SFit4 Updates for 2013

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Two foci of sfit4 Development

1. Flexibility – Exploratory analysis tool
   i. S_a (S_a^{-1}) definition / direct input
   ii. Background parameters (slope, curvature, zero)
   iii. Shifts, by species, by fit
   iv. Channeling
   v. SNR by region
   vi. Multiple regions / SZA
   vii. Fit gas by region
   viii. Phase, ME
   ix. Isotope separation
   x. Solar background /shift
   xi. Levenberg-Marquardt non-linear iteration scheme
   xii. Emission spectra
   xiii. Log(vmr) retrieval
   xiv. Line mixing (co2, ch4 soon…)
   xv. SDV speed dependent Voigt lineshape
   xvi. Spectra output by layer / gas
   xvii. O2 CIA line data included
2. Process & I/O Speed – NDACC operational processing
   i. Standard layering
   ii. Binary HITRAN input
   iii. Binary output for HDF ?

Sfit4 current version d0.9.2.1

- log scaling of vmr by gas
- include emission of atmosphere & source (moon)
- analytic derivatives for vmrs
- Levenberg-Marquardt iterative scheme
- internal raytracing module
- line mixing for CO2 (ch4…)
- speed dependent Voigt (from C Boone)
- tagged - variable input format
- arbitrary SZA / μwindow / resolution
  - Spectral process code to support it
- binary HITRAN input – end of cfgl files
- Pre-raytrace isotope separation scheme
- spectra-centric parameters in ascii spectra data file

required inputs

required output

sfit4.ctl
Retrieval specific params:
- *Region*
- *Species*
- *State vector*

t15asc4
- *Spectrum specific params:*
- *Date/Time*
- *Solar zenith angle*
- *N spectra*

stations.layers
- *Layering for each site*
- *From WACCM*

reference.prf
- *Z-p-T for reference profiles*
- *Reference (apriori) chemical profiles*

Binary (HITRAN) Line list file

sfit4
raytracing
retrieval

sit4.dtl (detail file)
- *Step-by-step of retrieval process*

auxiliary inputs

- *isotope separation data (new format)*
- instrument phase function
- instrument modulation function
- retrieval mixing ratio predefined covariance
- retrieval mixing ratio predefined inverse covariance
- solar line list

outputs

- Output can be set to 3 levels of detail
  - Plus any given output file can be switched off or on
- Any output file (other than sfit4.dtl – detail file) can be renamed
- Many output files have been reformatted for easy read / write by batch scripts
- All output files have version tag and timestamp
- *Direct binary or hdf output still planned*

output files

See: docs/output_descrip_v4.docx

- output level set to 1
  - Statevevctor file
  - Apriori profiles
  - Retrieved profiles
  - Final Calculated, observed and difference spectra
  - Fit summary
  - Averaging kernels
  - Complete Sa matrix
- output level set to 2
  - K matrix
  - K_b matrix
  - AB matrix
  - Measurement error
  - Sa Inverse matrix
  - Se inverse matrix
  - Shat matrix
  - Retrieval-Calculated Smoothing error
  - Parameter array by iteration
  - Spectra by gas
- output level set to 3
  - Channel spectra diagnostic
  - Raytracing diagnostics
  - Solar spectra calculation
  - L-M diagnostics
  - Cross-section diagnostics
- gas spectra type
  - =1 final spectra by gas, and fit
  - =2 and by atmospheric level
- raytrace type
  - =3 verbose output
  - =2 obsolete fastcode output

new HITRAN data input scheme

See: docs/hbin_descrip_v4.docx

Predefined directory structure:

```
001_H2O:
        01_hit08.par
        01_hit08.zip
        01_hit09.par
        01.H2O
002_CO2:
        02_hit08_f53.par
        02_hit08_f53+LM.par
        02_hit08.zip
        02.CO2
        co2_lm.dat
        read_out_example.txt
.
.
.
```

Stand alone code *hbin.f90* compiled with sfit4 is run before sfit4 call.

hbin is run once for a specified retrieval

hbin* reads files:

- sfit4.ctl
- hbin.input
- isotope.input
- Hitran files directly

Writes file: lllll.dddddd-hhhhh.dddddd.hbin
Sorts all lines in wavenumber order, edits id numbers, separates isotopes, can choose gases and adds flags for:

