

Interactive comment on “JIBox v1.0: A Julia based mixed-phase atmospheric chemistry box-model” by Langwen Huang and David Topping

Anonymous Referee #2

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This paper describes the 0D box-model JIBox, an atmospheric chemistry model to simulate gas phase kinetics and gas-particle partitioning. While plenty such models exist in the community, the innovation of this work is that it is written entirely in Julia geared towards high-performance computing. The paper presents version v1.0 of this model and highlights the advances compared to the python-based model PyBox, which serves as the basis for the JIBox model.

This is interesting work with a lot of potential for future atmospheric chemistry modeling endeavors. The paper is well written and fits well within the scope of GMD. I recommend publication and have some minor suggestions for revisions, mainly to improve the accessibility of this paper for a wider audience.

1. One of the biggest bottlenecks in updating gas/aerosol mechanisms is the interfac-
- C1

ing of the chemistry modules with the representation of aerosol microphysics (i.e. bins or modes, what exact bin structure, how many modes etc.) It would be helpful to have some more description in the paper how this is realized within JIBox.

2. Title and throughout the manuscript: The phrase “mixed-phase” to me sounds like referring to a cloud physics model (“mixed-phase clouds”). I suggest using the term “multi-phase” for referring to the combined gas-aerosol system.

3. Eq. (2)-(4): Typesetting of equations: Note that only the subscripts and superscripts that refer to variables should be in italics. Description subscripts and superscripts (eff, w, core, etc.) should be in textmode.

4. Eq. (3): Define variable `core_diss`, and what is considered as “core”.

5. Line 80: Rather than “size” of particles, this should read “radius”. This applies throughout the manuscript.

6. Line 82: surface tension: Is this the same for all size bins (i.e. taken to be the surface tension of water)?

7. Equation (10): It would be helpful to add some description around this equation and to split up the two equations into two lines. Also switch the lhs and the rhs of the first equation (so that m_k is on the lhs).

8. Line 289: “Validation” should be changed to “Verification”, since it refers to the benchmarking with another model.

9. Line 296/297: “average size of 0.2 microns” – I assume the authors mean “geometric mean diameter”.

10. Line 297: “microns” should be μm 11. Line 297: “standard deviation of 2.2 microns” – I assume that this should be the geometric standard deviation. If so, it has the unit 1 (not microns).

12. Line 297: Are the 16 bins logarithmically spaced? And over what radius size

range?

13. Line 317: "exponential growth of SOA mass": The growth doesn't look exponential.

14. Line 339: Regarding the high and low RH scenarios: How is water uptake simulated? Is water one of the n chemicals mentioned in line 86? And what is the reason for different run times depending on RH? Also, the system of equations (2)-(4) assume droplet solutions. Do you assume that the particles always contain water, even at the low RH of 10

15. Line 345: Something went wrong with this sentence, please rephrase.

16. Line 346: should read "cluster provides"

17. Figures 2 and 3: Suggest reporting the time in hours rather than in seconds.

18. Table 2: Suggest reducing the number of sig figs in the dSOA column and in the two last columns write the numbers as scientific notation 3.0×10^{17} etc.

19. Even though the simulation results are not of scientific interest in this paper, I suggest including a size distribution plot of the aerosol that undergoes condensational growth for at least the case shown in Figure 2.

20. Switch the order Tables A1 and A2 to make it consistent with the presentation of Figure 3 and 4.

Interactive comment on Geosci. Model Dev. Discuss., <https://doi.org/10.5194/gmd-2020-344>, 2020.