

A macroscale mixture theory analysis

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A macroscale mixture theory analysis of deposition and sublimation rates during heat and mass transfer in snow

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Abstract

The microstructure of a dry alpine snowpack is a dynamic environment where microstructural evolution is driven by seasonal density profiles and weather conditions. Notably, temperature gradients on the order of $10\text{--}20\text{ K m}^{-1}$, or larger, are known to produce a faceted snow microstructure exhibiting little strength. However, while strong temperature gradients are widely accepted as the primary driver for kinetic growth, they do not fully account for the range of experimental observations. An additional factor influencing snow metamorphism is believed to be the rate of mass transfer at the macroscale.

We develop a mixture theory capable of predicting macroscale deposition and/or sublimation in a snow cover under temperature gradient conditions. Temperature gradients and mass exchange are tracked over periods ranging from 1 to 10 days. Interesting heat and mass transfer behavior is observed near the ground, near the surface, as well as immediately above and below dense ice crusts. Information about deposition (condensation) and sublimation rates may help explain snow metamorphism phenomena that cannot be accounted for by temperature gradients alone.

The macroscale heat and mass transfer analysis requires accurate representations of the thermal conductivity and the effective mass diffusion coefficient for snow. We develop analytical models for these parameters based on first principles at the microscale. The expressions derived contain no empirical adjustments, and further, provide self consistent values for thermal conductivity and the effective diffusion coefficient for the limiting cases of air and solid ice. The predicted values for these macroscale material parameters are also in excellent agreement with numerical results based on microscale finite element analyses of representative volume elements generated from X-ray tomography.

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1 Introduction

The thermodynamically active nature of snow, coupled with unusual high porosities, poses significant challenges to modeling heat and mass transfer in a snow cover. A primary driver in much of the research on this subject has been efforts to explain the evolving microstructure of snow that often occurs in a matter of hours or days. Notably, snow metamorphism, induced by strong temperature gradients in a snow cover, is known to produce a highly faceted microstructure, the presence of which results in extremely weak layers in a snow cover. Weak layers have been observed near the ground, near the surface, as well as above and below dense layers (e.g., ice crusts) within a snow cover.

While strong temperature gradients are widely accepted as the primary driver in temperature gradient metamorphism (TGM), they do not fully account for the range of experimental observations. For instance, faceted crystal growth has been observed at low temperature gradients where rounded grains from sintering have normally been observed (Flin and Brzoska, 2008). In contrast, Pinzer and Schneebeli (2009) note that rounded grain forms have been observed in surface layers under temperature gradient conditions.

An additional factor influencing snow metamorphism is believed to be the rate of mass transfer at the macroscale. The influence of mass transfer at the macroscale is often neglected for the simple fact that deposition (condensation) and sublimation rates caused by vapor diffusion and phase changes are not known in a typical macroscale analysis. Vapor diffusion and the associated phase changes at the macroscale pose modeling challenges in that it forces the macroscopic analysis toward a mixture theory where the ice and humid air constituents retain their identity. Mixture theory itself is a subject that has yet to fully mature and many open questions remain.

Implementing a macroscopic continuum mixture theory to elucidate the coupled heat and mass transfer phenomena occurring in snow is the central focus of this paper. We study the effects of mass transfer near the ground, near the surface including diurnal

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temperature effects, as well as adjacent to an ice crust within the snow cover. Heat and mass transfer rates are tracked over several different time periods ranging up to 10 days.

The mixture theory analysis developed here-in requires an accurate assessment of macroscopic properties for thermal conductivity and the effective mass diffusion coefficient for snow. Determining these parameters requires an analysis of heat and mass transfer at the microscale. A major challenge in microstructural studies of snow metamorphism is the extremely complex three-dimensional structure of the ice phase.

Historically, generating an accurate geometric representation of the microstructure of snow and further connecting it to a subsequent heat and mass transfer analysis was simply not possible. However, in the last two decades, the use of X-ray computed tomography has profoundly altered experimental and theoretical research for snow at the microstructural level. Not only can one accurately capture the true 3-D snow microstructure, the evolution of the microstructure may be monitored in real time as metamorphism occurs. Furthermore, finite element analysis may be coupled to experimentally produced 3-D microstructures to model heat and mass transfer at the local scale.

High fidelity microscale numerical models, coupled with X-ray computer tomography, have been utilized by Riche and Schneebeli (2013) and Calonne et al. (2011) for predictions of macroscale thermal conductivity. Pinzer et al. (2012) and Flin and Brzoska (2008) use finite element analysis with X-ray tomography to address vapor diffusion. Evolution of the snow microstructure and determining an effective diffusion coefficient for snow are among their notable contributions.

We believe the finite element predictions based on computer generated X-ray tomography snow structures provide an excellent foundation for determining material properties for thermal conductivity and the effective diffusion coefficient for snow. However, instead of utilizing finite element micromechanics to generate macroscale material properties, we rely on an interesting mathematical model developed by Foslien (1994). The analytical model produces results for thermal conductivity and the effective

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diffusion coefficient for snow that are in remarkable agreement with the finite element predictions cited above. The model also accounts for thermal conductivity and effective diffusion coefficient properties over the entire range of densities and temperatures possible for snow. The strong correlation of thermal conductivity and diffusion coefficient for snow lends confidence to using parameters based on the model of Foslien in the macroscopic mixture theory analysis developed here-in.

2 Reflections on geometric scales: microscale vs. macroscale variables

The critical heat and mass transfer mechanisms for snow metamorphism play out at two distinctly different geometric and time scales. At the microscale (on the order of millimeters) snow exhibits an extremely complex and evolving microstructure consisting of ice grains and humid air. At the macroscale, the geometric scale of interest is associated with the depth of the snow cover (typically on the order of meters). Macroscopic variables of interest include density, temperature, temperature gradient, as well as the mass flux of water vapor and the resulting deposition and sublimation that will occur within a snow cover. These macroscopic variables are fundamental drivers for snow structure evolution occurring at the *microscale*, thereby coupling local phenomena driving snow metamorphism with macroscale heat and mass transfer.

When developing a theory that transcends multiple geometric scales, attention must be paid to the transition from the microscale to the macroscale, commonly referred to as homogenization. An implicit requirement necessary for homogenization in an up-scale process is appropriate separation of scales, both from a geometric and physical viewpoint. Auriault et al. (2009) provide extensive discussion of necessary conditions required for separation of scales, all of which are satisfied for the present work.

A notable aspect of the present homogenization process is that a mixture theory is introduced by defining snow at the macroscale to be a mixture composed of an *ice* constituent and a *humid air* constituent. The constituent variables may, in turn, be appropriately averaged to obtain the macroscale snow field variables. Allowing the

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constituents to retain their identity provides a vehicle to study mass transfer due to condensation and sublimation at the macroscale.

As a means of formalizing an upscaling process for snow, the concept of a *representative volume element* (RVE) is introduced. The RVE must be of sufficient size such that volume averages of the constituent variables do not change as the volume is increased.

Given an RVE, let ϕ_α denote the volume fraction of constituent α . The mixture constituents are immiscible and the constituent volume fractions are space filling, leading to the relation

$$\phi_i + \phi_{ha} = 1, \quad (1)$$

where subscripts (i) and (ha) denote the ice and humid air constituents, respectively.

