Comment on amt-2021-329
Anonymous Referee #1

Referee comment on "Sentinel-5P TROPOMI NO2 retrieval: impact of version v2.2 improvements and comparisons with OMI and ground-based data" by Jos van Geffen et al., Atmos. Meas. Tech. Discuss., https://doi.org/10.5194/amt-2021-329-RC1, 2021

Review of “Sentinel-5P TROPOMI NO2 retrieval: impact of version v2.2 improvements and comparisons with OMI and ground-based data” by van Geffen et al.

In this manuscript, the authors report on the latest versions of the operational TROPOMI NO2 retrieval, the changes relative to earlier versions and the effect they have on NO2 slant columns as well as vertical tropospheric and stratospheric columns for a so-called diagnostic data set (DDS). The v2.2 columns are then validated by comparison to ground-based zenith-sky, MAX-DOAS and Pandora observations and systematic improvements are found compared to the offline product in most cases.

The TROPOMI NO2 product is widely used in the scientific community and detailed description of algorithm changes and their impacts on the product are of interest to many users. The manuscript is overall well written, clearly structured and reports on relevant results and therefore should be published.

I am however surprised by the general lack of discussion of the results throughout the text and hope that the authors can improve on this in the revised version, taking into account the suggestions made below.

I also think that it is very unfortunate that separation of effects was apparently not possible for the cloud effects, which probably are the most relevant and would deserve a more detailed discussion. It is hard to believe that such an important change to the product was introduced without having an extended period of data processed with both FRESCO versions for comparison. Maybe this will be discussed in the manuscript by Eskes et al. (in preparation), but for the manuscript as it stands, this is a clear shortcoming which should be fixed.

Major comments

Discussion of new FRESCO version:

- As mentioned above, a scientific sound comparison separates independent effects and I therefore expect to see a comparison of NO2 columns for at least a few days where only the FRESCO version differs.
The discussion of Figure 7 is very superficial – although it is clear from the picture that high cloud pressures have again become more frequent from v1.4 to 2.2 this is not discussed. Also shown in the figure are results for O2-O2 which agree much better with FRESCO v1.2 than with FRESCO v2.2, but again this is not even mentioned. If you do not trust the O2-O2 results, then remove them. If you show them, then please discuss them.

**Discussion of surface albedo adjustment:**

I think that this is a very good idea and it is nice that it has been implemented. However, there is hardly any discussion provided in the text although many questions come to mind:

- How will radiance calibration issues and the known low bias in TROPOMI radiances impact on this correction?
- What about absorbing aerosols?
- Are the patterns found in the albedo correction stable over time and are they plausible in magnitude and pattern?
- What is the reason for the bias? Is it because the processor uses the mode instead of the minimum in the OMI reflectance data base? Is it because of the low bias in TROPOMI radiances? Is it because of cloud shadows? Or does BRDF play a role?

I think that more analysis and discussion is needed here.

**Discussion of uncertainties:**

- The manuscript uses relative changes of uncertainties in many places. In my opinion, this should be added by absolute changes in error at least in some places. For example, in Table 3, relative changes of the order of 2% in the SCD errors are reported. If I assume an original error of 10%, this would mean that the error now is 9.8%, right? I think that absolute values give a better impression of how large the improvement is.
- I could not find the definition of the RMS error, which is also given in the text and table. Please add the definition and explain why it makes sense that the RMS error sees larger reductions than the SCD error.
- One key aspect of the manuscript is the description of changes in the NO2 columns. For users, it is important to know if the algorithm changes lead to NO2 variations within the error bars or outside the error bars. In other words: Do they have to worry that conclusions they drew on old TROPOMI data have to be revised or was this already covered by the uncertainties given in the product?

**Comparison to QA4ECV OMI product:**

Comparison to OMI data is important and useful to identify problems. In version v2.2, the agreement between the operational TROPOMI product and the QA4ECV OMI product now is good for the vertical tropospheric columns which is nice. This has been achieved mainly through two changes: 1) the use of the wide FRESCO cloud pressure and 2) the correction of surface reflectance in cases of negative cloud fractions. However, neither of the two corrections is applied in the QA4ECV product. If a similar surface reflectance correction would be implemented in the QA4ECV+ product, differences would increase again.
Similarly, if Figure 7 can be taken as an indication, implementation of the O2-O2 cloud pressure in TROPOMI data would move NO2 vertical columns back towards values seen in v1.2, again increasing differences to OMI. I think that this needs to be acknowledged and discussed.

**Minor comments**

- The reference Eskes et al., 2021 appears three times in the bibliography for different manuscripts and it is unclear, which of the documents you are referring to in the citations given in the text.
- Page 4, line 16: Updated level1b v2.0 – surely, the updated level1 data will have a new version number?
- Page 5, line 11: is used => are used
- Page 6, line 13: "corrections for the absolute and relative (ir)radiances" this is very vague and also the distinction between absolute and relative (ir)radiances is unclear – to my knowledge, the lv1 product only contains absolute (ir)radiances. Please expand and clarify.
- Page 7, line 4: trace gas concentrations => trace gas columns
- Page 7, line 26: wavelengths varies => wavelength varies
- Page 7, line 30: If only two corrections are made to the spectral index selection, why does this have any effect on the other rows?
- Page 8, line 23: Why is it, that some rows always have outliers, and why at the beginning of the NO2 fitting window? Is there a reason for this unusual behaviour? Please expand.
- Figure 2: Please add matching figure for slant column differences
- Page 13, line 3: I assume that the RMS error is mainly affected by reflectance noise. You probably meant “by the assumed reflectance noise”
- Page 13, line 12: What do you base the conclusion on, that v2.x data have “much improved DOAS fit quality”? In the table, I see relative reductions of the uncertainty by around 2%, which is an improvement but a rather small one.
- Page 13, line 26: There is a clear sea-land contrast visible in the differences. Please discuss.
- Page 14, line 8: “lower spatial distribution => lower spatial resolution
- Page 16. Line 11: not sure how sun glint is related to the change in snow/ice map
- Page 16, line 16: Please provide some information on how the ECMWF product manages to be better than the NISE product in so many aspects. Is there a reference for how ECMWF does that? Is it using the same input data? Has it been validated?
- Page 17, line 6: “NO2 surface albedo is adjusted from the value of 0.62 in the climatology to a more realistic 0.04” I guess what you meant to say is, that because of the improved NISE, the normal albedo is used instead of the value appropriate for sea ice.
- Page 26, line 24: “The NO2 cloud (radiance) fraction is currently derived from the FRESCO cloud pressure”. This sentence does not make sense to me, please check.
- Page 27, line 10: data data
- Page 28, line 9: See above
- Page 28, line 19: "The use of the improved level-1b v2.0 leads a) to a somewhat lower cloud pressure for“ – I somehow fail to see where this has been shown in the paper
- Page 28, line 21: number fully => number of fully