Response to Reviewer 1 on tc-2020-317

We are thankful to the reviewer for reviewing and commenting our manuscript.

We have copied their specific and technical comments in blue. Our corresponding responses are available in black below each comment, with proposed modifications to the text written in *highlighted italics*.

Best Regards,
Kévin Fourteau on behalf of all co-authors

This manuscript presents compelling results of theoretical work and numerical simulations to demonstrate the latent heat effects of water vapor diffusion on the overall thermal conductivity of snow. The authors set up a theoretical model for the energy and vapor transport in snow. The work focuses on the effects of kinetics of sublimation/deposition by analyzing limiting cases of variation of the α parameter (sticking/accommodation coefficient) in the Hertz-Knudsen equation. Slow and fast kinetics are considered as bounds to the overall heat flux, with the bulk of the manuscript exploring the fast kinetics approach (as the slow kinetics approach has been considered in previous cited literature). As a result of the assumptions of their modeling, ultimately, the effects of latent heat from vapor transport can be incorporated into an expression for the conductivity in air, and the overall effective conductivity can be described as comprised of a conduction term and a vapor term, but the importantly authors note that these two terms are interdependent. Their theoretical work results in a linear relationship between the effective thermal conductivity and the normalized diffusion coefficient of water vapor.

Results are presented from numerical simulations using 34 micro-CT snow structures, spanning a range of densities, using the fast and slow kinetics approaches at a range of average temperatures. The complex interdependence of the overall heat transfer due to conduction in air, conduction in ice, and vapor kinetics effects are demonstrated by showing results for slow and fast kinetics and for different densities. The authors demonstrate that conductivity is significantly enhanced in the fast kinetics case at both high and low temperatures, but more so for high temperatures and for low densities. Useful relationships for thermal conductivity and normalized water vapor diffusion coefficient as a function of density are also presented and compared to published results. To assess if the fast kinetics approach is a reasonable model for snow, the authors compare their fast kinetics results to published work (measurements of thermal conductivity and normalized diffusion coefficient) and suggest that the fast kinetics approach may be reasonable model when temperature gradients are present.

Overall, I think that this work presents a strong contribution to the ability to effectively represent and conceptualize heat transfer in snow. Some clarification as to how the theoretical results differ from published work would be useful (see specific comments), but the combination of theoretical and numerical work presents a clear case for the potential of the fast kinetics approach to fairly simply represent complex heat transfer processes in temperature gradient scenarios. The methods implemented are appropriate and rigorous, citing appropriate precedent for both the theoretical and numerical portions of the work. I would appreciate some clarification on determining conditions for which the fast kinetics approach is valid given the assumptions that go into it (see specific comments). I believe that this work is significant and an important step in working from underlying physics to provide relevant information for snow modeling. The presentation of the work is clear and sufficiently structured, with only some minor points where writing could be clarified (as identified in the specific comments). I found the manuscript to be compelling, interesting, and fitting for The Cryosphere.

As detailed in our response below, our theory is derived under the condition of Temperature Gradient metamorphism (when metamorphism and vapor movement is driven by a macroscopic temperature gradient rather than curvature effects). This regime is usually observed for thermal gradients of 10K/m and above. We have added this information to the text **L92**, following the specific comments of the reviewer.

I recommend that this manuscript be accepted with minor revisions.

Specific Comments

Line 11: Consider listing which properties you are referring to here – effective thermal conductivity and water vapor diffusion coefficient, presumably?
We are indeed referring to the thermal conductivity and water vapor diffusion coefficient. We will rephrase **L11**:
"[…] could be a reasonable assumption for modeling heat and mass transfer in snow."

Line 44: Please indicate why neglecting convection in the pore space is a reasonable assumption in this case and cite appropriate references.
Convection might play a role in heat transfer in some specific cases, for instance in sub-arctic snowpacks (Sturm and Johnson, 1991). However developing a model of heat transfer in snow with convection is beyond the scope of this paper and the current formulation of our theory. We will clarify that it is a potential limit of our theory, and that the development of a theoretical model including convection would be beneficial.

