

Interactive comment on “Potential for the use of reconstructed IASI radiances in the detection of atmospheric trace gases” by N. C. Atkinson et al.

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The authors would like to thank the referee for the comments. These are reproduced below, along with the replies.

My main concern is with the generality of the conclusions drawn here. The authors only consider detection of trace gases (not retrievals) as stated in the title of the paper. Therefore, the authors should be more cautious in the abstract and conclusion before giving general conclusions concerning the use of PC scores for chemical and climate purposes: their results might be promising in terms of detection, but the lonely retrieval case presented here - without details on the retrieval procedure and with somehow limited results, is not sufficient to fully grasp the impact of using PC scores. Only a few case studies are presented, when a much longer trial and evaluation period, over all

seasons and areas, would be needed before judging the merits of using reconstructed radiances for chemistry and climate applications. The authors should try to present their arguments for what they are, without overselling their results.

REPLY: This study is a first step, and we will ensure that the text contains appropriate caveats and recommendations for further work.

Referring to the chemistry and climate community, the authors state “there is a concern that the signatures of trace gases may not be retained in the reconstructed spectra”. One of the major concerns of this community is indeed that the signatures of trace gases may not be retained in the reconstructed spectra. This question is partially addressed in this paper. However, this is by far not the only worrying point. Most pressing questions are: -To what extent are the signatures entirely retained in the reconstructed spectra, especially for weak signatures? -What would be the impact of using PC scores on both the precision and the accuracy of trace gas retrievals?

REPLY: We agree that these would be appropriate subjects for further studies.

Another major concern is what is called noise reduction: in a PCA, the diagonal noise is indeed reduced, but to the cost of increasing off-diagonal terms, something that could be seen as “noise spreading”. -In terms of retrieval, and not only detection, most techniques take advantage of the correlation existing between channels. This correlation will certainly be affected by the compression and will certainly depend on the training set used to compute the eigenvectors. These points should be mentioned and addressed in the paper.

REPLY: We feel that the referee’s comments are misleading as they imply that there is no real reduction in noise. This issue is addressed in some detail in the IASI Frequently Asked Questions (FAQ) page on the EUMETSAT web site (<http://www.eumetsat.int> Home > Access to Data > Metop & NOAA Services > Global Data Service > IASI). A reference to this document will be added. In brief, random (uncorrelated) noise will be spread evenly across all PCs, and will therefore be reduced by virtue of the fact that

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only the low-order PCs are retained. The remaining noise does show inter-channel correlations, as stated by the referee, and the noise covariance may be calculated according to $\mathbf{NEE}^T \mathbf{N}^{-1} \mathbf{RN}^{-1} \mathbf{EE}^T \mathbf{N}$. This noise covariance may, if required, be provided as input to retrieval schemes. For further discussion of correlated noise, see Hilton and Collard (2009).

Many trace gases (CO₂, CH₄, N₂O, etc) are characterized by strong seasonal cycles. Any compression scheme should thus be evaluated over at least one year, and periodically checked to account for any evolution of the instrument or of the atmospheric state. Accordingly, the IASI Sounding Science Working Group, which is the scientific advisory body to both CNES and EUMETSAT for all matters related to IASI, recognized that any set of eigenvectors “needs to be tested over a long time period (of order one year), in order to evaluate the impact of the data truncation on the user services. There is a risk that the data truncation based on a distinct threshold will be rejected and that a truncation of the data with a new threshold will have to be tested for another trial period, with an unpredictable outcome.” Such a statement should be added in the paper.

REPLY: Agreed. This point will be covered in Section 5 (discussed further below).

The paper strongly lacks a detailed description of the technique used to compute the principal components. Section 2 describes the general methodology but the authors do not explain how they adapted it to process IASI data. In particular, what noise normalisation matrix did they use? Did they work on apodized spectra? How was the scanning angle taken into account? Were the eigenvectors generated for each angle or not?

