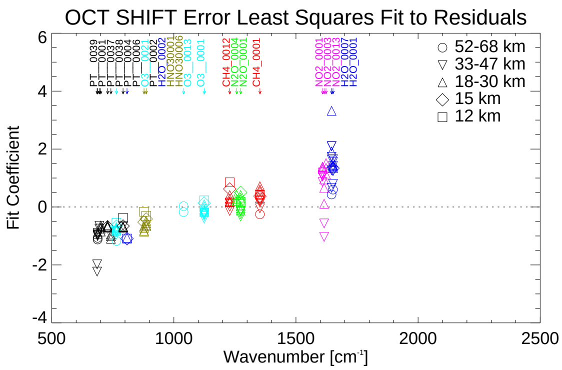
Recommendations

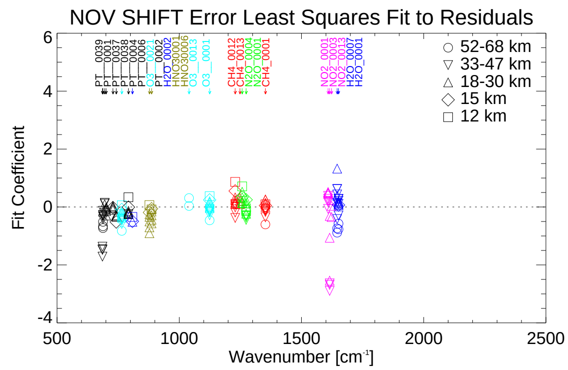
Investigate altitude dependence, and high residual in the NO_2 microwindow.

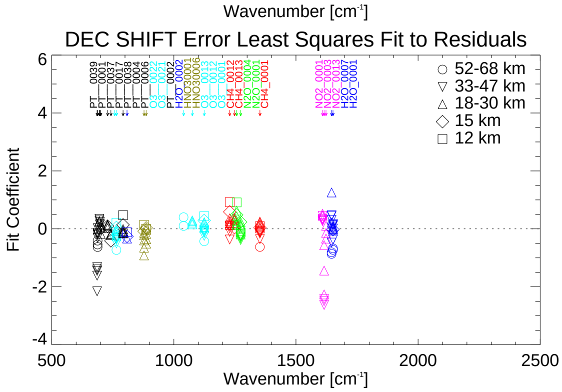
7.4 Spectral Shift (1st Derivative)

