Dear Editor / Dear Ilse,

Attached are our responses to the review reports.

When editing the manuscript to meet the reviews we took the opportunity to apply a few more technical updates, a list of which is given near the top of the responses to the review reports.

An updated version of the manuscript is uploaded, as well as a "diff" version with changes marked.

Best wishes,

Jos.

**Reply to Comment on egusphere-2025-5836 by Anonymous Referee #1**

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Referee comment on "Improved $NO_2$ spectral fits for TROPOMI and OMI by removing wavelengths around 430 nm" by Jos van Geffen et al., https://doi.org/10.5194/egusphere-2025-5836-RC1

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⟹ The referee report is copied below; the reply is preceeded by an arrow, like this text.

Apart from the changes resulting from the review process, we have carried out the following updates, which do not affect the conclusions of the paper:
– TROPOMI processor v2.9.1, which includes the "NO2-gap approach" of the paper, was activated on 22 November 2025; the text has been updated to represent this fact where appropriate.
– Since we now have a few months of v2.9.1 data, a quick comparison of results before and after the switch is added at the end of Sect. 4.2
– Fig. 2 in Sect. 2.2.2 is extended to include the year 2025; the figure caption was reformulated to improve readability.
– Fig. A1 in App. A is extended to contain the full year 2025.
– Meanwhile the OMI collection 4 $NO_2$ slant column data, named OMNO2A, are released by NASA; the URL of the download access is added to the "Data availability" section. NASA has assigned a DOI to both the dataset and the ATBD: https://doi.org/10.5067/AURA/OMI/DATA2433. Unfortunately, this DOI appears not yet activated; it should likely lead to a landing page such as the one for the collection 4 cloud data (OMCLDO2): https://doi.org/10.5067/AURA/OMI/DATA2407. Hopefully, NASA has activated the OMNO2A DOI by the time the paper is published.
– A few minor textual corrections were carried out.

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The paper "Improved $NO_2$ spectral fits for TROPOMI and OMI by removing wavelengths around 430 nm" by van Geffen et al. describes the improvement of the DOAS retrieval algorithms for the TROPOMI and OMI instruments by disabling a part of the fit-window that reduces the impact of vibrational Raman scattering on the spectral fit quality. The study updates the TROPOMI $NO_2$ retrieval algorithm described in van Geffen et al., 2020 and 2022. The "NO2-gap approach" is analysed for land- and water scenes and the impact on the stratospheric and tropospheric $NO_2$ columns is discussed.

