Updates in the forward model of PROFFAST Ver 2

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PROFFAST Ver 2 updates

Fiducial Reference Measurements for Ground-Based Infrared Greenhouse Gas Observations (FRM4GHG 2.0)

Introduction: One task of FRM4GHGII is to enhance the COCCON code suite. The COCCON processing chain has three steps:

- The pre-processing or L1-processing (performed by **PREPROCESS**): from raw OPUS interferograms to spectra. The resulting spectra are used for the quantitative trace gas analysis.
- The daily calculation of lookup tables with x-sections of gases for given atmospheric conditions (performed by **PCXS**)
- The trace gas retrievals (performed by **INVERS**)

This talk describes updates in PCXS as incorporated in Ver 2 of PROFFAST.

PROFFAST Ver 2 updates

Contents:

- Update + refined parameterization of TIPS
- Refined tabulation of x-sections as fct of airmass
- Spectroscopic improvements (line lists, line shape model)

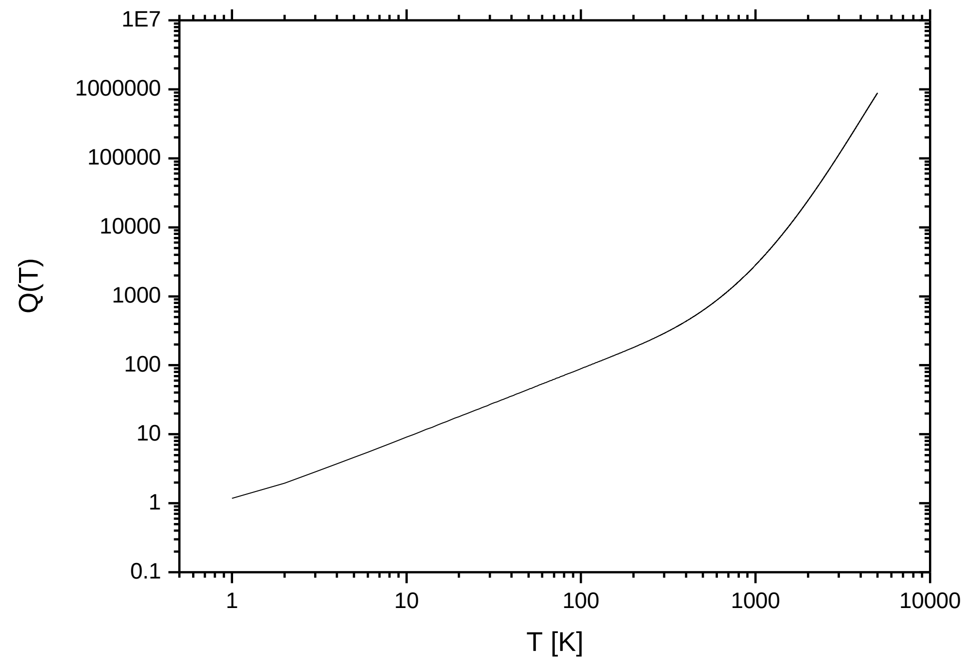
TIPS update

HITRAN tabulated TIPS: CO_2, main isotopologue

TIPS: Total Internal Partition Sum

The TIPS is used to determine the population of molecules as function of quantum state. These population factors are needed to determine the intensity of ro-vibrational transitions.

