Review "Impact of 3D Cloud Structures on the Atmospheric Trace Gas Products from UV-VIS Sounders – Part I: Synthetic dataset for validation of trace gas retrieval algorithms" by Emde et al.

The manuscript by Emde et al. (2021) presents a synthetic dataset of 3D radiative transfer simulations that can be used to investigate the effect of 3D cloud structures on trace gas retrievals. This is a relevant scientific topic, particularly in view of the increased spatial resolution of current and future satellite instruments. The effects of realistic 3D cloud structures have not been yet extensively investigated and quantified, so this study (and its companion papers) are of scientific significance. However, the presentation quality is just sufficient, and although the scientific approach and methods are valid, the results are not discussed in an appropriate way. Therefore, the manuscript is well suited for publication, but major revisions are needed.

General comments

The manuscript reads often like a technical report, sometimes difficult to follow. The fact that it presents a synthetic dataset as a part of three publications decreases the possibility of more in depth and detailed discussions. However, scientific discussion needs to be more extensive, otherwise it could just be published in a journal more suitable for datasets.

Two main issues that are of central importance (together with clouds) to trace gas retrievals are aerosols and NO2 profile. The aerosols and its correction on the retrieval algorithms is closely related to the clouds and their effects. Furthermore, the study uses the most realistic cloud field possible with 3D radiative transfer model but then uses a constant NO2 field throughout the domain. These two topics need to be discussed in the text, as currently is just mentioned as if this was of very little relevance.

Specific comments

Introduction:
The first two-three paragraphs as compared to the rest of the introduction are poorly written. The last sentence of the first paragraph does not add anything to the readability of the introduction and to the topic of the manuscript.

Page 2, lines 24-26: 'Here' referring to Schwaerzel et al? What do you mean by 3D box-airmass-factors? Calculated with 3D radiative transfer model? Please be more specific. This is the introduction and it is already somewhat confusing the naming of the AMFs. Later on, you also refer to 3D layer-AMFs (e.g. page 19, line 20), so please be consistent.

Page 3, line 33: what do you mean by inhomogeneous surface albedo? Spectral dependence? Reflection anisotropy?

Page 4, line 15: is the ALIS method influenced by the number of photons on the simulation?

Page 4, line 18-19: see my comment on the introduction about layer and box AMFs.

Last sentence on Sect. 2: maybe you can cite the paper of the series where this is actually analyzed. In this manuscript only one specific layer AMF has been analyzed (at 0.5 km).

Sect. 3:
Page , line 1: 'most of the NO2 located within the BL'. How high is the boundary layer for your base case? Have you investigated the effects in a non-polluted atmosphere? In connection to the apriori profile and the horizontal effects; the TROPOMI NO2 bias as reported by validation studies is different for urban and rural areas, so the 3D clouds effect may play a different role in these biases depending on the pollution level. See also your sentence in page 12, line 11. This needs further discussion, 'more or less affected' is not rigorous.

Later on the section it is also mentioned that 'Aerosols are not included'. Aerosols are a relevant topic for NO2 retrievals, so it needs further discussion. Even if it is not included, some motivation for this decision should be discussed, as well as the effect that the inclusion of an explicit aerosol treatment would have in the results.

What is the vertical discretization of the atmosphere? How does affect your simulations?

Sect. 3.1.2: what do you mean that in the y-direction the cloud layer extended to infinity? As I later understand the cloud has a geometrical dimension, right?

If half of the domain extending from 0 to 100km is cloud-free and the other half has a cloud, this does not match the schematic in Fig. 1.

Page 6, line 3: above the cloud as in the vertical dimension?

Page 7, line 7: 'the reflectance is higher than the clear sky reflectance near the cloud edge.'. Reads weird, please rephrase.

Page 6, line 7: 1D cloud layer setup. This is the first time this is mentioned. Do you mean just a cloud acting as a Lambertian reflector? Please explain.

Page 6, line 11: what are variance reduction methods, why are they needed? Please explain.

Reading of figure 1 could benefit from the addition of a grid. On page 9, line 31: do you mean larger than -15%?

Sect. 3.2.3. The explanation on this section could benefit from an Eq. that shows how the AMF is used in the retrieval.

Last sentence in page 12: it would be beneficial to include a discussion with few sentences on the main findings even though they are published in Yu et al.

Page 15 line 29: TROPOMI was not launch until October 2017.

Sect. 4.2.3: I would suggest to substitute the global maps of surface albedo for a zoom over the study for which the cloud simulations are done.

Sect. 4.2.4:

What about higher resolution than 7 km x 7 km? This is good for TROPOMI, but future sensors will definitely provide measurements at higher resolution. In Sect. 3 the simulations are done for higher resolution, and the ICON clouds resolution is 1.2 km x 1.2 km. The increased spatial resolution (as pointed in the manuscript) will enhance the impact of 3D clouds effects, so it would benefit the discussion to perform these simulations at higher resolution. If this is not feasible, then at least this should be discussed.

What is the effect on the results of reducing the number of photons with respect to the 1D/3D case? How will this affect the airmass factor calculation?

The study uses a very realistic cloud field from LES simulations, but then assumes a constant NO2 field over the whole domain, which is very unrealistic. The consequences of this assumption on NO2 needs to be discussed. How would the NO2 retrieval error on Fig. 12 look like if a realistic NO2 field would be used?

Editing

Figures and figure captions should be revised. Different sub-figures are specified differently in different figures, so please revise. See https://www.atmospheric-measurement-techniques.net/submission.html for figure guidelines. Using letters a,b,c etc. makes referencing on the text easier. Please mind the reader when creating the figures.
For example, Fig. 10: '(similar to TROPOMI on Sentinel-5P and Sentinel-5)' this is not relevant in a figure caption. Lower panels 'x = 256 km' is not relevant information and

makes the figure busier. Another example, Fig. 3 Top: legend ‘clear’ is better understood than ‘-1.5’ and ‘-10.5 km’, maybe add ‘shadow’ and ‘clear region’.

Name the O2 A band consistently throughout the manuscript (three names O2-A band, O2A-band, O2A band have been used)

Page 2, line 28: for->from TROPOMI/S5P obs.
Page 2, line 29: synthetic -> synthetic
Page 2, line 30: are-> were not included

Page3, line 3: incorrect grammar; the bias due to 3D clouds on what? And no need to start new paragraph if you talk about the same paper.

Page 18, limes 5-10: please write sentences in present tense. E.g., ‘pathlength is decreased’ -> ‘decreases’

Short paragraphs (1-2 sentences) just expressing technical details should be avoided.

Please include (at least) a reference when mentioning FRESCO cloud algorithm.

Page 22, line 6: what about the shadow effects?
Page 22, line 23: was this not at 1.2 km x 1.2 km?