Response to RC1 from Z.R. Courville on egusphere-2023-1947

We are thankful to Z.R. Courville for thorough and constructive review of our manuscript.

We have copied the comments of Z.R. Courville in blue. Our corresponding responses are available in black below each comment and proposed modifications to the manuscripts are written in yellow highlighted italics. The bold text line numbers correspond to the original manuscript.

Best regards

Anna Braun on behalf of all co-authors

The manuscript presents a very interesting physically-based modeling approach to the evolution of snow specific area during temperature gradient metamorphism, notably presenting results constraining the kinetic attachment coefficient, which is difficult to measure and has proved an elusive parameter in overall efforts at understanding temperature gradient metamorphism. I found the result that the kinetic coefficient varied between the two samples, and then over the course of one of the experiments particularly interesting, but intuitively makes sense in terms of the dependence of the kinetic coefficient on the morphology of snow grains. I also find the SSA modeling results presented in Fig 6 compelling with respect to the microCT data, with the match between model and experimental results remarkable. The manuscript is very well written. Below, I offer a few minor suggestions for consideration to improve clarity for a reader. The main suggestion I have is to use a consistent definition of alpha throughout the text. I also had a few questions about the specifics of the model mentioned that I think might warrant clarification.

Thanks a lot for the positive feedback. We are encouraged to confirm the intuitive understanding of temperature gradient metamorphism by a rigorous numerical approach. As detailed below, we will improve the naming of alpha, consistently calling it "condensation coefficient".

Line 64: "at the downside" is not quite the right phrase, I would suggest "at the expense" instead

We will change **Line 64** accordingly:

"[…], at the expense of microstructural realism."

Line 73: I would suggest writing: "While the interfacial curvature is a geometrical quantity, the interface growth velocity must be computed from a physical model." That is only a suggestion to make that sentence clearer vs. "first" and "second" term since that sentence has a lot of terms in it, and that's if I've interpreted the sentence correctly.

The sentence will be rewritten in the revised manuscript, removing the words "first" and "second". We also modified the sentence following a comment from Thomas Kaempfer. We will rephrase the text **Line 73** to:

"While the interfacial curvature is a purely geometrical quantity that can directly be computed from a µCT image, v_n is a physical quantity that further depends on the involved physical processes."

Line 88: I'm not sure "motion" is the best term for the interface, and would suggest "evolution" or maybe "migration" instead.

We propose to change **Lines 87-88** using the term "evolution":

"For an arbitrary snow structure, morphological changes during metamorphism are predominantly driven by the coupled diffusion of heat and mass together with ice-air interface evolution due to deposition and sublimation of vapor."

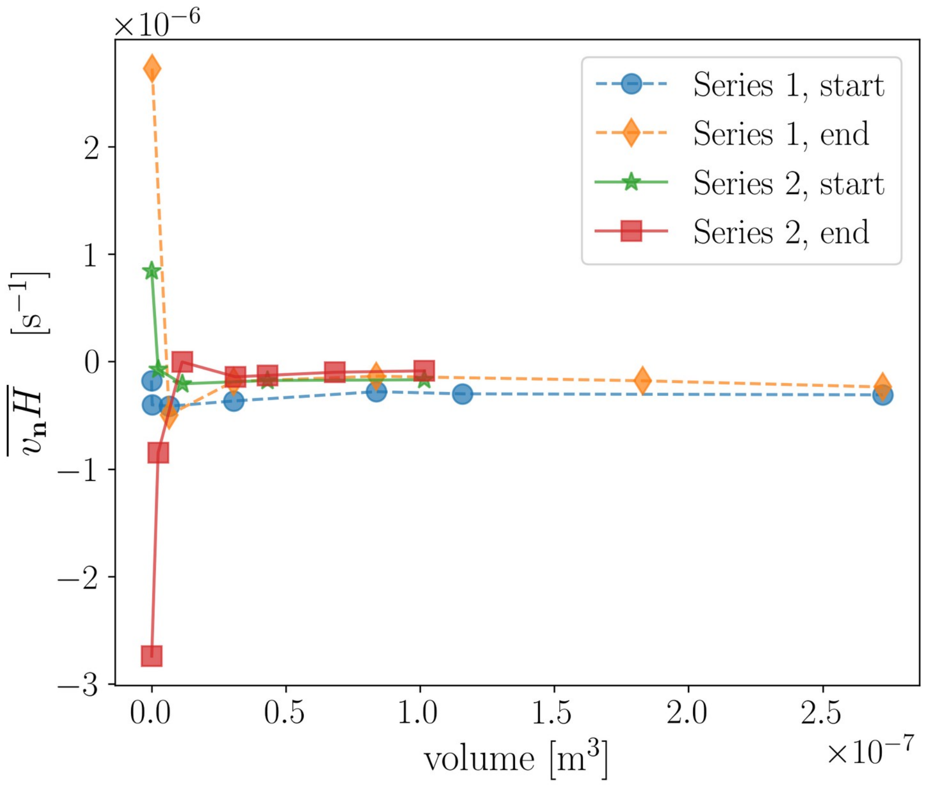
We will further rephrase "motion of the interface" in **Lines 92-93**:

"Due to the separation of time scales between heat and mass diffusion in the pores and the evolution of the interface due to crystal growth, [...]"

