Review of *A macroscale mixture theory analysis of deposition and sublimation rates during heat and mass transfer in snow* by Hansen and Foslien

General comments

The paper addresses homogenization of a phase-changing snowpack within a multi-constituent mixture theory and volume-fraction based closure for the transport coefficients. The upscaling is simplified to a one-dimensional problem which is solved numerically for an idealized snowpack containing a crust.

The paper is based on a sound methodology, well written and comprehensive. However, the work appears to be largely detached from many uncited contributions on upscaling and mixture theory put forward in the previous decades:

The main topic of the paper, mixture theory of snowpacks, has been addressed by various authors before e.g. [1, 2, 3]. All of them are multi-constituent approaches, some of them include phase changes. The present approach of heat and mass transfer is eventually reduced to 1D heat transfer, by coupling the vapor field tightly to the macroscopic temperature under the assumption of equilibrium. This strategy constitutes the foundation of all major operational snowpack models for a long time, cf. CROCUS [8], SNTHERM [7] or SNOWPACK [9]. These models have been used elsewhere to address test cases similar to the examples presented here. More recently, the problem of upscaling pore-scale heat and mass transfer in snow has also been studied within a two-scale expansion [6]. The latter approach confirms the commonly used form for the macroscopic equations (61,62) and touches, among other things, the role of latent heat. The two-scale expansion technique also provides the governing equations for the transport coefficients for arbitrary microstructures. Simplified models for the transport coefficients have been presented by [5] and [4] which can be contrasted to the present, volume fraction based approach (It is explicitly mentioned in the paper, though, that the present conductivity model is considered as a simplified approach, which does not include anisotropy). In addition, the derivation of the present, volume-fraction-based closure for the transport coefficient often refer to the MSc thesis (Foslien 1994) which is provided as a supplement. From my point of view this is not appropriate. If necessary, all relevant parts should be moved to the main manuscript.

I am not fundamentally against another contribution of another mixture-theory paper with another set of temperature-profile plots. But the benefit of the present approach should become more obvious. In any case, a major revision would be required to avoid repetition of previous developments and to carve out specialties of the present model for a particular application. There is certainly room for such an "intermediate complexity analysis". On one hand, operational snowpack models [8, 7, 9] are hardly been used anymore to study idealized situations. On the other hand, more recent advancements [6] have not been incorporated into operational models. Given the test cases, which are already included, it might e.g. be helpful to focus more on the details of heat and vapor transport near crusts. Crusts are discussed elsewhere in literature and constitute a key issue for operational snowpack

models due to near-crust metamorphism and implications for avalanche formation. Recently some high-res temperature measurements were conducted [11], revealing the emergence of a "super-gradient" near the crust as the potential origin of near-crust faceting. From my point of view, the present model could made a valuable contribution by providing careful, numerical evidence that the observed features *cannot* be recovered within the present coupling of heat and mass transfer (This is at least what I expect). This would have a strong implication on snowpack modeling which are in need to predict these things. Indeed, also the opposite outcome would give a good conclusion.

Henning Löwe

Authors' Response:

We would like to thank Henning Löwe for his detailed review of the manuscript and the thoughtful commentary provided. Reviews with this level of interest are genuinely appreciated.

Response to general comments:

We thank the reviewer for pointing out the previous contributions that have also studied heat and mass transfer of snow using a form of mixture theory. That said, we do not agree with the statement that the present work may be cast as, simply, "another mixture theory paper with another set of temperature profile plots."

A close review of references [1-3] will show such notable differences that it is difficult where to draw direct comparisons. We note these works involve the development of a 4 constituent mixture theory where one of the constituents is water. Phenomena such as percolation, melting, and freezing are addressed, and momentum balance plays a significant role in the work. The present work does not involve momentum balance, nor does it allow for a water constituent. Aside from the different focus, we note the mixture theories [1-3] are based on a classical theory of mixtures producing fundamentally different expressions for mass, momentum, and energy exchange as well as mixture variables.

