General Comments

This manuscript presents a validation study of the new TROPOMI Total Column Water Vapor (TCWV) retrieved from the 435-455 nm wavelength region. Validation involves comparing 2.5 of with AERONET Level 2 precipitable years data water vapour measurements. Comparisons are performed globally and in several zonal bands to determine the mean bias. The impact of viewing geometry (solar zenith angle, viewing zenith angle), cloud properties (cloud top pressure, cloud albedo, cloud fraction), and retrieval parameters (surface pressure, surface albedo, air mass factor, fit RMS, water vapour) on the comparisons are also examined.

The analysis is straightforward and provides a useful contribution to the evaluation of TROPOMI water vapor. However, the paper would be strengthened by making greater use of the validation dataset, examining the differences across the 351 stations rather averaging across zonal bands. Overall, I recommend publication after the comments below are addressed.

Thank you for recommending our paper for publication.

Specific Comments

Page 2, second last paragraph: The previous paragraph mentions the TROPOMI SWIR TCWV data product and its validation against TCCON. Why wasn't this new TROPOMI TCWV product compared against the SWIR product? Why wasn't TCCON included, or other available water vapour datasets such as GPS/RO? Explain why AERONET was chosen as the comparison dataset for this validation study.

Reply: We thank the reviewer for this comment.

The main reason for basing our work on AERONET water content observations is that, first of all, the network is very well established, with more than 25 years of operations and a transparent data quality assurance plan through its extensive cal/val routine operations, see here: <u>System Description - Aerosol Robotic Network (AERONET)</u> <u>Homepage (nasa.gov)</u>. Furthermore, the network offers a complete global coverage, covering the entire planet quite satisfactorily, see here: <u>AERONET Data Display</u> <u>Interface - WWW DEMONSTRAT (nasa.gov)</u>.

Even though it is true that AERONET has been extensively used for AOD validation, the AERONET water vapor observations have also been employed in space-born and ground-based instrumentation validation studies, see for e.g. https://doi.org/10.1016/j.atmosres.2019.04.005, https://doi.org/10.3390/rs13163246, https://doi.org/10.5194/amt-11-81-2018, etc. Due to the fact that a number of studies have already utilized the ground-based GPS datasets, and the same TCWV from TROPOMI/S5P product was also validated against GNSS (https://doi.org/10.3390/atmos13071079), in this work we aimed to start with the AERONET TCWV. Your suggestion is of course very welcome for future works.

Page 6, line 147: Define the equation used to calculate percentage difference, e.g., 100 x (TROPOMI – AERONET) / AERONET, so that this is clear. Also, this quantity should be called the relative difference. Is "minimize the noise" the best description? The choice of coincidence criteria is a trade-off between maximizing N for better statistics and minimizing space and time differences between the comparison datasets. No real justification is given for the choice of 10 km and 30 minutes; have these values been used in other water vapour validation studies or were trade-off curves constructed to find the optimum criteria? Do the comparisons involve single or multiple pairs, i.e., is each TROPOMI measurement compared with the closest AERONET measurement (or vice versa), or are multiple comparisons allowed the space and time criteria are met for a TROPOMI measurement and multiple AERONET measurements (or vice versa)?

Reply: The equation used to calculate the percentage difference was added in Section 3 and the manuscript was changed to refer to it as relative (percentage) difference.

The choice of the coincidence criteria was indeed the outcome of some studies we made in our effort to find the best trade-off between the number of co-locations and the results of their statistical analysis, taking into account the characteristics of the instruments, satellite and ground-based.

- It should be noted that the 10 km maximum search radius was only used for the extraction of the overpass files, taking under consideration the high spatial resolution of TROPOMI/S5P observations (3.5x7 km² until Aug. 2019 and 3.5 x 5.5 km² thereafter). Other studies, such as Borger et al. (2020), Xie et al. (2021) etc. used a similar distance for their validation work with respect to ground-based measurements. Besides, our aim was to use only the closest co-locations in space and in time for our statistical analysis, which leaded to a maximum spatial difference between the ground-based station and the satellite instrument of up to 5 km, as it is illustrated in Figure 1 of this document.
- As for the very strict criterion of up to 30' temporal difference between the satellite and ground-based observation, which is a much smaller time window than what other studies have used (for example, Chan et al. (2020) and Borger et

al. (2020) allow up to 2 hours, while Xie et al. (2021) also uses a 30' temporal difference), it was based on the fact that the AERONET dataset provides clear-sky measurements only, resulting to rather invariable temporally observation field.