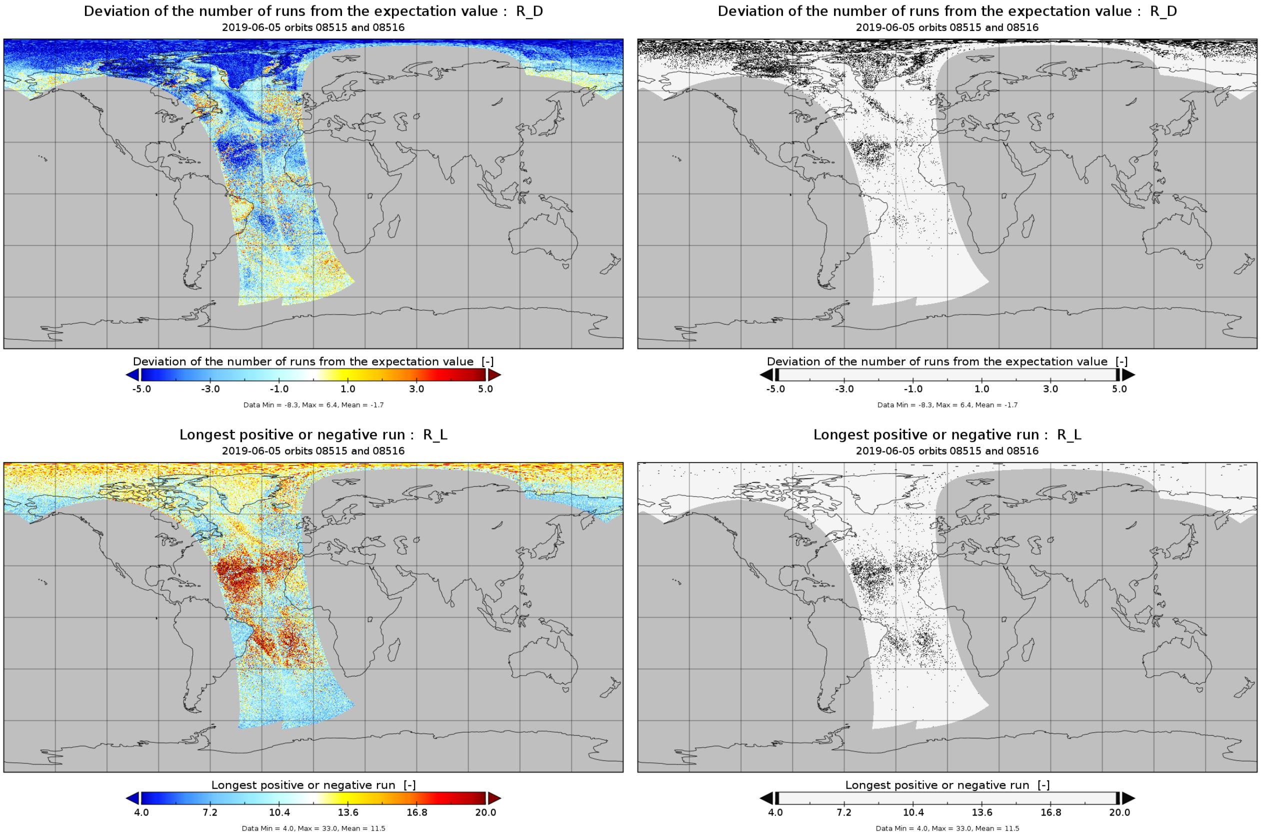
The topic of the manuscript is within the scope of AMT and it is of interest to the scientific community. It can be recommended for publication, if the authors make an effort to address the comments listed below, and improve the manuscript accordingly.

⟹ We thank the referee for these kind words.

**Specific comments**

*Section 1*
The authors explain that the remaining structures in the $NO_2$ fit residual around 430 nm for retrievals over clear-sky dry land indicate that the accounting for RRS effects (by including a Ring spectrum in the DOAS fit) may not be fully accurate. The possible effects of the RRS (besides the effects of VRS over water) are shortly discussed in Section 3. Could these RRS effects be further investigated by applying the TROPOMI DOAS algorithm on simulated reflectances calculated with a radiative transfer model with RRS (e.g. for some specific scenarios)?

⟹ It might be interesting to undertake such a study, but effect of the NO2-gap approach on the retrieval results is small, so that it is not clear whether such a study would provide additional information. In addition to that is will be a major effort since a lot of different circumstances are involved: land and water scenes, VRS (which is not easy to simulate, as it depends on aspects like the chlorophyll concentration as well as the viewing geometry), presence/absence of clouds, variation of the irradiance with solar activity, etc. In fact, using real data as done in the paper enables to have a close look at most possible cases without much effort, though of course it is then not possible to study the same case under irradiances at different moments in the solar cycle.




Fig_RC 1: Example plots of the runs test variables $R_D$ (top row) and $R_L$ (bottom row) using a colour scale between values considered to be tell-tale signs of possible problems (left column) and a black-and-white separation of the regimes (right column).

*Section 2.1.1*
Are there any other important algorithm improvements in the upcoming TROPOMI $NO_2$ processor v2.9.1 (besides the "NO2-gap approach" described in this manuscript) that are of interest to the reader and could be shortly mentioned here?

$\Longrightarrow$ Processor v2.9.1 is operational since 22 November 2025; the NO2-gap approach is the only update implemented; the text at the end of Sect. 2.1.1 has been updated to mention this.

*Section 2.2*
P4 Please include the definition of the geometric AMF used in this study.

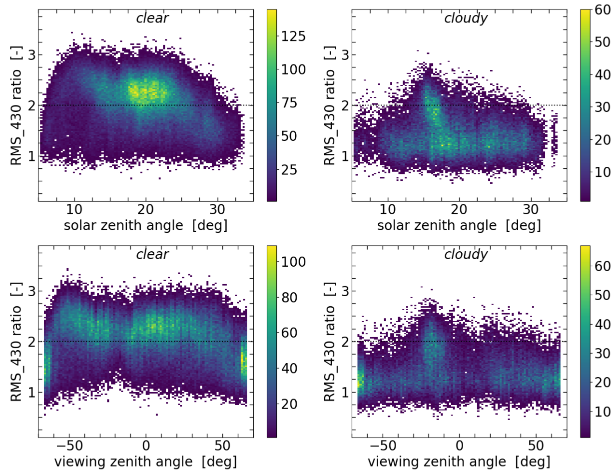
$\Longrightarrow$ Done.

