

***Interactive comment on “Information operator approach applied to the retrieval of the vertical distribution of atmospheric constituents from ground-based high-resolution FTIR measurements” by C. Senten et al.***

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General answers to the referees

We thank both referees for their constructive comments and have revised the paper accordingly.

All typographical corrections have been made and the clarifications that have been asked for are added.

C2018

Both referees made a comment regarding the fact that Tikhonov regularization (TR) was discussed only for O<sub>3</sub> and CH<sub>4</sub>, and not for N<sub>2</sub>O and CO. Therefore, we have now included also the retrieval results and corresponding error budgets for N<sub>2</sub>O and CO obtained with Tikhonov regularization. As such, for all molecules investigated in the paper, namely O<sub>3</sub>, N<sub>2</sub>O, CH<sub>4</sub>, and CO we now discuss the results for the three retrieval methods under investigation, namely OEM, IOA and TR.

In addition, we performed the theoretical study suggested by referee #1, in which an ensemble of virtual measurements was generated by a forward model calculation using a self-created set of VMR profiles. Gaussian distributed random noise was then added to these simulated spectra. Finally, we applied the three retrieval methods to this ensemble of synthetic spectra – assuming one a priori VMR profile and an a priori covariance matrix – to quantify the reconstruction of the initial VMR profiles. A table summarizing the quantitative results is included in the paper. As for the total columns we see that the OEM and IOA slightly better reproduce the original values than TR (i.e., mean relative differences of 0.11, 0.11 and 0.12%, respectively), although with larger standard deviations (i.e., 0.09, 0.09 and 0.06, respectively). For the second and fourth column, the IOA reproduces the input values best, whereas the first and third partial columns are better reconstructed by the TR and OEM, respectively. The standard deviations are smallest in the case of TR for each partial column. This test shows that the IOA is slightly better in reproducing the original input information, while TR produces more steady results.

For the discussion about whether or not the information operator approach provides ‘significant advantages’, we emphasize the fact that we are the first to present an implementation of the IOA for retrieving information about the vertical distribution of atmospheric constituents from ground-based FTIR measurements. We have shown the feasibility of this method and have found a few additional benefits with respect to the OEM and to a lesser extent to the TR. Therefore, we can conclude that it is a useful alternative to the OEM and TR, especially when limited a priori information is available.

C2019

Note however that we have not concluded that the IOA is unquestionably better.

Answers to the specific comments of the referees

Referee #1

Page 2: Please add a few references to clarify the significance of the NDACC.

The following two references have been added: Kurylo, M. J. and Solomon, S.: Network for the Detection of Stratospheric Change, NASA Rep, Code EEU, 1990. Kurylo, M. J.: Network for the detection of stratospheric change (NDSC), SPIE Proceedings 1991, Remote Sensing of Atmospheric Chemistry, 1491, 168–174, 1991.

Page 8: In the discussion of TR, you state "the parameter alpha we have used ... is ... the best compromise between DOFs and the total random error" - the total random error of which target quantity? Total column? The standard tuning method is the L-curve method: does the L-curve suggest a similar choice for alpha?

In the discussion of the Tikhonov regularization the determination of the constraint parameter  $\alpha$  is based on the fact that the DOFS as well as the total random error decrease with increasing  $\alpha$  (Steck, 2002). Thus, searching for the best compromise between both – i.e., the largest DOFS and the smallest total random error – is a straightforward method to find an optimal value of  $\alpha$ . Here we mean the total random error on the total column indeed. Ideally, the L-curve method should suggest a similar choice for  $\alpha$ , but it requires a larger effort.

Page 9: "The off-diagonal elements [of spectral noise covariance matrix] are set to zero,..." This is not valid unless care is taken that the spectrum is sampled on an appropriate spectral grid.

In the case of FTIR measurements the noise propagating into the spectrum can be assumed to be the same and independent for all spectral points. This can be explained by the fact that the discrete Fourier transform is orthogonal, such that the independence of the random noise in the interferogram points – which is the case because

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these points are measured from independent detector signals – is preserved during the Fourier transformation of the interferogram to the spectrum.