- CIA
- line mixing parameters
- Galatry parameters
- SVD parameters

(slightly) new isotope separation input scheme

See: docs/isotope_descrip_v4.docx

Main differences:

I. Profile for new gas is now on pre-raytrace or ‘refmod’ grid
II. There are no default pre-separated species
III. You can add subsequent isotopes to the new species that will use the new profile eg.
    a. H2O 1/4 -> HDO 80/1 ($HD^{16}O$)
    b. H2O 1/5 -> HDO 80/2 ($HD^{18}O$)
    c. H2O 1/6 -> HDO 80/3 (HD^{17}))

(slightly) new ascii spectral data file

header for each block:

```
 37.26100  6385.44500    40.03800   254.76000   402.3
      2011    6   23   16   24   11
06/23/2011 16:24:11UT Z:37.261 A:284.29 D:0101.7 R:0.0035 P:BX F:01.9139mr
 4881.8975000000000    4888.1025000000000    2.5000000000000005E-003    2483
0.315438E+00
0.293434E+00
0.285126E+00
0.271612E+00
0.240477E+00
.
.
.
```

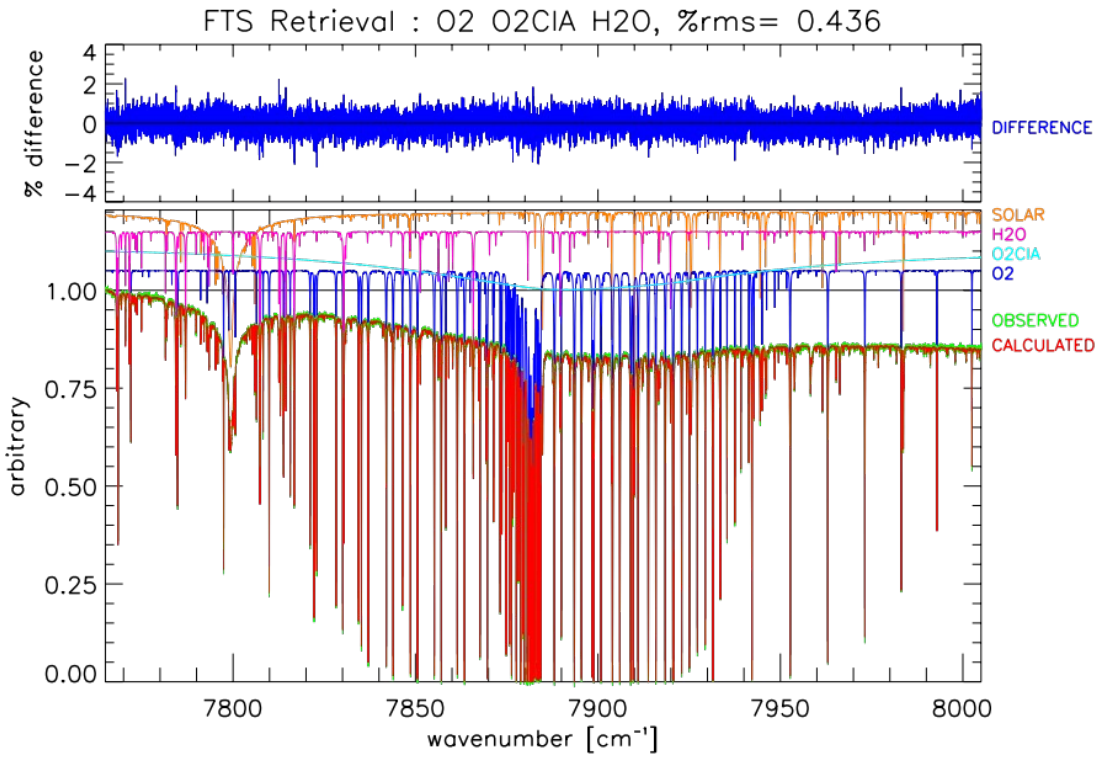
KEY:

SZA° radius_of_earth [km] latitude [°N] longitude [°E] SNR
YYYY MM DD HH MM SS
arbitrary ascii comment, 80 characters
start_wn end_wn point_spacing Npoints
spectra values…

