

SFIT4 – Retrieval parameters

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Retrieval parameters



Retrieval parameters

Overview

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

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

rt.convergence the iteration is considered converged when $\text{rt.convergence} > D_CHI = (CHI_2_MAX_{i-1} - CHI_2_MAX_i)$

rt.max_iteration maximum number of iterations



Retrieval parameters

Overview

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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
  4     5.1080   1.00E+03   0.038     32.608    32.646   134.166   101.519910
  5     2.6411   1.00E+02   0.105      6.402     6.507    32.646    26.139551
  6     1.9136   1.00E+01   0.217      2.831     3.048     6.507     3.458828
  7     1.8797   1.00E+00   0.281      2.594     2.875     3.048     0.172872
  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
    2      1           57.52           57.52           56.78           1.03
    3      1          154.48          154.48          110.55           1.95
    4      1          147.91           84.62           50.79           2.92

NEGATIVE MIXING RATIO VALUES FOUND FOR : 03668
NEGATIVE MIXING RATIO VALUES FOUND FOR : 03686
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rt.convergence the iteration is considered converged when $\text{rt.convergence} > D_CHI = (CHI_2_MAX_{i-1} - CHI_2_MAX_i)$

rt.max_iteration maximum number of iterations

For all retrieval parameters a priori 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 (!!!)



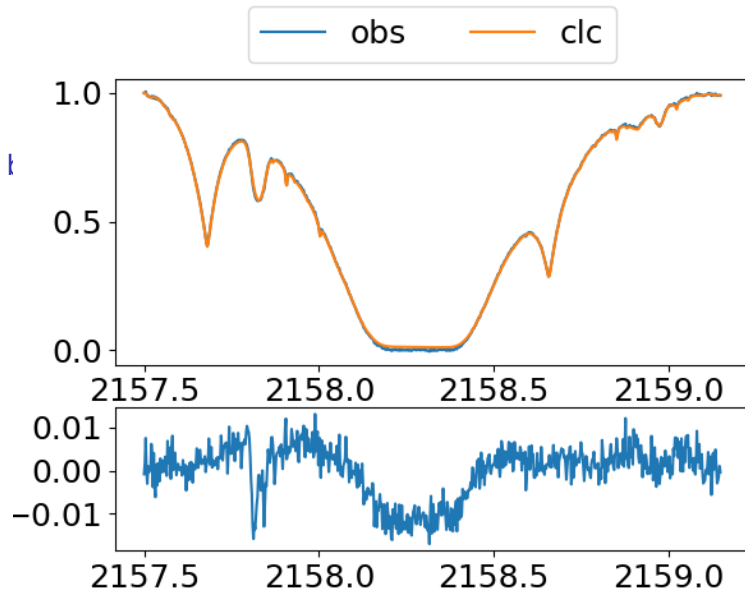
offset in window

`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



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- `.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.**



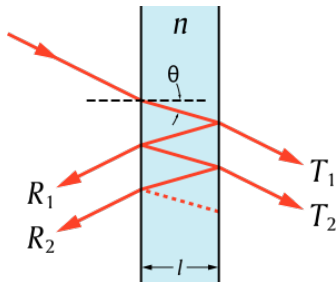
Theory

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



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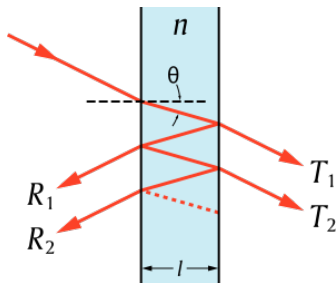
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The transmission $T = \sum_{n=1}^{\infty} T_n$ through an etalon l can be calculated by

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

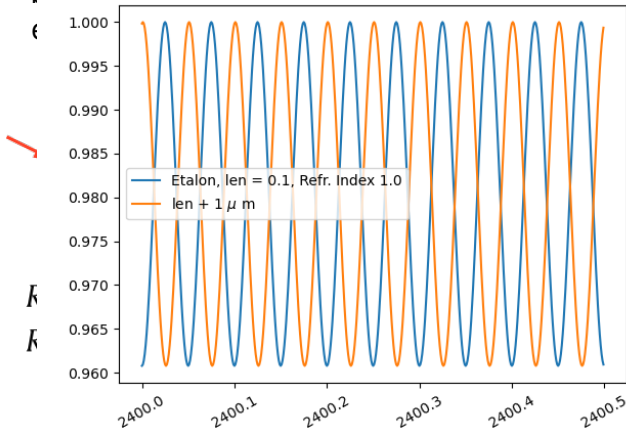
$$\delta = 400\pi\nu nl \quad (2)$$

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



Theory

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ces on the
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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 calculated

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

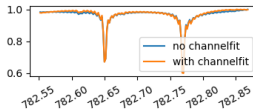
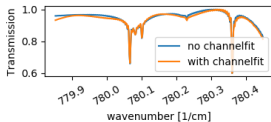
`band.x.beam.1.apriori` = AMP, FREQ, PHAS, SLOPE defines the apriori values of the beam 1

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

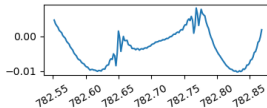
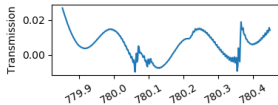


Channeling

Calculation in SFIT4

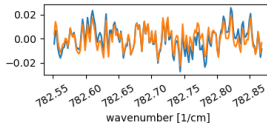
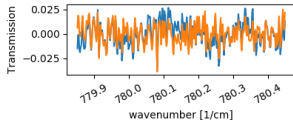


and 2 are



is to be

defines



rameters, i



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.

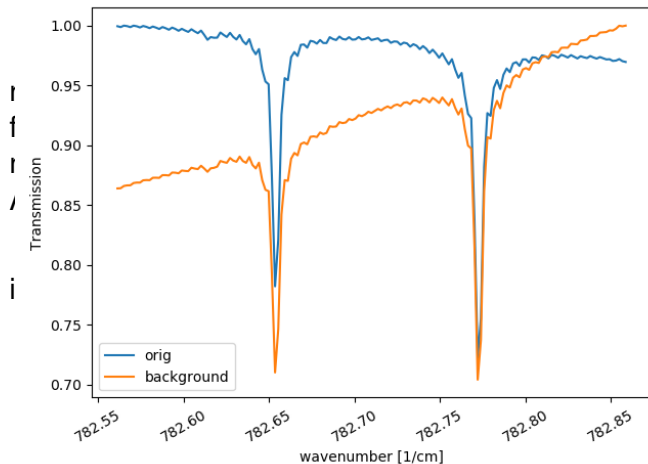
A function

$$\text{rt.slope} * \nu + \text{rt.background} * \nu^2 \quad (3)$$

is multiplied to the calculated spectrum.



rt.slope and rt.background



sensitivity
wave
f.

(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.



Retrieval parameters

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

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

$\chi_Y^2 = 1$ 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



Retrieval parameters

SFITT

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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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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

03	: T	H2O	: T	CO2	: F	03668	: F	03686	: 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	

Iter/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

