SFIT4 – Retrieval parameters

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Retrieval parameters

Retrieval parameters

Overview

rt The main parameter rt can be used to switch off and one the retrieval altogether.

rt.lm Switches on or off the Levenberg-Marquardt iteration scheme.

rt.convergence the iteration is considered converged when rt.convergence > D_CHI = (CHI_2_MAX$_{i-1}$ - CHI_2_MAX$_i$)

rt.max_iteration maximum number of iterations

Retrieval parameters

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ITER    FIT_RMS      GAMMA    CHI^2_X    CHI^2_Y      CHI^2 CHI^2_OLD       DCHI^2
   1    25.5294   1.00E+05      0.000    886.616
   2    15.7601   1.00E+05      0.000    332.528    332.528    886.616   554.088226
   3     9.8038   1.00E+04      0.004    134.162    134.166    332.528   198.361710
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   8     1.8844   1.00E-01      0.300      2.573      2.873      2.875     0.002286

 FINAL:     MEAN_SNR= 86.6267  MEAN_FIT_RMS(%)= 1.88443  NVAR= 185  NFIT= 3477

   BAND    SCAN    RMSSNR (CALCULATED)    (EFFECTIVE)    (RETRIEVED)          CHI^2
      1       1                  53.98          53.98          49.55           1.19
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      3       1                 154.48         154.48         110.55           1.95
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 NEGATIVE MIXING RATIO VALUES FOUND FOR : 03668
 NEGATIVE MIXING RATIO VALUES FOUND FOR : 03686
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- **rt** The main parameter rt can be used to switch off and one the retrieval altogether.
- **rt.lm** Switches on or off the Levenberg-Marquardt iteration scheme.
- **rt.convergence** the iteration is considered converged when rt.convergence > D_CHI = (CHI_2_MAX$_{i-1}$ - CHI_2_MAX$_i$)
- **rt.max_iteration** maximum number of iterations

For all retrieval parameters a apriori is given and a standard deviation sigma in the form

- **rt.x.apriori** the apriori of a given value. It is actually applied in the forward calculation. Meaning it can also be used in forward calculations.
- **rt.x.sigma** the entry in the S_A matrix corresponding to this parameter.

Retrieval parameters

Wave number scaling and shifting

rt.wshift wave number shift.

- Shift works on the internal grid **band.X.calc_point_space**
- This is only useful for microwindows (small) because the mismatch is a wavenumber dependent polynomial. For small wave number regions, this can be approximated by a shift.
- This is on top of rt.wave_factor, which is a scaling.
- The artificial grid needs to be more dense than the measured grid

rt.dwshift wave number shift for each retrieved gas separately, except the first retrieved one.

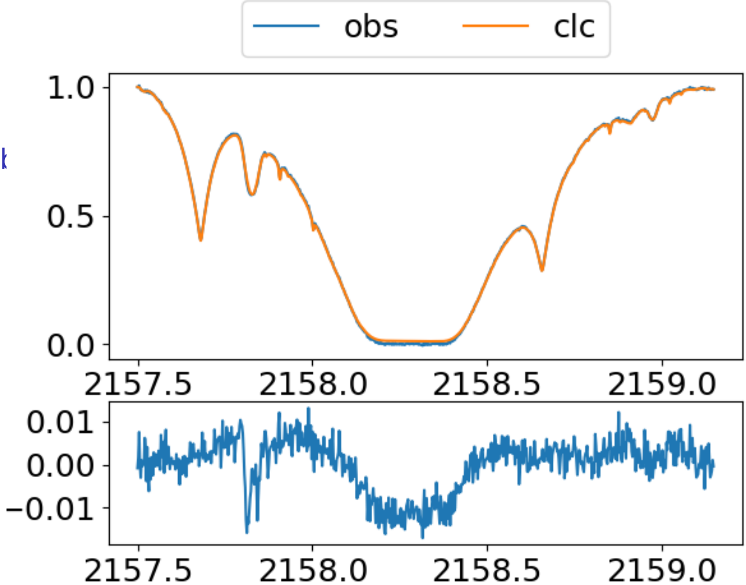
- all lines of each gas are shifted by the same amount (!!!)

offset in window

band.zshift calculates and retrieves an offset in the microwindow. Two types:

- .type = 1 retrieves the offset in this MW ONLY ONE!!!

offset in window



offset in window

band.zshift calculates and retrieves an offset in the microwindow. Two types:

- .type = 1 retrieves the offset in this MW ONLY ONE!!!
- .type = 2 uses the offset which is retrieved in another microwindow. THIS MUST BE LATER THAN THE MW USED FOR **ZSHIFT.TYPE=1**

band.zshift.apriori is also an **FW parameter**

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band.zshift.apriori is also an **FW parameter** RETRIEVAL ONLY POSSIBLE IF THERE IS AN SATURATED PART IN THE MW.

