Atmos. Meas. Tech. Discuss., 3, C2968-C2975, 2011

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## Interactive comment on "An effective method for the detection of trace species demonstrated using the MetOp Infrared Atmospheric Sounding Interferometer" by J. C. Walker et al.

J. C. Walker et al.

walker@atm.ox.ac.uk

Received and published: 31 March 2011

## 1 Replies to general comments

We thank the referee for their comments which we have found very useful.

RC: "The channel selection technique appears to be a powerful tool, and it is well presented. However, in the case studies all the channels in very broad bands are selected, which could have been done with just a quick examination of the spectrum; this rather weakens the demonstration of the technique".

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AC: The important thing is not the channel selection itself, but that the total measurement error covariance is well characterised, and enough channels have been used so that there is adequate information about all parameters which affect the measurement of the target species. Channel selection using this method is not the standard problem of avoiding channels which have a detrimental impact on the retrieval of the target species since using this method even channels which contain only contaminant contributions can contribute useful information by fixing the baseline. Therefore, channel selection is only a matter of efficiency, excluding channels which add negligible information, and is not strictly necessary. We found that broadband spectral regions work well in the case studies examined and further refinement of the channels was not needed. The insensitivity to the actual channels selected is an advantage for the operational user. A discussion about channel selection is included only as a check on information content of the channels chosen by eye. This is made clear in the revised paper and that section is renamed "Validation of channels".

RC: "the authors should expand the conclusion section with a discussion of the applicability of their methods and on the possibility of future work that would provide more quantitative retrievals".

AC: The authors have added a discussion of these issues in the amended paper. The main advantage of this method is that once the detection weights are derived, it is very fast and easy to apply to large datasets such as IASI where full retrievals would be very time consuming. In addition, false detections can be suppressed very effectively. The method may be useful in near-real-time applications such as the detection of volcanic  $SO_2$ , or to quickly scan large datasets for events of interest for further analysis. This is now mentioned in the conclusions. With regards to the possibility of more quantitative analysis, it would only be possible to provide a rough estimate the actual column amount, and only in circumstances where the shape of the profile is known to some degree, where radiative transfer is linear, i.e., in the weak absorption limit, and where the thermal contrast with the surface can be estimated, in cases where the surface is

visible. This is the case for NH<sub>3</sub> the profile shape is roughly known and absorption is weak. In fact, column amounts of this species have been estimated before using empirical detection methods by Clarisse et al. 2009 using a less sensitive filter. For this species, the main problem is likely to be thermal contrast with the surface, which can greatly affect the apparent concentration. This was identified as probably leading to differences in the estimated ammonia column between day and night, judging from the ammonia concentrations already derived in other studies for the same scene over the Indo-Gangetic Plane. In future, it may be possible to perform an improved estimate of the ammonia concentration by correcting for thermal contrast conditions using information from ECMWF data to scale the column. Because of the large uncertainty on the altitude distribution of a volcanic plume, a reasonable quantitative estimation of the column amount would probably not be possible without a full retrieval.

RC: "Page 4526, Line 16: Please justify how errors in the profile shape can be ignored".

AC: Uncertainties about the profile shape are only significant for volcanic  $SO_2$  which could have a peak of variable size at any given altitude. The shape of the assumed profile affects the column amount retrieved, but fortunately this is not expected to be accurate in a detection only method, so the profile shape can be considered an arbitrary parameter. This is the main reason why it would be difficult to extract any quantitative information about volcanic  $SO_2$  using this method.

## RC: "Page 4538, Line 8: Please explain how correlation in the covariance matrix suppresses systematic errors".

AC: The theoretical basis for this is explained in detail in the paper by von Clarmann, 2000. In a retrieval of a given parameter, measurements are typically only weighted according to the random noise error. However, as well as instrument noise, there are also errors arising from differences between the assumed forward model parameters and the physical radiative transfer process. These errors tend to be spectrally correlated whereas the error due to random instrument noise is only locally correlated. For

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a single target parameter, if the inversion is weighted by only the random error due to measurement noise, then the solution is not optimal because the systematic errors due to uncertainties in the forward model such as underestimating a contaminant, are not accounted for. Sometimes these errors are small enough to be ignored (not the case here). Otherwise, other uncertain parameters can be retrieved jointly with the target parameter increasing the size of the state vector to obtain an optimal solution. However, as explained in the paper by von Clarmann, 2000, in the linear regime, an equivalent optimal solution can be obtained without increasing the size of the state vector, but instead weighting the measurements according to the total error, including forward model errors. The diagonal elements of the  $S_y^{\text{tot}}$  matrix containing the total random and systematic error weight the spectral points appropriately, assigning less weight to points with a large total error. Now, in the case of  $SO_2$  where uncerainty in the water vapour concentration is a significant problem, instead of just weighting by random error, where each point essentially receives an equal weight, a point with a large uncertainty about water vapour is weighted less than a point with low uncertainty about water vapour. The long range correlations between the spectral points contained in the  $S_{u}^{\text{tot}}$  matrix, which arise from the forward model errors, then provide additional information about the expected behaviour of one spectral point relative to the others. Physically, correlations in  $S_y^{\text{tot}}$  mean that a spectral point with very little signal about SO<sub>2</sub> (and in our method, even zero SO<sub>2</sub> signal) can still add significant information about the target species because it helps to fix the baseline at other spectral points against which  $SO_2$  is determined. In the linear regime, a joint retrieval of all parameters affecting the measurement would achieve the same effect. For the retrieval of the target species, the suppression of errors in this way can be confirmed by comparison of the target retrieval error for the optimal inversion  $G_{tot}S_y^{tot}G_{tot}^T$  (where  $G_{\text{tot}} = (K^T S_y^{\text{tot}-1} K)^{-1} K^T S_y^{\text{tot}-1}) \text{ against the non-optimal case } G_{\text{rnd}} S_y^{\text{tot}} G_{\text{rnd}}^T \text{ (where } G_{\text{rnd}} = (K^T S_y^{\text{rnd}-1} K)^{-1} K^T S_y^{\text{rnd}-1}).$ 

RC: "Page 4544 Line 11: Provide the typical SO2 signal value".

