Optimization of model accuracy parameters

M. Höpfner and S. Kellmann

Abstract: For the discretization of the atmospheric radiative transfer problem a variety of parameters are necessary which determine the performance of the program. An adjustment of these parameters taking into account the trade-off between accuracy and run-time is required for routine applications of the processor. We present the model errors for all spectral bands of MIPAS-Envisat for different parameter settings compared to the expected noise of the measurements.

1 Introduction

A variety of parameters are necessary for the discretization of the atmospheric radiative transfer problem. For routine applications of the processor these parameters have to be adjusted by choosing a trade-off between accuracy and run-time. These parameters, which can be modified in $6 and $7 of the main Kopra input file, are:

- Ray-tracing step length ($7.11)
- Finest spectral grid ($6.1)
- Accuracy for cross-section calculation ($7.2)
- Width of the AILS function ($7.8)
- Number of cross-section recalculations for limb-scans ($7.7)
- Additional ray-paths for field-of-view ($7.9-7.10)
- Atmospheric layering ($7.3-7.6)
- Temperature for calculation of the Planck-function ($7.12)

We performed calculations over the entire spectral range of MIPAS-Envisat for different settings of each parameter and compared these to 'reference' cases where the parameters were set to very high accuracy. To give an impression on how these settings influence the total run-time of KOPRA a test was performed with a microwindow selection for ozone retrieval. It must be kept in mind, that these run-times are strictly valid only for the probed microwindows. However, the example should be sufficient to estimate the relative importance of the parameter settings (table 6). In the following we discuss the optimizations one by one. In tables 1 to 5 the mean, the standard deviation and the maximum relative error with respect to the MIPAS-Envisat noise (NESR, Noise Equivalent Signal Radiance) values are given for different tangent altitudes.

2 Ray-tracing step length

For modeling the atmospheric ray path and calculating partial column amounts and Curtis-Godson (C.G.) values of pressure and temperature the line of sight is subdivided into straight segments of equal length. The effect of the step length is twofold:

(a) Determining the accuracy of the refracted ray-path

(b) Determining the accuracy of the partial column and C.G. integrals and their derivatives with respect to retrieval parameters

Reference spectra were calculated with a step length of 0.1km. The main effect of enlarging this value is recognizable at the lowest tangent altitude. The errors are even for 10km steps below 10% of the NESR. For 1km the errors are below 1%. Therefore, step lengths between 1km and 5km are recommended for MIPAS-Envisat retrievals.

3 Finest spectral grid

Absorption cross-sections are calculated line-by-line on an irregular spectral grid which is an integer multiple of the finest spectral grid. Hence, the finest spectral grid is the minimum possible distance between two wavenumber grid points. If it is chosen too large, lines will not be sampled with a sufficient number of points. Due to this effect the error should increase with tangent altitude due to the narrower lines in the Doppler region. This can slightly be seen in band A. However, in the other bands this effect is not visible. This can be ascribed to the fact that at lower altitudes the radiance spectra are stronger and that in the tables the absolute errors with respect to the MIPAS noise are shown and no relative errors.
Reference spectra for the tables are made with a grid interval of $0.0001\mathrm{cm}^{-1}$. The coarsest grid tested was $0.001\mathrm{cm}^{-1}$. Also in this case the standard deviation of the error distribution is well below 10% of the NESR. However, for some tangent altitudes and wavenumbers the maximum error over the whole band can reach the NESR. Hence, we suggest to use settings between $0.0005\mathrm{cm}^{-1}$ and $0.0008\mathrm{cm}^{-1}$.

4 Accuracy for cross-section calculation

The line-by-line calculation of the absorption cross-sections is controlled by an accuracy parameter being the maximum error in optical depth allowed for each line when interpolating the irregular frequency grid to the finest spectral grid. From the tables it is evident that the largest errors occur at low tangent altitudes due to the strong overlap of many lines, a fact which is not considered by the accuracy coefficient since it is applied line by line.
The reference value for this accuracy coefficient has been 10^{-12}. A value of about 10^{-7} is sufficient to keep the errors for all cases well below 10% of the NESR.