We propose to rephrase **L44**:
"We also make the simplifying assumption that convection in the pore space does not occur or can be neglected (similarly to Riche and Schneebeli, 2013 or Calonne et al., 2014)."

and rephrase the concluding paragraph of Section 4.1, **L389**:
"Also, the derivation of a theoretical model able to describe heat and mass transfer with arbitrary surface kinetics would allow to investigate intermediary kinetics, in an effort to ultimately select the best modeling assumptions for snow. At the same time, this model could be formulated to explicitly take into account macroscopic convection, as this phenomenon has been observed in sub-artic shallow snowpacks (Trabant and Benson, 1972, Sturm and Johnson, 1991). Its derivation could be achieved using standard homogenization methods, such as the two-scale asymptotic expansion (e.g. Municchi and Icardi, 2020) or volume averaging methods (e.g. Whitaker, 1977)."

Lines 62-63: Please elaborate on which mechanisms specifically would invalidate the assumption that thermal conductivity and the vapor diffusion coefficient depend only on physical properties.
One of this reason could be the dependence of the sticking coefficient α to the local water vapor saturation. We will add **L63**:
"[…] depending on the nature of the mechanisms at play at the microscopic scale (for instance in the case of a dependence of the sticking coefficient of water molecules onto ice on the local saturation of water vapor, as discussed in Fourteau et al., 2021)."

Line 92: What constitutes a sufficiently large thermal gradient?
In our theory, we suppose that the thermal gradient is large enough so that variations in saturation concentration due to variations in curvatures are overridden by variations due to differences imposed by the thermal gradient. This limit corresponds to the limit between equi-temperature metamorphism (driven by curvature difference) and temperature gradient metamorphism, which is usually observed around 10K/m.

We will add to the text **L92**:

"Finally, when a sufficiently large thermal gradient is imposed on a snow sample, the variations of c_{sat} due to differences in curvature of the ice surface become negligible compared to variations due to temperature differences (Colbeck, 1983). This large temperature gradient condition, corresponds to the regime of Temperature Gradient metamorphism, usually observed for thermal gradients of 10 K m^{-1} and above (Sommerfeld and LaChappelle, 1970, Colbeck, 1982)."

In passing we also note that while in our theory, we assume the sole dependence of c_{sat} on the temperature thanks to large thermal gradient, it is possible that the same results could be obtained even in the case of small temperature gradients. This answer could be answered in the future with numerical simulations including curvature effects, and by explicitly keeping a dependence of the curvature to c_{sat} in theoretical derivations. We cannot however develop this point in the paper, as we do not have the appropriate numerical tools for it.

Line 121: Is it the magnitude or the rate of sublimation and deposition? Or is it both? Please clarify.

We are not sure to understand the implied difference between the magnitude and the rate of sublimation/deposition. For clarity, we propose to reformulate the sentence to:

"A macroscopic vapor flux might be present, but there is simply not enough mass than changes phase and release/absorption of latent heat to meaningfully impact the heat flux in the snow"

Line 146: The effective thermal conductivity in the fast kinetics approach does not depend on the macroscopic thermal gradient, but is it true that the thermal gradient must be sufficiently large to assume that the saturation concertation depends on temperature only?

It is indeed one of the assumptions of our theoretical development that the dependence of c_{sat} to curvatures can be neglected. As detailed in the answer about **L92**, it is however not clear at this point how the cases of small temperature gradient should be treated, and whether the effective thermal conductivity would actually be different than in the large gradient cases.

Lines 153-154 (and Equations 16): I think the reader could benefit from more explanation of the 〈∇TT ii〉 and 〈∇TT aa〉 terms. How are these terms computed in the numerical simulation portion of the work?

We will detail the definition of the temperature averages in the text **L154**:

"Note that the average thermal gradient in the ice (respectively the air) is defined by performing the volume average in the ice space only (respectively the air space only), and not in the entire snow volume."