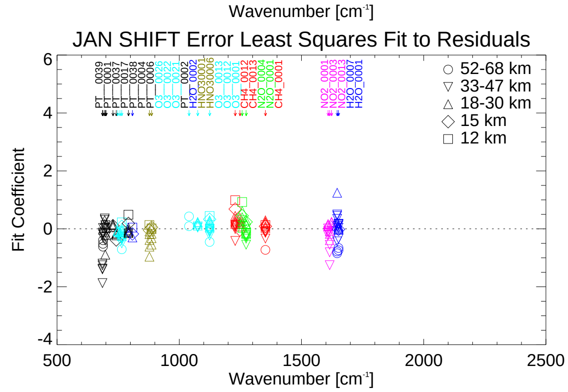


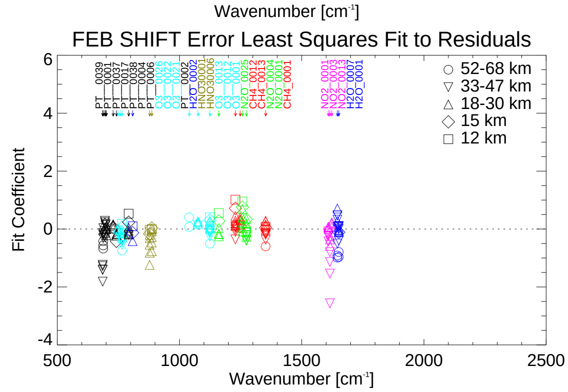












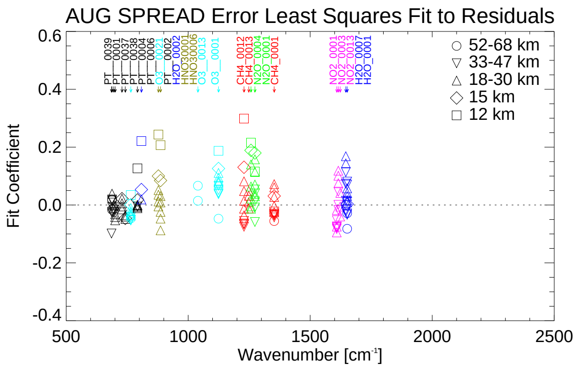
Comments

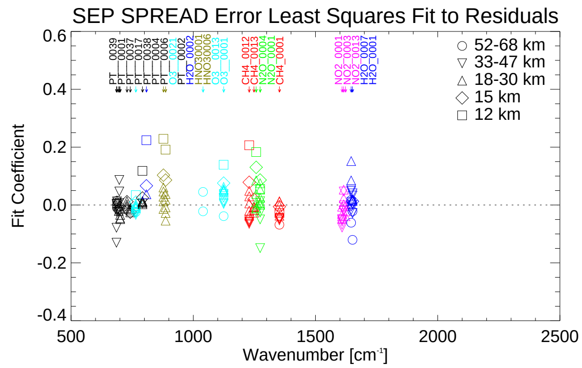
Fit coefficient +1 corresponds to a residual signature which is equivalent to the atmospheric spectrum shifted by +0.001 cm^{-1} relative to the modelled spectrum (the assumed uncertainty in spectral calibration is ±0.001 cm^{-1}). Prior to Nov 13th there is a persistent linear trend from −0.001 cm^{-1} in the lower A-band to +0.001 cm^{-1} in the C-band, which appears to have been removed in subsequent data. However superimposed on this is also an altitude trend: lower tangent height spectra appear to be shifted approximately +0.001 cm^{-1} relative to higher altitudes, particularly for NO_2.

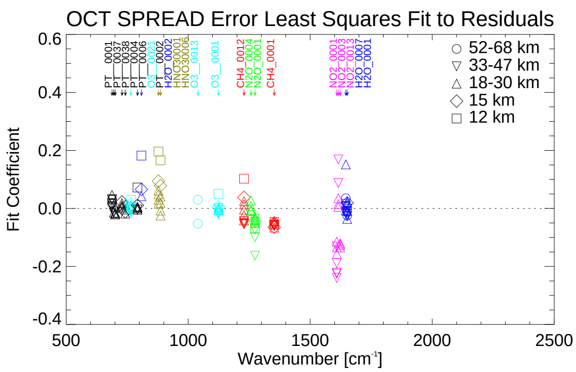
Recommendations

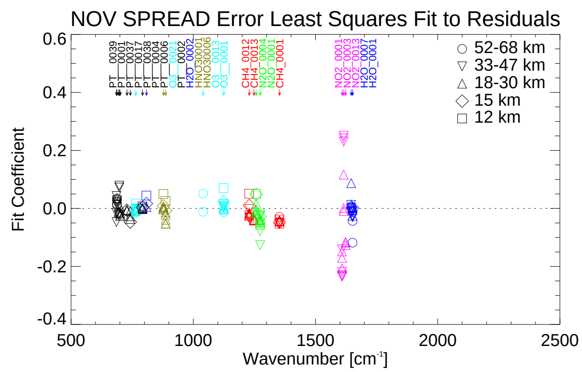
The instrument model assumes no altitude dependence of AILS, which is inconsistent with observed behaviour. However residual signatures are within the assumed uncertainties so not expected to affect retrieval accuracy significantly.

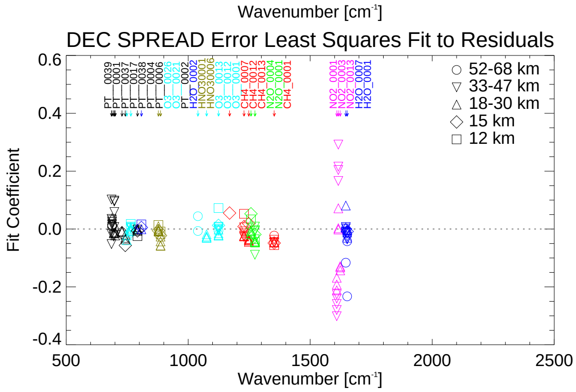
7.5 Spread (2nd Derivative)