The density of snow, ρ , is defined by the volume average of the local (microscale) density field, $\gamma_m(\mathbf{x})$, that varies throughout the RVE, i.e.,

$$\rho = \frac{1}{V} \int_V \gamma_m(\mathbf{x}) dV. \quad (2)$$

The subscript (m) on the local density field is used to emphasize that the variable is defined at the microscale. In the case of a mixture, the integral of Eq. (2) may be broken into an ice domain and a humid air domain as

$$\rho = \frac{1}{V} \int_{V_i} \gamma_m(\mathbf{x}) dV + \frac{1}{V} \int_{V_{ha}} \gamma_m(\mathbf{x}) dV. \quad (3)$$

Moreover, the following macroscale constituent densities are introduced as

$$\gamma_i = \frac{1}{V_i} \int_{V_i} \gamma_m(\mathbf{x}) dV, \quad (4)$$

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and

$$\gamma_{\text{ha}} = \frac{1}{V_{\text{ha}}} \int_{V_{\text{ha}}} \gamma_{\text{m}}(\mathbf{x}) dV. \quad (5)$$

Noting Eqs. (3)–(5) leads to a volume average expression for the density of snow given by

$$\rho = \phi_i \gamma_i + \phi_{\text{ha}} \gamma_{\text{ha}}. \quad (6)$$

We emphasize that the mixture formulation is defined entirely at the macroscale. Hence, all variables in Eq. (6) represent macroscale quantities.

Following Özdemir et al. (2008), we introduce heat transfer variables into the micro-macro upscaling process by defining the macroscopic heat capacity as

$$(\rho C^V) = \frac{1}{V} \int_V \gamma_{\text{m}}(C^V)_{\text{m}} dV, \quad (7)$$

where C^V is the specific heat at constant volume. This equation provides a definition for the specific heat of snow yielding consistent values of heat capacity at both scales. Following the same development as for the density of snow leads to the relation

$$(\rho C^V) = \phi_i (\gamma_i C_i^V) + \phi_{\text{ha}} (\gamma_{\text{ha}} C_{\text{ha}}^V), \quad (8)$$

where the heat capacity for constituent α is given by

$$(\gamma_{\alpha} C_{\alpha}^V) = \frac{1}{V_{\alpha}} \int_{V_{\alpha}} \gamma_{\text{m}}(C^V)_{\text{m}} dV. \quad (9)$$

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Özdemir et al. (2008) further enforces consistency of the stored heat at the microscale and macroscale through the relation

$$(\rho C^V)\theta = \frac{1}{V} \int_V \gamma_m(C^V)_m \theta_m dV, \quad (10)$$

where θ_m and θ represent the local temperature and macroscale temperature, respectively. Again, the integral of Eq. (10) may be separated into an ice constituent and a humid air constituent as

$$(\rho C^V) = \phi_i \left(\frac{1}{V_i} \int_{V_i} \gamma_m(C^V)_m \theta_m dV \right) + \phi_{ha} \left(\frac{1}{V_{ha}} \int_{V_{ha}} \gamma_m(C^V)_m \theta_m dV \right). \quad (11)$$

Constituent temperatures, θ_i and θ_{ha} , are introduced through the relations

$$\gamma_i C_i^V \theta_i = \frac{1}{V_i} \int_{V_i} \gamma_m(C^V)_m \theta_m dV, \quad (12)$$

and

$$\gamma_{ha} C_{ha}^V \theta_{ha} = \frac{1}{V_{ha}} \int_{V_{ha}} \gamma_m(C^V)_m \theta_m dV. \quad (13)$$

The heat capacity of the ice constituent is spatially homogeneous at the microscale, leading to a volume average temperature for ice given by

$$\theta_i = \frac{1}{V_i} \int_{V_i} \theta_m dV. \quad (14)$$

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For the range of temperatures of interest, the mass fraction of water vapor in dry air is on the order of 10^{-3} . Hence, the thermal properties of the humid air may be taken to be those of dry air and the heat capacity of dry air is constant for the temperature variations seen at the microscale. This condition leads to a volume average definition for the temperature of the humid air constituent given by

$$\theta_{\text{ha}} = \frac{1}{V_{\text{ha}}} \int_{V_{\text{ha}}} \theta_m dV. \quad (15)$$

The temperature of snow may be determined from

$$(\rho C^V) \theta = \phi_i (\gamma_i C_i^V) \theta_i + \phi_{\text{ha}} (\gamma_{\text{ha}} C_{\text{ha}}^V) \theta_{\text{ha}}. \quad (16)$$

Hence, the temperature of snow does not follow the constituent volume averaging found for the heat capacity (Eq. 8) and the density (Eq. 3) but rather is based on a volume average weighted by the constituent heat capacities.

The temperature gradient at the *microscale* is a critical parameter driving temperature gradient metamorphism. To this end, we introduce volume averaged temperature gradients for the ice and humid air constituents as

- $\nabla \theta_i$ ice temperature gradient, and
- $\nabla \theta_{\text{ha}}$ humid air temperature gradient,

where, for example,

$$\nabla \theta_i = \frac{1}{V_i} \int_{V_i} \nabla_x \theta_m(\mathbf{x}) dV. \quad (17)$$

The subscript x on the gradient operator in Eq. (17) is used to emphasize the gradient applies at the microscale.

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Given appropriate boundary conditions for the RVE, the macroscale temperature gradient for snow satisfies the volume weighted averaging:

$$\nabla\theta = \phi_i\nabla\theta_i + \phi_{ha}\nabla\theta_{ha}. \quad (18)$$

Özdemir et al. (2008) develop the specific boundary conditions for the RVE that are necessary to satisfy Eq. (18). These boundary conditions are precisely the ones used by Pinzer et al. (2012) and Riche and Schneebeli (2013) in their finite element analyses of heat and mass transfer at the microscale.

Finally, it is extremely important to recognize differences in behavior between local (microscale) temperature gradients and the volumed averaged macroscale temperature gradient. For instance, Pinzer et al. (2012) provide a figure of the local temperature gradients in an RVE for an applied macroscale temperature gradient of 50K m^{-1} . The color bar for the microscale temperature gradient indicates local values of the temperature gradient are as high as 300K m^{-1} . The high local values of the temperature gradient compared to the macroscopic temperature gradient must be kept in mind when interpreting macroscopic results, as it is the *local* temperature gradients that drive metamorphism. Hence, when macroscale temperature gradients are presented as computed by the mixture theory analysis, it is not unreasonable to assume the microscale temperature gradients may be an order of magnitude higher in some areas of the RVE.

3 A mixture theory model for macroscale heat and mass transfer

Adams and Brown (1990) studied heat and mass transfer in snow using a classical form of mixture theory. In contrast, the mixture theory analysis presented here-in largely follows the development of Hansen et al. (1991) and is referred to as a volume fraction theory. The theory produces the same balance equations found in the classical developments of mixture theory. However, the summed constituent balance equations are not forced to reduce to those of a single continuum except for the special case of

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a nondiffusing mixture. As a result of relaxing this constraint, the physical definitions of mixture variables as well as the constraints on mass, momentum, and energy interaction terms assume more appealing forms. We rely on the physical arguments of Sect. 2 to define mixture quantities of interest.

Consistent with the discussion on homogenization, we consider snow at the macroscale to be a two-constituent mixture consisting of *ice* and *humid air*. The humid air itself is treated as a mixture of water vapor and air. A schematic of the mixture theory analysis is shown in Fig. 1.

For the temperatures and pressures encountered in snow, the humid air may be treated as a mixture of two ideal gases where each gas occupies the same volume, i.e.,

$$\phi_{\text{ha}} = \phi_{\text{v}} = \phi_{\text{a}}, \quad (19)$$

where subscripts (v) and (a) represent *water vapor* and *dry air*, respectively. An important consequence of representing the humid air as a mixture of ideal gases is that both the water vapor and the air behave as though the other gas is not present, thereby greatly simplifying the analysis and allowing one to draw on classical results for ideal gases.