Line 89: How was the size of the representative snow volume determined? (or is that in the Pinzer article? If they do discuss how the representative volume was determined, I would mention that briefly.)

Following the reviews, we have performed additional simulations determining a representative elementary volume with respect to the growth rate.

In the figure below, the sample sizes used in the article correspond to the largest volumes for each sample. This shows that the estimated growth rates using these sample sizes are representative.



We will discuss this result, starting **Line 179**:

"The FE meshes of this article are based on the whole available µCT images. We verified that these selected volumes were large enough to yield representative results.. By varying sub-volumes extracted from the center of µCT images at the start and the end of both series ($I(t_1)$, $I(t_{49})$, $\hat{I}(t_1)$ and $\hat{I}(t_{83})$), we found that the simulated growth rate corresponds to a representative value for the sample sizes used in this study. This is consistent with the results of Calonne et al. (2011) for thermal conductivity, that report representativeness for sample side-lengths between 2.5 and 5mm."

Line 115: Throughout the text, there are several definitions/names of the parameter alpha (or at least I think they are all referring to alpha). As a suggestion, I recommend either being more consistent, or explaining at the first instance that alpha has been called different things. The first time it happened, I was wondering why the change from "vapor attachment coefficient" to "condensation coefficient", and recommended defining alpha as "the vapor attachment coefficient, or the condensation coefficient" at the first definition of alpha, but then I noted that there are several different forms of the definition used throughout the manuscript, including "kinetic coefficient" (line 293) and "attachment kinetics coefficient" (line 297). Again, I **think** these are all referring to alpha, but I am not sure.

We will introduce alpha in **Lines 39** and refer to it as the "condensation coefficient". We will also mention that other names of alpha appear in the literature:

"In this picture, one key parameter driving snow metamorphism is the condensation coefficient α, also called attachment, kinetic or sticking coefficient (Libbrecht, 2005; Kaempfer & Plapp, 2009; Krol & Loewe, 2016; Demange et al., 2017b; K. Fourteau et al., 2021a; L. Bouvet et al., 2022) that controls the kinetics of vapor deposition and sublimation."

We will further call alpha "condensation coefficient" in abstract (**Line 8**) and throughout the text.

Line 119: Ditto that last comment for the definition of alpha in this instance (I stopped noting all the different terms used for alpha as I went on in my review, see the above comment. I think either calling it the same thing or discussing all the different variations is warranted to alleviate confusion.)

We will change it according to the response to the previous comment.

Line 119: Suggest rewriting as "the kinetic coefficient α is defined as the probability of a water molecule sticking to an impinging surface." (this is only a minor grammar/usage suggestion)

From what we understand, the word impinging applies to the molecule rather than to the surface. We propose to rephrase **Line 119** as:

"In the Hertz-Knudsen equation, the condensation coefficient α is defined as the probability of a water molecule sticking to a surface after impinging on it."

Line 123: Is (7) referring to a reference in bibtex or some other citation managing software? Or is it referring to equation 7? Might be clearer if it said "eq. 7"

This should be a reference to Eq. 7. We will change **Line 123** accordingly:

"[…] as deviations from the local constitutive behavior (Eq. (7)) due to non-local surface processes (Libbrecht, 2005)."

Line 145: By "shorter" does that mean the sample is physically smaller, or that the time was shorter (I mean, I think I know the answer since the hours are greater for Series 2)? Suggest rewriting to clarify, maybe "Series 1 lasted 384 h and had a shorter sample height…" if that is what is meant. Also seems like the sample thicknesses/heights should be included as a well as the temperature gradients, even if the details are in the Pinzer paper.

No, just the duration is shorter. We will change **Line 145** to avoid confusion:

"Series 1 lasted 384 h, while Series 2 lasted 665 h."

We will further correct and rephrase **Line 155**, including the size of the samples:

"This corresponds to samples of 7.5x7.5x4.9mm^3 for series 1 and 5.4.x5.4x3.5mm^3 for series 2."

Line 146: Does mean T refer to the average air/ambient temperature for the experiment or the average temp throughout the sample?

Here, we mean the mean temperature throughout the sample. We will change **Line 146** accordingly:

"The mean temperature T of the sample [...]"

