

Geosci. Model Dev. Discuss., referee comment RC1
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Comment on gmd-2022-55

Anonymous Referee #1

Referee comment on "Atmospherically Relevant Chemistry and Aerosol box model – ARCA box (version 1.2)" by Petri Clusius et al., Geosci. Model Dev. Discuss.,
<https://doi.org/10.5194/gmd-2022-55-RC1>, 2022

In their article, Clusius et al. present the Atmospherically Relevant Chemistry and Aerosol box model (ARCA) representing atmospheric gas-phase chemistry and submicron aerosol processes. Its processes representation is mainly based on earlier model implementations but distinguishes itself by an extensive GUI and its focus on ease of use for scientists that have little experience in aerosol and chemical box modelling. Although the current manuscript provides already a good overview on the model itself, further elaborations are necessary before publication in GMD.

General Comments:

- At the beginning of the introduction, a very short overview on possible applications for aerosol and chemical box models is presented. However, the examples given are solely limited to the published work of the authors. The introduction would greatly benefit when discussing the ARCA model in the context of other aerosol and chemical box models in a technical and historical context. Especially, focusing on models and publications outside the authors' group.
- As the authors clearly state (Sect. 1.1), the model in its current state neglects important processes for aerosols (e.g., aqueous-phase chemistry). However, the targeted user group is scientists that have little to no experience in aerosol and chemical modelling. This user group would greatly benefit from a section discussing the implications of the missing processes on the model's results (e.g., before section 6).
- The authors claim that the GUI design is one of the main aspects that distinguishes ARCA from other box models. However, very little information on the GUI design is presented and is mainly limited to a series of figures from ARCA's GUI with very little information about it in the text (Sect. 3). Further elaboration on the GUI design is necessary in this section. This information should at least contain but is not limited to: (1) the GUI design principles, and (2) a workflow diagram and description of the GUI design/use including dependencies between the different tabs. At multiple locations in the text, the authors discuss possible errors. Since the targeted user group is expected to have little experience with box modelling, a proper error management is key to avoid

misconfiguration followed by potentially wrong conclusion. An elaboration on the error message management should be added.

- The verification of the model (Sect. 4) is poorly presented and e.g. in Sect. 4.3, it is limited to just presenting two plots. Some discussion of the results should be added.
- Before the authors provide a revised version of the manuscript, they should perform an editorial check focusing on the consistent use of the Copernicus rules (e.g., use of figure within the text), correct numbering of sections, etc.

Specific comments:

L20: Stating that “any compatible chemistry scheme” is ambiguous since currently the model is limited to gas-phase chemistry.

L109: Is the user notified of this if the time step is selected too large by the user? Is there an upper limit of the time step length?

Figure 1: The definition of PSD is missing in the caption.

L271: The last sentence seems to be out of place. Shouldn't this be specified in the introduction?

L285: Is the user made aware (e.g., in the GUI) that he is responsible to select the PSD size range? Is an error raised if he fails to do so? This could be used by the authors as an example for the error management (see general comment 3).

L397: What is your justification to select the same value for all compounds? Can the user change this value for single compounds? This would make it easier to tailor ARCA to individual chambers.

L432: The online user manual is nice. Adding a link to it here would be helpful.

L439: This statement is ambiguous, unspecific, and misleading. What distinguishes “good” and “better” science? I suggest rephrasing this statement focusing e.g. the avoidance of systematical errors when performing simulations or similar.

Section 5.3: In addition to the model code, please provide the modelling data of the

simulations used in the verification section (e.g., using Zenodo).

Section 6: In Sect. 1.1, you state that organic liquid phase chemistry is not considered in ARCA but may be important (e.g., on the thermodynamics, formation of secondary organic aerosols). Is there a reason why you currently do not plan to include this chemistry in future model versions? In the case when using MCM, the coupling to CLEPS (Mouchel-Vallon et al., 2017) should be strait forward.

References:

Mouchel-Vallon, C., Deguillaume, L., Monod, A., Perroux, H., Rose, C., Ghigo, G., Long, Y., Leriche, M., Aumont, B., Patryl, L., Armand, P., and Chaumerliac, N.: CLEPS 1.0: A new protocol for cloud aqueous phase oxidation of VOC mechanisms, *Geosci. Model Dev.*, 10, 1339–1362, <https://doi.org/10.5194/gmd-10-1339-2017>, 2017.