- ✓ *Any number of blocks are ok*
- ✓ *All blocks with spectra within sfit4.ctl band limits will be fit*
- ✓ *Spectra will be truncated to sfit4.ctl band limits*

Calculated Kb

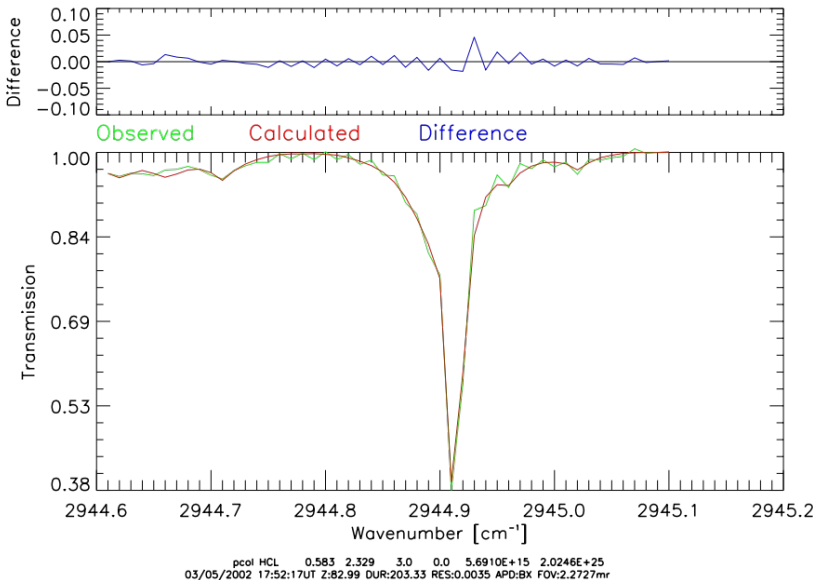
- temperature
- background
  - Slope
  - curvature
- solar shift
- solar line strength
- phase
- differential wavenumber shift
- wavenumber shift
- apodization function
- phase function
- zero level shift
- solar zenith angle
- field of view
- optical path difference
- hitran line parameters for retrieval or target gas
  - Strength
  - Pressure broadening
  - Broadening temperature depenence