Figure 1: The dependence of the relative difference between satellite and ground-based observations on the distance of their colocation. Each one of the gray data points consist of less than 3% for the total number of co-locations.

Please, note that in the process of the revision of our manuscript, it was found that a full re-analysis of our validation work had to be done. When the first validation exercises were performed, based on a limited dataset that was available at the time, we used the following co-location technique to increase the sample of the data to be evaluated:

Each satellite measurement from a specific pixel (the one spatially closest to the ground-based station within 10km), was compared to all instantaneous ground-based measurements that were performed within a $\pm 30'$ temporal interval with respect to the time of satellite observation. This way, for each overpass instance there were more than one matching pairs, explaining the high number of co-locations.

This approach is not necessary now that a significantly larger satellite dataset of 2.5 years, is available. Therefore, the co-location methodology was changed to <u>keeping</u> only the match with the minimum temporal difference between satellite and groundbased observations within a 10 km radius, if this temporal difference is up to 30 min. The resulting total number of co-locations is now about 70.000. The new methodology was applied throughout the manuscript and all plots and statistics were updated and the manuscript was revised accordingly. Additionally, a paragraph with a detailed description of the co-location methodology, giving all the above-mentioned details, is added in Section 3. **Page 7, line 156:** The 633,000 coincident measurements constitute a rich validation dataset that could be investigated in more detail. This large number would seem to be the justification for using AERONET for the validation, but the analysis doesn't take full advantage of the resulting information. Since a per-station analysis has already been done, there are 351 global comparisons – it would be interesting to examine these and to look more carefully for spatial differences and dependencies. For example, consider adding a panel to Figure 8 that shows the seasonal and latitudinal variability of the mean bias, and a similar figure showing latitudinal and longitudinal variability, using the results from all 351 stations. Another panel that could be added to Figure 8 is the seasonal and latitudinal variability of N, given the discussion on lines 228-233.

Reply: Thank you for the comment and your suggestions.

- A panel with a new contour plot was added in Figure 8, showing the seasonal and latitudinal variability of the mean bias, as it was suggested.
- Following the suggestions of Reviewer #1, the latitudinal and longitudinal variability of the mean relative bias was presented in the form of a world map, showing the relative mean bias of each station using a colorbar. To further investigate any possible patterns in relative bias over Europe and N. America, where the stations are very dense, the two areas were also plotted separately. The three maps (world, Europe and N. America) were added in Appendix A and commented in Section 4.
- As for the seasonal and latitudinal variability of the number of co-locations, we believe that the information was already given in the timeline plot shown in Figure 5.

Page 7, line 160 and Figures 3 and 4: State why monthly mean percentage differences are calculated and plotted (perhaps to provide more even annual coverage?). If the mean bias and standard deviation are calculated using all individual points for a station, do the results differ from those obtained using the monthly means?

Reply: The use of monthly means is adopted only when time series are shown, to keep the figures clear and to be able to detect any possible seasonal variability. For example, when a pole-to-pole graph is made, all individual (instantaneous) co-locations within each latitude belt are considered and, of course, they are not temporally averaged.

As for the difference in the statistics when using monthly means with respect to individual co-located data, you see in the example below (Figure 2 of this document), where:

- to the left, all individual co-locations for the station of Santa Cruz, Tenerife, are plotted in the form of time series, and
- to the right, the time series of the monthly means are depicted,

that the main difference between the two ways of illustration, as it is expected, is the standard deviation of the mean, which is almost double when all individual points are used for the statistics.



Figure 2: The time series of the relative differences between the co-located satellite and ground-based TCWV observations, in the form of raw, instantaneous percentage differences(left panel) and monthly means of the instantaneous differences (right panel), for the station of Santa Cruz, Tenerife.