5 Width of the AILS function

The apodized instrumental line shape (AILS) function is convolved with the monochromatic spectrum after radiative transfer. By this procedure information of transitions from outside the spectral region of interest is convolved into the range. In order to minimize the effect a Norton-Beer strong apodization was chosen. It is necessary to test how far the wings of this function have to be calculated. The width of the AILS in- fluences the run-time twofold:

(a) spectral microwindows have to be extended by the width of the AILS - hence, more time for the monochromatic calculation is needed

(b) the convolution time of the monochromatic spectrum with the AILS is increased

For simulations with many spectral microwindows (a) is the most important effect while for broadband calculations (b) is more relevant.
The reference was calculated with an width of the Norton-Beer strong apodization function of $7\mathrm{cm}^{-1}$ ($\$7.8 = 3$) where the apodization function decreases to 0.01% of it's center value. With an width of $0.15\mathrm{cm}^{-1}$ ($\$7.8 = 1$) the standard deviation of the error distribution is about 10% of the NESR, however, maximum errors of about the noise value can appear. With $1.4\mathrm{cm}^{-1}$ width ($\$7.8 = 2$) one is on the save side. However, for a distinct microwindow selection one should check if it is not possible to use $0.15\mathrm{cm}^{-1}$ ($\$7.8 = 1$) since the time saving can be substantial.

6 Number of cross-section recalculations for limb-scans

An entire limb-scan (16 tangent altitudes in the standard MIPAS mode) is calculated during one model-run. For minimization of cross-section determination cross-sections for all layers of the lowest line-of-sight are computed. For higher tangent altitudes cross-sections from the related layers of the lowest tangent path can be used since the Curtis-Godson p and T values vary only slightly[2] due to the bended layers of the atmosphere. Therefore, the differences in C.G. values of each path increase when approaching the tangent layer. With respect to a reference calculation where the cross-sections for all paths are calculated, it was tested how many 'extra' paths have to be recalculated for the geometries above the lowest one.
The result was that at least the tangent layers must be recalculated ($7.7 = 1). With this option the error standard deviation is around 4% of the NESR. A recalculation of the lowest two layers is recommended for more exact calculation ($7.7 = 2). A further enhancement of the recalculated layers seems to be unnecessary.

7 Additional ray-paths for field-of-view

For simulation of the finite field-of-view (FOV) of the instrument it is necessary to calculate additional ray-paths through the atmosphere. The FOV simulation is especially crucial at low tangent heights where the radiance profiles have strong gradients with respect to altitude. Therefore, KOPRA has the possibility to separate two altitude regions where the FOV simulation is performed with more or less additionally simulated ray-paths.
Reference calculations were performed with 13 geometries (6 on each side of the central ray) over the total FOV. In order to achieve standard deviations of the error of less than 10% above 14km tangent altitude one additional line of sight ($7.10 = -1) between the standard altitudes (with 3km spacing) is sufficient. With this setting maximum band errors of about 50% of the NESR can occur. Below 14km tangent altitude 2 additional ($7.10 = -2) geometries are necessary. At very low altitudes (8km) this even may not be sufficient and 3 ($7.10 = -3) could be necessary. Since the number of additional ray paths is an important factor determining the run-time it is surely worth to adjust it for used microwindow sets.

8 Atmospheric layering

The subdivision of the atmosphere into layers inside KOPRA determines the accuracy of the radiative transfer calculation. This is an important issue since the run-time of the program is nearly proportional to the number of layers.
Following options have been tested:

(a) US76 standard atmosphere layers
46 levels, with criteria:
$7.31 = 2
$7.32 = 46 levels: 1km up to 25km altitude, 2.5km up to 50km altitude, 5km up to 100km altitude

(b) automatic layering
75 levels with criteria:
$7.31 = 4

[2]The Curtis-Godson values would be exactly equal for plane-parallel layers.

$7.3 = 2, 5, 40 (ΔT 2K below 40km, 5K above)
$7.4 = 1.4 (maximum variation of the Lorentz line width between two model levels)
$7.5 = 100 2 (not relevant)
$7.6 = 0.4 (minimum layer thickness)

(c) automatic layering
66 levels with criteria:
$7.31 = 4
$7.3 = 2, 5, 25 (ΔT 2K below 25km, 5K above)
$7.4 = 1.4 (maximum variation of the Lorentz line width between two model levels)
$7.5 = 100 2 (not relevant)
$7.6 = 0.4 (minimum layer thickness)

(d) coarse layers 29 levels with criteria:
$7.31 = 2
$7.32 = 29 levels: 3km from 8 to 51km altitude, 5km above

(e) coarse layers and automatic layering
77 levels with criteria:
$7.31 = 3
$7.32 = 29 levels: 3km from 8 to 51km altitude, 5km above $7.3 = 2, 5, 40 (ΔT 2K below 40km, 5K above)
$7.4 = 1.4 (maximum variation of the Lorentz line width between two model levels)
$7.5 = 100 2 (not relevant)
$7.6 = 0.4 (minimum layer thickness)

(f) reference calculation
156 levels with criteria:
$7.31 = 2
$7.32 = 156 levels: 0.5km distance up to 75km altitude, 1km distance above

Below about 30km altitude the coarse layering with 3km width is not sufficient to reach error standard deviations of 10% of the noise. The 46 US76 standard levels reach this value down to 11km except for band AB. Below 11km (i.e. in the troposphere) a finer layering is needed, for example like in the case of 66 total levels.