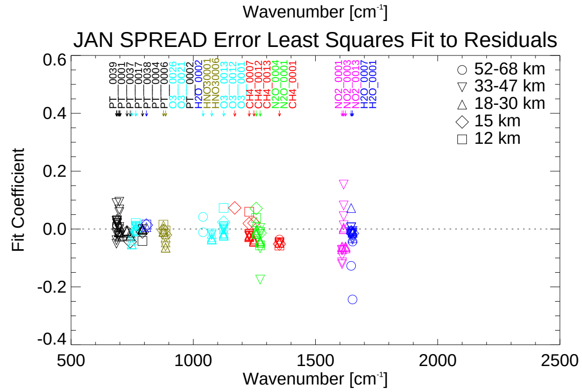


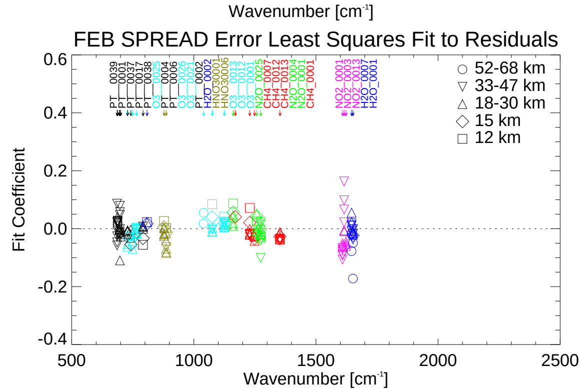












Comments

A fit coefficient of +0.02 corresponds to an increase in observed (apodised) line width of 1% compared to modelled width (±2% is the assumed uncertainty). Prior to Nov 13th low altitude linewidths in the A, AB and B bands were underestimated 10% (opposite sign to that expected from the pressure residuals, §3.2), while the C band widths were overestimated. Following Nov 13th the magnitude has been reduced to within 5% and the sign for the lower wavenumber A-band microwindows has been inverted (which is consistent with the pressure residuals). However the C band linewidths continue to be overestimated at low altitude and underestimated at high altitude.

Recommendations

Investigate modelling of AILS in C-band (NO_2 and H_2O) microwindows.

8 Summary

Summary comments refer to retrieved or assumed IG profiles compared to 'truth', excluding data prior to Nov 13th.

Residual	Ref	Summary	Possible problems	Priority
Target Species (T: target microwindows, O: other microwindows)				
Pressure	p.7	T: +3% 21–27 km, −1% $\geq$ 30km,	Retrieval or ILS	High
		O: (+10,−5,+10)% at (27,36,47)km.		
H_2O	p.9	T: +0.5ppmv at 12km, −3 ppmv at 60km	Convergence,	High
		O: +3ppmv at 12km, −3ppmv at 30km	High Alt Col or ILS	
O_3	p.11	T: ±0.2ppmv 12–47km, −0.5ppmv at 52km	High Alt Col	Medium
		O: (−1,+0.5,−0.5) ppmv at (30,42,52) km	IG or Spectroscopy	
HNO_3	p.13	T: −5 ppbv at 27km	Spectroscopy	High
		O: +10ppbv at 33km		
CH_4	p.15	T: −0.1ppmv at 27km, +0.05ppmv at 47km	Convergence	Low
		O: (−0.1,+0.1,−0.1) ppmv at (18,33,47) km		
N_2O	p.17	T: −25ppbv at 30km	Convergence	Medium
		O: ±10ppbv below 36km, +30ppbv(?) at 47km		
NO_2	p.19	T: ±0.5ppbv 21–42km	Climatology	Medium
		O: ±0.3ppbv $\leq$ 39km, +5ppbv(?) at 60 km		
Contaminant Species — Variable Profiles				
N_2O_5	p.22	Unreasonable REC fit at 40km	Residual signature	Low
$ClONO_2$	p.23	Unreasonable REC fit at 40km	Residual signature	Low
COF_2	p.24	−0.1ppbv at 33 km	Climatology	Medium
CFC-12	p.25	−0.2ppbv at 12km	Climatology	Low
HOCl	p.26	Order of magnitude too large, except low lat.	Climatology	Low
H_2O_2	p.27	(−0.05,+0.05,−0.5) ppbv at (12,27,36) km	Climatology	Low
HNO_4	p.28	−0.1ppbv at 12km, +0.1ppbv at 21km	Climatological SD	Low
C_2H_2	p.29	−0.05 ppbv at 15 km	Climatology	Low
C_2H_6	p.30	+0.2ppbv at 12km, −0.6ppbv at 15 km	Climatology	Low
ClO	p.31	−2ppmv(?) at 12km, +2ppmv(?) at 33 km	Residual signature	Low
Contaminant Species — Fixed Profiles				
SO_2	p.33	−0.2 ppbv at 12km, +0.1ppbv above 36km	Climatological SD	Medium
NH_3	p.34	Order of magnitude too large	Climatology	Medium
HCN	p.35	−0.2ppbv 30km, +0.2ppbv at 39km	Climatology & SD	Low
CCl_4	p.36	−0.1ppbv at 21km	Climatology & SD	Low
OCS	p.37	−0.5 ppbv at 12km, −1ppbv at 20 km	Climatology	Low
CFC-14	p.38	−0.1ppbv at 24km, +0.2ppbv at 36km	Climatology	Low
Forward Model Approximations				
Line-Mixing	p.40	0.5 of expected value, equat. and Feb variation	Resid. sig., Modelling	Low
Non-LTE	p.41	Unexpected seasonal/latitude variation	Modelling	Medium
Spectral Derivatives				
Gain	p.43	Altitude dependence, NO_2 microwindows	Gain, NO_2	High
Shift	p.44	Altitude dependence, NO_2 microwindows	AILS modelling, NO_2	Low
Spread	p.45	A,AB and B-band AILS widths deviate by ±2%	AILS modelling,	Low
		C-band widths deviate by ±5%	H_2O and NO_2	Medium