Page 7, line 167: "The mean relative bias per station (panels a) depends strongly on the ground-based instrument's calibration," Since all AERONET data is Level 2.0, what calibration issues are there? Nothing has been said about this elsewhere in the paper so this should be explained. Is there a parameter defining the calibration status for each station so that the dependence of the mean relative bias on the calibration can be determined?

Reply: We thank the reviewer for this comment. The wording used in the text does not reflect what we really meant. Of course, using Level 2.0 excludes any calibration issues from the discussion. The sentence was rephrased as follows:

"The monthly mean relative bias per station (panels a) depends strongly on the groundbased instrument's operation and maintenance, ..."

Technical Corrections

Page 1, line 9: here and elsewhere throughout the paper, delete "very". It is used too frequently and is not needed.

Reply: The use of the word "very" is minimized throughout the manuscript.

Page 1, line 11: (435-455 nm) **Reply:** Corrected.

Page 1, line 15: although AERONET has 1300 stations, data from only 351 are used in the study – this should be noted here

Reply: The number of stations was added in the sentence.

Page 1, line 18: "of the order of only -3% for the mid-latitudes and the tropics (+-60deg)" does not seem consistent with the mean bias numbers in Table 2 which are -4.0, -5.9, -9.6, -5.9, 2.4, and 5.8 for the six bands between 60N and 60S, nor with the NH, SH, and global biases in Table 1. Provide more specific results here.

Reply: This percentage referred to the mean relative bias for the mid-latitudes and the tropics and resulted from averaging the mean relative biases of all latitude belts within ±60°.

Hemisphere	Latitude belt	Mean Diff. ¹	Mean Rel.	Mean St.	Mean St.
		(kg/m^2)	Bias (%)	Dev. (%)	Err. ² (%)
NH	90°-60°	-0.4	1.2 ± 31.5	61.3	12.6
	60°-30°	-0.8	-4.0 ± 2.9	44.0	1.3
	30°-15°	-2.2	$\textbf{-5.9}\pm3.4$	23.6	1.6
	15°-0°	-3.7	$\textbf{-9.6}\pm3.0$	18.5	2.0
SH	0°-15°	-2.5	-5.9 ± 5.5	32.2	3.3
	15°-30°	-0.7	2.4 ± 8.3	52.3	3.6
	30°-60°	+0.5	5.8 ± 12.3	46.1	8.9
	60°-90°	+0.3	42.2 ± 4.9	84.8	16.5

Table 2: The zonal statistics of the co-located satellite and ground-based observations

¹ Satellite-Ground

² 99.7% CI

The abstract was revised and now the sentence refers to the overall mean relative bias, which is -2.7 %, after the new analysis that followed the revision of the colocation methodology:

"The Pearson correlation coefficient of the two products is found to be 0.91 and the mean bias of the overall relative percentage differences is of the order of only -2.7 %." Please note that the statistics in Table 2 were updated. Page 1, line 19: delete "influence" **Reply:** Deleted.

Page 1, line 21: define CTP, clarify what "low cloudiness" means – low cloud top pressure? **Reply**: The sentence was rephrased.

Page 1, lines 25-29 and elsewhere in the manuscript (lines 33, 70, 72, 208, etc.): change "earth" to "Earth" (the planet) throughout

Reply: Corrected.

Page 2, line 31: delete "very" **Reply**: Deleted.

Page 2, line 34: remove/replace one of the "therefore"s **Reply**: Corrected.

Page 2, line 37: delete line break **Reply**: Deleted.

Page 2, line 38: delete "very" **Reply:** Deleted.

Page 2, line 40: high-latitude **Reply**: Corrected.

Page 2, line 41: delete "key" (already say "important") **Reply**: Deleted.

Page 2, line 41: "for the evolution of the greenhouse effect and the projection ..." **Reply:** Corrected.

Page 2, line 41: climate change **Reply:** Corrected.

Page 2, line 45: (435-455 nm) **Reply**: Corrected. Page 2, line 45: delete "further" **Reply**: Deleted.

Page 2, line 47: delete "sensors" **Reply**: Deleted.

Page 2, lines 50, 54: clear-sky **Reply**: Corrected.

Page 3, line 66: delete "influence" **Reply**: Deleted.