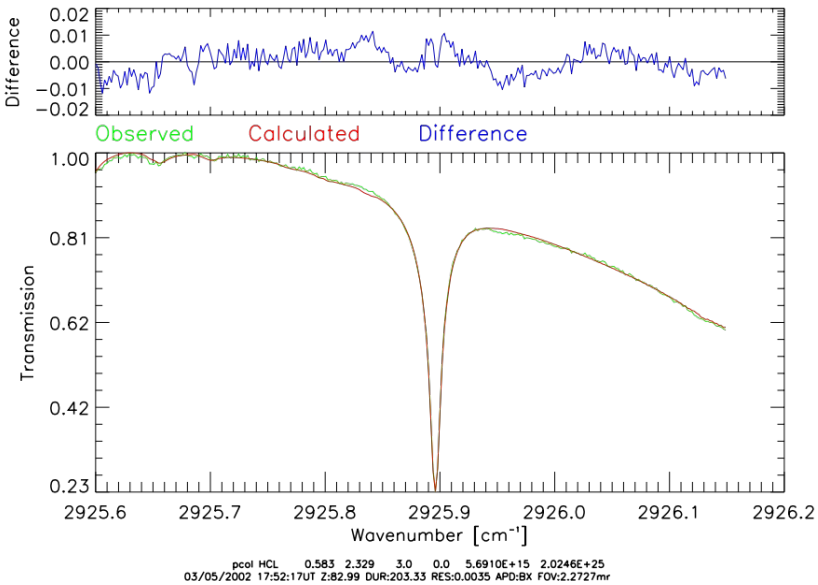


Sample Retrieval O_2, O_2CIA & H_20

Self & Foreign CIA lines use same O_2 profile

– Wollongong data

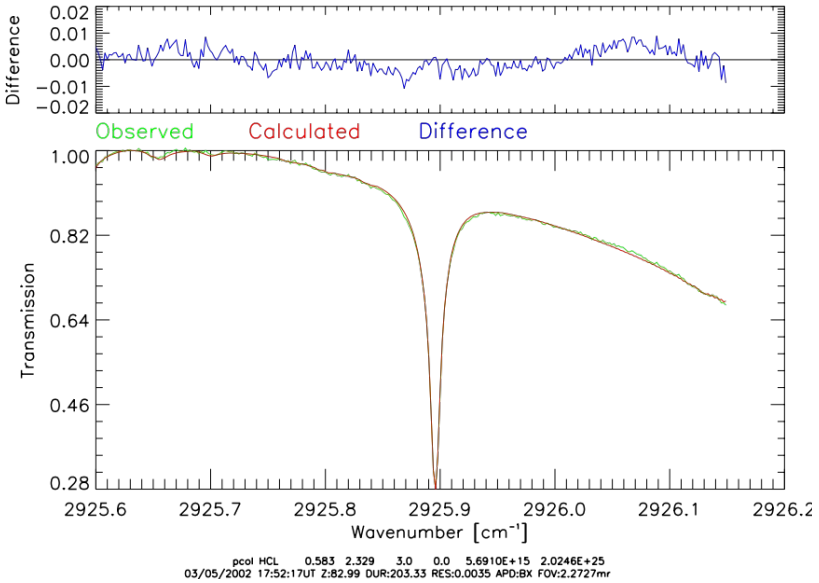


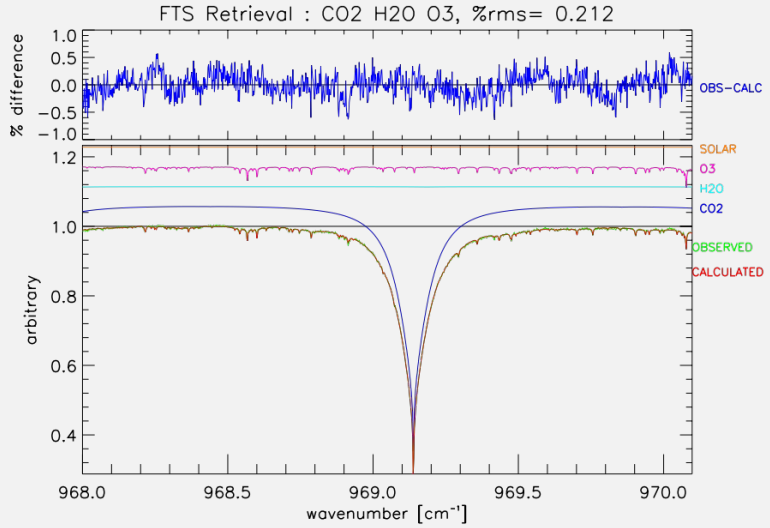


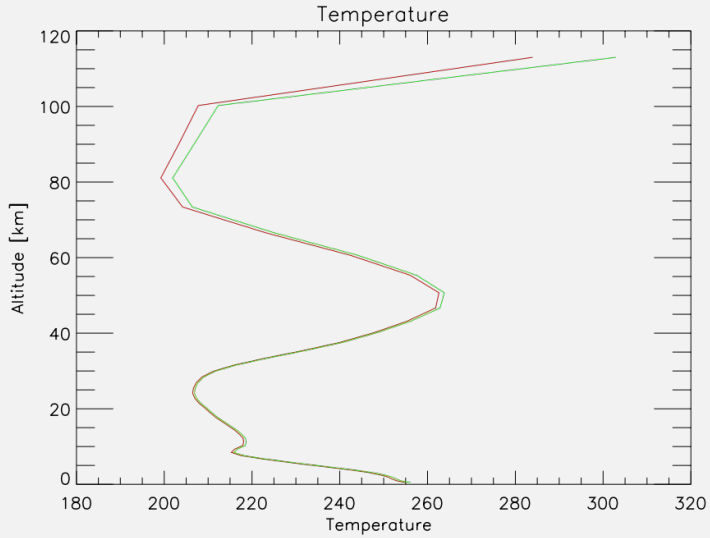
Example: HCl
2925 / 84.62 / 250cm
2925 / 83.11 / 250cm
2944 / 82.99 / 100cm

