Review of the manuscript "PyCHAM (v1.3.4): a Python box model for simulating aerosol chambers"

General comment:
This manuscript describes and assess the open source Chemistry with Aerosol Microphysics in Python (PyCHAM) box model software for aerosol chambers written in Python. The manuscript is generally very well written. I think PyCHAM has the potential to become a user friendly and widely used box model for analysis and interpretation of smog chamber experiments. The main concern I have is the long simulation time presented in Table 1. I consider that this manuscript should be accepted for publication in Geoscientific Model Development after some minor revision and appropriate answers to all comments.

Specific comments:
I could not find any clear description of how the gas-particle partitioning of multiple condensable organic and inorganic vapors are treated in PyCHAM. Do you consider the Kelvin effect and Raoult's law for ideal mixtures? Possible I just missed this information. I think you should add a separate section which describe more in detail how the gas-particle partitioning onto different size bins are treated and how you keep track of the chemical composition in each size bin over time.

Page 3, L78-79 and Fig. 1. Did you set the N_2O_5 activity coefficient to zero or should it be unity, e.g. assuming ideal solution for N_2O_5. What activity coefficients do you use for the dissolved inorganic ions, e.g. in this case NO_3^-, H^+? Which base neutralize the dissolved HNO_3? How did you calculate the particle water content? How do you calculate the $[H^+]$ in the aqueous phase? $[H^+]$ is needed in order to calculate the effective Henry's law coefficient which in turn is needed to derive the condensation and dissolution growth for HNO_3 and N_2O_5 I presume.

Based on the previous comments, does PyCHAM include any thermodynamics module which iteratively calculates the aqueous phase [H+] and particle water content etc., and if yes, how and when is it called?

P9-10, section 5.1 and Fig. 3. Considering that AtChem2 and PyCHAM use exactly the same MCM chemical scheme I am surprised that the deviation in the NO concentration is several percentage. Please discussion these results a bit more. What can the reasons be? Which error tolerances (solvers) did you use in PyCHAM and AtChem2?

P14, 307-308. First, does not particle wall losses also directly influence the particle number size concentration? Secondly, would it not be more appropriate to write particle number concentration size distribution or just particle number size distribution?

P14, L319-L322, I agree that the full-moving particle distribution technique is not ideal when consider addition of new particles to the particle size distribution over time, but it is not impossible to use the full-moving approach as long as you add new particle size bins during the course of the simulation see e.g. Sect. 3.3 in Roldin et al., Atmos. Chem. Phys., 15, 10777–10798, 2015. Hence, I would encourage you to add the option for users of PyCHAM to use the full-moving approach.

<u>Section 7, Fig. 7</u> I was expecting the accumulation mode in Fig 7a to move towards the right because of condensational growth during the course of the simulation. But maybe this is not apparent when only looking at the particle volume size distribution. Can you also add a panel illustrating the particle number size distribution at the start and in the end? I also think that it would have been more interesting and more appropriate, considering the intended use of PyCHAM, to show similar results from an idealized no-seed secondary organic aerosol formation experiment with new particle formation and consecutive growth.

<u>Section 8.</u> I generally do not like numerical methods which is not mass conserving but I can accept the choice of the semiimplicit method of solving the coagulation process since you show that it is almost mass conserving. Still, I wonder what the advantage is of using this method in front of a simple fixed section method which will be both mass and number conserving? Is the semiimplicit approach by Jacobson (2005) resulting in less numerical diffusion problems compared to methods which are both mass and number conserving, but which rely on redistribution of the exact new single particle volumes onto the existing size bins using a fixed section approach (see e.g. Korhonen et al., Atmos. Chem. Phys., 4, 757–771, 2004)? Since, coagulation in contrast to condensation only change the size of a minor fraction of the total particle concentration each time step, numerical diffusion should not be a major concern with this fixed section approach and hence, I would encourage you to consider using such a mass and number conserving approach in future PyCHAM versions.

<u>Section 11, Fig. 11.</u> To me this is the section which is least easy to understand. I think this is because Fig. 11 is not easy to follow. I think you should avoid to use a dark green background and red lines. I would suggest that you if possible replace this figure with one or several tables. You may then consider to mark the cells with less than 10 % deviation from the reference case.

<u>Table 1.</u> Please write out the actual simulation time in hours instead of log10(time). $10^{3.4}$ s ≈ 0.7 h for 2 size bins with 60 s time step is quite a long time for 6 hours of simulation I would say. I presume that this is mainly the gas-phase chemistry. I would like you to add the simulation time for a simulation without particles, e.g. only gas-phase chemistry and also add the simulation time for AtChem2 (no particles). I guess AtChem2 is written in Fortran or? Too me $10^{5.2}$ s ≈ 44 h for 32 size bins with 60 s time step is not very user friendly. I guess it must have to do with the ode-solver and the stiffness of the differential equation system when you add many particle size bins. I would like to see some more discussion about these results and how they could be solved in future versions.

Possible typos:
<u>P11, L255.</u> I do not understand the formulation ",with factor increases of 7 and 53 for 6×10^2 and 6×10^1 s resolutions, respectively."

<u>P12, L286.</u> "Third, k_w was held whilst" should it be Third, k_w was held <u>constant</u> whilst … ?