$$Q(T) = \sum g_k e^{-c_2 E''_k / T}$$



Handling of TIPS in PROFFAST ver 2

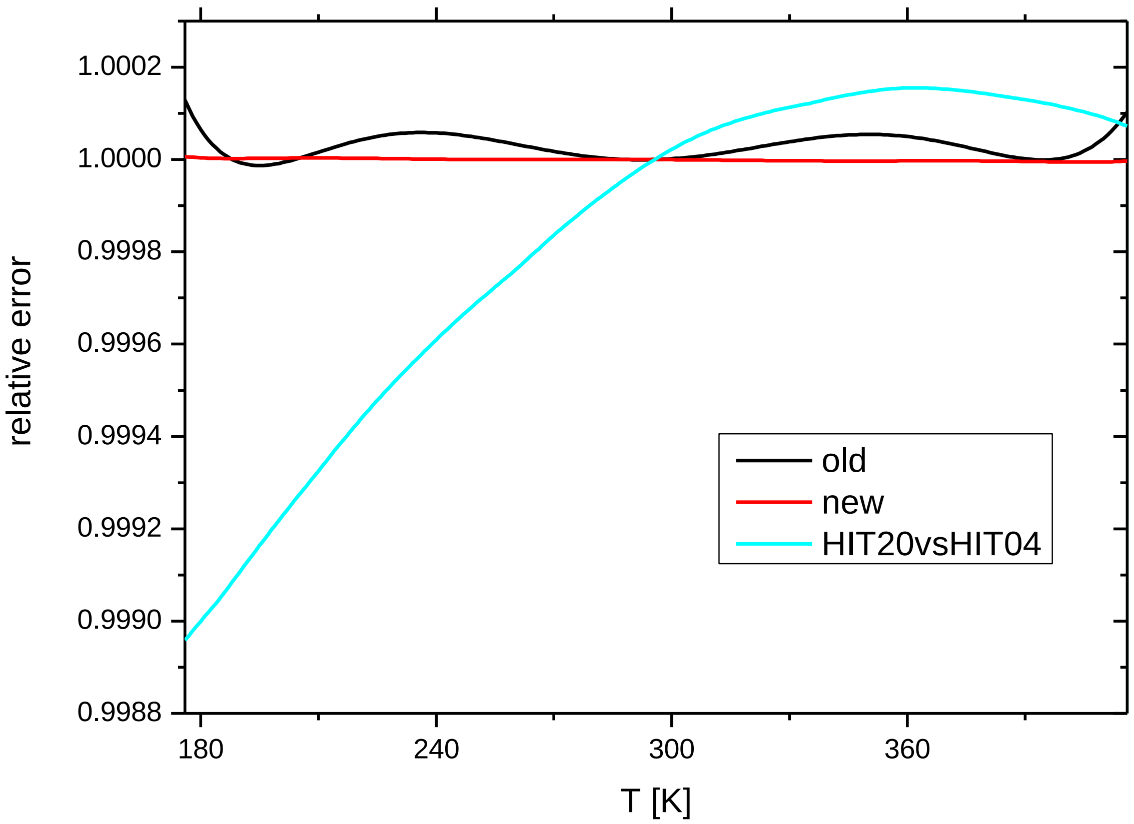
This table contains the masses and temperature parameterisations for Qvib(T)/Qvib(296), used by the forward model in the form

Qrel(x) = Qvib(296) / Qvib(T)
= exp(-(a1 * x + a2 * x**2 + a3 * x**3 + a4 * x**4 + a5 * x**5 + a6 * x**6 + a7 * x**7)).

x = (T[K] - 296.0) / 120.0, the fit to the tabellated values in parsum.dat is restricted to x=-1.0 to +1.0 (176K ... 416K)

HITRAN#	mass[amu]	a0	a1	a2	a3	a4	a5	a6	a7	species description
$										
11	18.010565	9.8819E-07	6.0605E-01	-1.1930E-01	3.3006E-02	-9.5289E-03	2.9598E-03	-1.3178E-03	4.8037E-04	H2O_161
....										
21	43.989830	7.0029E-07	5.1587E-01	-4.8593E-02	1.6248E-02	-6.8149E-03	2.7411E-03	-1.2363E-03	4.0896E-04	CO2_626
22	44.993185	7.2299E-07	5.2327E-01	-4.8421E-02	1.5669E-02	-6.5587E-03	2.6907E-03	-1.2581E-03	4.2542E-04	CO2_636
23	45.994076	6.9872E-07	5.1849E-01	-4.8090E-02	1.6110E-02	-6.8039E-03	2.7401E-03	-1.2376E-03	4.1061E-04	CO2_628

Resulting improvement



TIPS summary:

- ✓ Improved parameterisation
- ✓ Fits performed for all isotopologue TIPS provided in HITRAN 2020
- ✓ New species-ver2.inf file incorporated PROFFAST ver 2 distribution
- ✓ Handling in PROFFIT and LINEFIT updated accordingly

X-sections lookup table

Use of pre-calculated x-sections

Idea: store a table which does not keep any vertical information, but only allows to reconstruct $\tau_{igas,jnue}(\alpha_{obs})$!