The balance equations for mass, momentum, and energy for a constituent, α , are given by

Mass balance

$$\frac{\partial \rho_{\alpha}}{\partial t} + \nabla \cdot (\rho_{\alpha} \mathbf{v}_{\alpha}) = \hat{c}_{\alpha}, \quad (20)$$

Momentum balance

$$\rho_{\alpha} \mathbf{a}_{\alpha} = \nabla \cdot \mathbf{T}_{\alpha} + \rho_{\alpha} \mathbf{g} + \hat{\mathbf{p}}_{\alpha}, \quad (21)$$

Energy balance

$$\rho_{\alpha} \dot{u}_{\alpha} = tr(\mathbf{T}_{\alpha} \cdot \mathbf{L}_{\alpha}) + \rho_{\alpha} r_{\alpha} - \nabla \cdot \mathbf{q}_{\alpha} + \hat{e}_{\alpha}. \quad (22)$$

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In the above, \mathbf{v}_α and \mathbf{a}_α represent the velocity and acceleration of constituent α , respectively, while \mathbf{L}_α represents the velocity gradient; u_α is the internal energy, r_α is the heat supply (notably radiation), and \mathbf{g} is the gravity vector. The dispersed density of constituent α is denoted by ρ_α and is related to the true density, γ_α , as

$$\rho_\alpha = \phi_\alpha \gamma_\alpha. \quad (23)$$

Whereas the volume fraction, ϕ_α , appears explicitly in the definition of the dispersed density, ρ_α , the partial stress, \mathbf{T}_α , and the energy flux, \mathbf{q}_α , are implicitly scaled by the volume fraction. Finally, \hat{c}_α , $\hat{\mathbf{p}}_\alpha$, and \hat{e}_α represent mass, momentum, and energy supply terms that arise from interactions between constituents. Following Hansen et al. (1991), the mixture theory supply terms satisfy the appealing restrictions

$$\sum_\alpha \hat{c}_\alpha = 0, \quad (24)$$

$$\sum_\alpha \hat{\mathbf{p}}_\alpha = \mathbf{0}, \quad (25)$$

and

$$\sum_\alpha \hat{e}_\alpha = 0. \quad (26)$$

In what follows, the mixture theory balance equations are further specialized to study the macroscale coupled heat and mass transfer problem for snow.

3.1 Ice constituent mass balance

The balance of mass for the ice phase is given by

$$\frac{\partial \rho_i}{\partial t} + \nabla \cdot (\rho_i \mathbf{v}_i) = \hat{c}_i \quad (27)$$

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Assuming the mass supply is positive during condensation, we can write

$$\hat{c} = \hat{c}_i = -\hat{c}_{ha}. \quad (28)$$

Neglecting any settling velocity leads to a mass balance for the ice constituent given by

$$5 \quad \gamma_i \frac{\partial \phi_i}{\partial t} = \hat{c}, \quad (29)$$

where the mass density of ice is taken as constant at 917 kg m^{-3} .

3.2 Water vapor mass balance

The development for the humid air mass balance differs from that of the ice constituent in that we begin at the *microscale*. Furthermore, only the mass balance of the water vapor is considered because the air acts only as a medium through which the water vapor diffuses.

Mass transfer of the water vapor may be expressed as (Bird and Lightfoot, 1960)

$$10 \quad \gamma_v \mathbf{v}_v = \frac{\gamma_v}{\gamma_{ha}} (\gamma_a \mathbf{v}_a + \gamma_v \mathbf{v}_v) + \mathbf{j}_v. \quad (30)$$

Equation (30) says that the mass flux of the water vapor is due to the bulk fluid motion (the barycentric velocity) plus a relative velocity due to diffusion. In the absence of a pressure gradient, the barycentric velocity is zero, i.e.,

$$15 \quad \gamma_{ha} \mathbf{v}_{ha} = (\gamma_a \mathbf{v}_a + \gamma_v \mathbf{v}_v) = 0. \quad (31)$$

Mass balance due to diffusion may be expressed in the form of Fick's law (Bird and Lightfoot, 1960) as

$$20 \quad \mathbf{j}_v = -\gamma_{ha} D_{v-a} \nabla_x \left(\frac{\gamma_v}{\gamma_{ha}} \right), \quad (32)$$

where D_{v-a} is the binary diffusion coefficient for water vapor in air and ∇_x denotes the gradient operator at the microscale.

The diffusive flux can be expanded to give

$$\mathbf{j}_v = -D_{v-a} \nabla_x \gamma_v + \frac{\gamma_v}{\gamma_{ha}} D_{v-a} \nabla_x \gamma_{ha}, \quad (33)$$

5 but the second term on the right is negligibly small because the mass fraction of saturated water vapor in air at 273 K is about $4(10)^{-3}$. Hence, mass transfer of water vapor at the microscale may be described by

$$\gamma_v \mathbf{v}_v = -D_{v-a} \nabla_x \gamma_v. \quad (34)$$

10 In the transition to the macroscale, the same physical principles apply but one must now use an effective diffusion coefficient for water vapor. The need to introduce an effective diffusion coefficient for water vapor is attributed to the presence of the ice microstructure in snow. Specifically, the presence of the ice constituent introduces vapor transfer mechanisms that both enhance and retard mass transfer of water vapor when compared to a medium of humid air only. These mass transfer mechanisms are briefly
15 discussed in Sect. 5.3.

Defining D_s as the effective diffusion coefficient for the humid air constituent at the macroscale, there follows

$$\phi_v \gamma_v \mathbf{v}_v = \rho_v \mathbf{v}_v = -D_s \nabla \gamma_v, \quad (35)$$

20 where \mathbf{v}_v and γ_v now represent appropriately volume averaged macroscale variables. Note that the mass flux of water vapor is based on the dispersed density, ρ_v , in order to account for the reduced volume occupied by the humid air in the mixture. Finally, since only the humid air constituent is associated with diffusion in a mixture of ice and humid air, D_s also represents the effective diffusion coefficient for snow.

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Again, noting air is simply the medium for mass transfer of water vapor, the balance of mass for the vapor phase may be written as

$$\frac{\partial \rho_v}{\partial t} + \nabla \cdot (\rho_v \mathbf{v}_v) = \hat{c}_v. \quad (36)$$

Substitution of the diffusive flux into Eq. (36) and noting $\hat{c}_v = \hat{c}_{\text{ha}} = -\hat{c}$ leads to

$$\frac{\partial \rho_v}{\partial t} - \nabla \cdot (D_s \nabla \gamma_v) = -\hat{c}. \quad (37)$$

Expanding the time derivative of the dispersed density of the water vapor gives

$$\frac{\partial \rho_v}{\partial t} = \gamma_v \frac{\partial \phi_v}{\partial t} + \phi_v \frac{\partial \gamma_v}{\partial t}, \quad (38)$$

but

$$\frac{\partial \phi_v}{\partial t} = \frac{\partial \phi_{\text{ha}}}{\partial t} = -\frac{\partial \phi_i}{\partial t}. \quad (39)$$

The above results, along with the mass balance for the ice constituent (Eq. 29), can be used to write Eq. (37) as

$$\phi_v \frac{\partial \gamma_v}{\partial t} - \nabla \cdot (D_s \nabla \gamma_v) = \hat{c} \left(\frac{\gamma_v}{\gamma_i} - 1 \right), \quad (40)$$

but the quantity $\frac{\gamma_v}{\gamma_i} \ll 1$. Neglecting this term and noting $\phi_v = \phi_{\text{ha}}$, the mass balance equation for the water vapor becomes

$$\phi_{\text{ha}} \frac{\partial \gamma_v}{\partial t} - \nabla \cdot (D_s \nabla \gamma_v) = -\hat{c}. \quad (41)$$

Equation (41) states that changes in the water vapor density at the macroscale are due to the divergence of the water vapor flux and sublimation or condensation as defined through the mass supply.