9 Temperature for calculation of the Planck-function

In $7.12 of the main KOPRA input file one can decide which temperature is used for the Planck function of each atmospheric path[3]. For $7.12 = 0 the Planck functions with Curtis-Godson temperatures for each molecule are mixed and weighted by their optical depth at each wavenumber grid point. This option is used for reference calculation. For microwindow selections under $7.12 the number of the main absorbing molecule of these spectral regions can be inserted. $7.12 = -1 means that the Curtis-Godson temperatures of the different molecules will not be mixed but that just the Curtis-Godson temperature of total air is used. In this case the model errors are acceptable above the tropopause. For tangent altitudes in the troposphere it is recommended to perform tests for the specific microwindows in combination with a finer atmospheric layering.

[3]Paths are the segments cut by the internal layering out of the line-of-sight.

Band A: 685 – 970 cm^{-1}					
Mean, **standard deviation**, *maximum* relativ error in % with respect to MIPAS NESR for tangent altitudes					
		8 km	23 km	38 km	53 km
Ray–tracing	1 km	−0.210, **0.175**, *0.917*	0.006, **0.010**, *0.065*	0.002, **0.005**, *0.046*	−0.0002, **0.0009**,*0.026*
step length	10 km	−3.71, **2.77**, *11.77*	0.42, **0.78**, *5.19*	0.17, **0.47**, *4.01*	−0.02, **0.08**, *2.36*
Finest	0.0005 cm^{-1}	−0.20, **0.73**, *19.59*	−0.02, **0.89**, *16.87*	0.03, **0.14**, *1.22*	−0.02, **0.31**, *5.96*
spectral	0.0008 cm^{-1}	−0.32, **0.90**, *10.97*	−0.08, **1.13**, *22.09*	−0.04, **1.43**, *15.93*	−0.09, **3.16**, *53.80*
grid	0.001 cm^{-1}	−0.42, **2.19**, *37.76*	−0.10, **2.22**, *36.94*	0.06, **4.05**, *40.69*	0.10, **7.35**, *133.11*
Accuracy for	10^{-8}	−0.90, **0.79**, *2.97*	−0.26, **0.15**, *0.66*	−0.05, **0.03**, *0.21*	−0.01, **0.01**, *0.04*
cross–section	10^{-6}	−11.95, **13.02**, *53.85*	−3.26, **2.40**, *16.87*	−0.81, **0.64**, *3.92*	−0.13, **0.14**, *0.82*
calculation	10^{-4}	−195, **266**, *2353*	−51.51, **40.97**, *447*	−13.02, **11.58**, *76.23*	−2.17, **2059**, *21.18*
Width of	1.40 cm^{-1}	−2.71, **2.97**, *31.35*	−1.12, **4.90**, *25.42*	−0.42, **4.75**, *29.88*	−0.08, **1.98**, *13.22*
AILS function	0.15 cm^{-1}	7.91, **7.61**, *45.86*	3.29, **12.81**, *92.78*	1.20, **11.56**, *75.08*	0.23, **4.89**, *62.41*
Number of	3	−0.57, **0.65**, *4.99*	−0.83, **0.89**, *4.41*	−0.26, **0.41**, *3.21*	0.01, **0.06**, *1.49*
cross–section	2	−0.83, **0.98**, *7.57*	−2.28, **2.86**, *14.13*	−0.45, **0.84**, *6.76*	−0.01, **0.13**, *3.71*
recalculations	1	−1.81, **2.09**, *16.42*	−3.50, **4.09**, *19.90*	−1.13, **2.60**, *19.68*	−0.62, **1.85**, *26.73*
for limb–scans	0	−31.08, **48.28**, *300.98*	−9.49, **12.58**, *64.86*	−3.29, **6.83**, *44.05*	6.42, **26.97**, *408.11*
Additional	2	53.24, **52.41**, *324.54*	0.15, **3.81**, *22.79*	0.29, **1.73**, *21.30*	0.40, **0.96**, *12.30*
ray–paths	1	116.09, **104.05**, *464.04*	−0.36, **8.23**, *53.07*	0.61, **4.12**, *52.42*	0.92, **2.22**, *28.77*
for	0	687.4, **636.0**, *3238.5*	−2.53, **39.08**, *230.35*	3.11, **21.91**, *236.73*	4.49, **11.60**, *146.35*
field–of–view					
Atmospheric	a (46 levels)	−0.23, **18.44**, *174.84*	1.82, **9.49**, *80.95*	0.57, **5.98**, *94.85*	0.06, **1.96**, *47.60*
layering	b (75 levels)	5.37, **7.18**, *44.67*	2.65, **4.09**, *24.57*	0.76, **1.66**, *22.55*	0.19, **0.39**, *8.11*
	c (66 levels)	4.90, **9.28**, *46.56*	2.22, **9.98**, *61.67*	1.02, **2.54**, *40.27*	0.19, **0.39**, *8.11*
	d (29 levels)	−67.65, **197.82**, *1602.4*	1.36, **14.71**, *116.88*	0.33, **6.60**, *100.27*	0.08, **1.80**, *36.95*
	e (77 levels)	4.77, **7.48**, *43.72*	3.01, **4.26**, *25.28*	0.82, **1.83**, *28.07*	0.22, **0.43**, *8.73*
Gas/isotope number of the main gas	−1	−5.00, **11.43**, *119.13*	1.73, **1.95**, *10.45*	−0.07, **0.56**, *3.33*	−0.25, **0.67**, *8.87*

