Review of AMT-2024-28 “An advanced spatial co-registration of cloud properties for the atmospheric Sentinel missions: Application to TROPOMI”

28th April 2024

Review of the article submitted to AMT with the title “An advanced spatial co-registration of cloud properties for the atmospheric Sentinel missions: Application to TROPOMI”, by Athina Argyrouli, Diego Loyola, Fabian Romahn, Ronny Lutz, Víctor Molina García, Pascal Hedelt, Klaus-Peter Heue, and Richard Siddans. AMT article number “AMT-2024-28”.

In this review I will frequently refer to the L1B ATBD, which can be found in the Sentinel 5P document library. The article already refers to this document as (KNMI, 2022).

1 General comments

The article is generally well written. In some places details are left out that should in my view be included, in other places more detail than is perhaps desired can be found. The latter is especially the case when presenting the results. I’ll get back to these cases in the specific comments section. The article is long, and should be reduced in size. I will give some suggestions.

The mapping equations are introduced without much justification as to why one would want to use these specific quantities from VIIRS te aid in the transformations. That you use a derived fractional cloud cover from VIIRS to map the cloud fraction from UV-VIS to NIR is fairly logical, but why not use the γ factors derived from the VIIRS cloud fraction as well as the dimensionless scaling factor to aid in the mapping of the cloud height from NIR to UV-VIS? After all, you do get a weight that is related to the amount of clouds in the pixel, and therefore a means to obtain a weighted average.

This brings me to my second more important point. Using the cloud fractions would preclude extrapolation to row 0, but at the same time, how much of the information in row 0 is actually coming from the Tropomi instrument? A discussion on the effective contributions of the information from Tropomi and VIIRS in the final product is desired. Is the information from row 0 really VIIRS information that has been scaled locally by the ratio of Tropomi and VIIRS cloud heights to take into account the systematic model difference between the two instruments and retrieval methods? This discussion really needs to be added to the article before publication.

2 Specific comments

2.1 Spatial resolution

In the introduction, lines 33 to 37, the spatial resolution of Tropomi is discussed. For the bands used by OCRA/ROCINN the spatial resolution in the flight direction is unimportant. Because of the shared entrance slit between the VIS and NIR spectrometers (See L1B ATBD, section 7.2), there is no spatial misalignment between those spectrometers in the flight direction. That also means that the change of the spatial resolution in the flight direction is unimportant for the subject of this article. I suggest to shorten this discussion in the introduction.

2.2 Algorithm description

In section 2 of the article a description of the cloud retrieval algorithm is given. The algorithm is based on a pair of algorithms, OCRA for the cloud fraction, and ROCINN for the cloud top height and cloud albedo or cloud optical thickness, depending on the cloud model. Please explain how a cloud fraction can be derived from OCRA without assuming a cloud albedo, or put differently, show that the three parameters are independent, and the cloud albedo (or optical thickness) isn't (implicitly) assumed already in the cloud fraction derivation in OCRA.

2.3 Spatial alignment in the flight direction

In section 3, on lines 97 to 99, the authors mention that the static lookup tables used up to now indicate a very small mis-match in the flight directions. These are rounding errors in the algorithm used to calculate these tables. The design of the instrument itself (See L1B ATBD, section 7.2) *guarantees* that there is no spatial mismatch in the flight direction between the VIS and NIR spectrometers (bands 3 – 6). So the algorithm does not neglect anything, but it handles the situation correctly. Please adjust the text accordingly.

2.4 Previous treatment of the spatial mis-registration

In section 3.1 the previous treatment of the mis-registration is described. Here a "cloud co-registration inhomogeneity parameter" is introduced. This parameter involves the difference between the cloud fractions f_{ci} in the UV band and the cloud fraction f_{cj} in the NIR band. The source of the cloud fractions is not indicated. Up to this pont in the article only a cloud fraction in the UV that is derived by OCRA has been described. Please indicate the source for these cloud fractions, especially the source for f_{cj} in the NIR. If the cloud fractions are derived from the cloud mask information provided by the SNPP data, please indicate how the cloud fractions are calculated. Note specifically that equation 7 applies to the new method, so it does not apply here.

2.5 Unavailable reference

On line 116 a reference to (Sneep, 2015) is introduced. This is an unpublished and project-internal document with reference number S5P-KNMI-L2-0129-TN. Either use open literature, or find a way to make this document available to the readers of AMT, for instance by adding it to this article as supplementary material, or arrange for this document to be added to the Sentinel 5P document library.

