Response to Anonymous Referee 2

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Dear colleague. Thank you for taking the time to provide a review of our submitted manuscript, submitted on 2nd January 2021. We are pleased your review is supportive of our work and we are of course happy to response to points raised and revise the manuscript accordingly. Please find our responses with any suggested changes in the manuscript below.

General comment 1): 1. One of the biggest bottlenecks in updating gas/aerosol mechanisms is the interface 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 JlBox

Response: Yes, we agree this is one of the biggest bottlenecks. We hope the automated nature of JlBox at least removes some of the challenges in coupling the gaseous and condensed phases. Whilst we only include a fully moving sectional representation in v1.0, we suggest the following addition to the manuscript might help the reader better understand how this coupling is represented numerically. Please note the figure order in the manuscript reflects the new addition and this figure comes after the definitions of the variables displayed which are already defined in the main text:We extend the original ODE state y with concentrations of each chemicals on each size bins. A simple schematic is provided in Figure 1. Imagine there are $n = 800$ components in the gas phase. In the configuration displayed in figure 2, the first 800 cells hold the concentration of each component in the gas phase. If our simulation has 1 size bin, the proceeding cells hold the concentration of each component in the condensed phase. If our simulation has 2 size bins, the proceeding 800 cells hold the concentration of each component in the second size bin and so on.

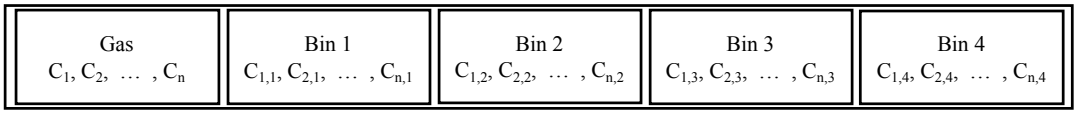

Figure 1. Array layout for ODE states y in Equation 5

General comment 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.

Response: This is a very good point, and we have changed this throughout the document, including the title.

Minor comments

Minor comment 1): 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

Response:. We have now changed the formatting in equations (2)-(4) and (10) to reflect this.

Minor comment 2): Eq. (3): Define variable $core\_diss$, and what is considered as "core".

Response: Apologies. The modified text in the manuscript now reads as follows: $[C_{\text{core},k}]$ is the molar concentration of an assumed involatile core in v1.0 that may dissociate into $core\_diss$ components. For example, for an ammonium sulphate core, $core\_diss$ is set to 3.0. $m_{\text{w},i}$ is the molecular weight of condensate i...

Minor comment 3): Line 80: Rather than "size" of particles, this should read "radius". This applies throughout the manuscript.

Response: We have replaced the instance of 'size' in the manuscript where the context is in relation to the size of the particles. Following the reviewers comment below, this has been changed to 'geometric mean diameter'.

Minor comment 4): 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 mk is on the lhs

Response: We have break Equation (10) into separate lines and added explanations of the equation. Yet we think the lhs and rhs of the first line is appropriate as a fully moving bin scheme has to calculate bin sizes at every time step according to that line.

Minor comment 5): Line 289: "Validation" should be changed to "Verification", since it refers to the benchmarking with another model.

Response: Yes we agree. This has now been changed in the manuscript.

Minor comment 6): - Line 296/297: "average size of 0.2 microns" – I assume the authors mean "geometric mean diameter".

Response: Yes this is correct and we have specified this in the manuscript.

Minor comment 7): - Line 297: "microns" should beμm11. 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).

Response: Yes apologies, this has now been removed.

Minor comment 8): - Line 297: Are the 16 bins logarithmically spaced? And over what radius size range?

Response: Yes, the bins are linearly separated in log space where a fixed volume ratio between bins defines the centre of the bin and bin width. The upper and lower size range and required number of bins define the centre (radius) of each bin accordingly. We have now added this description in section 4.2 as follows: ....discretized into 16 bins. The bins are linearly separated in

log-space where a fixed volume ratio between bins defines the centre of the bin and bin width. The upper and lower size range and required number of bins define the centre (radius) of each bin accordingly.

Minor comment 9): - Line 317: "exponential growth of SOA mass": The growth doesn't look exponential

Response: Yes, apologies for this lack of clarity. It is indeed sub-exponential growth. We have now removed this, and it should not affect the main point of this paper.

Minor comment 10): - 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

Response: This is a good point and we suggest some clarification is added to the manuscript. We explicitly simulate the partitioning of water between the gaseous and condensed phase following every other condensate. We appreciate this will, perhaps, significantly reduce the runtime of the box-model. However in this instance we wish to retain the explicit nature of the partitioning process before applying any simplifications such as assuming the mole fraction of water is equivalent to the relative humidity. One future expansion would be to run JlBox in a cloud parcel mode which would require the modification of the droplet growth equation to include latent heat release, but we feel the current architecture provides a good indication of the capability of a Julia based implementation. Likewise, with regards to the second comment on low RH, we assume an ideal solution. Another future development will include the ability to account for non-ideality. However this will also require subsequent treatment of dissociation of inorganic ions and a re-profiling of the subsequent computational cost. We suggest the following text is added to the end of section 3.2:

Please note we explicitly simulate the partitioning of water between the gaseous and condensed phase following every other condensate. We appreciate this may significantly reduce the run-time of the box-model. However, in this instance we wish to retain the explicit nature of the partitioning process before applying any simplifications as we briefly discuss in section 5.2

In section 5.2 'Future Developments' we then suggest the following modification: *...We could, and will, provide options for implementing simplified approaches to aerosol process, such as operator splitting and assume instantaneous equilibration for water in a range of sub-saturated humid conditions. Indeed, these methods..*

Minor comment 11): Line 345: Something went wrong with this sentence, please rephrase.

Response: We have now changed this sentence to the following: This represents a significant reduction when compared to the memory required to store a Jacobian matrix in a dense double precision format.

Minor comment 12): Line 346: should read "cluster provides"

Response: This has been changed.

Minor comment 13): Figures 2 and 3: Suggest reporting the time in hours rather than in seconds

Response: We agree, this has been changed.

Minor comment 14): 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 3.0×1017 etc

Response: This has now been changed.

Minor comment 15): 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

Response: Thanks for suggestion, we have now added an additional figure of size bin plot for one case in Figure 4.

Minor comment 16): Switch the order Tables A1 and A2 to make it consistent with the presentation of Figure 3 and 4.

Response: This has now been changed.