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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Technical Note: Impact of nonlinearity on changing the a prioriof trace gas profiles estimates from the Tropospheric Emission Spectrometer (TES)" *by* S. S. Kulawik et al.

S. S. Kulawik et al.

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Below contains the review from Thomas von Clarmann. Where a response is needed, a response statement is given with a description of the action taken. Thanks to Dr. von Clarmann for his detailed comments and suggestions.

General comments: This paper presents to my best knowledge the first thorough documentation of the retroactive exchange of a priori information in a set of retrievals without rerunning the nonlinear retrievals. This allows to constrain each single retrieval by its individual a priori and to use the a priori transformation to obtain a uniform dataset where artifacts due to changing a priori information are excluded. The authors conclude that for their TES retrievals the use of individual a priori information for each

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nonlinear retrieval and subsequent transformation behaves well compared to nonlinear retrievals using uniform a priori information. This paper is scientifically sound, well organized and written and fits well in ACP, of which one of four activity fields is remote sensing. The paper certainly has methodical focus but it is far more than a 'technical note'. The paper fulfils, to my judgement, every requirement of a regular journal paper. Thus, I recommend publication as a regular paper in ACP.

Response: We agree with the reviewer that the paper should have the status of a regular journal paper. The question of non-linearity in a retrieval and its impact on linear transformations of that geophysical quantity is of vital importance to researchers using data from most modern satellite sounders such as IASI, GOME2, AIRS, MOPITT, etc. in their comparison with models and in-situ data. Moreover, these results have significant implications for institutions that wish to assimilate geophysical quantities derived from optimal estimation by showing that the linearity assumption in the characterization of the retrieval, namely x^=x_a+A(x-x_a), is valid. This paper uses specially processed TES satellite data and is similar in purpose to other validation papers, such as validation of TES ozone.

Specific comments: Abstract: The abstract is concise and well written. Is the transformation of profile estimates to a common prior really a common strategy? The recipe how to do this might be common knowledge, but has this knowledge really been applied sufficiently often to justify to call this a 'common strategy'? The conclusion of the paper refers to maximum a posteriori retrievals in a Bayesian sense (optimal estimation). This assumption should be mentioned in the abstract, because the conclusion might be different for other types of constraint, and the reader of the abstract does not necessarily know that TES is analyzed with optimal estimation.

Response: The word "common" was replaced with "mitigation"; "One mitigation strategy is to transform profile estimates..."

Response: The first sentence now says, "non-linear maximum a posteriori (MAP) esti-

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mates of...."

Introduction: The introduction motivates the study, summarizes the necessary information on the TES instrument and introduces the averaging kernel representation of the retrieval. Some more information on the retrieval details may be useful already here. Currently the reader is referred to other papers, and some information is given in Section 3.1.2. Of particular interest are the sequence of operations and the elements of vector x beyond the obvious ones (if any). Are there joint-fit quantities beyond the profile values of the target species (e.g. surface emissivity) or have these been retrieved in a preceding step?

Response: This is a good point. We added text to describe the retrieval sequence and the full list of retrieved species in section 1. As surmised by the reviewer, there are additionally retrieved species, like surface emissivity, surface temperature, and cloud properties that are retrieved in combination with the trace gases of interest.

p 1264 l 5: "A is the averaging kernel"; I suggest "...averaging kernel matrix" (c.f. Backus and Gilbert, 1970, or Rodgers 2000). I suggest bold face A also in the text.

Response: These changes were made. The "A" in the original manuscript is bold faced following Equation (1); we will ensure that it is bold in the proofs.

p 1264 Eq 2 and lines 12/13: some sub- or superscripts are missing (at least on my screan and print-out), both with the ˆx and the xa. The current version of the equation certainly is correct (finally: ˆx=ˆx) but trivial.

Response: Thank you for catching this. The original manuscript is correct, but the proof for Equation 2 should have ˆx' on the left side, and the 2nd xa should be xa' on the right side of the equation. Additionally, the text following Equation 2 should read, "where and are the original and new priors, respectively, is the original retrieved value, and is the retrieved value with the new prior." We will ensure that this is corrected in the proofs.

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By the way: while the formalism of the transformation chosen here certainly is better suited for implementation, and is fully consistent with the concept introduced by Eq. 1, the equivalent transformation given by Rodgers (2000; Inverse Methods for... Eq. 10.48) might be more instructive for readers less experienced with the averaging kernel formalism. The post facto transformation as formulated by Rodgers (2000) can be understood without involving the averaging kernel representation of the retrieval, just on the basis of weighted means. Mentioning this representation may help to address a wider readership.

Response: Although Equation 10.48 in Rodgers (2000) is more generalized, as it allows exchange of the constraint matrix as well as the a priori vector, the Sˆ-1 matrix in Eq. 10.48 is not included in the TES products, whereas the averaging kernel is included in the TES products. Since it is not possible to use Eq. 10.48 with TES products, we do not feel it would significantly add to the paper to mention Eq. 10.48 in the paper.