Page 3, line 70: TROPOMI was launched on 13 October 2017 **Reply**: Corrected.

Page 3, line 79: (435-455 nm) **Reply**: Corrected.

Page 3, line 81: "in short, a two-step approach …" **Reply**: Corrected.

Page 3, line 84: air mass factor **Reply:** Corrected.

Page 3, lines 95-96: the seasons listed here (winter, spring, summer, autumn) only apply to the Northern hemisphere – either add NH before each season or remove the seasons from this sentence.

Reply: The seasons were removed from the sentence.

Page 4, line 99: "decreasing below 5-10 kg/m2 closer to the poles." **Reply:** Corrected.

Page 5, line 116: product **Reply:** Corrected.

Page 5, lines 130-131: for the 351 stations used in this study, AERONET coverage of all continents is not actually "very dense" spatially as seen in Figure 2 – revise this description.

Reply: The sentence was changed as follows: "The extended network of automatic and quality-controlled observations provides very dense (spatially and temporally) coverage of North & South America, Europe, South-East Asia, as well as Western Africa. This fact, in addition to the homogeneity of the retrieval algorithms, are strong advantages in favor of using the AERONET for this validation work."

Page 5, line 131: delete "very" **Reply:** Deleted.

Page 6, line 140: "resulted in the reduction ..." Describe the in-house quality control that reduced the number of stations with usable data from 1300 to 351.

Reply: The sentence was changed to clarify the methodology that was followed in the process of our quality-control:

"An in-house quality control based on the visual and statistical analysis of the available datasets per station, ensured that only stations with data that fully cover the time period of our study, and which offer observations within an expected range depending on the station's location, are contributing to the ground-based reference dataset. As a result, the number of stations to be used for the validation of TROPOMI/S5P TCWV was reduced to 369."

Please note that in the process of revising the manuscript, the ground-based dataset was also updated and the list of stations that are now used as reference numbers 369 stations. Moreover, the South Pole station (lat: -90°) was decided to be excluded from the reference dataset, since it was offering less than two months of observations to the study.

Page 6, line 142: "as can be …" **Reply:** The sentence is deleted.

Page 6, Figure 3 and page 7, Figure 4: The quality of the fonts is poor on these panels and hard to read – the fonts should be improved.

Reply: The figures were replaced by new ones of better quality.

Page 7, line 160: Why show monthly mean percentage differences **Reply:** This was answered above, in the section of the Specific Comments. Page 7, line 163: delete "very nice" (here and elsewhere, these subjective descriptions can be removed)

Reply: Deleted.

- Page 7, line 164: state whether the correlation coefficient is R or R^2 **Reply:** This is the Pearson correlation coefficient. It was clarified in the manuscript.
- Page 7, lines 165 and 167: delete "very" Reply: Deleted.

Page 8, Figure 5: The quality of this figure is poor; at a minimum, the y-axis should be extended beyond +-90 so that the highest latitude points are visible, the fonts should be improved, and "AERONET" removed from the top.

Reply: The figure was changed according to the reviewer's suggestions. The y-axis range was not changed beyond ±90° because in the process of the re-evaluation of our co-located data, the South Pole station was decided to be left out due to its limited temporal coverage (2 months of observations in 2018).

Page 8, line 180: 60S is mentioned here (and again on line 212) but line 177 says that the SH data only extend to 55S – should 60 be changed to 55?

Reply: Yes, the latitude was changed in both lines. Actually, after the re-evaluation of the stations that took place in this version of the analysis, the highest latitude Southern Hemisphere station available is at -46°S.

- Page 8, line 183: averaged **Reply:** Corrected.
- Page 9, line 191: on a global scale **Reply:** Corrected.
- Page 9, line 192: change "about" to "approximately" **Reply:** Corrected.
- Page 9, line 195: correlation coefficient R? delete "very"
 Reply: Yes, this is the Pearson correlation coefficient. The information was added to the text. "Very" was deleted.

Page 10, Figure 7: the legend (TROPOMI) on the lower left of the panels and "AERONET" in the lower right should be deleted. State in the figure caption what the errors bars are.

Reply: The figures were changed according to the reviewer's suggestions. A sentence is added in the figure caption to explain the error bars.

