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Interactive comment on "Accelerating simulations using Direct Relation Graphs for atmospheric chemistry mechanism reduction" *by* Zacharias M. Nikolaou et al.

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This is an interesting piece of work. Reduction of chemical mechanisms in chemistry transport models received relatively little attention, while there is a lot of computational effort to win. The paper is well written, and clearly organized. A solid introduction which sets the theory, and a short method section (some questions in the annotated pdf document). The results are spit in two parts (1) box model evaluation (2) full 3D model evaluation.

I have some problems with both approaches. The mechanisms are tested in a box model under relatively polluted conditions only, and at surface temperatures and pres-

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Discussion paper

sure. In a real setting, the scheme will also be applied to the upper atmosphere, where completely different conditions will prevail. I argue that the choice of scenarios is not balanced for a true atmospheric simulation. The same holds for the 3D validation, which uses unclearly formulated conditions for the initial and boundary conditions, and does not apply emissions. Furthermore, only the lowest 9 layers are analysed, which reinforces my point above.

An important point is made at the end of the result section. By removing species (i.e. reduced hydrocarbons), biases may be introduced that propagate through e.g. HO and CO. This is undesirable since these biases may accumulate in global models (not so much in regional models that apply boundary conditions). This is exactly the reason that lumped species have been introduced. This would involve the merger of species, instead of removal of species (and assumptions about similar effects on overall chemistry).

When the authors manage to address these main points, I think the paper is a valuable contribution to GMD. I guess it would also be good to provide the community with the tools the authors developed on top of the KPP code, but I guess this is mandatory in GMD.

Further comments can be found in the annotated manuscript.

Please also note the supplement to this comment:
https://www.geosci-model-dev-discuss.net/gmd-2018-106/gmd-2018-106-RC1-supplement.pdf

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