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

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Response to Anonymous Referee #2

We thank referee #2 for thoughtful and insightful questions.

Many comments by both reviewers can only be addressed appropriately with revisions to the text and/or figures in the manuscript. Therefore we have prepared a revised manuscript, which appears as a 'Supplement' to this comment, and will include it by reference below.

Introductory comment:

The reviewer prefers continued work rather than publication, but follows with numerous

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detailed suggestions which need to be addressed if publication is pursued at this time.

We believe publication of the work is appropriate after the requested revisions to the manuscript. The large-scale motivation for this study is improvement in our ability to monitor lower tropospheric CO2, specifically by retrieving some profile information from TCCON measurements. There is compelling theoretical justification for this approach, and a wealth of experience on related retrievals. However achieving satisfactory results at the accuracy required for tropospheric CO2 has proven much more difficult, and taken much longer, than expected.

Our work to date has provided numerous quantitative insights into the nature of the problem, documented difficulties, and suggested the directions of future work. As pointed out by Referee #1, there is a large community of researchers with the experience and interest who could contribute to achieving reliable CO2 profile information from TCCON. We believe that documenting our experience, and our partial results, will be valuable to this community and ultimately contribute to the large-scale goal.

Therefore we will address Referee #2's specific points in the remainder of this document.

General:

1. We have revised all panels of the figures showing profiles from atmospheric measurements, by adding horizontal 'error bars' indicating the standard deviation of the set of retrievals performed (typically 80). These are figure 9, 11, 14, 15, and 16 of the Supplement.

2. We have added a number of new references, and cited both them and existing ones in response to this suggestion. References requested in 'Specific' comments below have been supplied.

3. A pressure scale has been added to Figs. 1 and 2

4. A plot of a typical spectrum in the spectral region used, has been added and is Fig.

3 in the Supplement. It shows the individual gas contributions and the residuals.

5. The spectral residuals are barely changed by the various experiments, compared to the magnitude of the systematic residuals shown in Figures 12 and 13, so showing them repeatedly would not provide new insight. Therefore we have chosen not to include any new plots of residuals.

6. The reviewer asks about the parameters used in the retrieval and their constraints. This is addressed in the new sections 3.3 and 3.4 in the Supplement:

"3.3 State Vector and A priori Uncertainties

The full state vector consists of the CO2 profile, scale factors for the other gas profiles contributing to the spectrum in the band pass (H2O, HDO, and CH4 in the 6220 cm-1 band), the background continuum level, tilt, and curvature, a frequency shift and a zero level offset. This is identical to the standard GFIT scale factor, except for the CO2 profile itself. A scale factor multiplying a vector of systematic residuals, as described in 3.2, has been added to the state vector for the retrieval tests of section 4.4.

A critical input is the a priori covariance matrix Sa, specifying assumed uncertainties in the state vector and their correlations. The retrievals in this paper assume that Sa is diagonal. The a priori uncertainties assumed are guided by those used in the standard GFIT scaling, namely 1 for the three interfering species and the continuum level, 0.1 for the continuum tile and curvature, 2 for frequency shift, and 0.5% for zero level offset (which is expected to be approximately zero). The uncertainties range from 1-5%, are largest near the surface, and have been adjusted to improve the test results where possible. Finally the residual scale factor, when in use, has been assigned an uncertainty of 10%, based on the observed variability of the systematic residuals.

3.4 Other input parameters

The only other input parameters specific to profile retrieval concern convergence and

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goodness-of-fit. They include the convergence parameter defined in section 3.1, the maximum acceptable 2 of the spectral fit, and the maximum number of iterations allowed."