Line 159: How was "a reasonable volumetric division" determined or quantified? Specify the requirements.

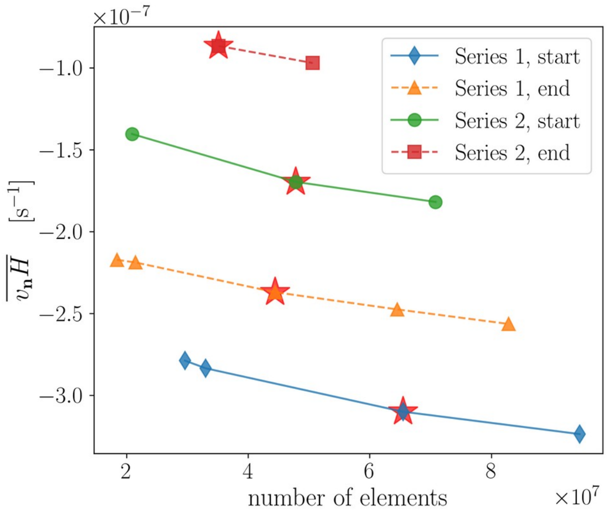
The main requirement of the mesh beside preserving the surfaces is the achievement of the accurate discretized numerical solution. There is no clear cut-off value here, apart from the general idea that the elements need to be small compared to the length-scale of the physical problem to be solved and that smaller elements *usually* yields less errors. A further constraint of the element size is the available computational power, as smaller elements means more elements.

We will rephrase **Lines 159-160** to be more specific:

"The production of an appropriate mesh that discretizes the air and ice domains, preserves the ice-air interface, and is fine enough to get accurate numerical solution (without overloading computational resources) is a key requirement for our problem."

To ensure that we used a sufficient degree of refinement, we have performed additional simulations with different degrees of refinement. This provides information about the sensitivity of our results to the FE mesh. As can be seen from the graph below (stars represent the number of elements that were used in the manuscript), the growth rate $v_n H$ is only reasonably impacted when increasing the number of elements. Moreover, as discussed later, the very good agreement between a FE simulation and the analytical solution for a spherical problem suggests that our meshing criteria yields an appropriate mesh. This will be stated **Line 170**:

"We have estimated the sensitivity of our results to the FE mesh. We found that doubling the number of elements in the mesh impacted the growth rate by about 10%. This is small in light of the dependence of the SSA values on the condensation coefficient α investigated in this study. Moreover, the very good agreement between a FE simulation and the analytical solution for a spherical problem (see Sect. 3.6) suggests that our meshing criteria yield an appropriate mesh."



Line 165: Likewise, define "small air padding" quantitatively, or if dependent on the size of the volume of interest/SSA or sample grain size, describe how that was determined.

The thickness of the air-padding layer is 3 voxels around the 300x300x196 snow image. This will be specified in the text **Line 160**:

"To this end, we employ the open-source Computational Geometry Algorithms Library (CGAL) (The CGAL Project, 2022). Specifically, we use the class Polyhedral_mesh_domain_with_features_3 that implements a tetrahedral mesh of a domain bounded by polyhedral surfaces that are preserved. The provided surfaces need to be closed and free of self-intersections. To obtain such surfaces, we extract the ice-air interface from the binary μCT data (Eq. (11) and (12)) following the procedure from (Krol and Löwe, 2018), namely by applying a Gaussian smoothing and the contour filter from the Visualization Toolkit (VTK) (Schroeder et al., 2006). However, by default this procedure applied to μCT images yields a surface that is open at the boundaries of the domain. In order to obtain closed surfaces, we added a small air-padding (three voxel-thick) around the image. This allowed us to properly define a closed outer boundary suitable for meshing. As detailed below, we provided special care to ensure that the introduction of this artificial air-padding does not perturb the simulation within the snow microstructure itself."

Line 189: For readers not familiar with Elmer, it would be good to add a brief description of what an ILU preconditioner is or does. I will note, though, that in general the authors have done a very good job of describing what the different functions in Elmer are for a non-Elmer user.

We will add a reference for the ILU preconditioner in **Line 188**:

"The equations are solved with the iterative biconjugate gradient stabilized method (BiCGSTAB; Van der Vorst, 1992) together with an ILU preconditioner, meant to facilitate the numerical solving by performing an incomplete LU factorization (Saad, 1996)."

Line 263: I would put in the length scale of the test case (0.9 mm) so the reader doesn't have to do the math, i.e., "In this way, the length scales of the test case (0.9 mm for the outer radius) are a similar order of magnitude…"

We add the lengths of the inner and outer radii **Line 264**:

"where the inner radius is set to R=21 voxel and the outer radius set to R_{\infty}=51 voxel with a voxel size of 18µm, corresponding to inner and outer radii of 0.38 and 0.92mm, respectively."