Page 11: Figure 1: Would you please note which DOF results for the OEM solution, shown in the upper left corner? It would be very instructive for the reader to show OEM solutions adjusted for the same NDOF as the IOA solutions. The current figure only tells that oscillations are reduced when NDOF is reduced, which is a rather trivial result.

The mean DOFS for the OEM profiles shown in Fig. 1 (a) is 3.1 (see text and Table 4). The fact that the oscillations are reduced when including fewer terms in the IOA sum – in turn reducing the DOFS – is indeed a trivial result, since the eigenvectors corresponding to small eigenvalues are the ones that cause the additional oscillations. However, the advantage of the IOA is that the best compromise between both is obtained automatically thanks to the well defined threshold, whereas the OEM does not exclude these oscillations, unless the user tunes the a priori covariance matrix for example to reduce the DOFS and to obtain less oscillating profiles. Hence, one can assume that the resulting DOFS from the IOA is a more realistic estimate of the true information content in the measurements.

Page 12 (+ Figure 2 + Table 2): If I correctly combine the results reported in Figure 2 and Table 2 the 0.8 threshold for  $g$  results in the use of e.g. 12 eigenvectors for O3 and even 22 (!) eigenvectors for CO. It is surprising to me that so many eigenvectors of the information matrix need to be taken into account to construct solutions which finally offer NDOF in the range of 3 (CO) to 4 (O3). Can such a scheme termed numerically effective? - If one would apply a truncated SVD, I would expect that the number of relevant contributions would equal NDOF.

The number of eigenvectors of  $P$  with significant eigenvalues corresponds to the number of DOFS of all fitted parameters and not of the target species' profile only. Indeed, as can be seen in Sect. 3.2.2, the number of terms in the IOA sum can be up to 22.

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Nevertheless, this does not imply a decrease in numerical efficiency. On the contrary, summing up 22 terms composed of simple matrix multiplications is numerically more efficient than calculating the inverse of a matrix (Eq. (1) versus Eq. (6)). The truncated SVD is another alternative method that could be used to perform retrievals from FTIR spectra. Singular vectors of the matrix  $F$  – representing the forward model – that introduce oscillations in the vertical profile are left out by truncating the SVD expansion. This approach is similar to the IOA and the remaining number of terms can indeed be expected to correspond to the total DOFS.

Figure 6: The IOA sensitivity curve shows considerable stronger overshooting at 18 km than does OEM?

Figure 8: All the IOA kernels look essentially the same - this retrieval seems to offer significantly less DOFS than OEM and TR (the table states DOFS 2.2/2.1/2.3 - hard to believe)? Why do the sensitivity curves show these sharp kinks (Fig 8a, c) and huge amplitudes (Fig 8b)? - In contrast, the CO sensitivities in Fig. 10 look plausible.

We have no clear explanation for the strange behavior of the averaging kernels and corresponding sensitivity curves for the CH<sub>4</sub> retrievals.

Table 1: CH<sub>4</sub> variability: "variable" What does this mean - variable as function of altitude? Or different settings used for different spectra?

"Variable" here means variable as function of altitude, more specifically, ranging from 4 to 70%.

Table 4: It would be appropriate to include TR for N<sub>2</sub>O and CO as well.

This has been done.

Conclusions: "Our findings proof that the IOA allows more stable vertical profiles". I do not see that the material proofs this claim, see, e.g. Fig 11, where TR solutions are obviously more stable over the relevant altitude range ".... and with generally lower error budgets" This also is an optimistic resume. The smoothing errors given in Table 5

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are generally smaller for OEM and TR, so obviously the solutions preserves more detail about the true state and this is probably the reason for less favorable partial column errors - essentially the same behavior would probably be observed in the comparison of two OEM setups with different DOFS.

Our conclusions concerning the stability of the retrievals and the error budgets have been revised based on the added TR results and theoretical study. For O<sub>3</sub>, the IOA still seems to give better results than the OEM and TR, whereas for N<sub>2</sub>O, CH<sub>4</sub> and CO the TR seems to provide slightly better results. In particular, comparisons of the OEM and IOA retrieval results with those obtained with TR have shown that the stability of the TR column values is somewhat better than the OEM and IOA stability. The information content of the IOA retrievals is slightly smaller than the information content of the OEM and TR retrievals, a quantity being about the same for the last two methods. So, the IOA performs well, i.e., similar to TR, and has some advantages with respect to the OEM, especially regarding profile stability and error budget evaluations. Based on this study, we can conclude that the IOA applied onto the OEM is a valuable alternative for the retrieval of vertical profile information of trace gases in the atmosphere from ground-based FTIR solar absorption measurements. It behaves better than the OEM from several points of view, but the significance of the improvements depends on the target species and on the chosen a priori information.