The constraints are discussed further in section 5:

"A simple alternative has been suggested, namely imposing a priori constraints on the profile shape by experimenting with explicit interlayer correlations in the a priori covariance matrix Sa. However it has been our experience in similar retrieval problems that interlayer correlations are best used to fine tune a successful algorithm, and may not be needed at all. This is fundamentally because in the Rodgers' algorithm the a priori profile shape implicitly imposes the profile fine structure, which is not strongly influenced by the measurement (see Rodgers, 1990). So, for example, the algorithm developed at Stony Brook University for ground-based microwave measurements of CIO has been used successfully for more than 20 years and has always used a diagonal Sa matrix (Solomon et al, 2000, Connor et al, 2013), and the OCO algorithm of Connor et al, 2008, on which the current OCO-2 algorithm is based, included interlayer correlations as a refinement after successful initial testing.

In light of past experience therefore we have deferred serious experimentation with interlayer correlations in the a priori of GFIT2, until either the forward model can be improved, or the sensitivity of the retrieval to forward model errors can be reduced, as described earlier in this section."

Specific:

The page numbers below are as cited by the reviewer, taken from the original manuscript. Where necessary the new page number in the Supplement (revised manuscript) is also cited.

Page 2

1. Captions to Figs. 1 and 2 have been expanded to address these issues:

"Fig. 1 Column averaging kernels for simulated retrievals. 'Profile Retrieval' and 'Profile Scaling' refer to a typical retrieval using GFIT2 on the 6220 cm-1 CO2 band observed operationally. 'Optically Thin', 'Optically Thick', and 'Intermediate' refer to an idealized, single, isolated spectral line. For these, we calculate a spectrum from a reference profile, perturb the profile at a single altitude, and calculate a new spectrum. We then perform a least-squares fit to this synthetic spectrum by deriving a scale factor for the reference profile. This scale factor, divided by the actual perturbation, produces a single element of the column averaging kernels shown."

"Fig. 2 Partial column averaging kernels for the profile retrieval algorithm of Fig. 1 (GFIT2 applied to the 6220 cm-1 spectral band, with assumed signal-to-noise ratio = 1000)."

2. Several references have been added here: "(Rodgers, 1976, Solomon et al, 2000, Dohe, 2013)"

Page 6 (page 7 of the Supplement)

Changed as suggested

Page 7: (page 8 of the Supplement)

There was a typographical error in the original submission, which was corrected before the manuscript was typeset. Eqn 5 is legible in my copy of the pdf taken from the AMT website.

Page 8: (page 9 of the Supplement)

- 1. Connor et al, 1995
- 2. Rodgers & Connor, 2003

3. We base this empirical correction on the OCO-2 algorithm, which has yet to be formally published, but is described in JPL, 2015.

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Page 19 (Page 21, Section 4.2.1 of the Supplement)

1. We believe our reference to 'lower troposphere' is imprecise and the wording will be changed to 'p > 0.5 atm'.

Page 20 (page 22 of the Supplement) The curve in Fig 8 of the original manuscript (Fig 10 as revised) is the measured spectra divided by the residual vector from the column retrieval, and is used as the diagonal of the new Se.

Page 21 (page 23 of the Supplement) 1. We have added the following sentence: "This result shows that the fundamental instability of the retrieval has not been adequately mitigated by the application of the variable SNR technique."

Page 32 (page 34, Section 5 of the Supplement)

1. The new section 4.1.4 in the revised manuscript suggests that ILS error is likely to be less important than error in spectroscopy, and the wording here will be changed to "Based on the tests shown in section 4.1, it would seem that our theoretical knowledge of the atmospheric spectra is inadequate to provide useful CO2 profiles at the accuracy required."

2. The 45 cm maximum OPD produces an ILS narrower than the atmospheric line in most of the troposphere, so should be adequate for improving altitude profiles in the mid- to lower troposphere. Experimenting with a larger OPD in the regard would be interesting but would require new, dedicated observations. The analyses presented and proposed in this paper can be applied to the entire body of existing TCCON observations.

Please also note the supplement to this comment: http://www.atmos-meas-tech-discuss.net/8/C5833/2016/amtd-8-C5833-2016supplement.pdf

Interactive comment on Atmos. Meas. Tech. Discuss., 8, 12263, 2015.