Geoscientific Model Development Discussions

Geosci. Model Dev. Discuss., referee comment RC2
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Comment on gmd-2022-55

Anonymous Referee #2

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-RC2, 2022

This manuscript presents the ARCA model, a fairly sophisticated box model with a graphical user interface that can be used to simulate atmospheric chemical processes. There are now several of these tools available but not all of them are aimed at researchers without a modelling background. I think the effort to simplify the process of setting up and running a complex chemical model is noteworthy and it seems ARCA fits into this description. The paper is well written and clearly outlines the inner workings of the model, referring the reader to the extensive online documentation for more detailed information. I think there are only a few minor points to clarify, otherwise I recommend publication in GMD.

The idea of using different timesteps for different processes is interesting. I am wondering if the authors can say how much computational time is saved compared, for example, to the fixed timestep mentioned on line 121. I imagine this is related to the chemical conditions used, but it would be good to have a ballpark idea. One things that is not clear to me is whether the possibility of using different timesteps for different processes is a consequence of the fact that the processes are run in a sequence (line 105). As a side note to this point, it would be good if the authors can comment on how the model ensures that mass is conserved when "moving" from one process/module (e.g. gas phase chemistry) to the next in the sequence (e.g. particle formation).

On line 94 it is said that all particles are considered to be liquid droplets, but on line 98 it is said they are void of water. This sounds like a contradiction.
Is is also not clear to me what is the difference between the aerosol module mentioned in this paragraph (lines 94-99) and the ACDC module. The following sentence (lines 100-101) implies they are both used in the model, but the text on page 2 (lines 73-76) seems to

suggest that the model uses the ACDC only. The APC scheme is also mentioned on page 2, but it is not clear whether it is part of the ARCA model or not.

I think there should be a little more explanation about the wall loss process described in section 2.7 (and also about the "gas-wall partitioning" in Figure 1. What is it meant for? Indoor studies and/or environmental chambers? Is it inactive in ambient studies?

line 81: delete "using"

line 99: instead of "restrictions" I suggest "limitations"

figure 1: I suggest changing "wall loss of particles" to "particle losses" for consistency with table 1 and related text (or viceversa, change the table).

line 226: can you clarify what is meant by "numerical diffusion"?

line 271: it is said here that "ARCA has slots for five ACDC modules". Does it means that there are 5 aerosol bins, as default? Related to this, does the ARCA GUI allow modification of the ACDC settings or one would need to modify those separately, following the ACDC user manual?

line 511: add link/reference to "UmanSysProp" and say what it is.

line 517: why do you say KPP is not necessary for ARCA? That seems to contradict the statements in section 2.1 and 2.1.2. The VODE (or DVODE? Is it the same thing?) solver is mentioned only once earlier in the paper. Please clarify if it is VODE or KPP (or perhaps both?) that are used to solve the differential equations system.

In Section 5.2. Are there any libraries or dependencies that need to be installed besides the netcdf libraries? e.g Python graphic libraries for the GUI and plotting?