

TCCON prescribed mode for HCl cell analysis

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A new test version of LINEFIT has been uploaded to the TCCON wiki. This supports a prescribed mode for HCl cell analysis, in order to facilitate the use of the software.

The new prescribed TCCON mode requires from the user only *(1) provision of a spectrum* recorded with $\text{OPD}_{\text{max}} = 45$ cm or higher, of sufficient spectral coverage ($5670 - 5805 \text{ cm}^{-1}$) and sufficient SNR (~ 2000) and *(2) to apply the demo input file* located in folder `examples\TCCON\lamp\HCl\prescribed`.

In the input file, only the *name of the spectrum file*, the *internal semi-field-of-view* ($\text{apt} / (2 * 418 \text{ mm})$), and the *correct temperature T and pressure values* (note: p_{tot} and p_{self} should be equal) have to be specified by the user. The reference p values for each cell are provided in the table of the TCCON wiki (note: a change of T will also affect the effective pressure values. If the temperature deviates from the reference $T = 296 \text{ K}$ of the table, the pressure values need to be updated according to the gas law).

When the code is started, the ***compatibility of input file settings*** with the prescribed mode is tested, if a deviation is found, the execution is stopped with a specific message.

E.g., the microwindow bounds, de-weighting sections, OPD-dependent constraints, ... , are compared with expected reference values.

Next, LINEFIT investigates whether the ***spectral coverage*** is sufficient and ***resamples*** the input spectrum. In this step, the resolution is limited to 45 cm, and the oversampling to a factor of 8.

The chosen sampling allows a visual inspection of retrieval results. A common choice for the spectral sampling of the fit is also useful as this interacts with the interpretation of constraints (as a larger number of spectral gridpoints will increase the spectral contribution to the cost function).

The SNR is tested on the resampled spectrum (range used: 5715.0 - 5716.5 cm^{-1}). The SNR deviation is determined wrt a local reference value, which is determined by applying a low-pass filter on the spectrum for creating the local reference (convolution with a window function of width $\sim 0.14 \text{ cm}^{-1}$). This SNR is slightly too optimistic, as it suppresses the spectrally broader contributions (extrapolation towards a total SNR based on a white noise assumption is not performed).

The high-pass SNR has been chosen as a measure of spectra quality because it allows spectra suffering from not too-high frequency channeling to pass the quality check. However, at the end of the inversion, the total SNR calculated from the fit residual is compared with the SNR derived from the measurement as described above. An error message is displayed if the fit SNR is below 70% of the previously determined high-pass SNR. In this case the user needs to check the measured spectrum, probably it contains channeling, which should be included when repeating the fit (for this purpose, the number of resonators to take into account and their channeling frequencies need to be determined from the fit residuals by, e.g., repeating the fit selecting ILS_choice = 3 (extended) instead of TCCON mode).

The mean value in the (5715.0 - 5716.5 cm^{-1}) window is used ***for normalizing the measured spectrum to unity***. A global scaling factor on the measured spectrum is applied - slope, curvature, etc. are imposed on the calculated spectrum during the retrieval (baseline parameters).

The normalisation of the background level is useful as this value interacts with the interpretation of constraints (higher values will increase the spectral contribution to the cost function).

Before the retrieval is started, the ***spectral calibration of the measured spectrum is checked and taken into account***, if required. A classical least-squares fit algorithm tends to fail when measured and calculated spectral lines do not overlap any more due to a mis-calibration of the measurement. For this reason, LINEFIT checks the spectral calibration of the measurement before the retrieval is started. In normal operation mode, the execution stops when the spectral detuning found is too big.

The standard behaviour is chosen because a general spectral scene might contain a dense forest of spectral lines, and allowing for larger range of the recalibration might lead to an incorrect assignment of lines. Therefore, the problem of checking the proper calibration of the measured spectrum is forwarded to the operator. In TCCON prescribed mode, the spectral scene is well-determined and simple. The HCl line located at $5739.262511\text{ cm}^{-1}$ is used for a pre-adjustment of the spectral calibration parameters before the retrieval is started. The line intensity is also evaluated. If the line is significantly weaker than expected for a TCCON cell, the program stops with the message: "HCl lines too weak or spectral calibration off!".

The global constraints (smoothness of modulation amplitude and phase) to be used by the retrieval ***are adjusted by the code*** using the relation $\text{reg} = 0.3 * (9000.0d0 / \text{high_pass_SNR})^{**2}$. Note that the phase error is clamped to zero at ZPD (zero path difference) for the TCCON prescribed mode.

Clamped phase: this is equivalent to the assuming the phase correction scheme used for the Fourier transform of the interferogram works perfectly. The modulation retrieved from the cell measurement will likely be incorporated in the GGG processing scheme in some future. As the atmospheric lines of interest are much broader than the HCl lines, their retrieval depends mainly of the modulation efficiency assumed for the section of the interferogram around ZPD.

If the **SNR** determined from the fit residual is worse than expected, the program is terminated with an ***error message***, otherwise the results are written to file. In TCCON prescribed mode, ***an additional output file TCCON.dat is generated***, which reports the high pass SNR and the global constraints used for the retrieval.