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3.3 Momentum balance

The momentum balance for the ice phase can be used to find the stress and strain in the ice phase. However, the effect that the ice stress has on the vapor density of the water is neglected, so the ice phase momentum balance is not considered further.

5 The momentum balance for the humid air phase becomes important when bulk fluid motion occurs as in the case of natural convection. Foslien (1994) has shown the Rayleigh number for a typical snow cover is more than an order of magnitude below the critical value for the onset of convection, so convection is unlikely to occur except in extreme circumstances. Therefore, the momentum balance of the humid air phase
10 is not considered further.

3.4 Energy balance for the ice constituent

The energy balance for the ice constituent may be expressed at the macroscale as

$$\rho_i \dot{u}_i = tr(\mathbf{T}_i \cdot \mathbf{L}_i) + \rho_i r_i - \nabla \cdot \mathbf{q}_i + \hat{e}_i. \quad (42)$$

In the above, any velocity gradient in the ice, \mathbf{L}_i , is attributed to settling and may be neglected. Moreover, heat generation from solar radiation is also neglected but could
15 easily be included as Colbeck (1989) and McComb et al. (1992) have done. These assumptions reduce the energy balance for ice to

$$\rho_i \dot{u}_i = -\nabla \cdot \mathbf{q}_i + \hat{e}_i. \quad (43)$$

The internal energy of the non-deforming ice is assumed to be a function of temperature only and is given by
20

$$u_i = C_i^V (\theta_i - \theta_{ref}), \quad (44)$$

where C_i^V is the specific heat of ice at constant volume and θ_{ref} is the reference temperature. The heat flux at the macroscale is expressed as Fourier's law of heat conduction

as

$$\mathbf{q}_i = -\phi_i k_i^{\text{eff}} \nabla \theta_i, \quad (45)$$

where k_i^{eff} is the effective thermal conductivity for the ice phase at the macroscale. This parameter should not be confused with the thermal conductivity of pure ice as differences arise due to the microstructure of ice implicitly present in snow.

Combining Eqs. (43)–(45), the energy balance for the ice phase is given by

$$\phi_i \gamma_i C_i^V \frac{\partial \theta_i}{\partial t} = \nabla \cdot (\phi_i k_i^{\text{eff}} \nabla \theta_i) + \hat{e}_i. \quad (46)$$

3.5 Humid air constituent energy balance

As with the ice phase, the work term and the energy source term of the humid air constituent are neglected, thereby reducing the energy equation to

$$\rho_{\text{ha}} \dot{u}_{\text{ha}} = -\nabla \cdot \mathbf{q}_{\text{ha}} + \hat{e}_{\text{ha}}. \quad (47)$$

The internal energy for the humid air mixture of ideal gases is given by

$$\gamma_{\text{ha}} u_{\text{ha}} = \gamma_a C_a^V (\theta_{\text{ha}} - \theta_{\text{ref}}) + \gamma_v (C_v^V (\theta_{\text{ha}} - \theta_{\text{ref}}) + u_{\text{sg}}), \quad (48)$$

where u_{sg} is the internal energy change when water changes from a solid to a vapor. The above assumes the reference value of the internal energy of ice was set to zero as was the case.

The definition of the energy flux vector for water vapor diffusing through air is (Bird and Lightfoot, 1960)

$$\mathbf{q}_{\text{ha}} = -\phi_{\text{ha}} k_{\text{ha}}^{\text{eff}} \nabla \theta_{\text{ha}} - u_{\text{sg}} D_s \nabla \gamma_v. \quad (49)$$

Again, one must recognize that $k_{\text{ha}}^{\text{eff}}$ and D_s represent the effective thermal conductivity for the humid air and the effective diffusion coefficient for snow, respectively; and these parameters apply at the macroscale.

Substituting Eqs. (48) and (49) into Eq. (47) leads to

$$\phi_{\text{ha}} \left(\gamma_{\text{a}} C_{\text{a}}^{\text{V}} + \gamma_{\text{v}} C_{\text{v}}^{\text{V}} \right) \frac{\partial \theta_{\text{ha}}}{\partial t} + u_{\text{sg}} \left(\phi_{\text{ha}} \frac{\partial \gamma_{\text{v}}}{\partial t} - \nabla \cdot (D_{\text{s}} \nabla \gamma_{\text{v}}) \right) = \nabla \cdot \left(\phi_{\text{ha}} k_{\text{ha}}^{\text{eff}} \nabla \theta_{\text{ha}} \right) + \hat{e}_{\text{ha}} \quad (50)$$

but

$$\hat{c} = \nabla \cdot (D_{\text{s}} \nabla \gamma_{\text{v}}) - \phi_{\text{ha}} \frac{\partial \gamma_{\text{v}}}{\partial t} \quad (51)$$

from the mass balance of the water vapor given by Eq. (41). Therefore, Eq. (50) governing the energy balance of humid air assumes the form

$$\phi_{\text{ha}} \left(\gamma_{\text{a}} C_{\text{a}}^{\text{V}} + \gamma_{\text{v}} C_{\text{v}}^{\text{V}} \right) \frac{\partial \theta_{\text{ha}}}{\partial t} = \nabla \cdot \left(\phi_{\text{ha}} k_{\text{ha}}^{\text{eff}} \nabla \theta_{\text{ha}} \right) + \hat{e}_{\text{ha}} + u_{\text{sg}} \hat{c}. \quad (52)$$

Hence, the change in internal energy for the humid air is attributed to the divergence of the heat flux, energy exchange with the ice constituent through the energy supply, and energy exchange through phase changes accounted for by the mass supply.

4 Separation of scales: macroscale observations

In this section, we discuss some observations that lead to important simplifications in the macroscale heat and mass transfer solution. Moreover, we demonstrate separation of the time scales for local and global heat and mass transfer, a condition required for homogenization.

4.1 Macroscale temperatures

An important simplification in the analysis of heat and mass transfer at the *macroscale* is to assume the constituent temperatures are equal and write

$$\theta = \theta_i = \theta_{\text{ha}},$$

where θ is the macroscale temperature of snow. Justification for assuming the ice and humid air temperatures are equal starts by writing a one-dimensional heat conduction equation at the microscale given by

$$\frac{\partial \theta_\alpha}{\partial t} = \left(\frac{k_\alpha}{\gamma_\alpha C_\alpha^V} \right) \frac{\partial^2 \theta_\alpha}{\partial x^2}. \quad (53)$$

5 Equation (53) is non-dimensionalized by introducing the following dimensionless variables:

$$t^* = t/t_o, \quad x^* = x/L_c, \quad \text{and} \quad \theta^* = \frac{\theta - \theta_{\text{init}}}{\theta_f - \theta_{\text{init}}}.$$

The resulting non-dimensional equation is

$$\frac{\partial \theta^*}{\partial t^*} = \left(\frac{t_o k_\alpha}{L_c^2 \gamma_\alpha C_\alpha^V} \right) \frac{\partial^2 \theta^*}{\partial x^{*2}}. \quad (54)$$

10 The time scale, t_o^{micro} , for heat conduction on the microscale is introduced as

$$t_o^{\text{micro}} = \frac{\gamma_\alpha C_\alpha^V L_c^2}{k_\alpha}. \quad (55)$$

The time scale, t_o^{macro} , for heat conduction in a snow cover is similarly defined as

$$t_o^{\text{macro}} = \frac{(\phi_i \gamma_i C_i^V + \phi_{\text{ha}} \gamma_{\text{ha}} C_{\text{ha}}^V) H^2}{k_s}, \quad (56)$$

15 where H is the height of the snowpack and k_s represents the thermal conductivity for snow.