Referee #2

Page 3746, line 4: Briefly define the upper Hessenberg form.

An upper Hessenberg matrix has zero entries below the first subdiagonal.

Page 3749, para 2 and Table 1: Explain why different spectral resolutions were used for the four gases.

For each target gas one or several well-chosen micro-windows are fitted. This choice mainly depends on where its well-resolved unsaturated absorption lines are situated

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and least effected by interfering species' lines. In order to measure different wavenumber ranges of the spectrum an FTIR instrument uses different optical filters, explaining the different spectral resolutions.

Page 3752, line 13: Was the Tikhonov regularization method tuned to give the same DOFS as the other two methods?

We did not tune the TR method to give the same DOFS as one of the other two methods, but the DOFS resulting from our selection criterion for  $\alpha$  appeared to be situated between both values in question.

Page 3754, line 13: Define the sense of the bias.

For O3 and CO each method gives about the same partial and total column values, i.e., without significant bias. For N2O the partial and total columns are distributed in a slightly different way. The biases between the OEM and IOA total columns are about -0.2% and the biases between the OEM and TR total columns are about -0.15%. The biases between the OEM and IOA first and second partial columns are -0.8 and +0.8%, respectively, whereas they are -0.5 and +0.5% between the respective OEM and TR partial columns. For CH4 there is a systematic bias of the order of +1.5% between the OEM and IOA daily mean first partial and total columns, while the bias between the OEM and TR column amounts is about +1%. So for the cases in which the IOA columns systematically deviate from the OEM columns, the same is observed for the TR columns, but with a smaller offset.

Page 3754, line 19: State which parameters are included in the forward model parameter error. Doesn't this include some of the other errors listed in this sentence (e.g., temperature, line intensity, pressure broadening, solar zenith angle, etc.)? Also on page 3755, lines 13-14, there appears to be redundancy in the list of errors.

In this article the temperature, solar zenith angle, line intensity and pressure broadening errors are all considered as separate error components and are not included

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in the forward model parameter error. Remaining forward model parameters that are comprised in the forward model parameter error are a wavenumber shift and scale multiplier, background slope and curvature parameters, etc.

Page 3756, line 4: Discuss possible reason(s) for the large systematic error for the CH4 partial columns retrieved using the TR method.

We have no unambiguous reason for the relatively large systematic error for the CH4 partial columns in the case of TR. Note that the error budget tables have now been extended with the N2O and CO results for TR as well. The conclusions have therefore been revised in the paper.

Page 3757, lines 5, 6: Discuss briefly the results of the sensitivity tests to retrieval grid, e.g., what grids were tested and the magnitude of the sensitivity.

To test the sensitivity of the OEM, IOA and TR retrieval results to the choice of the retrieval grid we have used different grids varying from a fine 44 layer grid to a coarse 7 layer grid. We have found the effect on the retrieval results to be similar for each method. More specifically, we observed a decreasing accuracy for a decreasing number of layers.

Page 3774, Figure 4: Why is the sensitivity for TR equal to unity for ozone?

For the particular choice of L1 as regularization matrix for the TR the averaging kernel matrix A becomes:  $A = (KrT Sy^{-1} Kr + \alpha L1T L1)^{-1} KrT Sy^{-1} Kr$ . Due to intrinsic properties of the used constraint matrix, the sum of all elements of each row of A equals 1, as can be seen from a simple matrix manipulation. This is valid for each choice of  $\alpha$ . Consequently, for the Tikhonov retrievals the sensitivity is always 1 at every altitude and is not a relevant parameter, in contrast to the OEM and IOA retrievals.

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Interactive comment on Atmos. Meas. Tech. Discuss., 4, 3739, 2011.

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