2.6 Choice for probably cloudy

In equation 4 the "probably cloudy" pixels are counted as cloud free. Please elaborate on this choice. The number of pixels in both "probably" classes is small, so the impact is limited, but even that should be mentioned.

2.7 Optimal Estimation reference

The authors use (Rodgers, 1976) as a reference for the optimal estimation. This reference points to: Rodgers, C. D.: Retrieval of atmospheric temperature and composition from remote measurements of thermal radiation, Reviews of Geophysics, 14, 609–624, DOI:10.1029/RG014i004p00609, 1976.

This is perhaps a little peculiar to use as a reference at this point in time, as the same author wrote *the* book on optimal estimation: Rodgers, C. D.: Inverse methods for atmospheric sounding. Theory and practice, volume 2 of Atmospheric, Oceanic and Planetary Physics. World Scientific, 2000. DOI:10.1142/3171.

I strongly suggest that the reference to the book is used instead of the much earlier article.

2.8 Cloud optical thickness handling

In lines 185 tot 190 and in equation 5 a transformation is provided to obtain a cloud albedo from a cloud optical thickness. Within the VIIRS mapping software, a similar transformation and its inverse must be used to translate the VIIRS cloud optical thickness into an albedo to be able to take the average, and then the inverse transformation to obtain an effective cloud optical thickness. Please add a statement whether the *same* transformation is used in the VIIRS remapping software (Siddans, 2026).

2.9 "Missing" three pixel mapping in NIR to UV-VIS scheme

In section 3.3.2 there is no equivalent to equations 10 – 12 in the UV-VIS to NIR mapping. I would expect such a three pixel equivalent near row 428 because of the symmetry of the binning factors in the Tropomi instrument and the shift between the detectors present in the instrument. A short remark about this absense can resolve the mystery. There is mention of a binning factor change at UV pixel 21, but the same change happens at the other side of the swath. Does that not have an impact, in a way that is similar to the UV-VIS to NIR mapping in section 3.3.1?

On lines 224 – 227 exceptions to the "normal" equations (13 and 14) are mentioned. However, for case (a) there is no explicit mention of *how* this affects the mapping. For clarity I advise to mention that UV/VIS pixel 21 is fully covered by one NIR pixel. The subsequent text makes a lot more sense with that knowledge.

2.10 Co-registration of cloud albedo and cloud optical thickness

On lines 240 – 242 the co-registration of cloud albedo and cloud optical thickness is mentioned, and the reader is referred to (Loyola et al., 2023). This is the algorithm theoretical baseline document for the cloud algorithm. In this reference, the only relevant statement to this subject that I can find is the following on page 31 of the reference:

> The basic principle is that the VIIRS and TROPOMI cloud data are interconnected and therefore, each point from the VIIRS dataset can be mapped to the respective TROPOMI point. The adjacent 15 pairs $(H_c^{\mathrm{UV}}[i], Z_c^{\mathrm{UV}})$, for $i \in [2, 17]$ are used to create the mapping function:
>
> $$Z_c^{\mathrm{UV}} = f_{Z_c}\left(H_c^{\mathrm{UV}}[i]\right)$$
>
> The mapping function for the cloud top height f_{Z_c} follows a linear regression model for the entire range of the cloud heights. The respective function for the cloud albedo f_{ω_c} and the cloud optical thickness f_{τ_c} is a two-way function (i.e., a combination of a linear model with a logarithmic model).

The reference used is insufficient to describe the method used. The statement in the article is essentially repeated without providing substantionally more details. Either complete and update the ATBD, or include an appropriate and reasonably complete description in this article.

2.11 More appropriate section

At the start of section 4.1 a listing is provided when the new scheme cannot be used. I think this information should be included in section 3, perhaps in a new sub-section.

2.12 Comparison results

I have several remarks about page 17 – 20 that I will group here.

1. In the caption of figure 12 it is not mentioned which day is shown.
2. On line 265 it is mentioned that the scheme can be successfully applied up to a certain latitude.
   (a) Is this a limit of the latitude, or of the solar zenith angle?
   (b) Which of the three reasons that cause failure of the new scheme are a cause of this limitation?
3. On line 267 a sequence of 5 figures is introduced, showing the correlation between the old and the new approach. Which is it obvious after reading the axis labels, please mention that this shows the correlation *after* the transformation.
4. Figures 13 – 17 do not show the units along the axes of the graphs.
5. The axis range of the histograms in figures 13 – 17 is probably too wide given the results, and the number of pixels in the comparison.
6. The vertical axis of the histograms in figures 13 – 17 is not a count but something else, probably a density. Please adjust the labels.
7. Indicate the number of pixels in each comparison, and indicate if the data was selected, for instance for filter out pixels that relied on the old scheme.