Theory

The channeling is due to etalons in the beampath. Such etalons may be windows iin a detector, filters, surfaces on the beamsplitter. In short, two partially reflecting surfaces create an etalon.

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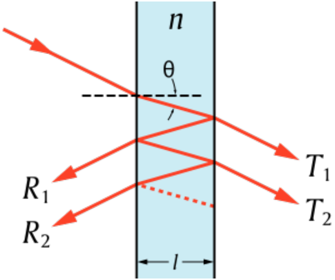

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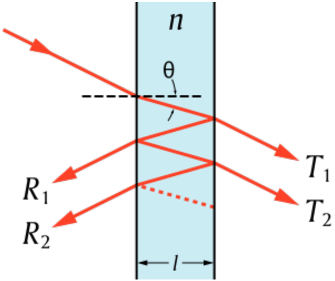

The transmission $T = \sum_{n=1}^{\infty} T_n$ through an etalon l can be calculated by

$$T = \frac{(1-R)^2}{1+2R\cos(\delta)+R^2} \quad (1)$$

$$\delta = 400\pi\nu n l \quad (2)$$

$R \sim 0$ is the reflectivty of the surface.
$n \sim 1.5$ is the refraction index.
$theta = 0$ (theta in figure), parallel beam

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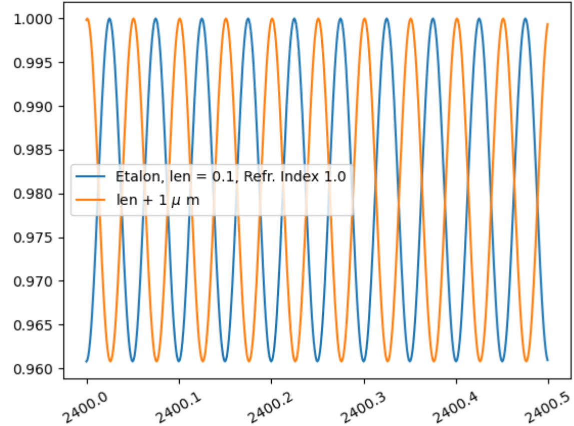

Channeling

Calculation in SFIT4

The channeling in a MW is calculated via

band.x.beam = 1,2 The beams with the numbers 1 and 2 are caclulated

band.x.beam.model = IP, PS which one is better has to be checked.

band.x.beam.1.apriori = AMP, FREQ,PHAS,SLOPE defines the apriori values of the beam 1

band.x.beam.1.sigma standard deviations for all parameters, i sigma = 0, parameter is not retrieved,

Channeling

Calculation in SFIT4

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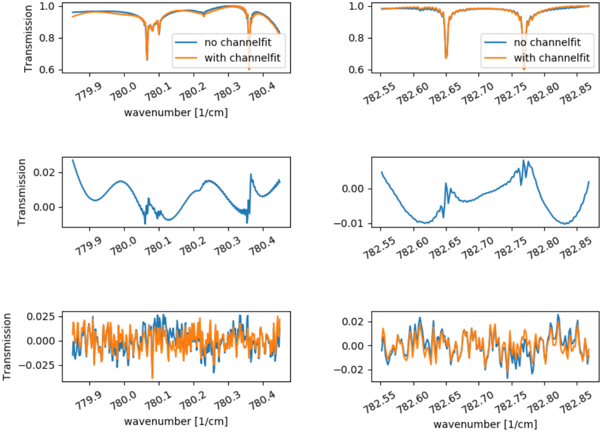