Adams and Brown [12] developed a mixture theory model for dry snow based on the classical theory of mixtures. In addition to the differences between a volume fraction theory and the classical theory of mixtures, their work differs from the present work in that it is based on non-equilibrium conditions of the constituents whereas the present work is based on equilibrium of the temperature field and a saturated vapor density.

In addition to noted theoretical differences, the present work also involves a fundamentally different approach in that balance of mass of the humid air phase is originally developed from first principles at the microscale where mass diffusion drives the vapor velocity. Specific outcomes of our approach that are unique from the works cited by the reviewer include:

- Analytical models, grounded in first principles, are developed for the effective thermal conductivity and the effective diffusion coefficient of snow. These models contain no empirical adjustments and are in remarkable agreement with high fidelity numerical predictions of these parameters based on snow microstructures obtained from X-ray tomography.

- The present work generates an analytical description of the separation of heat transfer due to mass diffusion and heat transfer due to conduction. References [1-3] do not separate these effects in their development.

- The focus of the present mixture theory analysis is on determining macroscale deposition/sublimation rates resulting from mass exchange of the constituents. By starting from first principles and introducing diffusion at the microscale, our expression for mass exchange again has no empirical coefficients, i.e. a constitutive law for the mass exchange is not needed.

A quantitatively correct *macroscale* analysis of constituent mass exchange brings out an interesting and, we think, important microscale analysis problem that is worthy of attention. In brief, recent numerical studies of heat and mass transfer at the microscale begin by solving the steady state diffusion equation for heat transfer with the appropriate thermal properties of ice and humid air. Dirichlet boundary conditions for temperature are specified at the top and bottom to simulate a desired temperature gradient. Once the local temperature field is determined, a solution for mass transport is obtained for the humid air phase. The vapor density boundary conditions are specified at the ice/air interface by assuming the vapor density is saturated, thereby a function of temperature only. In brief, the mass flux in such an analysis is essentially dictated by the macroscale temperature gradient.

The mixture theory results for macroscale deposition and or sublimation tell an entirely different story. For example, consider the effects of diurnal temperatures on heat and mass transfer near the surface as seen in Figures 14 and 15. Figure 14 shows strong negative temperature gradients at 6 and 24 hours between x=0.9 and x=1.0 (the region bounded by the ice crust and the surface). Now, examine Figure 15 showing mass exchange at the same time periods and snow depth. The 6 hour plot shows *condensation* is occurring while the 24 hour plot shows *sublimation* is occurring. The boundary conditions used for microscale analyses described above cannot capture this interesting phenomenon as the results are driven by temperature gradient only.

The decoupling of macroscale deposition/sublimation phenomena from the macroscale temperature gradient should come as no surprise from the mixture theory analysis. Indeed, the ability to show this phenomenon is the fundamental driver for developing a mixture theory to begin with. If this were not the case, one could simply generate a thermal profile from the energy equation and move on.

Given the mixture theory results described above, it would be interesting to investigate a transient microscale solution exploring the effects of imposing mass flux boundary conditions for the vapor while using the saturated vapor density (based on the temperature field) as an initial condition for the humid air. Perhaps such an analysis could help explain microstructural evolution (kinetic growth versus sintering) under conditions where specifying the temperature gradient alone is unable to do so. Christon et al. [17] developed a fully coupled heat and mass transfer formulation, although boundary conditions involved temperature and temperature gradient only.

The reviewer has also pointed out "operational" models of snow aimed at achieving similar information to the mixture theory references. Certainly, to some degree, the operational models have been replaced by the impressive direct numerical modeling of snow at the microstructural level using X-ray tomography. We have elected to draw comparisons with these high fidelity numerical models.