2.13 Not fully consistent terminology

When discussing the comparison of the cloud top height results on lines 374 – 375, the following statement is made: “The cloud-top heights at the original BD6 were 7600 m and 9400 m at points A and B respectively. After the co-registration at point A, the CTH at BD3 was 6900 m with the new scheme and 6600 m with the old scheme. At point B, the co-registered CTH at BD3 was 9300 m with the new scheme versus 9000 m with the old.” If the cloud top height at points A and B is already known, then why is the new co-registration scheme required? Given the location in the swath, there must be two pixels from band 6 contributing to each of the the result in band 3. The values of both contributing factors to both point A and point B should be mentioned for clarity.

The same point applies to table 4 and various other locations throughout the text. In particular the conclusion in lines 442 – 443 should probably be rephrased as well.

2.14 Caliop results

I strongly suggest to use the Caliop L1 backscatter intensity as a background for figure 35 – 37, as that provides more context, including – sometimes – the presence of multi-layer clouds. Caliop should also have information on the phase of the cloud top, allowing the authors to indicate where this may play a role.

2.15 Suggestion for shortening the article

The information presented in table 3, and the related figures 22 through 25, as well as the text in lines 284 – 312 are mostly descriptive, and the conclusions drawn from them are not very strong; mostly qualitative rather than quantitative. The article probably improves if this part is removed.

Reconsider if appendix A is really required.

2.16 Appendix B

Please provide a reference to the method used here. There are several method for calculating a great-circle distance between two points on a globe, with varying accuracy. This appears to be one of the spherical earth methods, rather than Vincenty's formular for an ellipsoid. Any method will be find, they all provide an answer with sufficient accuracy. At the very lease indicate that you are calculating the distance d between the location of the Caliop profile and the points within the selection boxes, and the $R = R_{\text{earth}}$. If the equations in appendix B are to be used without reference, at least provide names to the steps for readability.

3 Technical corrections

3.1 Spectrometer names

In table 1 on page 2 an overview is provided of the spectrometers in the Tropomi instrument. This table does not make it clear that there are in fact 4 spectrometers on board of the instrument, with 4 detectors (3 CCD's, 1 CMOS). Each of the detectors is split electronically into two halves, leading to a total of 8 bands. But each pair originating from the same detector share the same spatial coverage, and have *no* interband mis-registration. Bands 1 and 2 are special, because the spatial binning is different for band 1 compared to band 2. But the observations in band 2 can still be co-added on ground to a perfect match to band 1.

The suggested solution is to put the spectrometer names centred above the two columns of the bands that they measure, as "UV", "UV/VIS", "NIR", and "SWIR". Note that in the official Tropomi L1B documentation the UV-1 and UV-2 (etc) naming system is not used, see for instance table 1 on page 21 in the L1B ATBD. Using UV/VIS instead of UVIS as the documentation of the Tropomi team does is probably beneficial for clarity here. And of course the references in the text need to be adapted as well.

I believe vertical lines are against the design guidelines of the journal, but they may actually be appropriate here for clarity.

3.2 Using sun normalized radiances

In line 55 on page 3 the first instance of "sun-normalized radiances" is encountered. Does the algorithm really use sun-normalized radiances internally, or is the reflectance actually calculated? The difference is a factor π/μ_0, and especially look up tables and neural networks typically work better when using reflectances.

3.3 Ground pixel footprints

In figure 1 a section of an orbit is shown, to illustrate the spatial mismatch between the two bands involved in the retrieval. Please indicate the flight direction in this figure.

3.4 The A train

Line 104: Neither Sentinel 5P, nor Suomi-NPP are part of the A train, see atrain.nasa.gov.

3.5 Typography

In equation 4 on page 8 the superscripts are typeset in LaTeX mathematical typesetting mode. This is incorrect, compare the following two versions of the same equation, with the correct method used on the right:

$$M = \delta_{jk}^{ConfidentlyCloudy} \qquad M = \delta_{jk}^{\text{ConfidentlyCloudy}}$$

The *amsmath* package is part of the Copernicus document class. This means that the `\text{}` macro is available to typeset fragments that are text within an equation. This improves the readability. It isn't just the italics, but especially the spacing that is different. Please use `\text{}` in all mathematical notation where a superscript or subscript is not an index or exponent but an abbreviation or a name. The symbol $f_c^{\text{NIR}_{\text{old}}}$ can be coded as `$f_c^{\text{NIR}_{\text{old}}}$`.