Another issue: Eq. 2 assumes that the old and the new a priori information are characterized by the same statistics, i.e. that the related Sa matrices are identical. Most times this assumption may be - at least in approximation - valid, but I think this issue deserves some discussion.

Response: This is a good point. The following paragraph was added following Eq. 2:

"Additionally, the reader should be aware that the choice of prior will affect the predicted error in the retrieval through the smoothing error component, which depends on the a priori covariance matrix. The a priori covariance matrix is the expected covariance between the prior and the true state; if the global mean is chosen as the prior, the variance between the prior and the true state will increase as compared to choosing a more accurate prior that depends on latitude and longitude. It is apparent in Figs. 1 and 2 that the errors in the estimated state are much larger for the globally uniform prior than for the original prior, especially in the polar region where sensitivity is less and the prior has changed a great deal. The increased errors will be the same whether

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the profile was retrieved non-linearly or estimated using Eq. 2."

Method: The chosen analysis method is clearly documented. The chosen approach is appropriate. p 1265, text after ordered list (lines 15-18): I would expect SSC and SU to be equivalent only in the linear case; further I would expect SS and US to be equivalent only if full convergence is achieved (the latter seems to be an issue, c.f. differences in data versions v003 and v004). How is convergence of a log(VMR) retrieval defined in cases when the signal would - due to measurement noise - require a negative VMR? Could it be that this issue has something to do with the "non-global minimum issue" discussed later?

Response: Yes, the differences between SS and US is suspected to be from non-convergence to a global minimum. The following clause was added to clarify this, "Similarly, datasets SS and US should be equivalent since, as seen in Eq. (1), the initial guess should not impact the final answer, assuming convergence to the global minimum is achieved."

Response: If the global minimum for radiances occurs at negative VMR, it would cause the convergence location to rely on strength of the penalty imposed by the a priori information. Retrieving with a different prior should shift the penalty in a predictable way and the convergence location would vary in a predictable way. The concern is whether the old and new convergence locations have the same sensitivities, and if so that differences can be linearly predicted using Eq. 2. If the sensitivity increases with increasing retrieved value (which is true, except as the reviewer points out, for saturated lines), then larger changes in the prior would cause larger errors in the prediction by Eq. 2. However, it appears that the new answer is scattered around the predicted new answer, with no correlation to the direction of change of the prior. From the results of varying the initial guess, which have no theoretical impact on the convergence location, which results in the same sort of scatter, it seems most likely that the retrieval converges to a non-global minimum due to instability in the retrieval in some cases. It seems likely that the sheer number of retrieval parameters-130 for the joint TATM,H2O, O3,

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EMIS, TSUR, cloud retrieval step-could be responsible for the retrieval converging to local minima in some cases, or systematic or other errors could also be responsible, as discussed in the text.

Response: Text was added to section 3.1.1 to clarify the findings that the change in the prior is not likely causing the errors of the predictions by Eq. 2, "For the mean difference, the slope indicates if changes in the prior are correlated with the error in Eq. 2 predictions. If a positive slope is found, it would indicate that sensitivity is significantly increased at the new convergence location compared to the old location when the change in the prior is positive. The slope of the mean difference was found to be -0.02."

p 1265 l 13: The term Jacobian, while certainly known by most retrieval scientists, is not defined in this paper, particularly because the formalism used here does not explicitly involve the Jacobian. I suggest to avoid this technical term here and to argue in terms of 'relative sensitivities of the signal w.r.t. ...' instead. This will make the paper better accessible to a wider readership.

This change was made. The sentence now reads, "This gives an indication of the relative sensitivities of the signal to the trace gas profile amounts, and whether the error analysis is cross-applicable."

A general issue w.r.t. Section 2 (See also general comment to Section 1): Beyond the target variables (i.e. the profiles of the target species), often further variables are included in the vector x (e.g. further atmospheric state variables or instrument characterization variables). Is this also the case with TES retrievals? If so, it should be mentioned, and this issue then deserves some discussion, because this adds complication to the use of Eq. 2. I am asking this, because many space experiments (ATMOS, MIPAS, ACE-FTS...) make use of 'joint-fit variables'.

Response: A paragraph was added in section 1 describing the full set of variables retrieved at each step, and the ordering of steps. Some sentences were added following

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Eq.2 to describe the effects of retrieving more than the trace gas of interest on Eq. 2. "In the case of TES, the retrieval vector includes not only the trace gas of interest, but also surface and cloud properties, and for the ozone retrieval, also water and temperature. When is modified for only the trace gas of interest, Eq. 2 shows that the propagation to for the trace gas of interest is the same whether the full retrieval vector is considered or whether the matrices and vectors in Eq. 2 refers to just the trace gas of interest."

Results: The results are presented in a traceable way and are thoroughly discussed. p 1266 l 16: It is not clear to me why the Run ID is quoted, because it is not referred to later in the paper.