The reviewer has correctly drawn our attention to recent work on more refined thermal conductivity models as well as a multiscale analysis of heat and mass transfer [4-6]. Further discussion of the refinements in thermal conductivity will be included in our revised manuscript. The inclusion of microstructural effects beyond density (volume fraction) are notable as the model developed in the present work does not address this refinement. A notable result of Calonne [6] is that, through dimensional analysis, the source term arising from phase exchange is important to the macroscale analyses. This observation provides additional motivation for introducing this mass exchange source term as a boundary condition in the microscale problem.

The reviewer has provided some comments related to a "super gradient" in temperature at the microscale in areas near an ice crust. Specifically, Hammonds [11] reports local temperature gradients on the order of 3-6 times the gradient in an ice crust. We note with interest that, in the present work, we describe enhanced microstructural temperature gradients of this precise order (see pg. 1512, L8-19) as observed in Pinzer [13]. The mixture theory, in its base form, cannot capture these microscale temperature gradients as it is a macroscale analysis. However, it would be of great interest to use the data on temperature gradient and sublimation/deposition provided by the mixture theory as inputs to a microscale analysis of the snowpack adjacent to the crust. Macroscale deposition and sublimation are quite active adjacent to the ice crust.

Finally, the reviewer makes reference to our derivation for the transport coefficient as coming from Foslien's 1994 thesis when such a derivation should be in the paper. The derivation of the transport coefficient is, in fact, in the paper. However, clearly the derivation was poorly presented and we shall endeavor to significantly improve upon this in a revised manuscript. We do elaborate on the derivation in the specific comments below.

Response to Specific comments:

General comments

p1505,l14: What does "normally" refer to here?

Our intent was to convey that rounded grains from sintering are normally expected under equi-temperature conditions. We will modify the text to clarify this point.

p1508,l14: It might be advantageous to explicitly state $\gamma_m(x) = \gamma_i \chi_i(x) + \gamma_{ha}(1 - \chi_i(x))$ in terms of the indicator function $\chi_i(x)$ of the ice phase.

As suggested by the reviewer, we will add this equation to the paper in the interest of clarity.

p1510,l12: Ambiguous. Rather: the heat capacity is heterogeneous at the microscale, but homogeneous in the ice phase.

We agree with the suggestion of the reviewer and we will make the text change noted.

Eq 20-22: Are all equations similarly taken form Hansen (1991)? Maybe add the citation (again) in l.19.

The equations noted by the reviewer were, indeed, taken from Hansen [14] and we will add the citation to L.19 as suggested.

Eqs. (20-22) are standard forms that appear in the classical theory of mixtures. It is Eqs. (24-26) where the volume fraction mixture theory utilized here-in differs from the classical forms. Further differences arise in the definitions of mixture variables in terms of their constituents.

In addition to [14], we will add the reference of the original development found in Hansen [15]. This reference is interesting in that the differences between a volume fraction theory and the classical theory of mixtures are clearly drawn out and they are dramatic. That said, many of the simplifying assumptions imposed on the classical theory found in [1-3] bring the resulting equations more in line with the volume fraction theory used here-in.

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Finally, it should be noted that mixture theory is unsettled and many open questions remain. See, for example Klika [16].

p1514,l7: Here it might be helpful to replace the loose statement "are implicitly scaled the volume fraction" by a characterizing equation. I think this is important, also in view of the "effective diffusion" issue (see comment there)

The statement "implicitly scaled by the volume faction" is correct in this context and should not be replaced by a characterizing equation. A review of the history of mixture theories will show a rather standard convention of implicitly scaling the volume fraction for the partial stress and the heat flux at the constituent level. For example, see Morland [2] for an implicit scaling of the stress by the volume fraction; pg 274, Eqn. (14) and pg. 280 Eqn. (61). A similar discussion for the implicit scaling of the heat flux may be found in Hansen [15] in the text immediately surrounding Eqn. (68) on pg 1542.

Admittedly, the implicit scaling of these quantities by their volume fraction is a source of confusion, but history has perhaps won the day regarding changing this convention.

