Review of "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.

This paper is one of a set of three interconnected papers that discusses a) a publicly available synthetic dataset of 3D radiances, b) the sensitivity of vertical column density NO2 retrieval errors near box-clouds and observations, and c) 3D cloud biases and metrics. The reviewed paper is part a) of the full set of papers.

Since the paper is the first of a three-set collection, main findings are reserved for the other two papers. This produces the awkward situation that the main physical results, which one can derive from an analysis of the synthetic dataset, are not discussed in the reviewed paper. The reviewed paper is overly restrained. The reviewed paper is rather short of main findings, mainly stating that a synthetic data set is available, and therefore limited in informative results.

There are places in the text in which a terse one sentence paragraph is stated. Additional sentences can and should be added to the text in these portions of the text.

The paper should be revised. A suggested addition to the revised paper would be to include a figure or two that demonstrates the in-scattering and shadow curves (similar to Figure 2) for clouds of e.g. three heights in the LES cloud field, including panels in which (on the y axis) the reflectance is graphed as a function of distance from cloud edge, and panels in which retrieved NO2 is graphed (on the y axis) as a function of distance from cloud edge. These figures would help the research community better appreciate the quantitative importance of 3D cloud effects upon NO2 retrievals. Over what km range are 3D effects present as a function of cloud height, and what are the % errors in the NO2 column for these situations?

The paper is worthy of publication following revision.

Major comments

I would have liked to have seen in the Conclusions section a discussion of the major physical findings of the paper. The Figures provide instructive insights, yet these insights are barely touched upon in the Conclusions.

Minor comments

Page 3, line 12. Clarify what is meant by "bias" (the bias of what?)

Page 3, line 12. Replace by "In the third paper by Kylling..". The one sentence paragraph is a bit jarring since it is overly short in informative content.

Page 4, line 3. Clarify what is meant by "unbiased radiances"

Page 4, line 6. Replace "agreed perfectly" with a quantitative % value.

Page 4, lines 14-17. I am not convinced of the ability of the authors to "calculate the full spectrum based on photon path distributions sampled at a single wavelength". Atmospheric optical properties (Rayleigh scattering, aerosol optical depths, asymmetry and single scattering albedo) have a wavelength dependence in a real atmosphere. Please support your statements in the context of a real atmosphere with additional sentences. The sentence "The statistical error of

such a simulation is a bias for the complete spectrum" is not comprehensible. Add additional sentences which discuss the ALIS method. Replace with "This method allows one to calculate .."

Page 5, line 1. What is the boundary layer height, and how is NO2 vertically distributed in the troposphere?

Page 5, line 10. Change to "in the x-direction".

Page 5, line 14. The sentence implies just a single box-cloud geometry, while Table 1 lists several box-cloud heights. Rephrase to "For the liquid water cloud the primary cloud geometry has the base height set to 2 km ...".

Page 6, line 4. Why were aerosols not included in the calculations?

Page 6, line 11. Clarify what is meant by "variance reduction methods". Add sentences that describe the VROOM methods.

Page 9, line 12. Change to "Note that $D(\lambda)$ is a smooth function"

Page 11, line 8. Change to "layer-AMF as a function of"

Pager 13, line 2. Change to "realistic 3D clouds"

Page 15, line 17. Replace "sufficiently accurate" with a quantitative % accuracy.

Page 15, line 22. Change to "was analyzed, and it was found that SZA.."

Page 16, line 1. Change to "It was found that SZA varies.."

Page 17, line 1. Change to "Note that each simulated pixel includes 36 cloud pixels,.."

Page 17, line 5. Change to "Note that the number of .."

Page 18, Figure 11. What are the units of the NO2 retrieval error?

Page 19, line 16. Change to "Note that the complete LES.."

Page 23, line 7. Explain how the synthetic dataset can be used to "validate the various different trace gas retrieval approaches for Sentinel-S5P." This is an example of a terse one sentence paragraph that would benefit from additional sentences.

- 1. Does the paper address relevant scientific questions within the scope of AMT? yes
- 2. Does the paper present novel concepts, ideas, tools, or data? The box-cloud and LES 3D calculations are fairly unique
- 3. Are substantial conclusions reached? No (more discussion would add to the paper)
- 4. Are the scientific methods and assumptions valid and clearly outlined? Some additional sentences (e.g. on the ALIS method) should be added to the text
- 5. Are the results sufficient to support the interpretations and conclusions? yes

- 6. Is the description of experiments and calculations sufficiently complete and precise to allow their reproduction by fellow scientists (traceability of results)? yes
- 7. Do the authors give proper credit to related work and clearly indicate their own new/original contribution? yes
- 8. Does the title clearly reflect the contents of the paper? yes
- 9. Does the abstract provide a concise and complete summary? yes
- 10. Is the overall presentation well structured and clear? Some additional sentences should be added to the text to clarify the discussion
- 11. Is the language fluent and precise? yes
- 12. Are mathematical formulae, symbols, abbreviations, and units correctly defined and used? yes
- 13. Should any parts of the paper (text, formulae, figures, tables) be clarified, reduced, combined, or eliminated? There are several places in the text in which clarifications are suggested
- 14. Are the number and quality of references appropriate? yes
- 15. Is the amount and quality of supplementary material appropriate? Not applicable