Response: This run ID was referred to provide complete information to the reader regarding the data that was used in the analysis. However the date also uniquely identifies the data used so the run ID was dropped so as not to confuse the reader.

p 1266 l 16: 'target' is a very generic term. Wouldn't 'nadir' or 'subsatellite point' be more specific?

Response: The word "target" was changed to "nadir observation": "The TES nadir observation locations are shown..." "Target" was replaced by "Observation" everywhere else that it occurred.

p 1267 l 13: I do not quite understand what 'enhancements seen in the prior' mean. Meant: 'enhancements seen in the results after conversion of a priori'? Or 'regions where gas amounts were enhanced both in the original prior and the standard retrieval?'

Response: This wording was changed to be less confusing, "Poleward of 60N, patterns seen in the original prior and the standard retrieval are absent, indicating that TES retrievals are insensitive in those regions."

p 1268 l 9ff and elsewhere: since the effect of the quality flags is discussed here, it

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would be nice to know what the quality flags are based on, e.g. _2, or whatever.

Response: Sentences were added to describe the quality flag components. This was added to the new section describing the retrieval steps in section 1, "After each step is completed, the retrieval is assessed as to whether it has converged. Some of the quantities which are calculated and compared to thresholds are the radiance residual and mean, changes in the retrieved surface temperature or emissivity, the amount of signal remaining in the residual; and other known issues (Osterman et al., 2006). A master quality flag, speciesRetrievalQuality, combines the checks into a single quality flag, and is written to the TES product files."

p 1269 l 9ff: Here the authors expect that a large a priori change would lead to a breakdown of the linear transformation (Eq. 2). It should be noted that a moderate a priori change in a situation of a saturated emission line can also lead to the breakdown. In other words: the amount of the a priori change is not an unambiguous criterion for linearity, i.e. for applicability of Eq. 2.

Response: This statement was weakened from, "The lack of bias indicates that the differences are not a function of the choice of the uniform prior." to, "The lack of bias suggests that the differences are not a function of the choice of the uniform prior; further testing with a globally uniform initial guess in the next section strengthens this conclusion."

p 1269 l 17ff: This statement seems ambiguous to me: Do you mean "mean that a prior's change of less than 10% will end up as unbiased fluctuations..." or do you mean "10% of (each) prior's change (regardless how large it is) will end up as unbiased fluctuations (while the other 90% will cause a bias?)"? Or anything else? The first way to understand the statement seems to make more sense, but the second seems to be closer to the original text.

Response: Thanks for pointing out this ambiguity. This statement was clarified to, "Together these results mean that the error in the answer will be less than 10% of the

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prior's change, and will be unbiased with respect to the prior's direction of change."

p 1270 l 22: Is there any justification for the averaging kernel threshold of 0.04, or is this an ad hoc decision?

Response: This is an ad hoc cutoff which cuts out about half - the least sensitive half - of the data. The text now clarifies this, "...so statistics were calculated for only those points with a corresponding averaging kernel diagonal value of 0.04 or greater (retaining only the most sensitive half of the data)"

Conclusion: The conclusion is fully supported by the results section. A summarizing statement (such as lines 12-14 of the abstract) may help to get the main message without getting lost in details.

Response: The first sentence of the conclusion was changed to better mirror lines 12-14 of the abstract, "Linearly converting the prior following a non-linear retrieval is shown to have a minor effect on the TES trace gas retrievals as compared to a non-linear retrieval using a uniform prior, when compared to the expected total error."

Technical corrections: Since English is not my native language, I am not quite sure if my comments on wording and grammar issues are correct. Title: Since 'Impact' is specified ('of nonlinearity...') shouldn't it read 'The impact'?

Response: It seems like most other ACPD titles do not have the initial article, e.g. "Contribution of very short-lived organic substances..." rather than "The contribution of very short-lived...", "Assimilation of stratospheric and mesospheric temperatures..." rather than "The assimilation of...", "Seasonal variations in aerosol optical properties over China". Perhaps the Editor can advise.

Title: I suggest to use either a compound noun ('trace gas profile estimates', 'profile' singular) or a genetive plural (with an apostroph: 'trace gas profiles' estimates')

Response: Title changed as suggested, to, "Impact of nonlinearity on changing the a priori of trace gas profile estimates from the Tropospheric Emission Spectrometer

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(TES)"

Abstract l 7: examine (remove ’s’)

Response: Wording changed.

Abstract l-2: remove blank between ’10%’ and ’of’

Response: This is an error in the proof but not in the submitted manuscript; will check proofs.

p 1263 l 6: ’which’ ! ’who’ p 1263 l 8: ’which’ ! ’who’ p 1263 l 9: ’which’ ! ’who’

Response: Wording updated as suggested.

p 1263 l 16: I suggest blank before and after dash, before ’2260 cm-1’

Response: There are blanks in the submitted manuscript but not in the published ACPD paper; will check proofs.

p 1269 l 20: remove ’the’ (third word).

Response: Wording changed.

Thank you for the detailed comments and suggestions.

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