

## Reviewer 2

The presented manuscript has a well-thought structure and a fairly good scientific content. The implemented stochastic freezing method represents an important and valuable step towards an accurate description of the homogeneous freezing process although the final conclusions are somewhat limited by the absence of pre-existing ice in the idealized simulations. The step-by-step approach with incrementing complexity between the three presented ensemble sets is well thought and also the decision to vary always one variable at a time which keeps results and dependencies traceable in a simple manner. The following comments should be regarded before publication. If confirmed by the authors that there was a bug in the PySDM formula for the thermal conductivity correction used for the ICE-DEP simulations, it should be fixed and at least the high-CCN simulations with DEP-ICE be re-run before publication and the corresponding  $n_{ccn}$  ensemble plots re-rendered. Usually this would be clearly a recommendation for major revisions as part of the simulations need to be redone but in this case the conclusions might not change much or at all and therefore I'll leave it to the editor to decide if minor revisions could be okay as well.

### Major Comments

In section 2.2 the Eq.10 for the kinetic regime correction of the thermal conductivity is missing a factor of 4 in the right part of the denominator, it should be  $4 \cdot K_T$  instead of just  $K_T$  there (compare e.g. with Eq. 8.32 of Lamb & Verlinde / Eq. 5.2.13b of Khvorostyanov & Curry). Unfortunately this factor of 4 seems to be also absent in the PySDM code as well of the zenodo archive, meaning that there was a bug in the DEP-ICE part of the simulation code (under PySDM/physics/diffusion\_ice\_kinetics/standard.py at the bottom, although I could not understand which  $K_T$  kinetic effects correction the condensation uses, it should be the same as for DEP-ICE). This bug leads to an overestimation of the thermal conductivity for equivalent radii around  $2\mu m$  and smaller: a short jupyter-notebook-based analysis with copy-pasted formulas (see supplement) gave me an overestimation of  $K_T^*$  around 12% at  $r_i=2\mu m$ , 23% at  $1\mu m$  and 47% at  $0.5\mu m$  for the conditions of the simulations. Nevertheless the growth parameter  $G_v$  for ice deposition (you call it Howell-factor) doesn't seem to be too sensitive to the thermal conductivity for these conditions: I get a bug-introduced overestimation of  $G_v$  of just about 0.5% at  $r_i=2\mu m$ , 0.9% at  $1\mu m$  and 1.6% at  $0.5\mu m$  which seems almost negligible but should be considered enough to re-run the high-CCN simulations which lead to the smallest droplets/crystals.

**Response:** We thank the reviewer for this thorough review of the model equations, for checking the code, and for providing an extended example to highlight the magnitude of the error.

We fixed the equation in the manuscript and in the codebase. Overall, as expected by the reviewer, the changes are marginal. However, we decided to rerun all notebooks due to several changes in the plotting script. We also adjusted the ending condition of the simulation, which now triggers when at least one super-particle is frozen and either all super-particles are frozen or have returned to unactivated CCNs due to evaporation. These changes mostly only affect the simulations for the CCN ensemble quantitatively. The qualitative statements remain the same for all results. We revised all discussions of the results where necessary to reflect the new values.

## Minor Comments

In the title it says "in mixed-phase clouds" which might be a bit misleading since pre-existing ice is absent at the start of the homogeneous freezing process (it's a purely liquid-phase cloud). Something like "idealized developing cirrus clouds" could be clearer here.

The title should include the word "idealized" to clarify the idealized nature of the simulations.

**Response:** The pure liquid-phase state of the cloud represents only the initial condition. The cloud quickly develops into a mixed-phase cloud, and the competition between liquid droplets and ice crystals for vapour is the most important process affecting the freezing temperature distributions and the main conclusions of the manuscript. We therefore think that highlighting the mixed-phase state in the title is justified. Additionally, the phrases "homogeneous freezing" and "developing cirrus clouds" might imply cirrus formation by homogeneous nucleation of solution droplets — a distinct cirrus formation pathway not investigated in this manuscript.

We agree that the idealised nature of the simulations should be highlighted in the manuscript title, and have therefore changed it to:

“Stochastic homogeneous freezing of supercooled droplets in mixed-phase clouds in particle-based **idealised** microphysics framework (exemplified with PySDM v3.0)”

We also added the model version as per the GMD guidelines.

There is mixed spelling of vapour/vapor throughout the manuscript, it should be consistent and in line with other regional spelling choices (like idealised, discretise, emphasise).

**Response:** We checked the manuscript and improved spelling consistency.

Fig.1 in (a) and (b) the black lines representing JHOM-T seem both to coincide with each other but the red line in (a) and the 1.00 red line in (b) should also do so. It seems unexplainable that the black and red line in (a) diverge for  $T < 235\text{K}$  but they don't diverge in (b) for  $S_w = 1.00$ . It is stated that the temperature range below 235K is rarely relevant for the studied events which is okay but the lines should show the same thing in (a) and (b).

**Response:** The red line for JHOM-DWA  $S_w = 1.00$  in Fig. (a) was showing the wrong formulation for JHOM-DWA. We fixed it and both lines are now the same as expected. We also reformatted the labels for clarity.