Table 1: Mean-value, **standard deviation**, and *maximum* of the relative errors (%) with respect to MIPAS NESR in channel A for various model parameter settings and tangent altitudes.

Band AB: 1020 – 1170 cm^{-1}					
Mean, **standard deviation**, *maximum* relativ error in % with respect to MIPAS NESR for tangent altitudes					
		8 km	23 km	38 km	53 km
Ray–tracing step length	1 km	–0.010, **0.089**, *0.481*	0.016, **0.030**, *0.147*	0.008, **0.015**, *0.091*	0.0004, **0.0012**, *0.0106*
	10 km	–2.11, **1.82**, *6.73*	1.25, **2.09**, *11.85*	0.64, **1.28**, *7.70*	0.04, **0.12**, *1.02*
Finest spectral grid	0.0005 cm^{-1}	–0.30, **1.12**, *7.95*	–0.25, **0.34**, *2.05*	–0.36, **0.38**, *1.88*	–0.004, **0.081**, *0.687*
	0.0008 cm^{-1}	–0.45, **0.54**, *10.46*	–0.35, **0.37**, *3.37*	–0.29, **0.56**, *3.83*	–0.01, **2.26**, *24.32*
	0.001 cm^{-1}	–0.61, **1.39**, *9.19*	–0.47, **0.92**, *10.47*	–0.53, **1.78**, *13.50*	0.01, **6.47**, *62.57*
Accuracy for cross–section calculation	10^{-8}	–0.35, **0.31**, *1.70*	–0.20, **0.12**, *0.66*	–0.22, **0.15**, *0.74*	–0.03, **0.03**, *0.10*
	10^{-6}	–6.54, **6.37**, *34.79*	–2.96, **1.70**, *12.61*	–2.98, **2.46**, *10.96*	–0.36, **0.35**, *1.37*
	10^{-4}	–95.30, **98.97**, *869.46*	–41.47, **26.70**, *219.95*	–38.53, **30.24**, *195.59*	–5.81, **4.59**, *47.61*
Width of AILS function	1.40 cm^{-1}	–2.84, **5.19**, *30.13*	–2.08, **6.67**, *29.95*	–1.28, **9.46**, *47.46*	–0.23, **4.00**, *23.96*
	0.15 cm^{-1}	8.12, **12.77**, *72.28*	6.02, **16.79**, *74.29*	3.83, **22.94**, *120.62*	0.69, **9.88**, *55.50*
Number of cross–section recalculations for limb–scans	3	–0.45, **0.40**, *2.45*	–1.83, **1.23**, *5.07*	–0.62, **0.68**, *2.92*	–0.01, **0.02**, *0.16*
	2	–0.62, **0.59**, *3.34*	–3.71, **1.96**, *11.72*	–1.35, **1.72**, *7.72*	–0.06, **0.08**, *0.58*
	1	–1.12, **1.12**, *5.98*	–4.93, **2.65**, *16.35*	–4.29, **6.13**, *25.84*	–0.83, **1.19**, *6.82*
	0	–11.50, **16.34**, *121.04*	–10.62, **7.45**, *43.88*	–11.66, **14.05**, *66.14*	7.62, **14.22**, *97.34*
Additional ray–paths for field–of–view	2	21.99, **22.84**, *170.32*	–0.12, **2.76**, *14.58*	–1.68, **4.38**, *30.17*	1.27, **1.54**, *10.72*
	1	47.96, **44.87**, *236.85*	–0.29, **5.59**, *32.99*	–3.94, **10.34**, *72.08*	2.89, **3.50**, *24.59*
	0	270.7, **266.8**, *1637.6*	–1.01, **26.84**, *147.22*	–18.76, **49.99**, *325.67*	14.26, **17.22**, *119.03*
Atmospheric layering	a (46 levels)	–6.91, **15.71**, *101.77*	–10.81, **24.14**, *124.22*	–2.13, **11.65**, *110.93*	7.08, **17.94**, *139.82*
	b (75 levels)	1.22, **6.88**, *24.22*	–0.83, **7.21**, *27.36*	1.25, **3.72**, *27.70*	1.44, **2.38**, *16.58*
	c (66 levels)	–3.54, **16.07**, *63.06*	–9.70, **24.57**, *78.40*	1.16, **5.93**, *52.72*	1.44, **2.38**, *16.58*
	d (29 levels)	–44.28, **78.43**, *799.22*	–21.52, **44.41**, *202.84*	–6.62, **17.81**, *162.71*	6.09, **15.90**, *124.82*
	e (77 levels)	1.14, **6.76**, *24.27*	–0.67, **7.34**, *27.30*	1.10, **4.33**, *37.09*	1.41, **2.28**, *15.87*
Gas/isotope number of the main gas	–1	–2.35, **10.77**, *77.16*	–6.65, **7.00**, *43.67*	–0.19, **3.42**, *31.95*	–6.58, **11.75**, *79.35*