- For the spectral axis, a grid width $\Delta\nu \sim \nu$ is used (as width of Doppler core $\sim\nu$).
- For each gas, the complete spectral range is stored.
- A single-precision binary array is used to store the tabellated values.
- The angle argument used is the refracted (so apparent) SZA observed at the spectrometer α_{obs}.

X-sections lookup table

Designing the table …

Assume flat Earth, no refraction:

$$\tau(\alpha_{obs}) = \tau(0)/\cos(\alpha_{obs}) \qquad (1)$$

Assume flat Earth, allow refraction:

- Path length through layer extends with altitude

Assume spherical Earth, omit refraction:

- Path length through layer reduces with altitude

In reality both effects occur, so treating the effects as a perturbation of the simple reference equation (1) seems a reasonable approach.

X-sections lookup table

Designing the table …

So we use:

$$\tau(\alpha_{obs}) = [\tau(0) + K_2 \cdot \alpha_{obs}{}^2 + K_4 \cdot \alpha_{obs}{}^4 + \ ...] \,/\, \cos(\alpha) \qquad (2)$$

Procedure in PCXS:

- calculate $\tau_{ilayer}(0)$ for each model layer, perform a raytracing, calculate $\tau(\alpha_{obs,i})$ for a range of $i = 1\ ...M$ angles, covering the desired range of airmasses.

- Fit the N unknowns of the polynomial expansion $\tau(0)$, K_2, K_4, … .

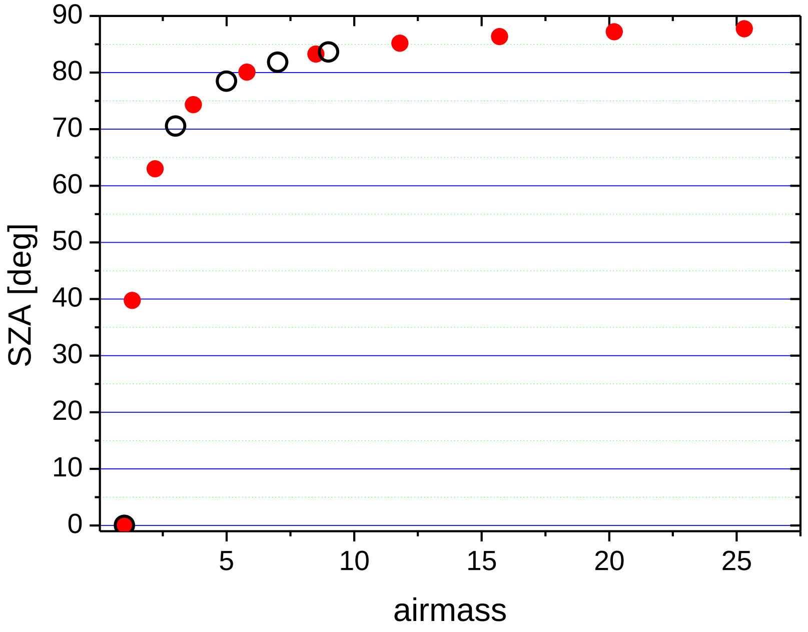
- Choose $N < M$ for an over-determined problem (residual fit errors can be exploited to specify quality of model).

X-sections lookup table

Adjusting the model quality …

Original implementation:
5 rays, 4 parameters fitted
($\alpha_{obs,max} = 83.6°$)

PROFFAST Ver 2:
10 rays, 5 parameters fitted
($\alpha_{obs,max} = 87.7°$)



X-sections lookup table

Quality of the model

Check for each species the maximum relative error of $\tau(\alpha_{obs})$ occuring in the fit (max values in complete table!):

H_2O:	8.3e-7
CO_2:	2.9e-5
N_2O:	7.9e-6
CO:	7.9e-5
CH_4:	9.6e-6
O_2:	1.8e-5
HF:	9.2e-5

Spectroscopic improvements:

Solar transmission (thanks to G. C. Toon!): GGG14 -> GGG20

Atmospheric gases:

Ver 1: wild mixture (HIT08 + empirical ad-hoc corrections, HIT12), O_2: GGG14

Ver 2: HIT20 (H_2O, CO_2 [+ LM + SDV], N_2O, CO, O_2 [+ SDV??])