Finally, we note this source of confusion does not appear in our mixture definitions of thermal conductivity and the effective diffusion coefficients in that the volume fractions of the mixture quantities are all explicit.

p1516,l12-14: Important sentence.

We agree with this assessment.

p1519,l14: Maybe refer explicitly to u_{sg} as "latent heat".

We will make explicit reference to u_{sg} as "latent heat" in this sentence.

Sec. 4.1: It might be helpful to actually evaluate the time scales with characteristic parameter values.

The time scales related to thermal equilibrium and the saturated vapor density were evaluated with characteristic parameter values in Foslien's 1994 thesis found in *The Supplement* of the submitted manuscript. The thermal equilibrium time scale evaluation is found on pg 41 while the saturated vapor density calculation is found on pg 38.

We omitted the development of these times scales from the paper in the interest of brevity as the paper was, in our view, already rather lengthy. We will include the time scale evaluations with characteristic parameters in our revised manuscript.

Sec. 5: If required, necessary details of the Foslien 94 model should be generally included in the paper. But the heat conductivity problem of laminate microstructures is a textbook example, where the effective properties are characterized by the arithmetic and harmonic average of the phase conductivities [10]. So it might be appropriate to directly state Eq.(74) with a such a citation, and noting that one of the phase conductivities is a modified one, which also includes the vapor term (according to eq 65).

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We respectfully disagree with shortening this portion of the paper through references as this work is at the core of the development of the thermal conductivity and transport parameters. While the snow properties developed come from "textbook" idealized microstructures, the introduction of diffusion and the process of connecting it to the mixture theory is nontrivial.

Eq. 75: Likewise, the conductivity model could be shortened: k_{pore} and k_{lam} are the well-known effective conductivities of a laminate (with volume fractions φ_i and φ_a and phase conductivities k_i and $k_{ha} + u_{sg}D_{va}d\gamma^{sat}/d\theta$) parallel and perpendicular to the laminate orientation, respectively. The final model for the effective conductivity of snow (eq. 75) is then a weighted average (with *ad hoc* weights) of both orientations. Or is the explanation given in l.12-19 (p1529) meant to be a justification for the coefficients φ_i, φ_{ha} in Eq (75)? (It's clear that the lineal fraction is equal to the volume fraction, but I can't relate this fact to eq 75).

L.12-19 (pg 1529) is, indeed, the intended justification for Eqn. 75. We are confused as to how to improve on the explanation. Referring to Figure 3, if one imagines one-dimensional heat transfer along the test line shown, heat transfer through the ice phase is dominated by the pore microstructure where some the thermal conductivity of ice is nearly 100 times that of air. Likewise, when the test line is in the air phase, heat transfer would be dominated by the lamellae microstructure. If one uses the lineal fraction as the weighted behavior of the thermal conductivity, Eq. 75 is the result. We believe the term *ad hoc* used to describe the weighting is a bit of a misnomer as we have provided sound physical arguments for the approach. It is certainly fair to argue against the merits of the model on physical grounds. We stand by the model, as the results generated by it in terms of predicted thermal conductivity and transport coefficients show very good agreement with high fidelity numerical models.

p1530,l10: Where does eq 78 come from?

This question serves to amplify the need for detail in the development of the thermal conductivity and transport parameters. Specifically, substituting Eqs. (69 & 74) into Eqn. (75) produces an effective thermal conductivity that includes the effects of mass diffusion. By comparing Eqn. (75) (with the noted substitutions) to Eqn. (65) one is immediately led to Eqn. (78) describing the effective diffusion coefficient defined for snow and labeled as D_s.

p.1531,1532: Regarding the discussion of effective diffusion: I think some confusion in literature about the effective diffusion in snow arised because the "effective diffusion coefficient" does not always refer exactly to the same thing. Sometimes it is defined as the diffusion coefficient in the phase averaged (dispersed) density equation, sometimes as the coefficient in the volume averaged equation (differing by a factor of volume fraction, that why the aforementioned "implicit scaling with volume fraction" should be made explicit) And sometimes it's meant to be a relation between the macroscopically applied vapor gradient and the resulting macroscopic flux (which would then also be affected by the source term in the diffusion equation). Here the present work should contribute to further clarify these things during the discussion here. This is also required to discuss Fig. 6. and the sentence (p1516,l12-14) in view of the statements in [6].