*Single retrieval from 3 spectra with different SZA and resolutions.**

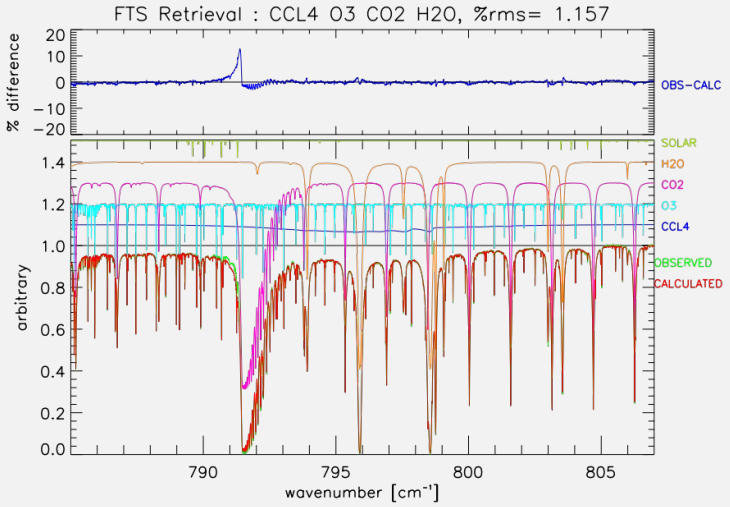
**all spectra from one μw must have same resolution & point spacing.*

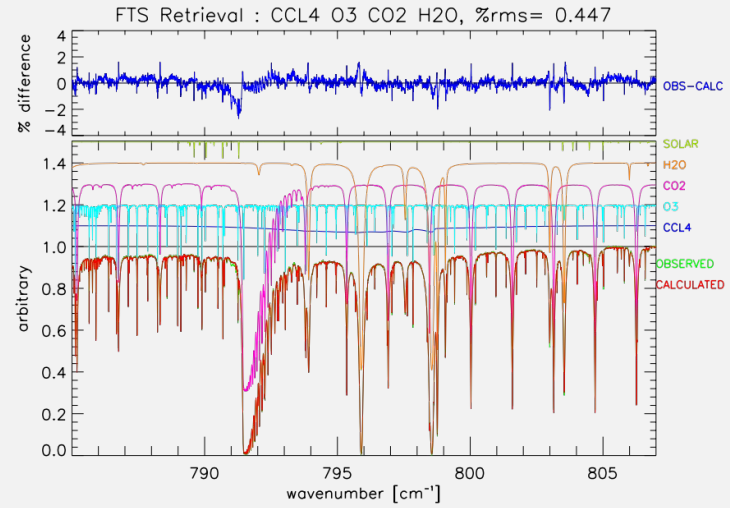




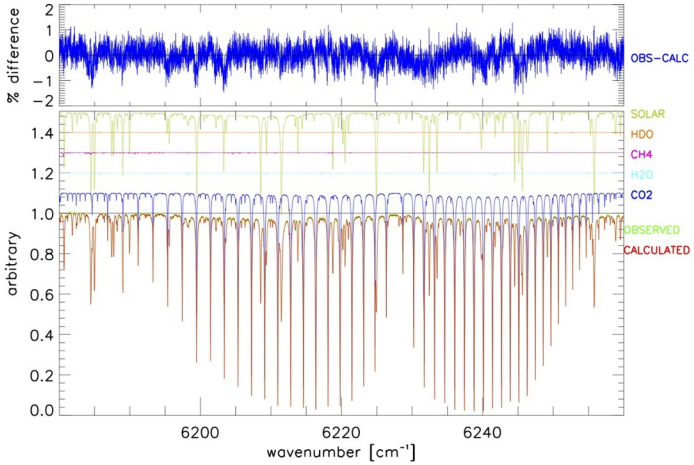


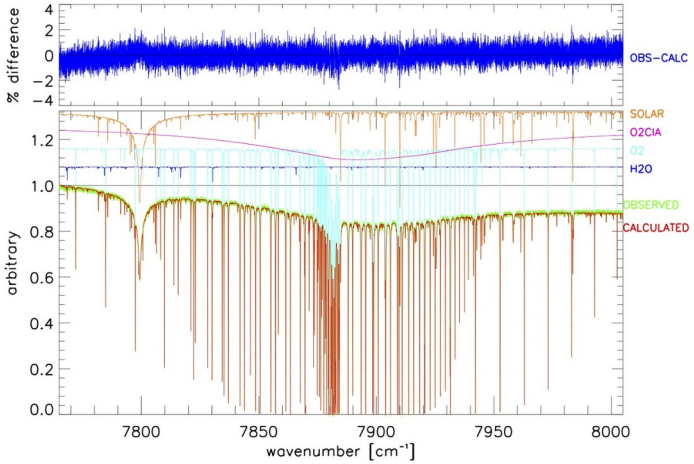
Work in progress
Retrieval of temperature profile from single CO_2 absorption feature