Table 2: Mean-value, **standard deviation**, and *maximum* of the relative errors (%) with respect to MIPAS NESR in channel AB for various model parameter settings and tangent altitudes.

Band B: 1215 – 1500 cm^{-1}					
Mean, **standard deviation**, *maximum* relativ error in % with respect to MIPAS NESR for tangent altitudes					
		8 km	23 km	38 km	53 km
Ray–tracing step length	1 km	–0.007, **0.094**, *0.527*	0.002, **0.004**, *0.045*	0.0002, **0.0015**,*0.0267*	–0.00003, **0.00018**,*0.00538*
	10 km	–1.00, **1.72**, *7.13*	0.09, **0.30**, *3.64*	0.01, **0.13**, *2.34*	–0.003, **0.017**, *0.466*
Finest spectral grid	0.0005 cm^{-1}	–0.18, **0.35**, *5.56*	0.003, **1.075**, *31.122*	–0.008, **0.055**, *0.603*	–0.003, **0.018**, *0.327*
	0.0008 cm^{-1}	–0.27, **0.16**, *1.39*	–0.07, **0.94**, *24.27*	–0.02, **0.08**, *0.92*	–0.004, **0.031**, *0.509*
	0.001 cm^{-1}	–0.36, **0.38**, *5.75*	–0.04, **1.07**, *30.90*	–0.02, **0.10**, *1.19*	–0.01, **0.04**, *0.95*
Accuracy for cross–section calculation	10^{-8}	–0.01, **1.27**, *0.96*	–0.08, **0.07**, *0.48*	–0.02, **0.02**, *0.07*	–0.002, **0.001**, *0.007*
	10^{-6}	0.35, **3.35**, *26.63*	–0.96, **6.33**, *36.25*	–0.36, **4.68**, *48.11*	–0.04, **1.59**, *17.51*
	10^{-4}	–4.16, **45.61**, *342.78*	–16.82, **15.19**, *77.12*	–5.79, **4.22**, *37.47*	–0.77, **0.63**, *5.02*
Width of AILS function	1.40 cm^{-1}	–1.26, **1.50**, *8.42*	–0.30, **2.31**, *26.68*	–0.07, **2.62**, *11.92*	–0.02, **1.06**, *5.36*
	0.15 cm^{-1}	3.83, **3.59**, *25.77*	0.89, **4.99**, *32.20*	0.21, **6.04**, *43.13*	0.05, **2.47**, *17.11*
Number of cross–section recalculations for limb–scans	3	0.06, **0.20**, *1.30*	–0.33, **0.33**, *2.11*	–0.07, **0.09**, *1.37*	0.0003, **0.0173**, *0.5458*
	2	0.18, **0.39**, *2.32*	–1.00, **1.08**, *5.65*	–0.12, **0.19**, *3.19*	–0.002, **0.044**, *1.363*
	1	0.21, **0.95**, *4.55*	–1.52, **1.59**, *8.33*	–0.25, **0.62**, *8.58*	–0.06, **0.20**, *3.44*
	0	–10.47, **19.14**, *133.76*	–5.51, **6.08**, *33.99*	–0.84, **1.97**, *21.66*	0.43, **2.40**, *50.39*
Additional ray–paths for field–of–view	2	7.64, **24.23**, *182.76*	0.50, **2.47**, *15.03*	0.21, **0.51**, *4.23*	0.11, **0.34**, *4.21*
	1	2.07, **49.76**, *274.79*	0.94, **5.22**, *33.26*	0.47, **1.16**, *10.00*	0.26, **0.79**, *9.85*
	0	35.7, **269.2**, *1887.8*	4.43, **24.41**, *131.90*	2.13, **7.38**, *72.45*	1.26, **4.28**, *44.83*
Atmospheric layering	a (46 levels)	28.63, **27.42**, *161.11*	–0.14, **6.82**, *80.34*	–0.13, **4.58**, *60.25*	0.27, **2.65**, *69.56*
	b (75 levels)	3.50, **5.12**, *26.33*	0.62, **2.38**, *20.17*	0.33, **1.09**, *14.29*	0.11, **0.32**, *7.99*
	c (66 levels)	3.08, **6.25**, *44.69*	0.12, **5.97**, *65.36*	0.34, **1.56**, *21.09*	0.11, **0.32**, *7.99*
	d (29 levels)	304.9, **254.4**, *1328.1*	–0.86, **11.07**, *122.62*	–0.44, **5.53**, *78.02*	0.22, **2.41**, *61.80*
	e (77 levels)	4.66, **4.27**, *24.10*	0.69, **2.42**, *19.76*	0.32, **1.20**, *16.08*	0.11, **0.30**, *7.58*
Gas/isotope number of the main gas	–1	–14.62, **16.69**, *97.48*	0.30, **2.60**, *27.48*	0.43, **1.74**, *21.00*	–0.24, **0.97**, *12.94*

Table 3: Mean-value, **standard deviation**, and *maximum* of the relative errors (%) with respect to MIPAS NESR in channel B for various model parameter settings and tangent altitudes.