AC: The typical signal for SO<sub>2</sub> at climatological levels is well below the noise threshold of the instrument with a signal of around 0.005 K in the  $\nu_1$  band and 0.025 K in the  $\nu_3$  band. These values are now mentioned in the text.

RC: "Page 4547 and following pages provide the value used to normalize to fractional units."

AC: The values are normalised with respect to the maximum values of  $SO_2$  detected inside the plume. These values were difficult to read by eye from the figures in the original paper, and so are now mentioned explicitly in the text for each case in the revised paper.

RC: "*Page 4542 Line 1: Provide a reference for the method (Dudhia et al., 2002?)*" in reference to the channel selection scheme.

AC: A reference is added to the Dudhia et al. 2002 paper for the use of the improvement in information content as a metric to judge whether a certain channel should be included. However, the channel selection problem is somewhat different to the one dealt with in that paper. Channel selection for detection is not the standard problem due to the fact that the total measurement error, rather than just the random measurement error, is used to weight the least squares inversion, which means that the addition of new channels adds information, since strong correlations between channels due to systematic errors mean that even channels where, for example, there is little contribution from the target species, and mainly contributions from interfering species, can add useful information about the presence of the target because it helps to fix the baseline due to the contribution of contaminants in other target channels. Channel selection is therefore just a question of optimising channels for the sake of efficiency, excluding channels which add little useful information, rather than of avoiding channels which could be detrimental to the retrieval of the target species.

RC:"The nu3 SO2 retrieval does not seem generally applicable. Water vapor is too strong an interferent for the modeling method and the ensemble method requires a

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## new filter for every scenario"

AC: Water vapour contamination can still be suppressed very well using the modelling method. The SO<sub>2</sub> detections using this method are about as accurate as current filters. So far, better accuracy than this has not been achieved in the  $\nu_3$  band using the modelling method due to not capturing the variability of the water vapour interference all the way across the band that has contributions from throughout the troposphere, as well as residual errors from changes in radiance due to viewing angle which are not entirely accounted for, also due to the complication of viewing all different levels through the troposphere. In the  $\nu_1$  band, these problems are not present because the atmosphere is optically thin in this region, but the SO<sub>2</sub> emission feature is not as strong, and so again detections are about as good as current filters using the  $\nu_3$  band.

However, it is possible to suppress errors in the  $\nu_3$  band using an ensemble of measured spectra to generate a realistic total measurement error covariance instead of attempting to model all the contributions. Once generated using the ensemble method, the same filter can be reused provided that the ensemble is large enough to capture the statistical variability of the water vapour, cloudiness and temperature signals where the detection is applied. It may even be possible to construct a global filter through consideration of a very large ensemble although the sensitivity would be reduced due to the greater variability encompassed by the ensemble. The statistical properties of the background field change over large distances for example polar, mid-latitude and equatorial regimes, and on the seasonal time scale. In the paper, even the small ensemble used is enough to capture the variability of these parameters, and thereby suppress water vapour, cloud and temperature effects at a distant location. Although some care is needed to ensure an appropriate ensemble is selected, there is no reason why one  $S_u^{obs}$  cannot be used over a fairly large geographical region for an extended period of time as long as the statistical properties of the water vapour, cloudiness and temperature variability are nearly the same. However, for a global  $SO_2$  detection, several different ensembles would probably be necessary e.g., deserts would require a separate filter from equatorial scenes, and seasonal changes would need to be accounted for, essentially constructing a climatology of water vapour, cloudiness and temperature conditions, stored as  $S^{obs}_{\ y}$  matrices. This would be an area for future work and is discussed in the revised paper.

RC: "Page 4550 Line 2: the NH3 band peaks at 967 cm $^{-1}$  not 950."

AC: This has been altered in the text.

In Technical comments:

RC:"Page 4531 Line 6: and "the" spectral background.

AC: This has been corrected in the revised Abstract.

RC: "Page 4535 Line 7: In "that" work, Line 14: "However" is not needed.

AC: Done.

RC: "Page 4538 Line 5: retrieval.

AC: Done.

RC: "Page 4539 Line 20: due "to".

AC: Done

RC:"Page 4542 Line 14: m-2".

AC: Done

RC: "Page 4544 Line 23: Internet reference? Line 28/29: "examine" used on both lines".

AC: Total column amounts for volcanic plumes observed by OMI derived in near-realtime are published on the internet for significant events. A value was not to my knowledge available for this particular day in the published literature for the Kasatochi event, but the values published online are thought in any case to be fairly reliable. A refer-

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ence to the retrieval algorithm used to derive the online values is added in the amended manuscript. Second "examine" replaced by "tested for".

RC:"Page 4546 and onwards (including figure captions): Use 'method' instead of 'case'. Line 21/23: 'however' used on both lines.

AC: Changed.

RC: "Page 4549 Line 25: Move 'on the time scale of days' to the beginning of sentence".

AC: Done.

RC: "Page 4545 Line 1 'if these other parameters have been suppressed' used in close succession. Line 12 "vicinity".

AC: Done

RC: "Figure labels and axes on figures 3 through 9 are very faint and hard to read".

AC: These have been made bigger and bolder in the revised manuscript.

RC: "Figures 10 and 13 captions: A map .... 'is' shown.

AC: Done.

Interactive comment on Atmos. Meas. Tech. Discuss., 3, 4531, 2010.