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Atmospheric Measurement Techniques Discussions

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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We thank referee #1 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.

The introductory comments raise questions about the forward model and inverse method and their implementation, which are addressed in more detail in Major Comment 2. We will respond to those questions below.

Major Comment #1:

The reviewer asks if the GFIT2 code is available for the community to test.

Unfortunately, it not available to the community as yet. We have added the following paragraph at the end of section 5:

"Finally, it is our intention to release GFIT2 to the community, as an option within the public version of GFIT. That would allow testing and development by a wider range of experienced researchers. So far that has proven impractical, but we hope to do so in the near future."

Major Comment #2:

The reviewer asks for details on the forward model, specifically how GFIT is used and which version.

We have added the following paragragh to the end of Section 2:

"Optimal estimation has been implemented as a user-selected option of inverse method added to the version of GFIT publically released in 2012; no other changes to the standard GFIT algorithm were made. The modified algorithm is known as GFIT2. GFIT is designed to treat each spectral band independently. All calculations in this paper are of the 1.61μ (6220 cm-1) spectral band; the use of other bands will be discussed briefly in section 5. Figure 3 shows a typical spectrum from the TCCON site at Lamont, OK, USA."

The solar Doppler shift is calculated using GFIT 2012 without modification, and will be discussed further under Major Comment #6, below.

Major Comment #3

The reviewer asks for more detail on implementation of the inverse method, We have edited the last paragraph of section 3.1 to improve clarity:

"To enable use of the Rodgers' algorithm, a modified GFIT code was developed which completely separates the forward model and inverse method, and allows integration of optimal estimation profile retrieval with the existing code. Conceptually, the experimental, integrated GFIT allows selection of the existing (profile scaling) or modified (profile retrieval) algorithm. This is simply accomplished by setting a parameter in an input file. The integrated algorithm has input and output files identical to the existing GFIT, plus new input and output files specific to profile retrieval, which are not required unless the modified algorithm is selected."

We have also written sections 3.3 and 3.4 to address the reviewer's questions:

"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 uncertainty in each of the 70 levels in the CO2 profile is set independently. These 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 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."

Major Comment #4:

The reviewer describes the value of regularisation of profile retrieval by imposing interlayer correlations or by use of alternative algorithms, such as Tikonov-Phillips, and comments that this issue has not been addressed. GFIT2 is capable of correlating layers by using a full (non-diagonal) Sa matrix, but we believe this is unlikely to provide much if any improvement in results. We have addressed this issue in section 5, Conclusions:

"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 ClO 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."

Connor, B.J., T. Mooney, G. E. Nedoluha, J. W. Barrett, A. Parrish, J. Koda, M. L. Santee, and R. M. Gomez (2013). Re-analysis of ground-based microwave ClO measurements fromMauna Kea, 1992 to early 2012. Atmos. Chem. Phys., 13, 8643–8650

Rodgers C D Characterization and error analysis of pro les retrieved from remote sounding measurements. J. Geophys Res 95, 5587-5595, 1990.

Solomon, P.M.; Barrett, J.; Connor, B.J.; Zoonematkermani, S.; Parrish, A.; Lee, A.; Pyle, J.; Chipperfield, M. (2000). Seasonal observations of chlorine monoxide in the stratosphere over Antarctica during the 1996-1998 ozone holes and comparison with the SLIMCAT 3D model. Journal of Geophysical Research 105: 28979-29001.

Major Comment #5:

The reviewer asks about correction of the solar Doppler shift to account for inaccurate telescope pointing. This was poorly explained in section 4.2. GFIT calculates the error observed in its solar Doppler shift, but does not apply it to the spectrum. We will modify the third paragraph of 4.2 as follows:

"Analysis of the data from these days immediately revealed significant errors in the solar Doppler shift. This is shown not only by simple examination of the residuals, but is also formally calculated, as the difference in the frequency shift observed for solar lines (after correcting for the calculated Doppler shift) and telluric lines. GFIT does not automatically take this error into account, by recalculating the spectrum with the correct Doppler shift. However, these errors can be corrected by using the retrieved solar/telluric difference to correct the calculated Doppler shift, and then re-running the retrieval. All measured spectra and retrievals used and/or shown in this paper have been 'Doppler shift corrected' in this way."

Major Comment #6:

The reviewer rightly points out that a discussion of the instrument line shape (ILS), as a source of spectral residuals, is needed. We have calculated the sensitivity of the GFIT2 profile to the estimated error in the ILS for a set of synthetic spectra, and include the relevant discussion and results in a new section on ILS error:

"4.1.4 ILS Error

Another potentially significant source of error is distortion of the measured line shape itself. For Fourier transform spectrometers (FTS, as used by TCCON) the instrument line shape (ILS) is a convolution of contributions from the finite path difference and the finite field-of-view (FOV) of the FTS. The path difference and its ILS contribution (a sinc function) are well known, but the FOV, which contributes a rectangular shape, has an uncertainty we estimate as 7%. This causes the observed line to be broader and weaker than the atmospheric line, and progressively has a larger effect as the line is narrower. I.e. the error due to finite aperture becomes more important at lower pressure where the intrinsic line shape is narrower. (See for example Davis, Abrams, and Brault, 2001.)

We illustrate this effect in Fig. 7, which is calculated for the same spectra as Fig. 6, and so is directly comparable to Fig. 6a. The net effect of this error is very small in the lower troposphere, and grows only to $\sim$1% in the stratosphere. We conclude that error in the measured line shape is unlikely to dominate error in the calculated line shape (section 4.1.3)."

Minor Comment:

The Kuai et al reference was incorrectly typeset on page 12280 as

Le, K., Wunch, D., Shia, R.-L., Connor, B., Miller, C., and Yung, Y.: Vertically constrained CO2 retrievals from TCCON measurements, J. Quant. Spectrosc. Ra., 113, 1753–1761, 2012

It appears correctly in the submitted manuscript:

Kuai, Le, Debra Wunch, Run-Lie Shia, Brian Connor, Charles Miller, Yuk Yung (2012), Vertically constrained CO2 retrievals from TCCON measurements. J. Quant. Spec. & Rad. Trans., 113 (14), 1753-1761.

Please also note the supplement to this comment:
http://www.atmos-meas-tech-discuss.net/8/C5826/2016/amtd-8-C5826-2016-supplement.pdf

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