Figure 1. Suggest putting a scale bar in for the sphere (in mm) if it doesn't clutter the figure too much since that will help a reader compare to typical snow grain sizes, or adding the outer sphere dimension to the caption.

We will add a scale bar to the Figure 1b. The revised Figure is displayed below.

Figure 1. For b) is the blue the "air padding" similar to what was added to the microCT volume?

The blue color in the Figure 1b does not correspond to an air-padding layer but to the outer sphere. It is blue as vapor sublimates from the outer sphere. We will state that more clearly in the caption of the Figure 1:

“Figure 1. [...] b) Clip of the outer and inner spherical shells with visible elements colored by the interface velocity v_n (sublimation in blue, deposition in red).”

Moreover, we will extent the text in **Lines 270** to discuss where sublimation and deposition occur:

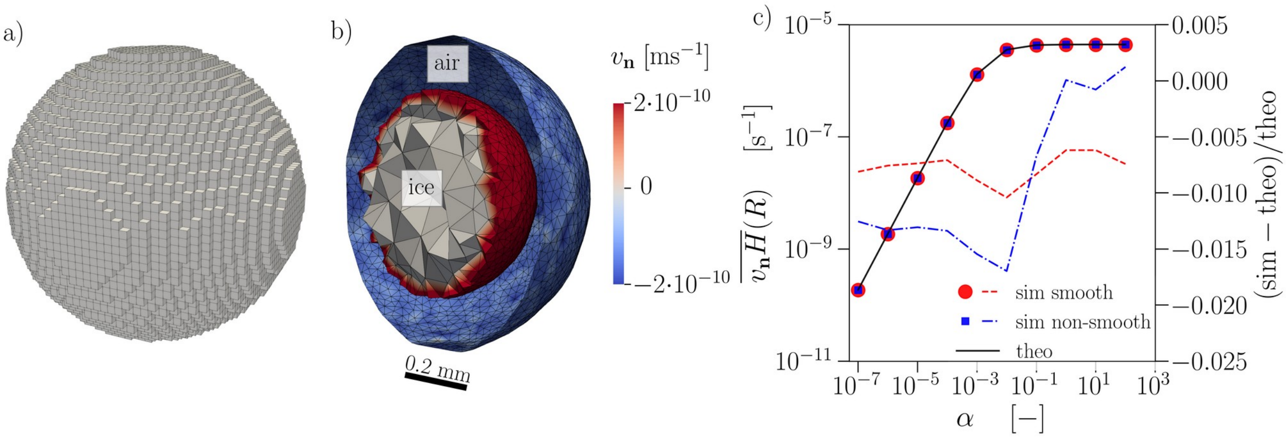
“*After solving the vapor equation, with appropriate boundary conditions, we obtain the interface velocity v_n, shown in Fig.1b. As expected, we observe a positive velocity on the inner shell, corresponding to vapor deposition, and a negative velocity on the outer shell, corresponding to sublimation.*”

Figure 1. For c) what are the red and blue dashed lines showing? I’m guessing that is the (sim-theo)/theo for values of alpha, but that should be called out in the legend, and which axis those values are plotted on should be indicated for easy of reading.

Indeed, the red and blue dashed lines corresponds to the relative errors.

This will be mentioned in the caption of **Fig. 1**:

“Figure 1. [...] c) Comparison of the growth rate v_nH on the inner radius R of theoretical (theo) and simulated (sim) solution of the spherical shell test case for different values of the condensation coefficient α. Two different surface mesh qualities with (smooth) and without (non-smooth) smoothing are employed. The red dots, blue squares and black solid line correspond to v_nH on the left y-axis while the dashed red and blue lines correspond to simulation error on the right y-axis.”



Line 308: what does the RMSE minimum “is deeper” mean? That the RMSE minimum is lower?

We will replace “deeper” with “lower” **Line 308** to:

“[…] the RMSE minimum for Series 2 is lower despite higher data scattering.”

Line 311: Should be “a time step refined down to the time interval between two microCT images…” or something (seems like there is a missing preposition after “down”).

We will change **Line 311** accordingly:

“[…] we performed simulations with a time step refined down to the time interval between […].”

ADDITIONAL REFERENCES:

Demange, G., Zapolsky, H., Patte, R., & Brunel, M.: A phase field model for snow crystal growth in three dimensions, Npj Computational Materials, 3(1), 1–7, https://doi.org/10.1038/s41524-017-0015-1, 2017b.

Saad, Y.: Iterative Methods for Sparse Linear Systems, Society for Industrial and Applied Mathematics, 2003.