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Riche and Schneebeli (2013) provide an expression for the thermal conductivity of snow as a function of snow density. Assuming a snow density of 200 kg m^{-3} , a depth of one meter, and a microscale characteristic length of one mm (Christon, 1990), the ratio of the time scale for heat conduction on the macroscale of the snowpack to the time scale for heat conduction on the microscale is on the order of 10^6 which suggests that macroscale thermal equilibrium between the ice and humid air constituents is a good assumption. Moreover, the large separation of scales in the time domain is consistent with the discussion of Auriault et al. (2009) regarding separation of time scales necessary for homogenization.

The assumption of uniform constituent temperatures at the macroscale should not be confused with the local (microscale) temperature. Under a macroscale temperature gradient, local constituent temperatures in the interior of the RVE differ due to different thermal conductivities of the ice and humid air. Further, temperature gradients within individual constituents are also present at the microscale. A warmer ice grain is separated from a colder ice grain by pore space, for example. These temperature differentials drive the mass transfer process at the microscale. Again, an excellent insight into microscale thermal behavior is provided in Fig. 4 of Pinzer et al. (2012).

Thermal equilibrium of the ice and humid air constituents at the macroscale allows the constituent energy equations, (Eqs. 46 and 52), to be added together to yield an energy equation for snow with a single temperature as

$$\left(\phi_{\text{ha}} \gamma_{\text{ha}} C_{\text{ha}}^V + \phi_{\text{i}} \gamma_{\text{i}} C_{\text{i}}^V \right) \frac{\partial \theta}{\partial t} = \nabla \cdot (k_{\text{s}} \nabla \theta) + \hat{c} u_{\text{sg}}, \quad (57)$$

where θ is the temperature of the snow. Notably, the constituent energy supply terms sum to zero in the energy equation for snow and the volume averaged constituent effective thermal conductivities have been combined into a thermal conductivity for snow (k_{s}).

Finally, recent research work has shown the thermal conductivity of snow to be anisotropic, see for example Schertzer and Adams (2011) and Riche and Schneebeli

beli (2013). We avoid this complexity at present as it becomes a non-issue for the one-dimensional heat and mass transfer theory developed subsequently.

4.2 Saturated vapor density at the macroscale

A physical interpretation of the mass supply term, \hat{c} , is the mass rate at which water vapor is condensing to form ice per unit volume of snow. Hobbs (1974) provides an expression for the condensation of water vapor to ice driven by a difference in the vapor pressure and the saturated vapor pressure over ice, $(p - p^{\text{sat}})$, as

$$\frac{\alpha_c m_{\text{mol}} (p - p^{\text{sat}})}{(2\pi m_{\text{mol}} \Omega \theta)^{1/2}} \text{ kg m}^{-2} \text{ s}^{-1}.$$

where m_{mol} is the mass per molecule of water, Ω is Boltzman's constant, and α_c is the condensation coefficient.

Multiplying the above expression by the specific surface area of snow, ξ , and utilizing the ideal gas law for water vapor provides an explicit expression for the mass supply driven by a difference in vapor density given by

$$\hat{c} = \frac{\xi R \theta \alpha_c m_{\text{mol}} (\gamma - \gamma^{\text{sat}})}{(2\pi m_{\text{mol}} \Omega \theta)^{1/2}}. \quad (58)$$

In the absence of diffusion, Eq. (58) can be combined with the mass balance equation (Eq. 41) for the water vapor as

$$\phi_v \frac{\partial \gamma_v}{\partial t} = \frac{\xi R \theta \alpha_c m_{\text{mol}} (\gamma - \gamma^{\text{sat}})}{(2\pi m_{\text{mol}} \Omega \theta)^{1/2}}. \quad (59)$$

If the saturated vapor density over the ice is held constant, the time for the vapor density difference between the pore density and the saturated vapor density to become

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0.1% of the initial density difference can be computed. Following Foslien (1994), for a snow density of 200 kg m^{-3} , the time for the vapor density to reach equilibrium is approximately 10^{-3} seconds. Hence, the vapor density in a pore can be assumed to be the saturated vapor density throughout the process of heat and mass transfer occurring at the macroscale where the time scale of interest is on the order of hours or days.

The knowledge that the vapor pressure may be assumed saturated in a macroscale analysis affords a critical simplification in the mixture theory analysis in that a constitutive law for the mass supply is no longer needed. Instead, the mass supply is computed from Eq. (41) by noting the water vapor is always saturated at the snow temperature, leading to

$$\hat{c} = \nabla \cdot (D_s \nabla \gamma_v^{\text{sat}}) - \phi_{\text{ha}} \frac{\partial \gamma_v^{\text{sat}}}{\partial t}. \quad (60)$$

4.3 Formulation summary

At this point, we restrict the development to a one-dimensional model and write the energy equation, (Eq. 57), as

$$\left(\phi_{\text{ha}} \gamma_{\text{ha}} C_{\text{ha}}^V + \phi_i \gamma_i C_i^V \right) \frac{\partial \theta}{\partial t} = \frac{\partial}{\partial x} \left(k_s \frac{\partial \theta}{\partial x} \right) + \hat{c} u_{\text{sg}}. \quad (61)$$

The mass supply equation, (Eq. 60), representing phase changes due to condensation or sublimation assumes the one-dimensional form

$$\hat{c} = \frac{\partial}{\partial x} \left(D_s \frac{\partial \gamma_v^{\text{sat}}}{\partial x} \right) - \phi_{\text{ha}} \frac{\partial \gamma_v^{\text{sat}}}{\partial t}. \quad (62)$$

The saturated vapor density may be expressed as purely a function of temperature (Dorsey, 1968) leading to

$$\frac{\partial \gamma^{\text{sat}}}{\partial x} = \frac{d\gamma^{\text{sat}}}{d\theta} \frac{\partial \theta}{\partial x} \quad \text{and} \quad \frac{\partial \gamma^{\text{sat}}}{\partial t} = \frac{d\gamma^{\text{sat}}}{d\theta} \frac{\partial \theta}{\partial t}.$$

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Noting the above, the mass supply equation, (Eq. 62), is expressed as

$$\hat{c} = \frac{\partial}{\partial x} \left(D_s \frac{d\gamma_v^{\text{sat}}}{d\theta} \frac{\partial \theta}{\partial x} \right) - \phi_{\text{ha}} \frac{d\gamma_v^{\text{sat}}}{d\theta} \frac{\partial \theta}{\partial t}. \quad (63)$$

Finally, substituting Eq. (63) into Eq. (61) leads to a single partial differential equation governing the energy balance for snow given by

$$5 \left(\phi_{\text{ha}} \gamma_{\text{ha}} C_{\text{ha}}^V + \phi_i \gamma_i C_i^V + u_{\text{sg}} \phi_{\text{ha}} \frac{d\gamma_v^{\text{sat}}}{d\theta} \right) \frac{\partial \theta}{\partial t} = \frac{\partial}{\partial x} \left(k_s^{\text{con}+d} \frac{\partial \theta}{\partial x} \right), \quad (64)$$

where

$$k_s^{\text{con}+d} = k_s + u_{\text{sg}} D_s \frac{d\gamma_v^{\text{sat}}}{d\theta}. \quad (65)$$

The thermal conductivity $k_s^{\text{con}+d}$ is the thermal conductivity that would be measured experimentally when studying heat transfer through a snow cover. It involves a thermal conductivity due to conduction, k_s , with an added term resulting from mass latent heat transfer due to mass diffusion.

