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Interactive comment on "PyCHAM (v1.3.4): a Python box model for simulating aerosol chambers" *by* Simon Patrick O'Meara et al.

Anonymous Referee #2

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O'Meara et al. described in detail about the structure and demos of an open-source python box model for simulating aerosol chambers (PyCHAM). Comparisons were made with the results from other models. Sensitivities of different parameters were also tested. The manuscript is overall well written and the PyCHAM could be very helpful for both experimentalists and modelers. I suggest for publication in GMD after some minor revisions:

1. What is the file format of MCM that PyCHAM is taking, i.e., can it be directly used after downloaded the specific file from the MCM website or some formatting has to be made to the file before imported?

2. Fig. 1: since the size distribution uses $dN/dlog_{10}(D_p)$, the y-axis should be in log_{10} scale instead of linear scale.

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Discussion paper

3. Is the chamber temperature coupled with the vapor molecule thermodynamic properties (e.g., the vapor pressure, diffusivity, etc.) in the PyCHAM?

4. What is the ODE solver used in the PyCHAM since most of the ODEs are very stiff? Are Jacobian matrices specified or numerically calculated in the code? What are the units used when simulating, e.g., ppm/min or pg/s or not the same for compounds in different phases?

5. L282: 0.5 μm seed particles are usually too big in a chamber experiment, which can cause significant particle-wall loss. Usually, the seed particles are around 100 nm. If no particle-wall loss is considered in this section, suggest using a smaller size of particles but with the same particle surface area concentration to test.

6. Given different C_w values are used in Sec.6 for sensitivity test, Krechmer et al. (2016, DOI: 10.1021/acs.est.6b00606, Krechmer 2017 cited in the manuscript is not on this topic) have shown the vapor pressure-dependent C_w. Since the PyCHAM couples the molecule structure with the UManSysProp module, this character can be easily incorporated.

7. For both α-pinene and isoprene SOA experiments, please list the compounds (as well as their corresponding vapor pressures) that are allowed to partition to the particle phase.

8. L390: What are the timescales of coagulation versus condensation growth?

9. Fig. 10: Which experiment does this figure correspond to, α-pinene or isoprene?

10. Eq. 11: What is the unit of P_1? From the description, it looks like a rate. But Fig. 10 indicates it is a number concentration. If as a concentration, the nucleation rate would be changing over time (reaching the maximum around 150 s by differentiating curves in Fig. 10), how does that happen? Maybe explain this a bit more in this section.

11. Sec. 11: The title "... spatial resolution" is confusing, which is actually "size" resolution. When appearing together with "temporal", one could think it as in a 3D

space. Suggest to change it to an appropriate word.

12. L471: Which method is used to interpolate the data points?

13. Eq. 13: Maybe use a different symbol (or sub-/super-scripts) for σ_g since it has been used to evaluate the Z & Y.

14. Fig. 11 is a little bit difficult to follow: a). The simulation time in the context means the time consumed by the processor to finish the simulation, but one could think it as the time in the model to simulate. Maybe change to a different name. b). What is the number of size bin for different time interval simulation? c). If possible, contour plots of derivation/consuming time with the x-axis of the time interval and the y-axis of the number of size bin would be appreciated.

15. Table 1: Instead of using log_{10} unit, units of hr or min are more intuitive to the readers.

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