Implementation of 1st order LM + SDV in PROFFAST Ver 2

Special item: CH_4
HITRAN: LM under construction ~ 1 a
Recent DLR line list covers only TROPOMI window (uses HTP + 2nd order LM)

Spectroscopic improvements

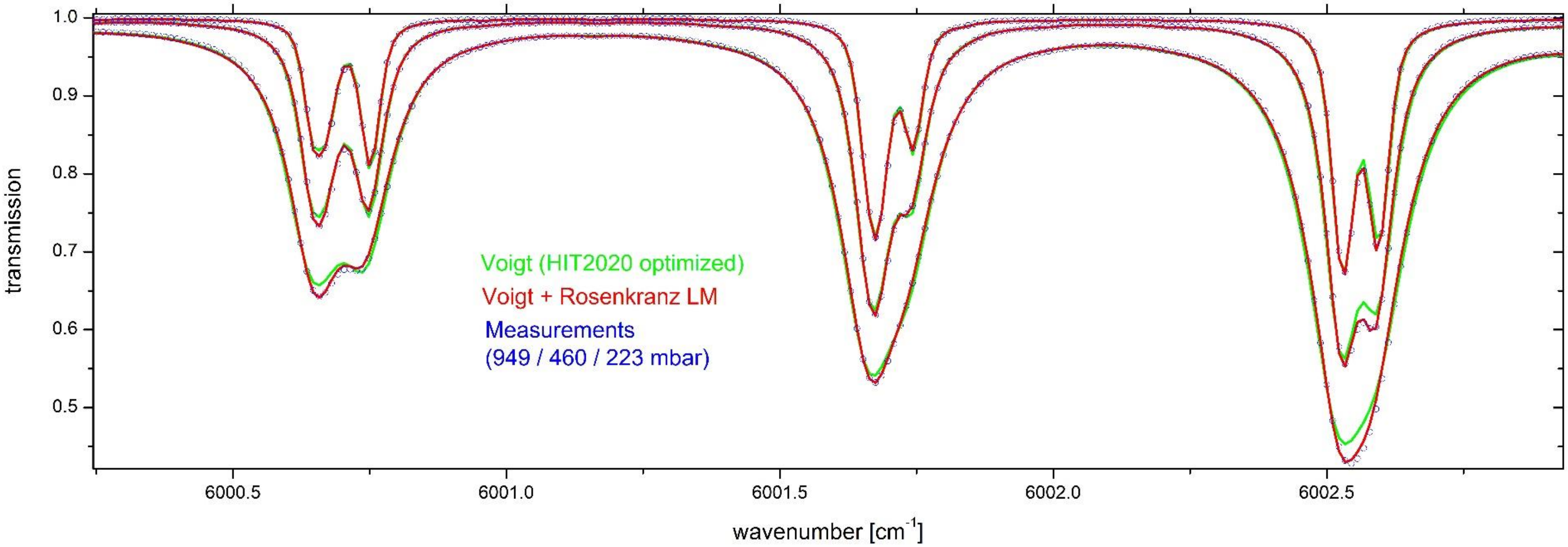
- Collect room-temperature cell measurements: pure CH_4 and CH_4 in air (~ 1000, 500, 250, 125 mbar), use a "poor-man's" measurement strategy

pressure	Fitted CH_4 column	ratio
949.0	5.293e+23	--
460.0	2.566e+23	0.4848
223.0	1.244e+23	0.4848
108.0	6.031e+22	0.4848