REPLY: We will include the following information in Section 2: “Set 1: Used de-apodized radiances. The noise normalisation was the RMS reconstruction error after an initial set of PCs had been generated using a CNES pre-launch noise covariance. Set 2 & 3: Used apodized radiances. The noise normalisation was the CNES post-launch noise covariance. In all three cases a random selection of scanning angles was

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used.”

A general description of the characteristics of IASI instruments (3 spectral bands, spectral and spatial resolutions, number of FOVs, etc) should be given at some point and linked to the choices the authors made to compute the principal components.

REPLY: A general description of IASI will be added to Section 1.

The choice of the eigenvectors is quite mysterious, and not clear at all for the average reader. Some information should be given on the way the training sets and the number of eigenvectors have been chosen. This is particularly true for sets 2 and 3, since neither reference nor detail is given for them.

REPLY: This point was also raised by referee #1. We will add an explanatory paragraph: “For sets 2 and 3, the optimal number of PCs was selected for each band by plotting the PC score spatial correlation as a function of eigenvector rank, as described in Atkinson et al. (2009). Low-order eigenvectors show high spatial correlation as they mainly represent atmospheric structure, whereas high-order eigenvectors show low spatial correlation as they are dominated by random noise. In the case of Set 1 a simpler method was used: a plot of the eigenvalues was examined and PCs were selected up to the point where the slope of the curve stabilised.”

Concerning set 4, described in Section 4, some precision on the iterative selection of outliers should be given to fully grasp how the set is built.

REPLY: We feel that the level of detail described in this paper is sufficient to give most users a good general understanding of the processes used by EUMETSAT to select outliers. If some users require more details then it is hoped that this would be covered in the EUMETSAT operational documentation. The Product Validation Report might be a natural place to include information about the choice of training set, noise normalisation and number of scores used for the generation of the eigenvectors.

Since it is said that this set works better than the 3 previous ones, results obtained with

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this set should be presented (at least in terms of score) for all the cases studied before. This is particularly the case for SO₂ since the authors claim in Section 3.2 that set 4 improves the residual structures found with set 3, but do not refer to it at all in Section 4.

REPLY: We agree. We will include a plot showing the residual structures with Set 4, for the SO₂ case.

Concerning the figures, I find it particularly hard – and dangerous, to only compare raw radiances in one panel with reconstructed radiances in another. A better way to present the results would be to plot the differences between raw radiances and reconstructed radiances. This would reveal to what extent the intensities of the plumes are similar, and the denoising of the radiances would be highlighted.

REPLY: On the contrary, we feel that raw and reconstructed radiances are easier to interpret than reconstruction errors, which is why the initial plots are of radiance or brightness temperature. For example, in Figure 1 it is clear that the set 3 reconstruction gives a similar intensity to the raw radiances, with lower noise. Later in the paper, reconstruction scores are shown (Figures 7 and 13).

Specific comments

Abstract

p. 502, l. 7: “the technique can also be used to generate reconstructed radiances in which random instrument noise has been suppressed.” This is an overstatement. The noise is reduced to some extent, but at the cost of spreading the noise from diagonal terms to off-diagonal terms and changing the correlation between channels.

REPLY: This point has been addressed in the general comments. We have used the word “suppressed”, meaning “reduced” – not “eliminated”.

p. 502, l. 17-19: Some features of the chemical signatures are retained in the reconstructed radiances, but it is not clear from the results presented in the paper, to what

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extent the whole signatures are actually retained. Even a slight under/over-estimation could have huge impact on the precision and accuracy of the retrievals based on these signatures.

REPLY: We will change this phrase in the abstract to “key features of the chemical signatures are retained”.

p. 502, l. 22-23: “The paper describes the generation of the reference eigenvectors for this new service.” Since this paper aims at being the reference for one part of the new EARS-IASI service, the generation of the eigenvectors should be more described in Section 4 (see above).

REPLY: This point has been addressed in the general comments. The best place for detailed information on EARS-IASI would be in the EUMETSAT operational documentation.