We do not need to compute these temperature averages for the simulations and their analysis. We only compute the total heat flux Q, which yields the effective thermal conductivity K^{eff} by dividing with the macroscopic thermal gradient. Then, the values of K^{cond}, K^{ice}, K^{air} can be derived from K^{eff} using Equations 11 and 12.

We have however checked on a few samples that explicitly computing the temperature gradients in the individual phases, yielded the same values for K^{cond}, K^{ice} and K^{air}.

We will precise how the macroscopic heat flux Q is computed **L229**:

"The macroscopic heat flux Q is computed as the volume average of the microscopic heat fluxes using the Paraview software."

We will precise how K^{cond}, K^{ice} and K^{air} are obtained **L267:**

"With our simulations, the values of K^{cond}, K^{ice}, K^{air} are computed directly from K^{eff}, k_i, k_a, and k_v, and using Equations 11 and 12."

Line 170: The text notes that a similar expression to Equation 9 was reported by Jordan (1991) and Sturm and Johnson (1992). Please clarify if their work was based on the same modeling assumptions or how your results differ.

The equations of Jordan (1991) and Sturm and Johnson (1992) were obtained by considering energy balance and transport directly at the macroscopic scale, assuming saturated vapor, and that pure conduction and mass transport could be represented with constant effective coefficients, relating the fluxes to the driving gradients. In our case, we have demonstrated starting from the microscopic scale that these constant effective coefficients are indeed well-defined, and how they can be computed from the microscopic scale.

We will add to the text **L170**:
"[…] has notably been reported by Jordan (1991) and Sturm and Johnson (1992), by directly considering energy balance and transport at the macroscopic scale and pre-supposing the existence of well-defined (i.e. independent of the macroscopic thermal gradient) K^{cond} and D^{eff}."

Lines 175-178: I think the explanation here just needs a bit of clarification in the wording. The sentence that starts "This increases the average..." – Is it the reduced contrast in conductivity what increases in the average temperature gradient? Or is it just the increased effective conductivity in the pore space?
It is the reduced contrast in thermal conductivity that increases the temperature gradient in the pores and decreases it in the ice. However, as the thermal conductivity of ice is constant, increasing the apparent thermal conductivity of the air directly reduces the thermal contrast between both phases. We will rephrase **L175**:
"The presence of latent heat increases the apparent thermal conductivity of the pore space, and thus reduces the thermal conductivity contrast between the two phases. In turn, this reduced thermal contrast increases the average temperature gradient [...]"

Lines 205-206 (and Figure 2): Does this relationship represent an upper limit because of the fast kinetics assumption? Please clarify.
Vapor diffusion increases with faster kinetics, and the infinitely fast kinetics represents an upper boundary for a given structure. Figure 2 thus indeed represents the maximum values of effective diffusion coefficient at a given thermal conductivity.

We will add to **L206**:
"Moreover, as the macroscopic vapor flux decreases with slower kinetics (Pinzer et al., 2012, Fourteau et al., 2021), this curve represents an upper limit for the effective diffusion coefficient."

Line 227: Is there a reason that a thermal gradient of 50 K m -1 was chosen? There is a discussion earlier about how the magnitude of the gradient does not affect the ultimate thermal conductivity results, but must be sufficient to warrant the fast kinetics approach.
The value of the imposed thermal gradient is purely arbitrary and was chosen for its similarity with Riche and Schneebeli (2013). Since we do not include curvature effects in our simulations, all microscopic heat fluxes are strictly proportional to the imposed gradient, and therefore so is the resulting macroscopic heat flux. The effective thermal conductivity, i.e. the ratio between the macroscopic heat flux and the imposed thermal gradient, is thus independent of the magnitude of the thermal gradient (as theoretically expected).

We will clarify the text by adding **L229**:
"Note that the chosen value of 50 K m^{-1} for the imposed gradient is purely arbitrary and does not impact our results, as the resulting effective thermal conductivity does not depend on the magnitude of the gradient."

