

Interactive comment on “GFIT2: an experimental algorithm for vertical profile retrieval from near IR spectra” by B. J. Connor et al.

Anonymous Referee #1

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The paper by Connor et al reports on progress made in developing a new software tool for processing FTIR spectra as part of TCCON. The software is a modification of the existing official TCCON algorithm GFIT, adding a new inverse profile retrieval capability. GFIT is a community used algorithm to retrieve total column amounts of atmospheric gases. There is more information in the IR spectra than just a total column, depending on the gas, and as the authors explain there are a number of advantages worth exploiting if this can be realised for CO₂.

What puzzles the referee is the purpose of this paper. The authors do not describe the forward model in any detail (indeed there not a definitive GFIT paper) which is not expected here but how is the GFIT forward model adapted for their purpose? Nor do they explain how the inverse method is used in any detail other than a very brief

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description based on another paper. So this current paper is not a full description or reference paper for GFIT2, but more of a report on a series experiments (as the title suggests) on various difficulties the authors have had using the software on real spectra. It is therefore not clear how the software was implemented, what specific version of GFIT was used and any modifications made (is this the 2012 or 2014 GFIT version or earlier?), and what choices of constraints/regularisations were used in the inverse method (some but not all discussed or mentioned).

Generally the paper is well written and clear in its content, with figures that are also clear and easy to read. This paper needs to address a number of issues listed below before the paper is ready to publish. Below are comments/suggestions in order of page number.

Major Comments:

1. Is this code available for the TCCON community to test? The authors clearly make a strong argument why such an analysis tools would be really useful, but there is also considerable expertise using optimal estimation algorithms within the TCCON (and NDACC) communities that may well sort out the instability problems that seem to be a major problem in the examples tested.
2. Section 2. How is the GFIT algorithm used? Which version? Is it really just a standard version as used by the community or are there specific additions? For example, it is mentioned that the solar Doppler shift was a problem and was “formally retrieved”, page 12273. So this must be added to the forward model (this is not in the 2014 version?), and added to the state vector as a retrieved parameter (more on this later). Is the standard 70 layer atmosphere used or something else? Are the standard CO2 micro windows fitted simultaneously (as is possible using PROFFIT or SFIT4) or concurrently (which is the normal GFIT practise)?
3. Section 3. Large parts of this description are essentially identical to sections in Connor et al (2008). This is probably ok or should it be reworded? The title of this

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section says “implementation”. So how was it implemented in practise? What are the critical components that are required to run the retrieval and need to be stated up front in the running of the code? The authors clearly state and experiment with S_e , the measurement signal to noise. What about S_a ? How is this implemented in the code? What apriori covariances are assumed for CO_2 ? What about the assumed uncertainties for a range of other parameters, for example line shifts, solar zenith angle, background slope and curvature, and interfering gases to name a few. In an optimal estimator all of these have assumed uncertainties that form part of the inverse method.

4. Section 3.1. There is a nice discussion here on the effects of measurement error on the stability of the profile, and various methods to remove its effects. This part of a broader practise when using optimal estimators in terms of how codes (like PROFFIT and SFIT4) use regularisation to help dampen down oscillations. This applies to the S_a used as well. GFIT2 does not seem to have (at least at this point in its development), the ability to correlate layers, and methods like Tikonov-Phillips (TP) that can have significant impacts on profile stability. The former, the layer correlations, is particularly useful when using either a Gaussian or exponential type fall off between layers with correlative widths of order 4 to 6 km. It has the added advantage of not reducing the dof as well. TP on the other hand maybe better at smoothing instabilities, but reduces the dof to about 1.5 in the case of CO_2 . These regularisation schemes are a very useful tool for these problems and have not been explored at all here.

5. Section 4.2. In this section the issue with the Doppler shift in the solar lines being different to the telluric line shift is discussed. GFIT has always assumed that the instrument pointing was accurate, and the appropriate solar Doppler shift computed per spectrum. A procedure is outlined on page 12273 which seems to imply that the Doppler shift is added to the state vector as a retrieved quantify (as it should be), but then the original spectra are corrected and the retrieval re-run? Why do this when the spectra are effectively corrected in the first run by shifting the solar lines as a fitted parameter? Has this step been misunderstood here?

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6. Sections 4.3 and 4.4. A lot of work has gone into this section of the paper, identifying residual structures in the spectra that are common to both Lauder and Lamont spectra. These structures are explained in terms of errors in spectroscopic parameters (linewidths for example), and also the physics of the lineshape model (or missing physics) used in the forward model. The mean bias correction is a nice way of dealing with these unknowns, a practise used in other fields of spectroscopy (uv/vis for example) to account for similar shortcomings in the forward model physics and/or unknown absorbers. This approach in this paper has mixed results. What is missing in this section of the paper, and indeed in the testing with real spectra, is any discussion or testing of the effects of instrument lineshape (ILS). While spectra from a Bruker 125HR, carefully aligned, will in general be adequately described by the known optical path difference and field of view, just how sensitive is the CO₂ profile retrieved with GFIT2 to any changes in the ILS, however small? The authors after all note on page 12272 in section 4.3.1 on linewidth errors, that the CO₂ profile is extremely sensitive to errors in the pressure broadening coefficient, "... and by extention to other sources of lineshape error...". Perhaps this is not an issue at the OPD used in TCCON (50cm) compared with a typical NDACC spectrum (180-250cm), but the levels of precision and accuracy demanded of the analysis for CO₂ is very high. Even so, this should be explored and its effects demonstrated one way or the other. This does pose a challenge with the GFIT forward model, as the model assumes a well aligned instrument, with a limited range of apodisation functions. In other words, are the authors convinced that the instability they are experiencing in the CO₂ profile is being driven solely by spectroscopic and lineshape (defined here excluding ILS) errors and not by potential small errors in the ILS?

Minor Comment

1. The Kuia et al paper, page 12265, is missing in the references

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