- Page 11, Figure 8: delete "TROPOMI" and "AERONET" from the panel **Reply:** The figure was changed according to the reviewer's suggestions.
- Page 12, lines 235, 236, 245, 252: delete "very", etc. **Reply**: Deleted.
- Page 12, line 253: 80deg S to 90deg S **Reply:** Corrected.
- Page 12, line 261: location **Reply:** Corrected.
- Page 12, line 264: regarded as [very] good. **Reply**: Corrected.
- Page 12, line 265: rewrite this sentence for clarity it is not clear what is meant **Reply:** The sentence was changed to: *"Howbeit, the performance of the TROPOMI/S5P TCWV retrieval algorithm, mainly on the aspect of the surface albedo parameter, which significantly changes with latitude, is adequate and could be further improved in the future."*
- Page 13, line 273: delete "influence", change "quantities" to parameters or variables **Reply**: The term "influence quantity" was replaced by "parameter"

Page 13, line 274-275: "detailed results" is a strange term – how is air mass factor a detailed result? Are these outputs from the retrieval algorithm?

Reply: The sentence was changed as follows:

"These quantities can be parameters that are used as inputs for the TCWV retrieval algorithm, such as cloud and surface information, or algorithm-related parameters, like the air mass factor." Page 13, line 276 and Figures 10-13: the numbers at the top of each panel are unreadable – revise these plots to show this information in another way.

Reply: The figures were changed and we used the following sentences in Section 4.2, 1st paragraph, to clarify the new way of illustration:

"Note that, in the following figures, when the number of co-locations that are averaged for each bin is less than 3% of the total, the respective the data point is shown in gray (instead of blue). This is a way to distinguish the data points in terms of relative importance."

Page 13, line 276: change "of each figure" to "Figures 10-13"

Reply: Due to re-phrasing of the sentence (see above) this correction is not needed anymore.

Page 13, line 280: specify whether the SZA and VZA are for TROPOMI or AERONET. Define what is meant by the viewing zenith angle.

Reply: These are parameters coming from the TROPOMI dataset and it was clarified in the manuscript. Following the suggestion of Reviewer #1, the VZA dependence figure was replaced with another one showing the dependence on the satellite pixel, to investigate if a West-East dependence exists in the TROPOMI swath. Therefore, a definition is not needed now.

Page 13, line 281: delete line break

Reply: This is probably an issue of different word versions used, as in our document no line break is included at that location. If you mean that the first sentence of the section and the following paragraph should be joined, that was done.

Page 13, line 285: it's not clear what is meant by "the dependence of the percentage differences on SZA is ~13%". The differences in Figure 10(a) vary from approximately -10% to +10% so where is 13% coming from? Has a line been fitted to the data? If so, should it be added to the plot? Discussion of these results should be clarified.

Reply: Thank you for your comment. The difference (now 15%) that is mentioned here is the peak-to-peak difference seen for the total range of SZAs, since below 45° the co-locations' mean relative biases are negative, up to -6 %, and above 70° they have a mean relative bias of ~ +8%. The sentence was re-phrased as follows: *"Overall, the dependence of the relative differences on SZA is ~15 % peak-to-peak."*

Page 13, line 285: "of the mean increases for larger/smaller SZA" "higher SZA" is ambiguous – specify whether larger or smaller

Reply: The word "larger" was used instead of "higher".

Figures 10-14: Improve the presentation of numbers as noted above. Delete the legend (TROPOMI) on the lower left of the panels and "AERONET" in the lower right. State in the figure caption what the errors bars are. Revise the figure captions so that they are consistent between figures and fully describe what is shown in the panels.

Reply: The suggested improvements for the figures were adopted. Thank you. An extensive description of what is seen in the plots that follow and how it is calculated (monthly means and error bars) is given in the last paragraph of Section 3. Nevertheless, the information for the error bars representation is also added in the figure captions. All figure captions were carefully reviewed and corrected where necessary.