Line 233: For the c sat equation that follows the Clausius-Clapeyron and ideal gas laws, perhaps include a reference to the Fourteau et al. 2020 paper which contains the c sat equation or include the equation here.
We will include a reference to Fourteau et al. (2021) **L233**:
"[…] by assuming that water vapor follows the Clausius-Clapeyron and ideal gas laws (Eq. 11 in Fourteau et al., 2021)"

Lines 303-304: Here you reference the absolute difference in thermal conductivity between the fast and slow kinetics. Perhaps the results of the slow kinetics simulations could be included in the Supplement along with the fast kinetics results?
We will add the values of the vertical components of K^{eff} at 248 and 273K as a Supplementary material.

Figure 8: Would it make sense to also include the polynomial fit for slow kinetics from your numerical experiments as well, since this is more directly comparable to the work done by Calonne et al. (2011) and Riche et al. (2013)? I understand the desire to show the difference between the slow and fast kinetics approaches, but showing that your slow kinetics results agree with their work (or explaining why if they do not agree) might be useful.
In the slow kinetics regime we only computed the vertical component at 248 and 273K, and we thus cannot add slow kinetics values to Figure 8.

The potential difference between slow kinetics values computed with our samples and the results of Calonne et al. (2011) and Riche and Schneebeli (2013) would come from the microstructural variability of snow at a given density. Such a study would be interesting to study the impact of the snow microstructure beyond density (as in Löwe et al., 2013) but would go beyond the scope of our study.

Line 377: It is not quite clear which "reported experimental values" you are referencing here? The ones from Sokratov and Maeno (2000) which are discussed in the next sentence? Or others? Please clarify.
Yes we are referring to the experiments of Sokratov and Maneo (2000). We will rephrase the **L377**:
"While direct measurements of the effective diffusion coefficient are difficult and should therefore be analyzed with caution, the reported experimental values of Sokratov and Maeno (2000) reports an average normalized diffusion coefficient of 0.64 for snow densities of [...]"

Line 386: This calls back to previous comments, but again I am curious if there is some limit of the magnitude of thermal gradient that should be considered to employ the fast kinetics approach. I understand that your simulations cannot directly answer that question, but addressing the question at the level of the assumptions that go into the modeling might help this work be implemented more readily.
The magnitude of the thermal gradient does not influence the fast kinetics versus slow kinetics aspect, but rather if vapor concentration gradients at the microscopic scale are governed by the imposed thermal gradient, or if curvatures effects should also be considered.

As proposed before, we will clarify that the large thermal gradient regime corresponds to the Temperature Gradient metamorphism regime, observed for macroscopic thermal gradients above 10 K/m.

Line 429: Please clarify the conditions under which this approach is well suited to model snow.
We will modify the sentence **L429** to:
"This suggests that the fast kinetics option might be well suited to model heat and mass transport in snow during temperature gradient metamorphism."

Technical Corrections

The technical corrections of the reviewer not copied below will be implemented into the text, in the form proposed by the reviewer.

Line 3: (and throughout) I think because kinetics is plural, this should read "...case where kinetics are fast...". Please revise subject/verb agreement here and throughout the manuscript.
Kinetics is an uncountable word and should thus be treated as a singular.

Line 258: suggest restructuring to clarify this sentence. Maybe removing comma after "causes" is sufficient
We will rephrase **L258** to:
"The temperature dependence of K^{eff} is due to the temperature dependence of the underlying materials. Indeed, an increasing temperature results in the decrease of the ice thermal conductivity k_i and the increase of the apparent thermal conductivity of the air k_v due to both the increase [...]"

Line 422: clarify that it us up to 50% more than for the slow kinetics case
We will rephrase **L422** to:
"[…] can lead to a significant increase of the effective thermal conductivity compared to the slow kinetics case, up to 50%for low-density snow near the melting point."

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