Geosci. Model Dev. Discuss.,
https://doi.org/10.5194/gmd-2020-337-RC3, 2020

Geoscientific Model Development Discussions

Interactive comment on "Oxidation of low-molecular weight organic compounds in cloud droplets: development of the JAMOC chemical mechanism in CAABA/MECCA (version 4.5.0gmdd)" *by* Simon Rosanka et al.

Anonymous Referee #2

Received and published: 27 November 2020

The paper "Oxidation of low-molecular weight organic compounds in cloud droplets: development of the JAMOC chemical mechanism in CAABA/MECCA (version 4.5.0gmdd)" by Rosanka et al. presents JAMOC, a cloud chemical mechanism. The paper fits within the scope of GMD and I recommend publication once the authors address a couple of points and provide additional information.

General Comments

I have a little difficulty in understanding how JAMOC fits within the whole

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Discussion paper

MECCA/CAABA/MESSy/EMAC ecosystem and while I am sure this has been described previously in the corresponding papers, I think it should be mentioned repeated here. A few points come to mind:

1. As I understand it, the JAMOC module is part of MECCA and MECCA itself is a module that can be used in the CAABA box-model and/or in the EMAC global model. In this case, it is perhaps better to remove CAABA from the title (and elsewhere in the text)?

2. If I am not mistaken, MECCA already includes an aqueous-phase chemical mechanism. Is JAMOC an upgrade/extension to it or is it supposed to replace it or run alongside it? This relationship should be clarified, and it should be explained, for example, why it is necessary to create a new module and not simply add reactions to the pre-existing aqueous-phase module.

3. On page 3 the authors say: "The inorganic chemistry for the proposed mechanism is very similar to the inorganic chemistry of the standard aqueous-phase mechanism used in EMAC (Tost et al., 2007; Jockel et al., 2016) and reactions included in MECCA (e.g. Fenton chemistry), which are not yet implemented in EMAC." This is a bit confusing, as it implies that the reactions in JAMOC are already in MECCA and some, but not all, are already in EMAC. Howeverm it does not say which ones, so it is difficult to understand how much of a change has been made. This also suggests that JAMOC is meant to replace the current aqueous-phase mechanism in MECCA and/or EMAC. As per my previous point, the relationship between the different parts of the system needs to be clarified.

The other major comment I have is about CLEPS. The authors describe JAMOC as derived from CLEPS but they don't say how this was done. Were the reactions "hand-picked" from CLEPS (if so on which basis?) or was some reduction procedure applied? It is important that the process is described and the rationale behind certain choices is explained.

I also think it would be more useful and, more informative perhaps, to compare the output of "CAABA with JAMOC" to the output of CLEPS, rather than to the output of "CAABA without JAMOC" (Figure 3 and related discussion). This would allow a better understanding of the accuracy of the reduction procedure, and how much information (if any) is lost when the more explicit mechanism CLEPS is condensed into the smaller mechanism JAMOC.

Minor Comments

line48: "only a selection of species containing up to four carbon atoms react within the aqueous-phase". Can you explain why this choice was made? I understand one of the reasons is to keep the size of the mechanism relatively small, but why only up to C4 species react and up to C10 species undergo phase transfer? Is the reaction of molecules with high carbon number too slow to matter? Do you actually need to transfer C5-C10 into the aqueous-phase if they don't react and you need to keep the mechanism small?

line 71: can you clarify the difference between apparent and intrinsic Henry's law constant?

line 86: "Pseudo-first order rate constants for the hydration and dehydration are mainly obtained from the literature". This implies that some were obtained or estimated in another way, please clarify.

line 141: "In all cases, branching ratios are rescaled to 100%." Can you explain this point better?

line 149: how much faster is R11 with respect to R12?

line 182: correct "modells"

figure 3: the first panel should be sum of OVOC rather than sum of VOCs

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2020.