Equation (65) is useful to study the significance of heat transfer due to mass diffusion. However, rather than combining Eqs. (61) and (63) and solving Eq. (64), it is more insightful to solve Eqs. (61) and (63) separately. Retaining a separate equation for the mass supply allows one to quantify macroscale deposition and sublimation rates, a fundamental objective of the theory developed here-in.

5 Evaluation of the effective thermal conductivity and the effective diffusion coefficient for snow

Solution of the energy equation (Eq. 61) and the mass balance equation (Eq. 63) requires knowledge of macroscale parameters for thermal conductivity as well as the

effective diffusion coefficient for snow. Calonne et al. (2011) and Riche and Schneebeli (2013) have performed extensive numerical studies using finite element analysis coupled with X-ray computer tomography to quantify the thermal conductivity for snow as a function of density at a fixed temperature. Calonne et al. (2011) also provide thermal conductivity predictions at two separate temperatures. Pinzer et al. (2012) performed similar numerical studies aimed at determining the effective diffusion coefficient for snow.

Regardless of the parameter being studied, a drawback of microscale finite element analysis (micromechanics) is that the results provide heat and mass transfer properties at a single temperature and density. Hence, a complete characterization of these parameters as a function of density and temperature requires a significant number of micromechanics solutions at multiple densities and temperatures followed by a curve fitting exercise.

Rather than relying on finite element micromechanics solutions, we present an analytical approach developed by Foslien (1994) to predict values for the thermal conductivity and the effective diffusion coefficient of snow. Foslien's model has several attractive features including:

- excellent correlation with the cited finite element results for thermal conductivity and effective diffusion coefficient for snow,
- density effects are explicitly introduced in the analytical model through volume fractions while temperature effects appear implicitly through thermal conductivity properties for ice and air,
- the effects of mass diffusion on the energy flux are explicit and the relative influence on the energy flux is readily determined,
- the model provides self-consistent results for thermal conductivity and effective diffusion coefficient for the limiting cases of air and ice,

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- the model is developed from first principles and contains no empirical coefficients of adjustment.

Foslien's development begins by formulating microscale heat and mass transfer models for classic microstructures consisting of ice and humid air acting in parallel and series, respectively. Heat and mass transfer properties for snow are then proposed using arguments from quantitative stereology.

Figure 2a shows an ice matrix with humid air pores in parallel to an applied temperature gradient. In this *pore* microstructure, energy is transferred in parallel through the snowpack. The energy fluxes for the ice (q_i) and humid air (q_{ha}) constituents are simply added together to obtain the total energy flux through the snowpack. Because the thermal conductivity of ice is roughly 100 times larger than for the humid air, the ice phase plays a dominant role in heat transfer for this microstructure.

The second microstructure studied, referred to as a *lamellae* microstructure, consisted of ice and humid air layers oriented perpendicular to the energy flux, Fig. 2b. In this case, energy flows in series through the respective layers. Hence, the energy flux in the humid air constituent must equal the energy flux through the ice constituent. An interesting feature of mass transfer in the lamellae microstructure is that diffusion via the "hand to hand" model described by Yosida (1955) is naturally present and accounted for in the development. Specifically, diffusion is enhanced as the total path length for diffusion is reduced by the ice layer which acts as both a source and sink for water vapor.

The two microstructures studied by Foslien (1994) were first considered by de Quervain (1963) and produce two very different heat and mass transfer results that are believed to represent the extremes possible for ice and humid air mixtures.

5.1 Pore microstructure

Foslien's heat and mass transfer analysis of the pore microstructure begins by writing energy flux expressions for the ice and humid air constituents at the macroscale. The

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energy flux of the ice is attributed to heat conduction leading to

$$q_i = -k_i \frac{\partial \theta}{\partial x}. \quad (66)$$

The energy flux of the humid air is attributed to conduction of the humid air and the mass flux of water vapor. Following Bird and Lightfoot (1960) we can write

$$q_{ha} = -k_{ha} \frac{\partial \theta}{\partial x} - u_{sg} D_{v-a} \frac{d\gamma^{sat}}{d\theta} \frac{\partial \theta}{\partial x}. \quad (67)$$

The energy flux of the pore microstructure is introduced as

$$q_{pore} = -k_{pore} \frac{\partial \theta}{\partial x}, \quad (68)$$

Energy transfer in the pore microstructure occurs in parallel and the energy flux is simply the volume average of the energy fluxes of the ice and humid air leading to

$$k_{pore} = \phi_i k_i + \phi_{ha} k_{ha} + \phi_{ha} u_{sg} D_{v-a} \frac{d\gamma^{sat}}{d\theta}. \quad (69)$$

5.2 Lamellae microstructure

The discontinuous nature of the lamellae microstructure in the direction of interest introduces a complexity in the spatial gradients as the constituent gradients must be defined with respect to a differential length, dx_α . Hence the constituent energy fluxes assume the form

$$q_i = -k_i \frac{\partial \theta}{\partial x_i}, \quad (70)$$

and

$$q_{ha} = -k_{ha} \frac{\partial \theta}{\partial x_{ha}} - u_{sg} D_{v-a} \frac{d\gamma^{sat}}{d\theta} \frac{\partial \theta}{\partial x_{ha}}. \quad (71)$$

The average temperature gradient expressed in terms of the macroscale coordinate x is given by

$$\frac{\partial \theta}{\partial x} = \phi_i \frac{\partial \theta}{\partial x_i} + \phi_{ha} \frac{\partial \theta}{\partial x_{ha}}. \quad (72)$$

The energy flux through the lamellae microstructure is introduced as

$$q_{lam} = -k_{lam} \frac{\partial \theta}{\partial x}. \quad (73)$$

Equations (70)–(73) may be combined to arrive at

$$k_{lam} = \frac{k_i \left(k_{ha} + u_{sg} D_{v-a} \frac{dy_v^{sat}}{d\theta} \right)}{\phi_i \left(k_a + u_{sg} D_{v-a} \frac{dy_v^{sat}}{d\theta} \right) + \phi_{ha} k_i}. \quad (74)$$

5.3 Snow properties

Foslien proposed an effective thermal conductivity for snow that includes energy transfer due to mass transport of water vapor given by

$$k_s^{con+d} = \phi_i k_{pore} + \phi_{ha} k_{lam}. \quad (75)$$

Justification for Eq. (75) is provided by considering a snow surface section as shown in Fig. 3. When a test line is arbitrarily drawn through the surface section, a fraction of the total length will pass through the ice constituent and the remainder will pass through the humid air constituent. If one imagines *one-dimensional* heat transfer occurring along the test line; anytime the line passes through ice, heat transfer along that portion of the line is dominated by the pore microstructural model where the thermal conductivity of ice plays the dominant role in energy transfer. In contrast, anytime the test line passes through the humid air constituent, heat transfer is occurring in a manner similar to

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the lamellae microstructure. Finally, under conditions of isotropy, the lineal fraction is identical to the volume fraction (Underwood, 1970) leading directly to Eq. (75).