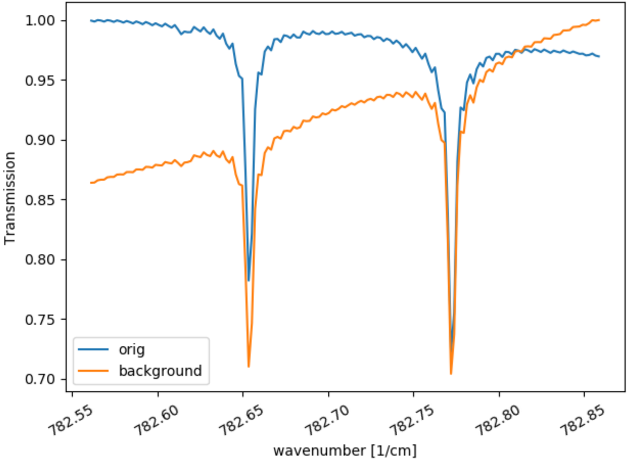
rt.slope and rt.background

rt.slope and rt.background can be used to model a sensitivity function of the instrument, caused by a filter or the wave number dependent sensitivity of the instrument itself.
A function

$$\text{rt.slope} * \nu + \text{rt.background} * \nu^2 \tag{3}$$

is multiplied to the calculated spectrum.

rt.slope and rt.background



sensitivity
wave
lf.

(3)

Retrieval parameters

Construction of the S_A matrix.

The S_A matrix is constructed from the sigma values given. How this is actually done, depends on the parameters. In principle the S_A is constructed as a diagonal matrix and inverted in the code to yield the S_A^{-1} matrix. Some caveats:

gas.profile.x.correlation off diagonals using the sigma values as maxima

- .type = 1 gaussian with FWHM = .width
- .type = 2 exponentially with FWHM = .width
- .type = 3 not used
- .type = 4 the S_A matrix is read in from file.sa_matrix
- .type = 5 the S_A^{-1} matrix is read in from file.sa_matrix

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gas.profile.x.regmethod lets you chose between OE optimization and the Thikonov-Phillips regularization with L1 constraint (smoothness constraint)

- **.type = 'OE'** optimal estimation (Rodgers, 2000)
- **.type = 'TP'** Thikonov-Phillips with smoothness constraint
  - **.lambda** strength of the regularization in TP. The higher the value the less is the regularization.

  The smoothness constraint is calculated from file.stalayers in order to adapt for non-unique altitude layering. The matrix is scaled using the gas.profile.x.sigma values.

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SFIT

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FIT_RMS mean variance of the residuum

GAMMA the Levenberg Marquardt Parameter

CHI_2_X A measure of the deviation of the retrieved state from the A PRIORI

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CHI_2_Y A measure for the retrieval quality

$$\chi^2_Y = \frac{(y_M - y_C)^T S_\epsilon (y_M - y_C)}{m}$$

$\chi^2_Y = 1$ if the residuum is reduced to the noise as specified in S_ϵ

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- In the lower half, the retrieval diagnostics for the last calculation are shown for each MW.
- A warning if retrieved profiles have negative parts

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Iteration stopped if either DCHI < rt.convergence or ITER > rt.max_iteration, what ever comes first.

The finish

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  BAND    SCAN    RMSSNR (CALCULATED)    (EFFECTIVE)    (RETRIEVED)         CHI^2
     1       1                 138.44         138.44         113.72          1.48
     2       1                 146.53         146.53         143.52          1.04
     3       1                 327.50         327.50         185.55          3.12
     4       1                 319.57         146.69          81.72          2.40

 NEGATIVE MIXING RATIO VALUES FOUND FOR : H2O
 NEGATIVE MIXING RATIO VALUES FOUND FOR : C2H4

  O3      : T   H2O     : T   CO2     : F   O3668   : F   O3686   : F   C2H4    : F
  9.5734E+18  5.2139E+22  7.9696E+21  1.6077E+19  1.6077E+19  9.8413E+14
  1.0921E+19  4.1944E+22  1.4369E+22  1.6255E+19  1.5224E+19 -9.1080E+14

Itr/Mx:05/15 %RMS=1.125 FitPrm=117 CVRG:T DIVW:F DOFS=4.755 SNR=  162. CHI_2_Y=   2.2875

 RDRV: DONE. ELAPSED TIME =    200.01916800000001
```