*Section 2.2.2*
The statistical DOAS uncertainty is derived from the standard deviation on the slant columns in 2°x2° grid cells. Since the SCD also depends on the viewing geometry, it might be better to use geometrical corrected slant columns (GCD). The question is if there are significant differences between the statistical uncertainties based on the SCD or GCD.

$\Longrightarrow$ For consistency sake we have followed the same approach as used by Zara et al.,2018 (who refers to earlier papers regarding the adopted method) and average the SCD over 2°x2° boxes, which is OK as Zara et al. write "as long as the geometric AMFs within the box show little variability". And also following Zara et al.: "Boxes with relative AMF variability of more than 5% are discarded to prevent variability in viewing geometry influencing the results." A remark representing the latter has been added to the text. Also added is that boxes with less then 10 ground pixels in them are discarded as well.

*Section 3 → 2.2.3*
P9 Please include a global map of RD and RL

$\Longrightarrow$ Such maps do not provide much information: depending on the scale used, they show a




Fig_RC 2: Scatter plots of the RMS_430 ratio (y-axis) as function of the solar zenith angle (top row) and viewing zenith angle (bottom row) for clear-sky pixels (left column) and cloudy pixels (right colomn) for the Atlantic Ocean orbit section of Sect. 3.1.

scatter of many points or hardly any points. Fig_RC 1 above gives an example using two orbits. Obviously, one could select boundaries between the regions other than $|R_D| > 5$ and $R_L > 20$ to indicate possible problems. As the text of Sect. 2.2.3 stresses both $R_D$ and $R_L$ are *additional independent* sources of information on possible problems with retrieval results: they do not on their own signal problems.
The plots of Fig_RC 1 are made using Panoply and the graphs are exported in the "Extra large" size; if you would like to see the individual graphs in PNG format, you can download them: `http://www.josvg.dds.nl/downloads/20190605_example_runs.zip` – that file will be deleted once the review process is finished.

*Section 3.1*
A possible dependence of the RMS_430 ratio on the viewing/scattering geometry is not really discussed in the manuscript. It would be useful to include scatter plots of the RMS_430 ratio as a function of solar-, viewing or scattering angles for clear-sky pixels over the Atlantic Ocean.

$\Longrightarrow$ There is no apparent relationship between the RMS_430 ratio and SZA or VZA, as Fig_RC 2 shows (VZA values for the left side of the track are shown as negative angles); a remark to this effect is added to the end of Sect. 3.1. (The "peak" in RMS_430 around SZA $\approx 15°$ and VZA $\approx 15°$ are related to a cloud complex in the Atlantic Ocean orbit section.)

*Section 3.4*
Fig. 6 Why are the RMS_430 ratios only plotted in black ($> 2$) and white ($< 2$)? A color map would provide more information, e.g. about the RMS_430 ratios over different water scenes. Measurements with cloud radiance fractions $> 0.5$ could be marked as well.

$\Longrightarrow$ The map of Fig. 6 is intended to show the areas where we consider the RMS_430 ratio to indicate problems and this is most clearly shown in this black-and-white version. Upon your request, a colour scale version of the map has been added in the new App. C, with separate maps for clear and cloudy pixels.

*Section 4.1*
Is there also a significant impact of the NO2-gap fit on the statistical SCD uncertainty? This parameter could be included in Tables 2 and 3 as well.

$\Longrightarrow$ There is indeed an impact on the statistical SCD uncertainty – this is discussed in Sect. 4.2 and listed in Table 4 on the basis of Pacific Ocean orbits from the two test months. As mentioned at the beginning, we've added to Table 4 also results of the first comparison of before/after the operational switch.

*Section 4.2*
Fig. 10 Please include a global map of the relative change in the $NO_2$ SCD as well. The scatter plot on Fig. 11 show small changes in the SCD for most pixels but there seems to be a fairly large

scatter in the SCD change as well.