- coding of a multispectrum fitting tool

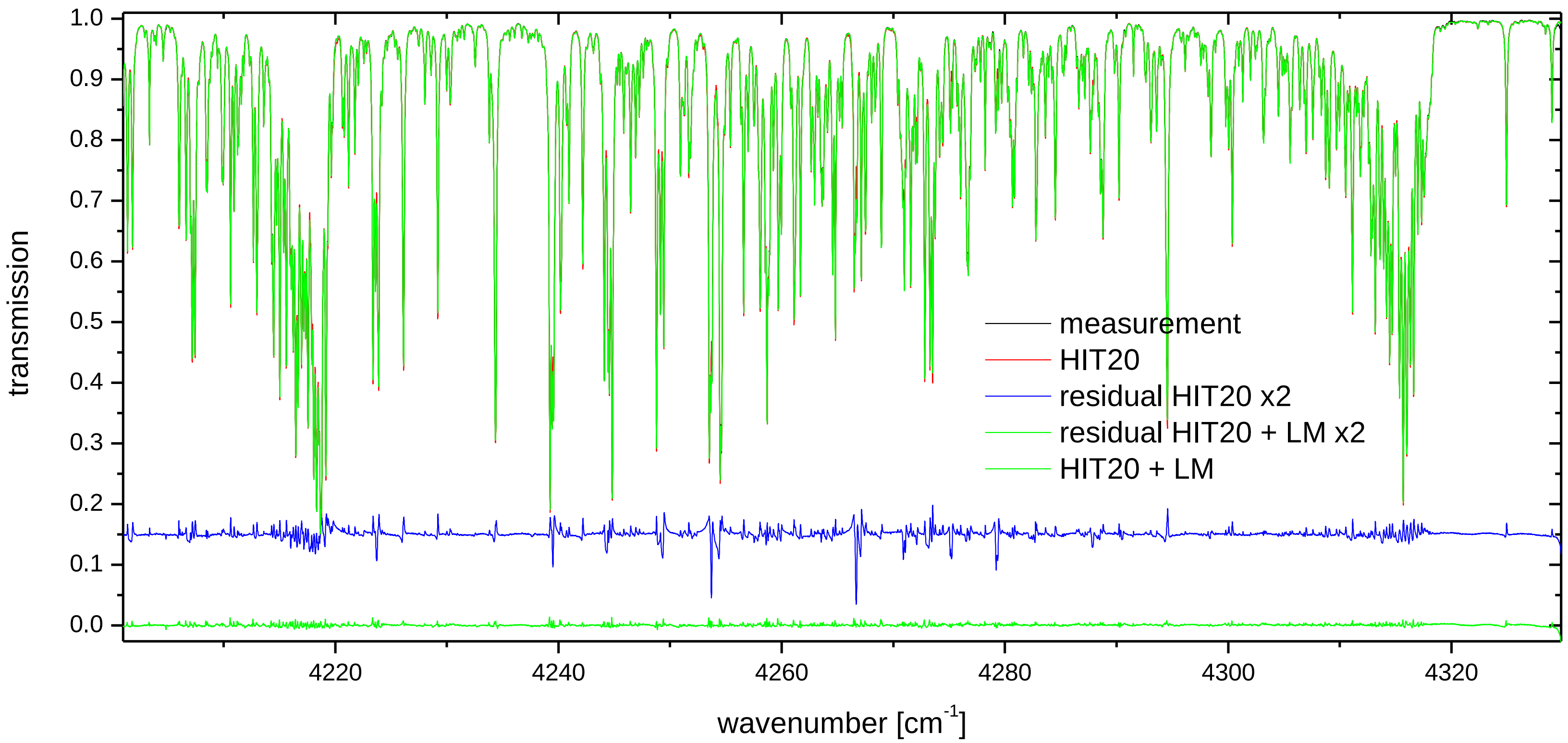
- Retrieval of optimized spectral parameters from available line lists and own measurements (*TROPOMI range:* DLR line positions + intensities consistent, only fit of p-dependent parameters, *TCCON range:* HIT20 line positions + intensities not satisfactory, ATM20 line list: significantly better than HIT20, not on DLR quality level, re-fit positions and intensities)

Spectroscopic improvements



Spectroscopic improvements

Fit quality on 1000 mbar spectrum (note: multispectrum fit was performed).