Band C: 1570 – 1750 cm^{-1}					
Mean, **standard deviation**, *maximum* relativ error in % with respect to MIPAS NESR for tangent altitudes					
		8 km	23 km	38 km	53 km
Ray–tracing step length	1 km	–0.008, **0.013**, *0.071*	0.003, **0.010**, *0.154*	0.001, **0.006**, *0.099*	–0.00002, **0.00028**, *0.00497*
	10 km	0.34, **0.47**, *5.22*	0.25, **0.84**, *12.42*	0.09, **0.50**, *8.60*	–0.002, **0.025**, *0.443*
Finest spectral grid	0.0005 cm^{-1}	–0.14, **0.32**, *1.61*	–0.12, **0.80**, *19.32*	–0.12, **0.09**, *0.74*	–0.02, **0.03**, *0.41*
	0.0008 cm^{-1}	–0.23, **0.15**, *0.38*	–0.08, **0.72**, *17.18*	–0.03, **0.09**, *1.03*	–0.01, **0.04**, *0.74*
	0.001 cm^{-1}	–0.29, **0.33**, *1.87*	–0.17, **0.80**, *19.21*	–0.14, **0.13**, *1.38*	–0.02, **0.05**, *0.95*
Accuracy for cross–section calculation	10^{-8}	–0.001, **0.017**, *0.091*	–0.06, **0.03**, *0.14*	–0.03, **0.01**, *0.07*	–0.003, **0.001**, *0.008*
	10^{-6}	0.04, **0.37**, *2.43*	–0.97, **0.48**, *2.51*	–0.58, **0.18**, *1.44*	–0.06, **0.02**, *0.19*
	10^{-4}	0.24 **5.98**, *43.09*	–14.42, **7.05**, *42.43*	–9.70, **4.54**, *33.23*	–1.18, **0.81**, *7.07*
Width of AILS function	1.40 cm^{-1}	–0.92, **1.39**, *6.44*	–0.30, **1.97**, *18.19*	–0.11, **2.20**, *7.90*	–0.02, **1.30**, *5.32*
	0.15 cm^{-1}	2.48, **3.30**, *20.52*	0.77, **4.55**, *21.72*	0.31, **5.63**, *28.92*	0.05, **3.19**, *17.86*
Number of cross–section recalculations for limb–scans	3	0.15, **0.16**, *0.72*	–0.57, **0.50**, *2.75*	–0.16, **0.31**, *5.28*	–0.002, **0.023**, *0.438*
	2	0.29, **0.28**, *1.12*	–1.50, **1.05**, *7.02*	–0.31, **0.72**, *11.78*	–0.0002, **0.053**, *1.042*
	1	0.42, **0.45**, *1.68*	–2.08, **1.42**, *9.99*	–0.77, **2.12**, *29.46*	–0.11, **0.43**, *10.44*
	0	–0.02, **0.26**, *1.50*	–6.91, **4.47**, *32.69*	–1.97, **4.17**, *52.06*	1.23, **7.99**, *210.82*
Additional ray–paths for field–of–view	2	6.51, **6.40**, *18.70*	0.82, **2.10**, *13.03*	–0.07, **0.85**, *12.91*	0.19, **0.59**, *12.55*
	1	–2.73, **2.94**, *10.05*	1.78, **4.68**, *30.00*	–0.18, **2.05**, *31.56*	0.44, **1.35**, *28.83*
	0	–14.29, **15.82**, *81.16*	8.46, **21.79**, *122.86*	–0.82, **10.33**, *151.81*	2.18, **6.78**, *140.97*
Atmospheric layering	a (46 levels)	36.74, **31.35**, *99.48*	–0.03, **4.47**, *70.27*	1.11, **4.88**, *56.25*	1.09, **7.23**, *87.28*
	b (75 levels)	12.77, **8.27**, *33.84*	0.39, **1.80**, *18.16*	0.71, **1.05**, *21.61*	0.22, **0.74**, *8.76*
	c (66 levels)	12.47, **9.37**, *55.07*	–0.50, **6.35**, *79.51*	0.87, **1.64**, *42.89*	0.22, **0.74**, *8.76*
	d (29 levels)	504.0, **398.9**, *1140.7*	–1.22, **8.56**, *123.88*	0.72, **4.59**, *66.78*	0.99, **6.70**, *81.98*
	e (77 levels)	7.48, **5.94**, *20.67*	0.44, **1.84**, *16.46*	0.72, **1.22**, *29.76*	0.22, **0.67**, *9.12*
Gas/isotope number of the main gas	–1	–11.97, **8.93**, *32.94*	–1.36, **2.08**, *27.08*	0.21, **1.87**, *25.14*	–0.32, **1.00**, *15.45*

Table 4: Mean-value, **standard deviation**, and *maximum* of the relative errors (%) with respect to MIPAS NESR in channel C for various model parameter settings and tangent altitudes.

