



EGUsphere, author comment AC2
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Reply on RC1

Joanna Joiner et al.

Author comment on "Use of machine learning and principal component analysis to retrieve nitrogen dioxide (NO₂) with hyperspectral imagers and reduce noise in spectral fitting" by Joanna Joiner et al., EGU sphere, <https://doi.org/10.5194/egusphere-2022-806-AC2>, 2022

We thank the reviewer for their careful review that has helped to improve the manuscript and reply to each comment (repeated below) in bold face.

The paper by Joiner et al. is a carefully, well written paper. It contains interesting results. First of all, it shows that a meaningful retrieval of NO₂ is possible at a moderate spectral resolution of about 5 nm as provided by OCI. Secondly, it demonstrates a neural net PCA approach as a fast way to do the retrievals, an approach with interesting properties. As such I am in favour of publishing these results. However, I have several questions I would ask the authors to address in the final version of the paper.

page 5, line 108: "The conversion of SCD to total or tropospheric VCD can be accomplished in a straight-forward and computationally efficient manner as in current algorithms and is not addressed further here. " Nevertheless, I understand that the largest contributions to the overall error is in the conversion to vertical columns. Information on the clouds, aerosols and albedo is important for this step. It would be of interest to comment if such information is available from OCI/PACE.

Such information will be available from OCI/PACE. We add this to the discussion: "Information about the surface, aerosol, and cloud, such as cloud/aerosol radiance fraction and effective pressure needed for calculation of the AMF (e.g., from the O₂ A band), will be available from OCI itself (Werdell et al., 2019)."

line 158: "independent of radiance value." The cloud-free scenes are the most relevant ones, and these have lower radiance levels than cloud covered scenes. Does this assumption not lead to an over-optimistic representation of the results?

We do not believe that the first SNR model we used (independent of radiance value) produces over-optimistic results for OCI. Compared to the second more refined SNR model based on more recent measurements, the SNRs for the radiance-independent model are overall lower, except when radiances values drop below 50 W/m²/sr/um. We included PDFs of OMI measured radiance in the appendix (Figure A1) that show that for all wavelengths, only a small fraction of scenes has radiances below 50 W/m²/sr/um. The radiance-independent SNR model may be in fact pessimistic as shown by the comparisons with the more refined SNR model (see Figs. 5-6 and Table 2 in the revised manuscript and those in our original manuscript). To avoid confusion, we have removed results with the OCI radiance-independent SNR model and now show only results from

the most recent radiance-dependent SNR model. For GLIMR, we have only a radiance-independent model, but we also now include the most optimistic results for GLIMR with no noise added. In addition, we added "Note that for determination of NO₂ tropospheric vertical columns, cloudy observations are used to help estimate stratospheric column amounts, so that the full range of radiance values is needed, not just clear-sky observations (Bucsela et al., 2013)."

line 172: "The PCA concentrates the spectral features" -> The PCA concentrates on the spectral features

fixed, thank you.

line 275 "nominal"

fixed, thank you.

line 280: "GLIMR, even with no noise, were not satisfactory .. are not shown". I would like to ask the authors to consider to provide them anyway, or add a few lines to table 1 or 2. Linked to figure 1, this would more explicitly show that meaningful retrievals are possible up to 5nm resolution, but that 10nm is removing much of the useful NO₂ information.

We provided GLIMR results with and without noise in Table 2 (the old Table 1) as requested and added text to go along with it.

How does the NN-OMNO₂ RMS compare to the OMNO₂ retrieval uncertainty?

We have provided maps of the fitting uncertainties from the OMNO₂ retrieval in the revised manuscript (Fig. 6e and Fig. 9e) with explanatory text. In comparison with the difference maps, these new uncertainty maps now provide context. In areas of low pollution, the differences are of the same order as the fitting uncertainties. However, in polluted regions, the differences may be larger than the uncertainties.

It seems there is still quite a spread and some systematic effects caused by the NN approach (Fig.4). Please comment and put the results in perspective.

Instead of showing results with the nominal SNR model in Fig. 4, we now show results with the more refined SNR model assuming 4 pixels are averaged (as we expect to do averaging over time and/or space). We also now show the results in terms of normalized slant column (close to the total column) rather than slant column as researchers are more familiar with this quantity. As noted, there is still significant spread and systematic effects (also seen in the figures with maps). The addition of the fitting uncertainties to the figures with maps helps to put the results in perspective as discussed on the previous point.