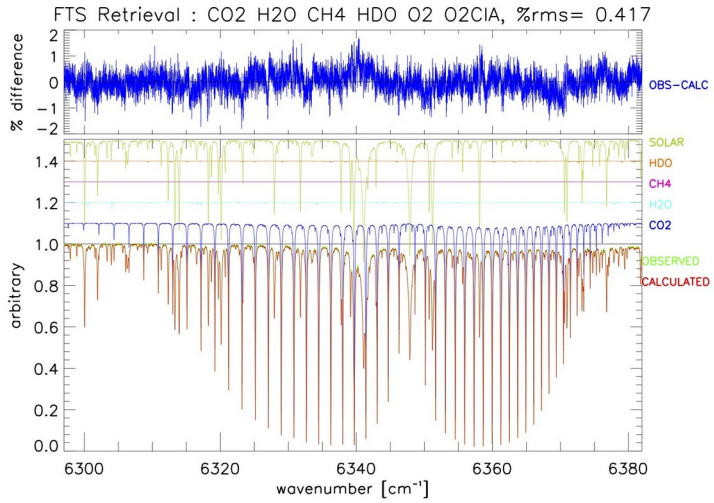




Line Mixing required for CCl_4
Only CO_2 so far







Simultaneous fit CO2, CO2 & O2

Bialystok, Poland

Status

- Current version d0.9.2.1 with several testcases available :
  - *ftp://acd.ucar.edu//user/jamesw/IRWG_NORS_EW/sfit4/delta*
- Input / output files & formats complete
- Derivatives of several retrieval / model parameters calculated for error analysis (K_b)
- Temperature retrieval in process
- Testing / bug fixes in process
- Suite of testcases for IRWG windows in process
- Python based spectral processing environment in process
  - *A hot topic next week!*
- Some (but not complete) documentation available

end

Latest Release Version SFIT2 V3.94

- SFIT2 v394 delivered Winter ’09
  - Primarily HITRAN 08 & molecular database
- But also
  - Perturbation ability: Added flags to make small changes in
    - line intensity
    - Air broadened halfwidth
  - Use CH_3CH from H08 and previous pseudolines as CH_3CNPL
  - Bug fixes eg writing second Sa off diag elements
  - Intensity scaling in isotope substitution
  - Output Sa.complete, Parm.out, Prfs.out
  - Better use of matrix intrinsics
- Lapack version available 3.94LP
  - Matrix inversion
  - direct output: AK & AK Eigenvectors, Smoothing error

Log scaling of Retrieval Gases

- New flag in binput to switch on or off
- vmr → ln(vmr)
- Output (K-matrices and AVK) changed accordingly
- Schneider and Hase (2009) for more information
- Retrieval of ratio (e.g. HDO/H2O; Schneider et. al., 2006) only possible via extra SA matrix, not checked yet…

Schneider, M.; Hase, F. & Blumenstock, T. Ground-based remote sensing of HDO/H2O ratio profiles: introduction and validation of an innovative retrieval approach Atmos. Chem. Phys., 2006, 6, 4705-4722
Schneider, M. & Hase, F. Ground-based FTIR water vapour profile analyses Atmos. Meas. Tech., 2009, 2, 609 - 619

Emission modelling

- New switch emission modelling off or on
- Input Temperature of blackbody radiation at TOA
- Switch: E – emission, M - for reflection of sunlight on moon)
- Switch: Units Watt/(cm^-1 sr cmr^2)
- Switch: - spectrum normalized

V 4.00 *continued*

What do the changes mean?