⟹ There is indeed large scatter for the changes in GCD values, but the pattern is the same as for the SCD error shown in Fig. 10; upon your request a map has been added to Fig. 10.

*Section 6*
The authors discuss the unexpected large TROPOMI tropospheric $NO_2$ columns over the Tibetian lakes that are likely due to unreliable DOAS retrievals and they also propose an (experimental) approach to improve the spectral fit over small areas like the lakes. I agree that such an approach to construct the missing reference spectrum might not be suitable for global retrievals and operational use. However, a case study for the Tibetian lakes would fit in the manuscript and enhance the scientific significance of the paper.

⟹ Such a case study for these lakes would indeed be interesting but the same time complex to carry out, and was discussed in the context of the Labzovskii et al. (2024) paper. However, this is a research topic on its own and falls ouside the score of our paper.

**Reply to Comment on egusphere-2025-5836 by Anonymous Referee #2**

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Referee comment on "Improved $NO_2$ spectral fits for TROPOMI and OMI by removing wavelengths around 430 nm" by Jos van Geffen et al., `https://doi.org/10.5194/egusphere-2025-5836-RC2`

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⟹ The referee report is copied below; the reply is preceeded by an arrow, like this text.

Apart from the changes resulting from the review process, we have carried out the following updates, which do not affect the conclusions of the paper:
– TROPOMI processor v2.9.1, which includes the "NO2-gap approach" of the paper, was activated on 22 November 2025; the text has been updated to represent this fact where appropriate.
– Since we now have a few months of v2.9.1 data, a quick comparison of results before and after the switch is added at the end of Sect. 4.2
– Fig. 2 in Sect. 2.2.2 is extended to include the year 2025; the figure caption was reformulated to improve readability.
– Fig. A1 in App. A is extended to contain the full year 2025.
– Meanwhile the OMI collection 4 $NO_2$ slant column data, named OMNO2A, are released by NASA; the URL of the download access is added to the "Data availability" section. NASA has assigned a DOI to both the dataset and the ATBD: `https://doi.org/10.5067/AURA/OMI/DATA2433`. Unfortunately, this DOI appears not yet activated; it should likely lead to a landing page such as the one for the collection 4 cloud data (OMCLDO2): `https://doi.org/10.5067/AURA/OMI/DATA2407`. Hopefully, NASA has activated the OMNO2A DOI by the time the paper is published.
– A few minor textual corrections were carried out.

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**General comments**

This manuscript presents a detailed investigation of the $NO_2$ slant column fitting results from TROPOMI and OMI. Fitting residuals are carefully inspected showing that spectral misfits are systematically encountered around 430 nm, i.e. approximately in the middle of the retrieval range used for operational $NO_2$ retrieval from both satellite sensors. These misfits are mostly observed above open water scenes (primarily Pacific, Atlantic and Indian oceans) and are attributed to the combined effect of inaccurate corrections for rotational Raman scattering (RRS) in air and vibrational Raman scattering (VRS) in water, the latter effect being ignored in the retrieval settings due to its complexity.

The authors present a convincing quantitative analysis of the dependency of the fit residuals on various parameters which clearly shows that the discrepancy is systematic and observed mainly above the water in a similar way for OMI and TROPOMI. This reinforces the interpretation of the nature of the problem. To solve the issue, they propose to introduce a 5-nm gap (428-433 nm) in the spectral range used for $NO_2$ retrieval. The introduction of this gap is shown to reduce fitting RMS and SCD errors by about 10% while the $NO_2$ SCD is seen to decrease by a few percent over oceans. Overall, the proposed algorithm adaptation only affects the retrieved $NO_2$ columns by a few $\mu$mol/m$^2$ (equivalent to a few $10^{14}$ molec/cm$^2$) and is therefore essentially cosmetic.

⟹ We thank the referee for these kind words.
Though the overall impact of the adaptation is not large in terms of numbers or percentages, it is in the end quite an important improvement, evidenced by the 10After all, we are at a stage where improvements in the $NO_2$ retrieval with large impact have been well studied, so that further improvements will be smaller and smaller in magnitude.