Band D: 1820 – 2410 cm^{-1}					
Mean, **standard deviation**, *maximum* relativ error in % with respect to MIPAS NESR for tangent altitudes					
		8 km	23 km	38 km	53 km
Ray–tracing step length	1 km	–0.030, **0.035**, *0.129*	0.0004, **0.0019**, *0.0365*	0.0005, **0.0016**, *0.0211*	–0.0001, **0.0004**, *0.0052*
	10 km	–0.26, **0.37**, *1.88*	0.03, **0.15**, *3.06*	0.04, **0.14**, *1.86*	–0.01, **0.03**, *0.46*
Finest	0.0005 cm^{-1}	–0.028, **0.211**, *2.585*	–0.002, **0.014**, *0.234*	–0.001, **0.015**, *0.263*	–0.001, **0.005**, *0.179*
spectral	0.0008 cm^{-1}	–0.024, **0.074**, *0.397*	–0.004, **0.019**, *0.398*	–0.002, **0.018**, *0.409*	–0.0003, **0.008**, *0.315*
grid	0.001 cm^{-1}	–0.047, **0.215**, *2.602*	–0.005, **0.022**, *0.516*	–0.003, **0.024**, *0.552*	–0.002, **0.013**, *0.406*
Accuracy for	10^{-8}	–0.004, **0.011**, *0.083*	–0.010, **0.008**, *0.051*	–0.010, **0.008**, *0.046*	–0.001, **0.001**, *0.004*
cross–section	10^{-6}	–0.052, **0.187**, *1.324*	–0.142, **0.105**, *0.829*	–0.130, **0.098**, *0.566*	–0.017, **0.010**, *0.070*
calculation	10^{-4}	–1.01, **2.84**, *22.00*	–2.38, **1.90**, *26.53*	–2.43, **1.89**, *35.00*	–0.42, **0.34**, *7.77*
Width of	1.40 cm^{-1}	–0.16, **0.47**, *3.61*	–0.04, **0.47**, *2.83*	–0.03, **0.61**, *3.49*	–0.009, **0.308**, *2.340*
AILS function	0.15 cm^{-1}	0.24, **0.94**, *8.38*	0.03, **1.07**, *9.03*	0.02, **1.42**, *11.14*	0.004, **0.701**, *7.807*
Number of	3	0.005, **0.027**, *0.122*	–0.07, **0.08**, *1.30*	–0.05, **0.11**, *0.93*	0.005, **0.023**, *0.340*
cross–section	2	0.02, **0.08**, *0.50*	–0.13, **0.16**, *1.95*	–0.09, **0.18**, *2.06*	0.015, **0.083**, *1.136*
recalculations	1	0.02, **0.20**, *1.30*	–0.17, **0.21**, *2.74*	–0.18, **0.36**, *6.20*	–0.05, **0.24**, *2.82*
for limb–scans	0	–3.05, **5.07**, *29.02*	–0.38, **0.56**, *7.97*	–0.27, **0.47**, *9.74*	1.59, **4.32**, *36.65*