Page 15, lines 297 and 304-307: discuss the dependence on cloud fraction above 0.3

Reply: The paragraph discussion cloud fraction was changed as follows: "The cloud fraction figure (panel c) shows that the vast majority of the co-locations have cloud fraction values below 0.3, which is expected since both satellite and ground-based observations are filtered for cloudiness (satellite data are filtered for cloud fraction < 0.5). Within the cloud fraction range of 0 to 0.3, no particular dependence is seen. The colocations that are characterized with cloud fraction between 0.3 and 0.5 are very few in population but they introduce high positive mean relative biases. Filtering-out the colocation dataset for cloud fraction > 0.3 was also investigated, resulting to no major differences in the validation results. Nevertheless, it is advisable to not use this small portion of TCWV data for future scientific studies."

Page 16, lines 326-327: change the title of this section – "Detailed results" is not informative. Are these outputs from the TROPOMI retrieval algorithm?

Reply: The title of the section was changed to "Dependency on algorithm-related parameters".

Page 16, line 332: from Figure 13(a), the largest negative value for AMFs of 2-4 looks like approx.. 25%, not 18%

Reply: Thank you for the comment. The percentage was changed to 20% according to the updated figure 13(a).

Page 16, line 336: "with a low ..." **Reply:** Corrected Page 16, line 338: delete "result" **Reply:** Deleted

Page 16, line 342: areas **Reply:** Corrected

Page 16, line 343: this sentence is unclear – what does "they" refer to and what "should be treated with caution? Revise for clarity.

Reply: The sentence was changed as follows:

"Even though very few retrievals are based on an AMF value of less than 1, we note that comparisons to these pixels result in extremely high relative differences with respect to ground-based measurements, up to -100 %."

Page 17, line 346: "namely: TROPOMI (a)..." **Reply:** Corrected

- Page 17, line 348: is "statistics" needed in the title of this section? **Reply:** Section 5 was renamed to "Summary and conclusions".
- Page 17, line 350: consistency with **Reply:** Corrected
- Page 17, line 353: corresponding to clear-sky **Reply:** Corrected
- Page 17, line 355: summarized as follows **Reply:** Corrected
- Page 18, line 358: delete "excellent", change "their" to "the" **Reply:** Corrected
- Page 18, line 359: mean bias is -4.7%
 Reply: After the new analysis, the overall mean relative bias resulted to -2.7 %. The hemispherical mean relative biases are now -3.1 % for the NH and +0.9 % for the SH.

Page 18, line 363: should "accuracy" be "consistency"?

Reply: Thank you for the comment. The sentence was re-phrased to: *"The mean standard error of the comparisons, at a 99.7% CI, is 0.5 %, highlighting the consistency of the results. "*

Page 18, line 381: does "low cloudiness" mean low cloud top pressure? **Reply:** The term "low cloudiness" was changed to "low cloud top height".

Page 18, line 386: Is 2.5 years of comparisons sufficient to claim temporal stability? What is the basis for claiming high precision? Accuracy appears to be -9% to -13% based on line 365. Revise this sentence.

Reply: Thank you for your comment.

The issue of the temporal stability refers to the time period of available data only, and that is clarified in various parts of the text, but it will be clarified here as well.

The wording in this final paragraph was is re-phrased as follows:

"To conclude, as shown from the validation of 2.5 years of available satellite observations, with respect to ground-based observations from AERONET, the TROPOMI/S5P TCWV product retrieved from the blue spectral range, is a temporally stable product of high quality and precision, especially at the tropics. Also, it is not significantly affected by any other parameters, except from clouds when and if some cloudiness at lower atmospheric layers is present in the measurement field."

The high precision of the product refers mainly to the tropics, where (as seen in Figure 8b) the standard deviation of the mean bias has a very low variability.

Page 18, line 388: delete "very"

Reply: Deleted

Page 18, line 389: list other "blue-band satellites"

Reply: The following satellites were listed in the sentence:

- Global Ozone Monitoring Experience (GOME) mission (Burrows et al., 1999),
- SCanning Imaging Absorption SpectroMeter for Atmospheric CHartographY (SCIAMACHY; Bovensmann et al., 1999),
- Global Ozone Monitoring Experience 2 (GOME-2; Callies et al., 2000)
- Ozone Monitoring Instrument (OMI; Levelt et al., 2006),

Thank you very much for your constructive feedbacks and questions. The authors