The energy flux through snow is introduced as

$$q_s = k_s \frac{\partial \theta}{\partial x} + u_{sg} D_s \frac{d\gamma_v^{\text{sat}}}{d\theta} \frac{\partial \theta}{\partial x}. \quad (76)$$

- 5 Combining Eqs. (69), (74) with (75) and comparing the results with Eq. (76) leads to the following expressions for the thermal conductivity of snow and the effective diffusion coefficient for snow given by

$$k_s = \phi_i (\phi_{ha} k_{ha} + \phi_i k_i) + \phi_{ha} \frac{k_i k_{ha}}{\phi_i \left(k_a + u_{sg} D_{v-a} \frac{d\gamma_v^{\text{sat}}}{d\theta} \right) + \phi_{ha} k_i}, \quad (77)$$

and

$$10 D_s = \phi_i (\phi_{ha} D_{v-a}) + \phi_{ha} \left(\frac{k_i D_{v-a}}{\phi_i \left(k_a + u_{sg} D_{v-a} \frac{d\gamma_v^{\text{sat}}}{d\theta} \right) + \phi_{ha} k_i} \right). \quad (78)$$

Despite the presence of the binary diffusion coefficient of water vapor in air, it should be emphasized that the result given in Eq. (77) represents the thermal conductivity for snow as predicted by the analytical model. The effective thermal conductivity including enhancement due to diffusion is given by Eq. (65).

- 15 Calonne et al. (2011) and Riche and Schneebeli (2013) provide curve fits of snow thermal conductivity as a function of density based on their finite element micromechanics analyses. Calonne's data included analysis of crystal structures of all types while Riche's data was limited to depth hoar and faceted crystals which produce higher thermal conductivities in the direction of interest (normal to the ground).

- 20 Figure 4 provides the predictions of Eq. (77) for a temperature of 253 K against the curve fits of Calonne et al. (2011) and Riche and Schneebeli (2013). The correlation

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of the analytical model is excellent as the model virtually tracks the numerical results of Riche and Schneebeli (2013) whose data were also generated at 253 K. Fosliens predicted curve at 271 K shifts downward toward the curve generated by Calonne et al. (2011), also generated at 271 K, but remains well within the bounds of both curves generated through finite element analysis of real microstructures. Furthermore, the most significant deviation of the analytical model occurs at a density for solid ice where Foslien's model predicts the self-consistent correct result of thermal conductivity for ice.

Changes in thermal conductivity as a function of temperature were observed by Calonne et al. (2011) for temperatures of 271 and 203 K, respectively. Figure 5 shows the thermal conductivity line predicted by Foslien along with the numerical micromechanics predictions of Calonne et al. (2011). Excellent correlation of the analytical model and the finite element analyses is again observed.

The value of the effective diffusion coefficient, D_s , for snow has a long history of dispute. Giddings and LaChapelle (1962) claimed D_s to be less than the diffusion coefficient of water vapor in air due to the fact that ice grains interfere with diffusion paths. In contrast, Yosida (1955) conducted experiments where the diffusion coefficient was estimated to be 3.5–5 times larger than that for air while experiments by Sommerfeld et al. (1987) found that the diffusion coefficient was about twice that for air. Yosida (1955) provided a classic description of diffusion being enhanced by water vapor moving between ice grains in a “hand to hand” fashion, thereby shortening the pathway required for water vapor to travel. It is interesting to note that the mechanisms for diffusion argued by Giddings and LaChapelle (1962) and Yosida (1955) both have merit and are competing against one another.

Christon et al. (1994) provided some of the first micromechanics finite element work on mass transfer for snow and generated predictions for the effective diffusion coefficient ranging from 1.0–1.93 times the diffusion coefficient for water vapor in air. Christon's results have been criticized, perhaps unfairly in our view, due to the simplistic microstructure models that he was forced to work with at that time. Pinzer et al. (2012)

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have laid any questions about the influence of microstructure to rest by performing finite element analysis on real snow microstructures generated through X-ray computer tomography. Their finite element predictions show a diffusion coefficient for snow to be very nearly that of diffusion of water vapor in air, perhaps an enhancement of 5–13% for snow compared to diffusion of water vapor in air based on the data provided in Fig. 11 of their work. Despite wildly more complex microstructures, the results of Pinzer et al. (2012) are largely consistent with Christon’s results. Indeed, in reference to studies on the vapor flux and its dependence on microstructure over time, Pinzer et al. (2012) note that “*the flux stays constant in time, despite the dramatic changes in the structure*”.

The diffusion coefficient given by Eq. (78) divided by the diffusion coefficient of water vapor in air is plotted in Fig. 6 to show Foslien’s predicted diffusion enhancement as a function of density at a snow temperature of 263 K. Also plotted in Fig. 6 are the diffusion enhancement ratios of Christon (1990) for two microstructural geometries in their applicable density ranges as well as the more recent predictions of Pinzer et al. (2012) based on real snow microstructures determined from X-ray tomography. Pinzer’s results show a range of diffusion enhancement at any given density that represents the range of diffusion enhancement computed over time as the microstructure evolved.

Foslien’s model predicted a maximum diffusion enhancement for snow compared to air of 1.23 with enhancements for typical snow densities in the range from 1.0–1.2. These values are in excellent agreement with the numerical predictions of Christon (1990) and the more recent results of Pinzer et al. (2012). In brief, we agree with view of Pinzer et al. (2012) in that any enhancement of water vapor diffusion in snow compared to diffusion of water vapor in air is minimal.

5.3.1 Thermal conductivity with diffusion

The effective thermal conductivity for snow including the enhancement of heat transfer due to mass diffusion is given by Eq. (65). Figure 7 shows the enhancement of the effective thermal conductivity incorporating diffusion effects as a function of density at

three different temperatures. For instance, at a density of 250 kg m^{-3} , the heat transfer enhancement due to diffusion is 9 and 3% for temperatures of 268 and 257 K, respectively. These values are reasonably consistent with calculated values provided by Riche and Schneebeli (2013) showing latent heat transfer contributions to be approximately 14 and 1% for temperatures of 268 and 257 K, respectively. Specific densities were not provided for the calculations of Riche and Schneebeli (2013) but the average density of their samples was 254 kg m^{-3} .

The analytical predictions of Foslien shown in Fig. 7 suggest the importance of latent heat transfer by diffusion is most prominent in low density snow at temperatures near freezing. In this case, the enhancement of heat transfer due to diffusion may be as high as 30–40% for low density snow. These results are consistent with the numerical studies of Christon et al. (1994) who note: “*the enhancement due to the transport of latent energy is seen to peak at about 40% of the conduction for the lowest density and the highest base temperature*”.

In closing, results from the analytical model for the thermal conductivity of snow, k_s , and the effective diffusion coefficient for snow, D_s , proposed by Foslien are in excellent agreement with cited finite element micromechanics analyses and, further, the parameter predictions are self-consistent with the limiting cases of air and solid ice. The results lend confidence to using the predicted parameters for k_s and D_s over the entire spectrum of temperatures and densities encountered in the macroscale heat and mass transfer analyses presented in Sect. 6.

6 Numerical results for macroscale heat and mass transfer

In this section, numerical results of the nonlinear equations (Eqs. 61 and 63) governing heat and mass transfer in a snowpack are presented. The specific problem at hand is to model the heat and mass transfer in a one-meter deep snow cover with complexities associated with a real snowpack such as dense layers and a time varying surface boundary condition for temperature. Figure 8 shows a schematic of the anal-

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also has the effect of producing a much higher temperature gradient in the near surface fresh snow cover in the pack. Figure 11 shows that, even after 10 days, the temperature gradient near the surface is approximately $60^{\circ}\text{C m}^{-1}$, three times the average temperature gradient. The high temperature gradients near the surface are even more notable when one considers the significant amplification of temperature gradients that occur at the microscale as discussed in Sect. 2 and demonstrated in Fig. 4 of Pinzer et al. (2012).