To expand a bit on this response: in order to achieve a unified JHOM formulation that depends on DWA while still coinciding with JHOM-T for  $T > 235\text{K}$ , there are two possible approaches: (1) add a constant to the KP00 formulation to shift the curve toward JHOM-T at  $S_w = 1.00$ , or (2) reformulate JHOM-T so that it depends on DWA. We originally used the first approach but later switched to the second, since it is more consistent to use JHOM-T as the starting point when we consider JHOM-T to be the “correct” curve for micrometer-sized droplets at  $S_w = 1.00$ . The red curve in Fig. (a) still reflects the first approach, while Fig. (b) reflects the second. It remains unclear what the slope of JHOM for  $T < 235\text{K}$  should look like at  $S_w = 1.00$ ; however, this discussion is beyond the scope of this manuscript, and we refer interested readers to Spichtinger et al. (2023).

Do the CCN concentration numbers in the manuscript and figures get always downscaled to the air density of the simulations (so around -40%) in general? I guess this is implied in L.247 but it would be a lot clearer to mention this explicitly there and add an "(STP)" note to the y-axis descriptions of the CCN number concentrations plots.

**Response:** The local CCN concentration used as an input variable for super-droplet initialisation is given as CCN concentration at STP scaled by local air density / STP air density. Hence, the local CCN concentration is indeed lower than the STP CCN concentration displayed on the y-axis and discussed in the text. We added the recommended label on y-axis and extended the text description.

#### Shorter/Technical Comments

1.

L.26-27 "liquid-origin pathway" appears twice in the comparison

**Response:** We corrected the mistake.

L.55 as WRF has a whole range of different options for microphysical models e.g. mentioning "P3" instead of "WRF" would be more specific, the given reference is referring to P3 anyway

**Response:** We clarified that we reference the P3 scheme used in the WRF model similar to how we describe the options of microphysics schemes for the Unified Model and ICON.

2.

L.113 there's a typo in the exponent sign of the  $J_{\text{hom}}$  value, should be positive

**Response:** We corrected the mistake.

L.196 nanometer size range is probably not the best word here (there are no droplets 1-10nm in size and the mean droplet radii in the later figures are in the range of 0.5-10 $\mu\text{m}$ ), sub-micrometer size range would be more precise

**Response:** We changed nanometer to sub-micrometer as suggested. However, note that we do not investigate the freezing of aqueous solution droplets in this work. These aqueous solution droplets are usually in the size range of 10 – 50nm and important for the in-situ-formation pathway of cirrus. We highlight their relevance, as it is an important conclusion of this study that the approach of using an unified  $J_{\text{hom}}$  formulation (water activity dependent) for both size ranges –  $\mu\text{m}$ -sized cloud droplets and nm-sized aqueous solution droplets – is not feasible.

L.188 Eq.6 is missing a  $\pi$  factor (although the  $\pi$  factor seems to be present in the code of the zenodo archive and no introduced bug here)

**Response:** We added the missing  $\pi$  factor.

L.222 should be "an" adiabatic parcel

**Response:** We corrected the mistake.

3.

Fig.2 in (h) the solid and dashed of the blue and red lines should be switched (JHOM-DWA is active, JHOM-T not)

**Response:** We fixed the bug in the plotting script; the inactive JHOM formulations are now correctly displayed as dashed lines.

L.289 it seems slightly confusing that the reference value is mentioned as JHOM-T, with JHOM-DWA being higher than the reference, the relative error should be positive then, not negative. Negative relative errors are fine and maybe also better readable in the plots but then the reference (to compare against) should be JHOM-DWA.

**Response:** We calculate the relative error here as:  $(\text{value} - \text{reference value}) / \text{reference value}$ . Hence, a negative relative error corresponds to an underestimation. In Fig. 2, which shows the simulations without vapour deposition on ice (DEP), JHOM-DWA is always larger than JHOM-T, corresponding to a positive relative error. In Fig. S1 (with DEP active), the relative error changes sign during the simulation: JHOM is initially overestimated and later underestimated, due to the transition from super- to subsaturation with respect to water. Note that both figures are affected by the aforementioned fixes to the plot script and now show the correct relative errors.

L.300 & L.371 leave out the word "solid" as only the black line is solid and the other two are dashed/dotted.

**Response:** We removed "solid" in both lines.

L.322/323 The strong updrafts of supercells can reach easily over 30m/s, sometimes even 50m/s or more (e.g. Marinescu et al., 2020, MWR). In this context, calling "very strong updrafts of 5 and 10m/s" representative of the conditions in deep convective systems might also be a bit of an overstatement. Maybe calling it just "strong updrafts" instead of "very strong updrafts" would be an easy midway here.

**Response:** The "very strong updrafts" are now only considered as "strong".

L.403 hard to tell if it increases actually exponentially, as  $w$  is on a logarithmic y-axis, so it could be also linear to  $w$ .

**Response:** We changed the y-axis in Fig. 5(c,d) to linear scaling and revised the discussion.

L.420 should probably be "narrower range" rather than now being "broader range" if referring to the histograms of JHOM-T

**Response:** We corrected the mistake.

L.443 missing reference at the end of the line

**Response:** We fixed the label of the reference in the tex file.

L.450 ambiguous reference to "the literature", at least a reference should be given

**Response:** We removed the reference to literature here.

L.491 referring to Fig. 5 (g) and (h) which don't exist in the manuscript. This should probably be Fig. S5 (a) and (b)

**Response:** We fixed the reference.

4.

L.519 in section 2. the droplet volume was named uppercase  $V$  (or  $V_l$ ), here it's called lowercase  $v$ , the variable names should be consistent.

**Response:** We updated all references to the droplet volume to be uppercase  $V$ .