Data is shown for 28 January over the US, when both the solar angle and NO₂ column amount is relatively high. It would be interesting to show also an example (maybe in the tables only) for the summer to check the seasonality of the differences.

We now provide results in Table 1 (now Table 2) for a summer date as suggested where we removed this date from the training and used it for independent evaluation. In looking at the initial results, we decided to add more training data, so all results have been recomputed using one day each month instead of every other month (plus additional high pollution days) and choosing every third sample. We added a paragraph to explain the results: "Most results in Table 2

are shown for 28 January 2005, a day not used in the training. For comparison, we also show results for a model with all predictors where we withheld data from 15 June 2005 from the training and instead used it for evaluation. On this day, the correlation is significantly lower as compared with 28 January 2005 and root mean squared difference (RMSD) slightly higher. In the northern hemisphere, there are high anthropogenic NO_x emissions generally in populated regions. These emissions lead to higher NO₂ column amounts in the winter when lifetimes are generally longer. The solar zenith angles are also higher in winter than in summer. These factors lead to higher SCDs in winter in the northern hemisphere populated regions than in summer. The higher NO₂ SCDs and variability in the northern hemisphere winter result in higher sensitivities and improved global statistics." We added new results also in Table 2 for the winter month, but for a sample in clean air and saw a similar drop in correlation.

line 313: "generally low bias over highly polluted areas" What is the reason for this low bias? I would expect instrument noise to lead to random effects, not a systematic bias.

There may be systematic errors in the training data that lead the neural network to reduce the fitting errors in a certain way that may lead to spatially dependent differences. It is possible that a separate training could be done and applied for cases of high pollution if we are to completely trust the OMNO2 results. We revised this paragraph to replace the words "error" and "bias" with "differences" as OMNO2 used as the target of the training may not represent the absolute truth. We expanded the mapped area over the US to more clearly show both positive and negative differences that can be spatially correlated. We also added a histogram of the low column amounts over the mapped area that encompasses the US to illustrate a possible noise reduction for these cases as a preview of the additional analysis we conduct later for the tropical Pacific. We added text to describe the additional panels. We also added, "The effect of adding random noise to the spectra causes the neural network to draw less closely to the input data, and the ultimate effect may be to produce systematic or spatially dependent errors as well as random errors."

line 364: "convolved with a 1 nm boxcar function" Could you explain why this is done, instead of using OMI radiances at their spectral resolution?

To assure that we weren't fitting to the noise, we chose to do this convolution. However, the use of leading PCA coefficients should ensure that we are not fitting the noise. As stated in the response to the next comment, we have revised this part to remove the convolution.

Figure 9: It was confusing to me what can be concluded from these plots. Several things were changed: wider spectral range, change of spectral resolution, NN versus standard retrieval. Is the effect due to the wider window, or could the NN procedure cause a lowering of the apparent noise? Is the NN distribution of SCD values more realistic than the OMNO2 one?

We thank the reviewer for this question. To make this aspect clearer, we replaced the previous results with new experiments, now using exactly the same training days as for the OCI simulations. We try to disentangle the impact of using the NN with PCA coefficients as inputs as well as increasing the spectral range and decreasing the spectral resolution. We don't know what the true SCD values or distributions are but based on visual analysis in the clean region shown in Figure 9, we believe that we have reduced the effects of random noise in the original spectra that produced random noise in the retrievals. For example, we have reduced what is believed to be erroneously low values in the lower tail of

the OMNO2 distribution (for example, the unphysical negative values). We added a table (Table 4 in the revised manuscript) that shows the standard deviation of normalized SCDs over the mapped region for the different experiments and reworked this section. The new experiments suggest that it is not the increased wavelength range that produces lower standard deviations or even the spectral resolution, but rather the approach of using leading PCA coefficients as inputs to the NN.

line 403: "could be used for emissions estimates". Most emission estimation methods make use of daily data, basically identifying the plume from a localised source, which then allows the estimation of the source (and these daily values may then be averaged in time). Would monthly-averaged maps be of use for emission estimates?

Yes, averaged maps can be used for emission estimates using for example the method of Liu et al. (2022) as referenced rather than averaging emissions estimates from individual days. We added "based on averaged maps" here to make this clearer.