- More versatile, faster!
- New inputs: binput, fastcode, t15asc
  - Some new coding for you
  - Ease for new users
  - Zypher2 future's is unknown?
- Support code
  - Preping spectra
  - Simple scripts for running – not quite batch processing

- Users Meeting Planned

Levenberg-Marquardt Iteration Scheme

- New flags in binput:
- Switch: for Gauss-Newton iteration or Levenberg-Marquardt iteration-scheme
- Value of start for gamma
- Value for decrease of gamma if successful
- Value for increase of gamma if not successful
- Value to break off if cost does not decrease more than 0.5

Sample Output:

```
ITER= 8 RMS(%)= 0.0718869 NVAR=117 NFIT=   311
chi2_x   =  9.7670E-01                  cost for state vector
chi_2_y  =  2.0671E+00                  cost for spectrum
chi2     =  3.0438E+00                  cost sum
chi2_old =  3.4307E+00                  cost of last successful iteration
d chi_2  =  3.8689E-01                  change in cost (decrease is positive)
gamma    = 1.0e3                        actual value of gamma
```

- Chi_2_y is set up in a way, that it is 1 if the noise given (in binput) is the same as spectral noise and residual is perfect.

map of Input & output files … needs to be cleaned up

```
! --- SET DEFAULT FILENAMES

     TFILE(08) = 'pbpfile'

! --- ISOTOPE SEPARATION FILE
     TFILE(09) = 'isotope.input'

     TFILE(15) = 't15asc'

     TFILE(16) = 'detail'

! --- STATEVEC
     TFILE(18) = 'statevec'

! --- SET MIXOUTPUT FILENAME AS STATE VECTOR FILENAME + .MXF
     TFILE(17) = TRIM(TFILE(18))//'.mxf'

! --- SAVED SYNTHETIC SPECTRUM
     TFILE(19) = 'synspec.out'

! --- SUMMARY
     TFILE(20) = 'summary'

! --- SET PARTICAL COLUMN OUTPUT FILENAME AS STATE VECTOR FILENAME + .PRC
     TFILE(22) = TRIM(TFILE(18))//'.prc'

! --- EMPIRICAL MODULATION FUNCTION
     TFILE(23) = 'ils.dat'

! --- EMPIRICAL PHASE FUNCTION
     TFILE(24) = 'ils.dat'

! --- CHANNEL OUTPUT
     TFILE(30) = 'chnspec.data1'

     TFILE(40) = 'chnspec.data2'

! --- SET SHORT FILENAME AS SUMMARY FILENAME + .ST
     TFILE(31) = TRIM(TFILE(20))//'.st'

! --- DEFAULT FIRST RETRIEVAL GAS SA OUTPUT FILENAME
! --- OUTPUT DEPENDS ON NAME SA .NORM, .VMR, .PCOL
     TFILE(61) = 'Sa.norm'

! --- DEFAULT SAINV INPUT FILENAME
     TFILE(62) = 'Sainv.input'

! --- DEFAULT COMPLETE SA OUTPUT FILENAME
     TFILE(63) = 'Sa.complete'

! --- DEFAULT K,SE,SA MATRICES OUTPUT FILENAME
     TFILE(66) = 'K.out'

! --- SE OUTPUT
     TFILE(67) = 'Se.out'

! --- DEFAULT K TRANSPOSED FILENAME
     TFILE(68) =  'KT.out'

! ---  LEVENBERG-MARQUARDT DETAILS
     TFILE(70) = 'detail.opt'

! --- LAYERING SCHEME - OUTPUT FROM WACCM PROFILES
     TFILE(71) = 'station.layers'

! --- REFERENCE VMR PROFILES
     TFILE(72) = 'reference.prf'

! --- RAYTRACE DETAILED OUTPUT AKA TAPE6
     TFILE(73) = 'raytrace.out'

     TFILE(74) = 'raytrace.pt'
     TFILE(75) = 'raytrace.ms'
     TFILE(76) = 'raytrace.mix'
     TFILE(77) = 'raytrace.sa'
     TFILE(78) = 'raytrace.pnch'

! --- RESERVED FOR GASOUT NAME CHANGES - SEE FRWDMDL.F90
     !TFILE(80)

     TFILE(81) = 'AK.out'
     TFILE(82) = 'SM.out'
     TFILE(83) = 'SS.out'
     TFILE(84) = 'A-S.out'
     TFILE(85) = 'AEIGEN.out'

     TFILE(88) = 'PRFS.out'
     TFILE(89) = 'Parm.out'

     TFILE(91) = 'Spec.out'
```