The manuscript is well written and organized, and figures are all clear. The scientific approach to characterize fitting residuals and their variations is sound and appropriate. However, I remain unconvinced by the approach chosen to resolve the issue. In my view, especially considering the discussion in section 6.2, the intensity offset correction seems to provide an equally good correction while conserving the full spectral information.

⟹ As we argue in Sect. 6.2 the IOC indeed gives similar results at the NO2-gap approach, but the IOC will still introduce artifacts because (a) it has a narrower peak around 430 nm than the problem seen in the residual, (b) the (solar) reference spectrum has structures outside that peak which affect the retrieval as well, and (c) the physical interpretation of the intensity offset term is unclear. These three issues are avoided by the NO2-gap approach.

Another possible approach could have been to perform a PCA analysis of the spectral residuals over oceans and use it to generate an additional pseudo cross-section accounting for the misfit. Similar approaches have been recently exploited with success in correcting other misfit problems (e.g. the impact of scene inhomogeneities affecting the effective instrumental response function at the edge of bright scenes).

⟹ A priciple component analysis (PCA) is indeed another option for $NO_2$ retrieval, and it has been done by some groups but it is not a common practice for the groups involved in the TROPOMI and OMI retrieval. PCA should then, however, be applied to the reflectance spectrum, not on the spectral residual, as the shape of the spectral residual is determined by the fit results, i.e. by, for example, an incorrect $NO_2$ column value.
In a retrieval such as ours, we prescribe a selected set of physical quantities we know are involved, though we at the same time know that we do not actually include all quantities that are involved, simply because we do not know all in detail and because reference spectra of different components may not be fully independent (orthogonal).
Given the nature of the paper, we consider a discussion of these points beyond the scope of the paper.

In the end, the main benefit of the change in algorithm is to provide more realistic estimates of the random uncertainties in the retrieved slant columns. This aspect could be better stressed in the conclusions of the study.

⟹ The wording in the 5th paragraph of Sect. 7 has been expanded a little in the light of this remark.

That said, this article is of high quality and interesting in many respects, and it should certainly be published in AMT, once the comments below have been considered.

### Detailed comments

*Pg. 1, line 8 and pg. 2, line 23*
The authors repeatedly state that VRS cannot be corrected by way of a scalable reference spectrum, however it is not clear why it is so. References given for other VRS studies show that corrections can be implemented in some cases. Please make it clear in which way the correction that would be needed for $NO_2$ is different from what has been successfully applied in other studies.

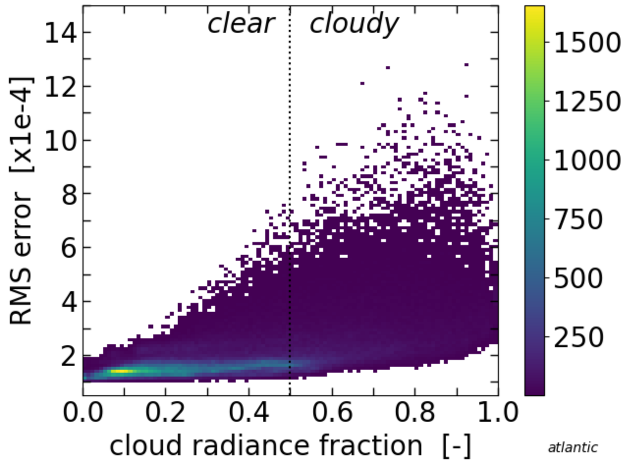
⟹ The argument is given on page 2, at the line you mention, as well as in the last section: the effect of VRS depends on the viewing geometry and conditions of the water an each situation would thus require its own reference spectrum and thus on-the-fly radiative calculations, which is not an option for operational world-wide processing. The 2nd paragraph in Sect. 7 has been updated.

*Pg. 3, line 17*
As written, this sentence sounds a bit weird. I would suggest: "The Tropospheric Monitoring Instrument, sole payload aboard ESA's Sentinel-5 Precursor (S5P) spacecraft, was launched on 13 October 2017 into an..."

⟹ Thank you for this suggestion, the text has been updated accordingly. The first sentence of Sect. 2.1.2 on OMI has been changed in the same way.

*Pg. 5, line 20*
The Ring vector was calculated using the Dobber et al. atlas. Have you checked the potential impact of using another (more recent) solar reference spectrum for the calculation of the Ring cross-section (e.g. TSIS-1, or Chance and Kurucz)?