Introduction

p. 503, l. 14: could the authors specify whether the same subset of channels is used by all NWP centres or not, and, if not, what the differences are? In case these NWP centres used principal components, would they use the same set?

REPLY: Details of the channel selection are outside the scope of this paper. But in reply to the question, most NWP centres use channels selected either from EUMETSAT’s 314 channels or from NOAA’s 616 channels. The pilot EARS-IASI data will include both PC scores and a channel selection (as stated in Sect. 1 – we will add that this will comprise 366 channels). If the use of IASI reconstructed radiances gains acceptance in NWP, then the expectation is that centres would all use the same PCs. But note that any scheme that assimilates PCs directly will *not* use the EUMETSAT PCs: a matrix transformation would be necessary, whether starting with raw radiances or EUMETSAT PCs.

p. 503, l. 17-24: MACC is the atmospheric service of the European GMES pro-

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gramme. Therefore, the sentence should be modified according to: “: : in the context of the international efforts under the Global Monitoring for Environment and Security (GMES) initiative, in particular through its atmospheric service designed in the framework of the Monitoring Atmospheric Composition and Climate (MACC) project (<http://www.gmesatmosphere.eu/>).”.

REPLY: Accepted. The text will be changed.

p. 504, l. 9-12: the authors present the use of principal components as unavoidable. Another possibility to distribute IASI data would be to increase the bandwidth of the communication channels, or to distribute a reduced subset of channels selected by the users.

REPLY: We will make the point that bandwidth costs money, so data transmission methods that reduce unnecessary data (i.e. data that contains no useful information) are always of interest to us. Furthermore, the use of PCs has been decided by the EUMETSAT delegate bodies: a parallel stream of PC-compressed global MetOp-A IASI data is due to start in mid-2010, and the pilot EARS-IASI service will also use PC-compressed data.

p. 504, l. 18: “This could occur if the trace gas signal is very weak (significantly below instrument noise level)” This question has not been addressed in the paper, the authors focusing on rather strong signals; usually well above the noise level. A comment should be added on the performance of PCA for weak signal which are of the same level as the noise (as it is the case for CO₂ or N₂O for instance).

REPLY: We would not describe ammonia signals as being “rather strong”; to generate an accurate ammonia climatology currently requires extensive averaging of the data. We have not looked at CO₂ or N₂O, and will mention this as an area for further study.

p. 505, l. 2-6: as explained in Razavi et al., 2009, the nu3 band MAY add information on CH₄ but only in specific conditions. The sentence should be rephrase accordingly.

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REPLY: Accepted. The sentence will be re-phrased.

Section 2: PC methodology

p. 506, l. 20: what represents location i ?

REPLY: We assume the reviewer is referring to page 505. Subscript i just means the location of a particular IASI observation, as stated.

p. 506, l. 3-4: “To simplify the computation, the noise normalisation matrix is usually assumed to be diagonal.” Is it the case here? What is the reference for this matrix?

REPLY: Yes, it is assumed diagonal. Revised text has been given in an earlier reply.

p. 506, l. 25: a brief description of the three bands of IASI should be given.

REPLY: This will be added to Section 1.

p. 507, l. 10: it would be helpful to explain what an elevated or particularly low value of a Reconstruction Score mean.

REPLY: We propose to add the following explanatory text: “In qualitative terms, a value of R much greater than 1.0 implies that the reconstruction is not fitting the raw spectrum to the expected level, whilst a value consistently less than 1.0 implies that the assumed noise is greater than the actual random noise”.

Section 3.1: Detection of ammonia

Fig. 1 and 2: could it be possible to indicate on Fig. 1 the spots used to plot Fig. 2?

