Comment on "Retrieval of atmospheric CO_2 vertical profiles from ground-based near-infrared spectra".

By Frank Hase

The authors address a very relevant topic in their investigation, as it would be highly desirable to gain the capability of deriving vertical mixing ratios of CO_2 from high-resolution ground-based solar absorption spectra as recorded by TCCON. It needs to be noted, that the involved researchers at University of Toronto work enduringly since many years on improvements of the required spectroscopic data sets, which is an important pre-requisite for developing successful profile retrievals of atmospheric carbon dioxide.

However, I would like to add a few technical comments on the manuscript. Perhaps the authors might find these suggestions useful for further enhancing this study.

Page 2, line 66: "Scaling retrievals do not require inter-level constraints on a–priori concentration uncertainties" – I agree that a scaling retrieval does not require the explicit construction of inter-level constraints, but actually scaling equals the assumption of very strong inter-level constraints.

I would suggest to rephrase the notion on how GFIT handles a scaling retrieval (I hope I understand the authors correctly), as, e.g. "Technically, GFIT handles the scaling retrieval by weakly constraining the fitted VSF factor. The approach is equivalent to performing an optimal estimation of the VSF, assigning a value of unity to the a-priori VSF and a value of 1e6 as its expected range of variability."

Page 3, line 96: the line mixing referred to by the authors is (I believe) Rosenkranz line mixing and should be referred to as such.

Page 6, line 147: "We see no advantage to fitting non-contiguous windows in parallel, rather than in series, and then averaging the results." In my opinion, this is a misjudgement. Especially for retrieving profile information, combining weak and strong bands in a simultaneous fit is known to be potentially very advantageous. While the line wings of saturated lines in a strong band carry information about the lowermost atmospheric layers, weaker lines contribute information on higher atmospheric levels. We tried combination of bands in the context of the cited work by Dohe, which improved the uniformity of partial column sensitivities significantly over what is shown in Fig. 8.3 in the work of Dohe (using only the strong band). At that time, spectroscopic inconsistencies hindered a successful combined fit of weak and strong bands, given the progress on spectroscopic data this might look different today. In any case, the general statement that such a capability does not offer an advantage is in my opinion highly questionable. (The method of sequential estimation would be equivalent to a combined fit (if linearity can be assumed) and could be used as a makeshift solution if a fit of several windows is not supported by the code, but I assume this is not what the authors describe by "averaging the results".)

Section 3.1: In my feeling, this section would better correspond to the following investigation using measured spectra if a similar (not much higher) SNR and a similar and more realistic a-priori covariance would be used. I miss a sensitivity study concerning ILS in section 3.1 (this should be possible to realize although the code does not yet explicitly support ILS parameters by using slightly different acceptance cones in the forward calculation and in the retrieval, thereby modelling a modulation loss via the self-apodisation). I also miss a sensitivity study with respect to the offset (as it cannot be fitted in the non-saturated bands). By the way: as a DC-correction is implemented and as the non-linearity is well controlled (I assume), why is an offset observed in the saturated band? Does this offset behave like noise – varying from spectrum to spectrum – or is this a systematic offset? It would be interesting to provide a figure showing the behaviour of the fitted offset for a larger number of spectra (could be included in fig E2?).

I find the fact that the fit residuals of the unperturbed spectrum shows these oscillatory high-resolution features in the residuals very irritating. Why is it not possible to achieve a self-consistent code configuration that applies the same approximations in the simulation of the spectrum as in the forward calculation performed as part of the retrieval? Note that for the disturbance of line parameters (panels e and f in figure 7), these artificial features seem to be of similar size as those invoked by the perturbation.

Figure 11: it might be instructive to add a further panel displaying XCO_2 for each retrieval setup.

Figure 13: Why is GGG XCO2 so significantly off from the in situ value (scaling retrievals in the TCCON bands are off by about 4 ppm)? I assume that required calibration factors have not yet been applied?

Note that this problem of bias is connected to a significant problem in your retrieval setup: as far as I oversee, the CO_2 a-priori profiles used are intended to match with the actual CO_2 mixing ratios in the atmosphere. But the CO_2 becomes calibrated to WMO scale only further down the processing line (by rationing CO_2 column over the O_2 column and application of ADCFs + AICFs). Let's assume the calibration is off: this poses no problem for a scaling retrieval (same residuals, same solution, only a different scaling factor is reported). However, an optimal estimation setup will misbehave if the a-priori is biased: it will try to approach the a-priori values in altitudes where the sensitivity is low and in effect the retrieved profile will oscillate significantly. I think it would be superior to apply a pure smoothness constraint as used by Dohe instead of an optimal estimation with diagonal constraint and just some correlation on top. If a pure smoothness constraint is used, a bias of the a-priori remains without effect even for a profile retrieval (same residuals, same solution, only different scaling factors on identical profile shapes). Moreover, this setup is preferable because it allows a smooth transition between the profile retrieval and the simple scaling retrieval (just increase the smoothing constraint further and further).