3.6 Figure size

While the schematic overview in figures 3, 5, 6, 8, 9, and 10 is much appreciated in explaining the method, the vertical spacing of these seem rather large. Reducing the vertical spacing of the "source" and "target" panels is likely to provide a better spacing in the article, and allow for easier reference to the figures while reading the description of the method in section 3.3.1, especially for the baseline case (equations 6 and 7).

3.7 Readability of equation 12

Suggestion to split the contribution of γ_1 and γ_2 to emphasize the symmetry on the equation.

3.8 Missing introduction of the H_c symbol

In equation the symbols H_c^{UV} and H_c^{NIR} are used, but this symbol is never properly introduced. Extending table 2 to also introduce the symbols for the quantities taken from VIIRS is a possible solution.

3.9 Language

I'm not a native speaker, but the following sentences (line 314 – 316) do not seem to be correct English, or at least a slight rephrasing may make them more readable: "The first TROPOMI UV detector pixels were lacking of cloud height and cloud optical thickness properties up to now due to the missing TROPOMI NIR overlap detector pixels. The use of VIIRS data made possible to re-construct the UV/VIS cloud height information for these pixels through the mapping linear function of Equation 17."

I'll group this under language as well: on lines 324, 325, 327, and 487 the chemical symbol for ozone is given as "O3" rather than "O_3".

In the conclusions, on line 421 – 422, "...from UV/VIS to NIR with the new scheme results to a lower cloud fraction compared to the old scheme ..." should probably be "...from UV/VIS to NIR with the new scheme results *in* a lower cloud fraction compared to the old scheme ...".

In the conclusions, on line 432 – 433, "...allows the restructuring of the ROCINN retrieved parameters...", I would suggest "...allows the reconstruction of the ROCINN retrieved parameters...".

In the conclusions, on lines 444 – 445, "The old co-registration scheme is applied when the old scheme for co-registering the OCRA CF when the VIIRS CF at both UV/VIS and NIR bands are equal to 1.". Please check and rephrase, there is a repeated part in this sentence.

3.10 Figures 26, 27, 30 through 37, and table 4

While the difference between figures 26 and 27 is obvious if you can switch between them on a computer screen, if they are on adjacent pages and share the same position on the page, once printed it is nearly impossible to spot the difference between these two figures. This is an issue either for the journal, to make sure that these pages end up in a location where switching between them is possible (as in the current pre-print), or to combine these figures in a three pane single figure, showing both figures and adding a difference plot.

In figure 30 there are 6 pixels that are highlighted. At the printed scale these highlights are hardly visible. Either zoom in further or select another display technique. A zoomed in inset in the top-left of the figure may be an option.

In figures 31 through 37 the locations are displayed only with their longitude *or* their latitude. Please add a second axis with the other coordinate of the data points. Given the importance of the 20 % cloud fraction for trace gas retrievals, I suggest to add a thin horizontal line to figures 30 through 33 to indicate that level as a visual guide to see the impact of the new scheme. The 5 % level is important for the ROCINN retrieval, and may require an additional grid line in these figures. For clarity I suggest to use a consistent line style for band 6 and a different, but also consistent one for band 3, one continuous, and one dashed for instance. At the moment this is *almost* the case, except for the old band 6 lines.

The same additional coordinate – i.e. latitude – is required in table 4.

In Figure 35 I suggest to plot the "old" and "new" traces in reverse order. Right now the "new" trace is almost completely obscured by the "old" trace. Combined with the intensity of the colours of both traces it is somewhat hard to spot the "new" data. A suggestion specifically for figure 35 is to reduce the vertical scale to 0,- 15 km.

3.11 Caliop

In section 4.3 on Caliop, there are some confusing statements, please double check them.

1. On line 384 the altitude of Caliop is given as 685 km. On line 385 and 386 Caliop is moved the a *lower* orbit at 688 km. The emphasis is mine.
2. On line 386 it is stated that "Caliop is a two-wavelength. . . ". Unfortunately Caliop is no longer active since August 1st, 2023. Consider to use the past tense.
3. On line 460 the time coverage of version 4.21 of the Caliop processing is listed at up to the present. Please update this with the actual availability.