REPLY: We will add this information to the figure.

p. 508, l. 18-21: “we conclude that the inability of set 1 to detect the ammonia signal is due primarily to a lack of significant ammonia episodes within the relatively small set 1 training set” This is quite an important comment, which shows a weakness of the methodology: as in any compression/retrieval scheme, the training dataset is a crucial element. If some events (here, signatures of key elements) are missing, the com-

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pression will fail. In case that some signatures appear to be missing (especially from unexpected species – let’s remind here that one of the biggest discovery made from IASI observations was the ability to detect new species that were generally thought to be out of reach), a new dataset will have to be generated and tested. This should be included in the discussion.

REPLY: The advantage of using real spectra as the training set is that unexpected species will automatically be included. It is not necessary to identify these species before computing the eigenvectors (as would be necessary if forward-modelled radiances were used). We believe that the methodology is robust – and have shown the importance of iterative refinement of the training set. We accept that the current set training set may not include the signatures of all possible trace gases, and will make the point that when specific cases of outlier emission are identified, they should be added to the training set and a new eigenvector set should be generated and tested.

p. 509, l. 2: what are the reconstruction scores obtained in band 1 with sets 2 and 3 and how does it compare with the reconstruction scores obtained with set 1?

REPLY: We will replace the sentence beginning “Clearly the inclusion . . .” with the following: “When analyzed using *set 3*, the peak reconstruction score dropped to 1.2, confirming that the inclusion of these spectra has added an ammonia signal to the eigenvectors (though the residual is still somewhat elevated compared with neighbouring spots). For reference, the peak reconstruction score for *set 1* was 4.6.”

p. 509, l. 3-4: “Clearly the inclusion of these outliers is adding an ammonia signal to the eigenvectors.” This sentence is quite vague and leads to the question of how big the added ammonia signal needs to be to add enough information in the data sets. Could it be possible to detail more carefully what is the level of detection that is achievable with IASI using raw radiances or reconstructed radiances?

REPLY: See previous reply. A quantitative assessment of the detection ability for ammonia is beyond the scope of this study. What we have shown is that for specific cases

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the ammonia signature is detectable in both the raw radiances and the reconstructed radiances, with lower noise in the reconstructed radiances.

Section 3.2: Detection of volcanic SO₂

Could the authors provide some insights on the reasons for an overestimation of SO₂ with set 2?

REPLY: This point was also raised by Referee #1. We would speculate that the training set 2 contains some low-level SO₂ content, but with poor signal to noise. So when a high SO₂ situation is encountered the errors are amplified. But we would not wish to put anything definitive in the final paper.

Section 3.4: Retrieval of carbon monoxide

The results presented in this section are particularly hard to evaluate since the retrieval scheme is not detailed, nor even published. Details on the retrieval methodology should be given here (prior information, covariance matrices, spectroscopic databases, etc).

REPLY: We propose to add the following text in Sect. 3.4 (together with additional references): “The University of Leicester IASI Retrieval Scheme (ULIRS) has been developed at the University of Leicester to specifically retrieve CO from IASI measured Top of Atmosphere (TOA) radiances, utilising an Optimal Estimation Method (OEM) (Rodgers2000). As with any OEM it makes use of an a priori profile and covariance matrix to restrain the ill-conditioned nature of the retrieval problem. The ULIRS utilises the Oxford RFM as a forward model, which itself is based on the line-by-line model GENLN2 (Edwards, 1992). The CO a priori profile and covariance matrix have been constructed using over 8000 profiles from the TOMCAT CTM (Chipperfield, 2006), which incorporate a wide variety of CO scenarios, and the retrieval scheme makes use of the spectral interval 2143–2181 cm⁻¹, for reasons outlined in Barret (2005). The ULIRS utilises a spatially precise surface elevation and emissivity (Seeman, 2008), as well as incorporating a quantified back-scattered solar radiation component into the

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retrieval process. More details of the ULIRS can be found in Illingworth (2010), which is currently in preparation.”

The choice of the covariance matrices is particularly crucial in such an approach, since retrieval methods based on the so-called optimal method make use of the correlations existing between channels. Now, using principal components changes the covariance between channels. Therefore, the authors should indicate how they dealt with this issue.