Spectroscopic improvements

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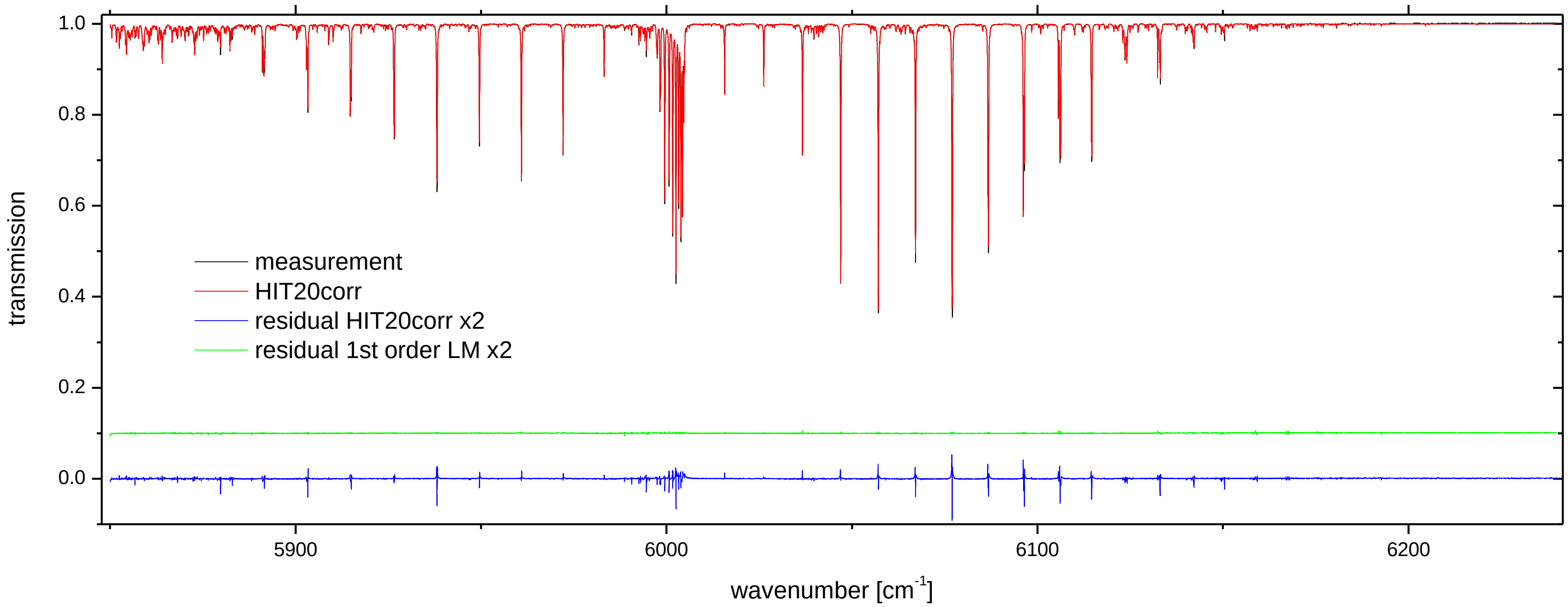
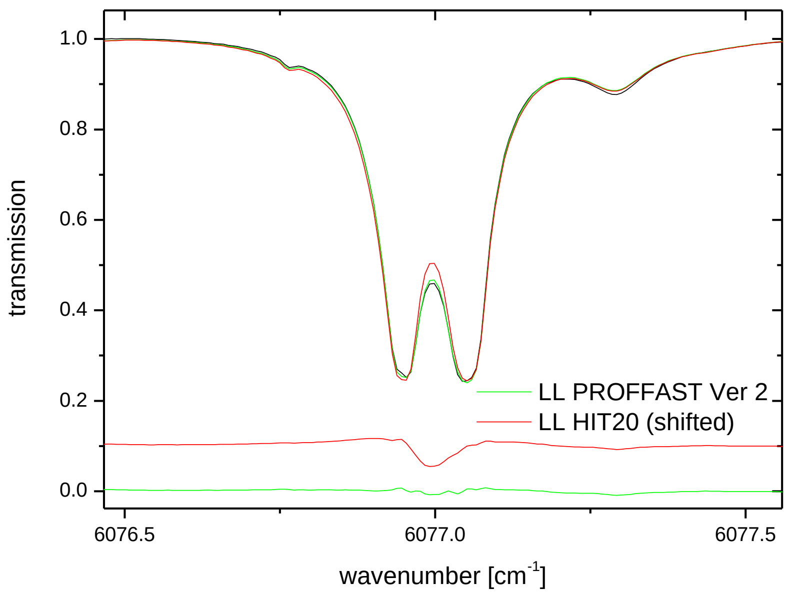
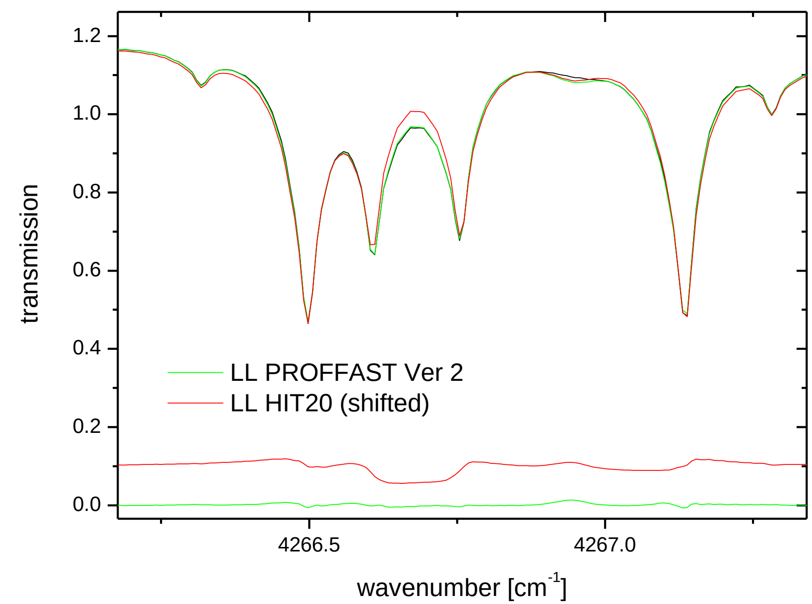