(Very new) sfit4.ctl
General I/O files

Retrieval Gases

Forward Model Parameters

```
# General

file.stalayers              = station.layers
file.refprofile             = reference.prf
file.spectrum               = t15asc.4
file.eap_dat                = ils.dat
file.ephs_dat               = ils.dat
file.sa_matrix              = sa.input
file.isotope                = isotope.input
file.solarlines             = ..//linelist/solar/120621/solar.dat
file.linelist               = ./02723.690800-02930.039200.hbin

# Definition for retrieval gases

gas.layers                  =              47
gas                         = HCL CH4 O3 HDO N2O NO2
gas.HCL.ifoff               =               1
gas.HCL.zwid                =           3.000
gas.HCL.zmin                =           0.225
gas.HCL.zmax                =         120.000
gas.HCL.logstate            =               F
gas.HCL.ifprf               =               T
gas.HCL.sigma               =
  0.62398   0.33613   0.33382   0.22898   0.14726
  0.14435   0.14265   0.14204   0.14226   0.14383
  0.14538   0.14531   0.14490   0.14430   0.14320
  0.14272   0.14354   0.14652   0.15191   0.15851
  0.16395   0.16691   0.17080   0.17993   0.19615
  0.21887   0.24784   0.27969   0.30479   0.32309
  0.34501   0.37861   0.42903   0.50225   0.58601
  0.62527   0.61862   0.63071   0.73872   0.92782
  1.08104   1.19786   1.28879   1.35951   1.42124
  1.46301   1.48165
gas.CH4.ifprf               =               F
gas.CH4.sigma               =
  1.00000   1.00000

# Forward model parameters

fw.delnu                    =           0.10000
fw.lshapemodel              =               0
fw.linemixing               =               T
fw.linemixing.gas           = CO2
fw.solar                    =               T
fw.solar.shift              =           0.00000
fw.ifps                     =               F
fw.ieap                     =               4
fw.neap                     =               0
fw.iephs                    =               4
fw.nephs                    =               0
fw.emission                 =               F
fw.ifiso                    =               T
fw.write_k                  =               T
fw.write_gasfiles           =               T
fw.write_gasfiles.type      =               1
```

Retrieval parameters

```
# Retrieval parameter

 rt                          =              T
 rt.write_sa                 =              F
 rt.lm                       =              F
 rt.lm.gamma_start           =         100000.
 rt.lm.gamma_dec             =           10.0
 rt.lm.gamma_inc             =           10.0
 rt.convergence              =            0.1
 rt.tolerance              =             0.05
 rt.max_iteration            =             15
 rt.wshift                   =              2
 rt.wshift.apriori           =          0.000
 rt.wshift.sa                =          0.100
 rt.slope                    =              T
 rt.slope.apriori            =          0.000
 rt.slope.sa                 =          0.100
 rt.solar                    =              T
 rt.solar.apriori            =          1.000
 rt.solar.sa                 =          0.500
 rt.ifdiff                   =              T
 rt.temperature              =              F
 rt.raytonly                 =              F

 # Microwindows and their parameters
```

Band Parameters

```
 band                        =   1 2
 band.1.nu_start             =        2727.730
 band.1.nu_stop              =        2727.830
 band.1.zshift               =               0
 band.1.zshift.apriori       =           0.000
 band.1.zshift.sa            =           0.200
 band.1.beam                 =               0
 band.1.dn                   =       0.800E-03
 band.1.wavfac               =           1.000
 band.1.pmax                 =         257.143
 band.1.omega                =           2.273
 band.1.iap                  =               0
 band.1.snr                  =         200.000
 band.1.gasb                 = HCL    O3     HDO

 band.2.nu_start             =        2775.700
 band.2.nu_stop              =        2775.800
 band.2.zshift               =               0
 band.2.zshift.apriori       =           0.000
 band.2.zshift.sa            =           0.200
 band.2.beam                 =               0
 band.2.dn                   =       0.800E-03
 band.2.wavfac               =           1.000
 band.2.pmax                 =         257.143
 band.2.omega                =           2.273
 band.2.iap                  =               0
 band.2.snr                  =         200.000
 band.2.gasb                 = HCL    O3    , N2O
```