REPLY: The purpose of the paper is to verify that reconstructed radiances can be used as raw radiances without damaging results to any great extent, and so they have been used as a direct replacement in the tests without modifying the procedure at all.

Fig. 10: it would be interesting to add the noise level on the right panel to see how the BT difference compares to it.

REPLY: We assume the referee is referring to Fig. 9. The noise level will be added.

p. 511, l. 21-25: “The differences between raw and set 3 radiances produce differences in retrieved values which are generally less than 25-50% of the retrieval error.” The typical retrieval error should be indicated, to give a feeling of what 50% of the error stands for in ppb.

REPLY: The mean retrieval error was 24.4% of the total column, with a standard deviation of 3.4%. This will be added to the text.

A striking feature displayed in Fig. 10 that is not addressed in the text, is the shape of the distribution of the error. It seems that there is a negative bias of about -20%, with an associated standard deviation of 25%. Could the author comment on that bias? What would be the implication of such a bias on the retrieved fields?

REPLY: We assume the referee is referring to Fig. 11. From a one-off case study we do not attribute any significance to the apparent small negative bias. We will mention that further studies would be needed to assess whether there are any statistically significant

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biases between retrieved CO amounts for raw/reconstructed radiances.

pp. 511-512: “In both cases, the residual fit is within the instrument noise across the spectral region, indicating that the principal component compression has had no major effect on the behaviour of the retrieval scheme.” This statement seems particularly misleading to me and should be rephrased. As already said, PCA decreases diagonal noise but increases off-diagonal terms of the noise matrix and changes the correlation between channels. Therefore, random noise has been traded for a reconstruction noise with specific characteristics that could influence the results.

REPLY: We do not see that this statement is misleading. The experiment tested direct substitution of reconstructed radiances for raw radiances in the retrieval scheme, keeping everything else constant. The figure and text compare the residual fits with the raw instrument noise (same in both cases). We will ensure that this is made clear in the text.

Section 4: Further refinement of the eigenvectors

p. 512, l. 8-9: “The previous section has shown that the set of eigenvectors generated through the addition of outliers to the initial training set generally performs well.” This is overstated – it has been shown that some features could still be detected, but with no quantitative evaluation of the level of agreement.

REPLY: We will change the text to: “The previous sections have shown that by adding outliers to the initial training set, the resulting reconstructed radiances retain qualitatively many of the trace gas features observed in the raw radiances, for these case studies.”

Section 5: Conclusions

As said previously, the conclusions seem rather optimistic and definitive, despite all the questions that remain to be addressed. Here is the wording I object to: p. 513, l. 23-24: “and additionally reduces the amount of random instrument noise in the reconstructed

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spectra considerably” As explained before, the noise reduction has undesirable effects that should also be given here.

REPLY: We will change this to “and additionally reduces considerably the overall amount of instrument noise in the reconstructed spectra. Random noise is much reduced, though there is an increase in correlated noise.”

p. 514, l. 9: “However, an iterative procedure, involving refinement of a base training set by the addition of outlier spectra, is successful.” I would prefer the wording: : : : by the addition of outlier spectra, helps improving the residuals.

REPLY: We will change this to “However, an iterative procedure, involving refinement of a base training set by the addition of outlier spectra, is successful in improving the residuals, such that there is good qualitative agreement between raw and reconstructed spectra.”

p. 514, l. 10: “will be used in the EARS-IASI system”. It should be clearly said that the training set will need to be 1) fully tested by the community; 2) refined on a regular basis to account for unaccounted signatures or for any evolution of the instrument of the atmospheric state.

REPLY: We will change this to “will be used in the pilot phase of the EARS-IASI system and in the trial parallel dissemination of PC-compressed global IASI data. The performance of the scheme will need to be fully tested by the IASI user community. Updates to the eigenvectors may be needed in the future if deficiencies are found in the training set, or if there are changes in the instrument characteristics, ground processing or atmospheric state.”

Interactive comment on Atmos. Meas. Tech. Discuss., 3, 501, 2010.

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