⟹ No, we have not investigated other solar reference spectra. But even with another solar reference, there will be only a single Ring reference, i.e. with a fixed peak at 430 nm, which thus will still not reflect the variation of the Fraunhofer lines with the solar activity cycle. From the general point of view of TROPOMI retrievals, the possible use of the TSIS reference will be investigated,




Fig_RC 1: Scatter plot of the RMS error as function of the cloud radiance fraction for the Atlantic Ocean section.

and likely before the next update (scheduled in Nov. 2026 to v3.0.0 and in preparation for the full mission reprocessing).

*Pg. 11, line 19*
Here, I would expect the RMS to be smaller over cloudy pixels, due to the increased S/N ratio over bright scenes (more photons being reflected to the satellite). Maybe the reason for the low RMS_430 ratio is simply that water is hidden by clouds. Please clarify.

⟹ Fig_RC 1 shows the RMS error as function of the cloud radiance fraction for the Atlantic Ocean section of Sect. 3.1: although there is indeed more light over cloudy scenes (and thus the SNR is higher there), the fit residual is (much) more noisy over cloudy scenes. The text at the end of Sect. 3.1 has been updated to mention this.

*Pg. 27, line 16*
I follow the reasoning here, but the residual plot in Fig.17 still does show an almost complete compensation. As mentioned later in the text, the broad-band structures visible in the fit residual themselves do not represent the missing reference spectrum, because the shape of the residual is the result of DOAS adjusting all fit parameters so as to minimise the residual. Therefore, although the peak at 430 nm is narrower than found in the residuals, it might well be that the IOC compensates well for the effect over the full interval.

⟹ As mentioned above in the General Comments, the IOC does indeed give similar results, but we are affraid that the IOC may introduce additional features in the fit, because it has a structure outside the peak, while the NO2-gap approach seems a more physically sound approach because it is simply a matter of (re)defining the fit window limits to the optimal range(s).

*Section 4.2, table 4*
In my understanding, the main benefit of the NO2-gap is to improve residuals and therefore to bring the SCD errors closer to the statistical noise. It would be interesting to further discuss this point and maybe add values in table 4 showing how close the resulting SCD errors are to statistical errors.

⟹ Improving the fit residuals, in terms of reducing the DOAS SCD uncertainty estimate and the RMS error, is indeed the objective. But this does not necessarily mean that the DOAS and statistical uncertainty will lie closer together: how close these are together also depends on the accuracy of the statistical uncertainty.
Whether the two uncertainties are closer together or not due to the NO2-gap approach can in pinciple be seen from the numbers in Table 4.
– For the clear-sky case the DOAS uncertainty changes by a factor of about 0.95, while the statistical uncertainty remains almost unchanged (factor 0.99), so that for this case the two uncertainties have come somewhat closer togheter.
– For the cloudy case, however, the two have gone further apart: the DOAS uncertainty has changed a little (factor 0.98) while the statistical uncertainty has been improved by a factor of 0.91.

The important conclusion is that the NO2-gap approach either reduces the uncertainties or leaves them more or less uneffected, without deteriorating the results. The text of Sect. 4.2 has been modified a little.

*Section 6.1*
I understand that the spectral features over Tibetan lakes are related to a different mechanism, than those found more generally over oceans. Their impact on the $NO_2$ SCDs is also more significant. It is not fully clear from the text whether the "NO2-gap" approach is able to reduce the observed bias on the $NO_2$ SCDs. Please clarify.

$\Longrightarrow$ As mentioned at the end of Sect. 6.1 the effect of the NO2-gap approach on the GCD values is minimal, so no: the approach does not solve the observed bias, though the fit quality is improved (lower SCD and RMS error). To solve the bias, we need to know the characteristics of the dissolved matter. The end of Sect. 6.1 has been expanded somewhat to express this.

**Spelling, typos**

*Pg. 3, line 4* – Remove the 's' at the end of 'shows' in "Residuals may also shows broad-band.."

*Pg. 7, line 7* – Replace 'encounted' by 'encountered'

*Pg. 19, line 8* – Replace "where" by "were"

*Pg. 24, line 33* – Replace "deaper" by "deeper"

$\Longrightarrow$ Thanks for spotting these typos – they have been corrected.