Additional	2	4.77, **10.08**, *42.13*	0.01, **0.16**, *2.90*	–0.05, **0.16**, *2.42*	0.15, **0.26**, *2.39*
ray–paths	1	6.09, **16.94**, *58.08*	0.02, **0.33**, *6.52*	–0.11, **0.39**, *5.87*	0.35, **0.59**, *5.55*
for field–of–view	0	28.46, **92.63**, *405.01*	0.14, **1.91**, *29.98*	–0.76, **2.26**, *37.22*	1.73, **2.93**, *24.51*
Atmospheric	a (46 levels)	4.98, **13.26**, *70.81*	–1.25, **3.03**, *21.93*	–1.39, **3.92**, *32.38*	–0.14, **2.07**, *49.84*
layering	b (75 levels)	0.32, **1.70**, *13.24*	–0.13, **0.70**, *6.16*	–0.21, **1.07**, *8.64*	0.03, **0.33**, *5.83*
	c (66 levels)	0.08, **1.97**, *13.29*	–0.55, **1.37**, *16.07*	–0.36, **1.39**, *9.22*	0.03, **0.33**, *5.83*
	d (29 levels)	61.97, **118.58**, *591.82*	–1.92, **4.00**, *29.88*	–1.74, **4.52**, *31.59*	–0.13, **1.76**, *46.48*
	e (77 levels)	0.88, **2.17**, *11.59*	–0.14, **0.69**, *5.60*	–0.23, **1.07**, *7.84*	0.03, **0.32**, *5.67*
Gas/isotope number of the main gas	–1	–7.24, **11.70**, *44.30*	–0.09, **0.44**, *8.64*	0.05, **0.45**, *6.99*	–0.08, **0.61**, *10.13*

Table 5: Mean-value, **standard deviation**, and *maximum* of the relative errors (%) with respect to MIPAS NESR in channel D for various model parameter settings and tangent altitudes.

Relative run-times		
		Relative time
Ray–tracing step length	1 km	1
	10 km	0.96
Finest spectral grid	0.0005 cm^{-1}	1
	0.0008 cm^{-1}	0.92
	0.001 cm^{-1}	0.86
Accuracy for cross–section calculation	10^{-8}	1
	10^{-6}	0.64
	10^{-4}	0.44
Width of AILS function	1.40 cm^{-1}	1
	0.15 cm^{-1}	0.74
Number of cross–section recalculations for limb–scans	3	1
	2	0.86
	1	0.72
	0	0.58
Additional ray–paths for field–of–view	2	1
	1	0.73
	0	0.46
Atmospheric layering	a (46 levels)	1
	b (75 levels)	1.43
	c (66 levels)	1.27
	d (29 levels)	0.93
	e (77 levels)	1.43
Temperature for Planck function calculation	0	1
	–1	0.85

Table 6: Relative run-times for a microwindow selection for ozone retrieval.