

Review of: Three-dimensional radiative transfer effects on airborne, satellite and ground-based trace gas remote sensing (Schwaerzel et al., 2020)

The manuscript discusses the study of 3D RT/geometric effects on trace gas remote sensing. The 3D distribution of the instrument sensitivity to a certain pollutant is a very relevant problem when observing a heterogeneous atmosphere at high resolution from ground-based, airborne, spaceborne instruments. 3D-BOX AMFs are implemented into the Monte Carlo MYSTIC RTM and validated against 1D-layer AMFs computed by other RTMs. The geometric effects are demonstrated based on a ground-based and airborne case with a focus on NO₂ and based on simulated data. The scientific content of the paper fits well within the scope of AMT and will be valuable to a wide community. The manuscript is well-written and generally well-structured. Therefore I highly recommend its publication in AMT. However, some revisions (detailed below) need to be conducted in the paper before publication.

General comments

-On p.3, l.43 the authors state that the assumption of horizontal homogeneity (1D-BOX AMF) is not valid in polluted environments. In theory, I fully agree with this statement. However, in case of real-world observations I'm doubting that all relevant data will be available for most regions in order to fully benefit of the 3D-BOX AMF calculations. It requires accurate and high-resolution 3D trace gas and aerosol fields, while it is now often already difficult to get the proper high-resolution a priori for the 1D layer geometry. This has not been discussed in the paper. It would be an added-value to add a paragraph, e.g. in the conclusion, to discuss what is currently missing or needed in order to fully benefit of the 3D BOX-AMF geometry in case of real-world observations.

-I assume it is most likely subject of a future study but I'm also strongly interested to see the impact on total AMFs and VCDs when using 3D BOX-AMFs instead of "typical" 1D layer AMFs in case of real-world MAX-DOAS and airborne/spaceborne observations. In case this is subject of future work, it could be mentioned in the conclusion.

-A quantification of the horizontal smoothing of the plume due to geometric effects when 1-d layer AMFs are used would be an added-value in addition to Fig. 10 and 11. For example, a table could be added quantifying the horizontal smoothing for different scenarios of SZA, VZA, plume size and plume altitude.

-The reader might also be interested to get some info on absolute computation time and difference between MYSTIC 1D layer AMF and MYSTIC 3D box AMF computation time for a typical satellite or airborne scene.

Minor comments

-p.2, l.35 I understand you want to make a distinction between layer-AMFs (1D) and BOX-AMFs (3D). However, in past studies eg Wagner et al. 2007, "BOX-AMFs" were used for what is defined in this work as layer-AMFs. I would add a short statement to clarify. I noticed that you clarify this later on in p.5. I propose to switch it to the introduction.

-p.3, l.68: SCD and VCD acronyms were already defined in the introduction. No need to do it here again. There is some repetition here as well like explaining again what a VCD and AMF is. I suggest to remove it from the introduction or remove it here.

-In Fig. 8b I would expect the two SCD maxima to be east and west of the true VCD at first glance (also when looking at Fig. 9). However, they both seem to be east of the true VCD, with the most western SCD maximum falling together with the VCD maximum. Or do you assume VZA is 0°? In that case it isn't consistent with the example in Fig. 7. Could you please clarify?

Technical corrections

-p.1, l.6: MYSTIC acronym stands for ...?

-p.2, l.45: I would add "at high resolution" after "trace gas remote sensing"

-p.3, l.63: It depends also on the molecule and aerosol properties (e.g. SSA)

-p.3, l.75: remove "and" after VCD

-p.5, l.87: an aircraft

-p.5, l.88: sensitivity to NO₂ → it is a general discussion. I suggest replacing "NO₂" by "the trace gas - under investigation"

-p.5, l.110: "computationally efficiency" → computational

-p.6, l.133: 577nm → add space

-p.6, l.137: mostly 1000m resolution → maybe more clear to describe it as a layer thickness instead of vertical resolution.

-p.8, l.161: The upper row of Figures 3 (**scenario at 577 nm**) and 4 (**scenario at 360 nm**)

-p.8, l.162: shows

-p.11, l.13: for → at

-p.13, l.257: For clarity, mention explicitly GRAL is a dispersion model, eg. Graz Lagrangian dispersion model

-p.14, l.289: planet boundary layer (PBL) -> boundary layer has occurred many times earlier in the paper. Please explain PBL acronym at first occurrence and use the acronym in the continuation of the work.

-p.15, l.294: SCCs → SCDs

-p.16, l.302: ...3 instrument zenith angles -- > 3 viewing zenith angles (VZA)

-p.16, l.310: (Fig 8 2nd row) → (Fig. 8d, 8e, 8f) (same for line 312)

-p.18, l.339: The VCD cross sections

-p.21; l.374: the application of

-Figure 2: The spherical regression line and points are not clear at all. Maybe consider having two scatter plots. However, the main message of the plot stays clear based on the 5% deviation lines

-Figure 5 caption: Decay of vertically integrated AMFs with distance to the instrument (c) → please add “is visualized” after “instrument”

-Figure 8: ...located at $x=19$ km and $y=13$ km. → should be $x=1.9$ km and $y = 1.3$ km?

-Figure 12: maybe put “NO₂ concentration” instead of “VCD” in plot and caption.

-Table 2: Maybe better to give RAA instead of SAA in order to be consistent with the discussion at the end of p.19

Section 6 (Conclusion): I assume there is no need to define acronyms again here, e.g. AMF, RTM, VCD, SCD, etc.