Spectroscopic improvements

Do the new CH_4 line parameters really work? - Tests on high-res solar spectra.

(Shown here: fits to average noon spectrum TCCON Ka 01-Aug-2019)





Summary spectroscopic improvements:

- ✓ PROFFAST Ver 2 supports 1st order LM + SDV
- ✓ Solar transmission model updated
- ✓ HIT2020 O_2 line list
- ✓ HIT2020 CO_2 line list (+ LM + SDV)
- ✓ Homebrewn CH_4 line list (+ LM)

X-sections lookup table

Use of pre-calculated x-sections

Model limitations accepted for PROFFAST implementation:

- Assume horizontal atmospheric homogeneity, local sphericity of Earth
- Neglect atmospheric dispersion

Technical limitations accepted in PROFFAST implementation:

- Supports only fit of scaling factors on a-priori trace gas profiles (no profile retrievals)
- Vertical sensitivities cannot be calculated in INVERS

X-sections lookup table

Limitations, residual errors

- The INVERS code uses a closed refraction formula:
  10% (1 arcmin) error @85° -> relative change in airmass 0.3%

- Radius of curvature function of azimuthal direction:
  0.06% variation of airmass @ 85 deg (Equator)

- Atmospheric dispersion (Ciddor, 1996):
  O_2 @ 7900 cm-1 : $n_{air} \approx 1.00027358$
  CH_4 @ 6000 cm-1: $n_{air} \approx 1.00027318$
  change of bending power 0.15% -> angular spread @85° 0.015'
  -> relative change in airmass: 5e-5

Improved x-sections lookup table summary

- New implementation supports the SZA range up to ~ 85°
- Remaining possible refinements:

  replace closed formula for atmospheric refraction