Our definition of the effective diffusion coefficient is best spelled out in Eqn. (35)—it is the coefficient when multiplied by the gradient of the vapor density leads to the mass flux at the macroscale for snow, so we believe it is the latter of the three descriptions provided above. Eqn. (63) then shows the deposition/sublimation rate at a point in the macroscale is governed by diffusion of mass as well as the time rate of change of the saturated vapor density as caused by local changes in the temperature. There is no implicit dependence of the diffusion coefficient on volume fractions as all volume fractions are explicitly introduced in the development of thermal and transport coefficients.

We certainly agree with the reviewer's description of possible sources of confusion in this parameter and we will provide clarification in our revision.

p1534,l8-12: I don't understand the comment about the boundary condition here. I think a subtle point about the model (eq 63-65) is behavior of the vapor phase at the boundary. By saying $\gamma_v(x) = \gamma^{sat}(\theta(x))$, the mass supply is automatically prescribed by the temperature gradient at the boundary, isn't it?

We elaborated on this point in significant detail in our opening discussion. Altering this boundary condition to a Neumann condition for the mass flux is necessary to independently account for condensation/sublimation effects occurring at the macroscale.

fig. 6: What does "no branch", "vertical branch" mean?

The terms "no branch" and "vertical branch" are taken directly from Christon [17]. They are terms used to describe the microstructures developed for the numerical heat and mass transfer analyses at the microscale. An example of a "vertical branch" geometry is provided below. Christon's microstructures produced numerical values for the diffusion coefficient that are quite close to the values developed by Pinzer [13] using real snow microstructures.
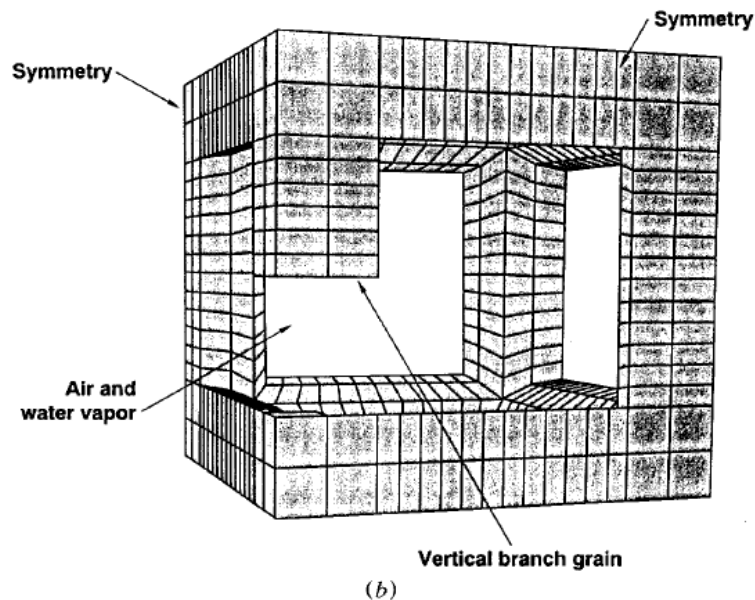

(b)

fig. 10/11/12: Why not including 1,5,10 days curves in *all* of the plots.

In our initial draft of the manuscript, we included 1, 5, and 10 day curves in all plots as suggested by

the reviewer. However, our discussion of the results did not focus on day 5 in Figures 11 and 12 and, as a result, we removed the data for day 5 to reduce clutter in the Figures.

We will show results for 1, 5, and 10 days in all plots in our subsequent revision of the paper, as suggested by the review.

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