Figure 12 shows both condensation and sublimation occurring in the snowpack with significant activity near the dense ice crust. Near the surface, condensation is occurring because water vapor is diffusing toward the surface which is colder and, therefore, an area of lower saturation for the vapor density. The water vapor must then condense if the air is not to become supersaturated. Just below the dense layer, Fig. 12 shows another area of condensation near the dense ice crust. Condensation occurs here due to the decrease in humid air volume fraction in the direction of the water vapor diffusion. If the amount of air available to hold water decreases, then the amount of water vapor must also decrease. Just above the dense layer, the opposite is true. Here, Fig. 12 shows that sublimation is occurring because the vapor volume fraction is increasing in the direction of vapor flow. Sublimation must occur to keep the increasing amount of air saturated.

Local weakening above and below dense layers in a snow cover have been observed (Adams and Brown, 1982). If condensation is known to enhance depth hoar growth (Colbeck, 1983), then the condensation occurring below the dense layer in Fig. 12 could contribute to the weakening observed in this region of a snowpack. We note that temperature gradients are relatively low below the ice crust, although in the range of where faceted crystal growth has been observed in field studies. The sublimation occurring above the dense layer may contribute to any snowpack weakness observed here.

Sublimation is also observed near the ground after 10 days and appears to be increasing with time. At a sublimation rate of $4\text{ mg m}^{-3}\text{ s}^{-1}$ occurring just above the

ground after 10 days, a decrease in density of 1 kg m^{-3} would take about 3 days. This slow rate of change in density is consistent with experimental studies on temperature gradient metamorphism, where little change in density is observed despite the dramatic changes in the crystal structure of snow (Pinzer et al., 2012).

6.2 Effect of diurnal temperatures

To study diurnal temperature effects, the surface of the snowpack was subjected to a harmonic temperature boundary condition given by

$$\theta(1, t) = -20 - 10 \sin \frac{\pi t}{43200}, \quad (79)$$

with the lower surface temperature held fixed at 0°C . The boundary condition given by Eq. (79) has a mean value of -20°C with a 10°C fluctuation about the mean. Initial conditions for the temperature through the snowpack were specified based on the average temperature gradient of -20°C m^{-1} at time $t = 0$.

Figure 13 shows the temperature profile over a 24 h period at day 5, after any transients have disappeared. Only the upper half-meter of the snowpack is shown. Strong temperature gradients are observed in the fresh snow near the surface, with gradients as high as $-150^\circ\text{C m}^{-1}$ as shown in Fig. 14. The large temperature gradients found near the surface are also accompanied by active condensation and sublimation throughout a 24 h cycle, Fig. 15. Both the temperature gradient and the mass exchange are likely to impact microstructural changes that occur in the near surface snow cover.

7 Summary

We have developed a macroscale mixture theory analysis for modeling condensation and sublimation rates in a snow cover under temperature gradient conditions. The theory is general enough to accommodate arbitrary density profiles with any desired time

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dependent surface boundary conditions. Condensation and/or sublimation is observed near the ground and the surface as well as immediately above and below dense layers such as ice crusts. Macroscale temperature gradients can be surprisingly high compared to the average temperature gradient in the snowpack.

Strong macroscale temperature gradients coupled with enhanced condensation/sublimation rates warrant further studies of heat and mass transfer at the microscale. In current finite element micromechanics analyses, the vapor flux at the microscale is driven by microscale temperature gradients. The local temperature gradients are induced by imposing a specified macroscopic temperature gradient formed by specifying a temperature differential on the lower and upper surfaces of the RVE.

Just as the temperature gradient is specified in the aforementioned micromechanical analysis, it is also possible to specify an independent net mass transfer boundary condition on the RVE. Specifying an independent mass flux allows one to represent either condensation or sublimation based on macroscale conditions. In brief, knowledge of the condensation or sublimation rates at the macroscale provides the foundation for a fully coupled solution of heat and mass transfer at the microscale.

Finally, analytical expressions of thermal conductivity and the effective diffusion coefficient for snow were developed from first principles of heat and mass transfer phenomena at the microscale. The equations developed provide an elegant path to modeling thermal conductivity and the effective diffusion coefficient of snow that are needed for the macroscale mixture theory analysis. The model is also capable of quantifying the significance of latent heat transfer to the total energy flux.

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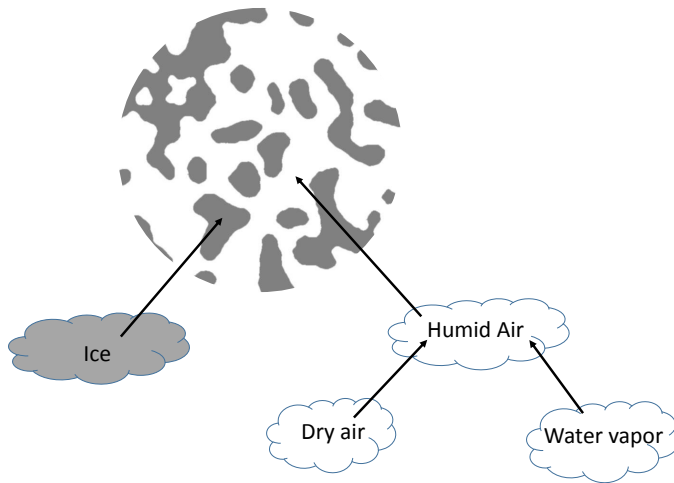


Figure 1. Schematic showing a continuum point of snow with the associated constituents for a mixture theory analysis.

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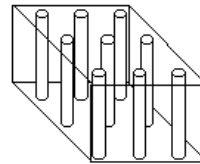
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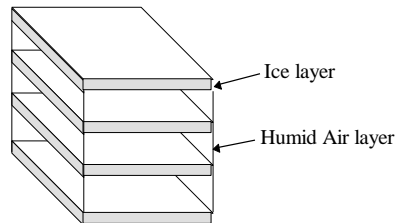


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(a) Pore Microstructure

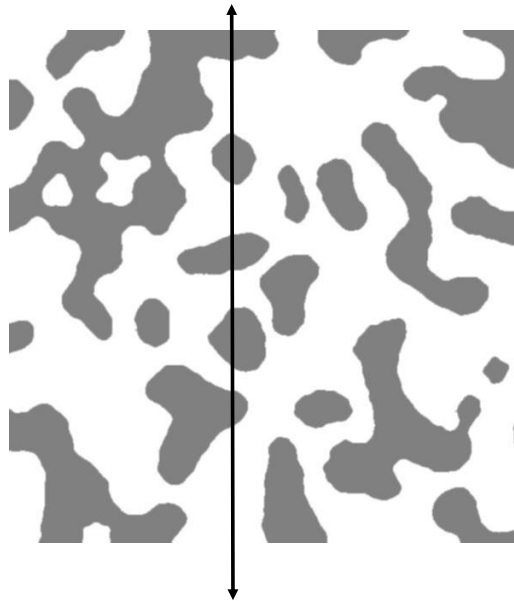


(b) Lamellae Microstructure

Figure 2. Idealized microstructures used to model heat and mass transfer in parallel **(a)** and series **(b)**.

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1-D Heat Transfer

Figure 3. Test line through a snow surface section showing one-dimensional heat and mass transfer at the microscale.

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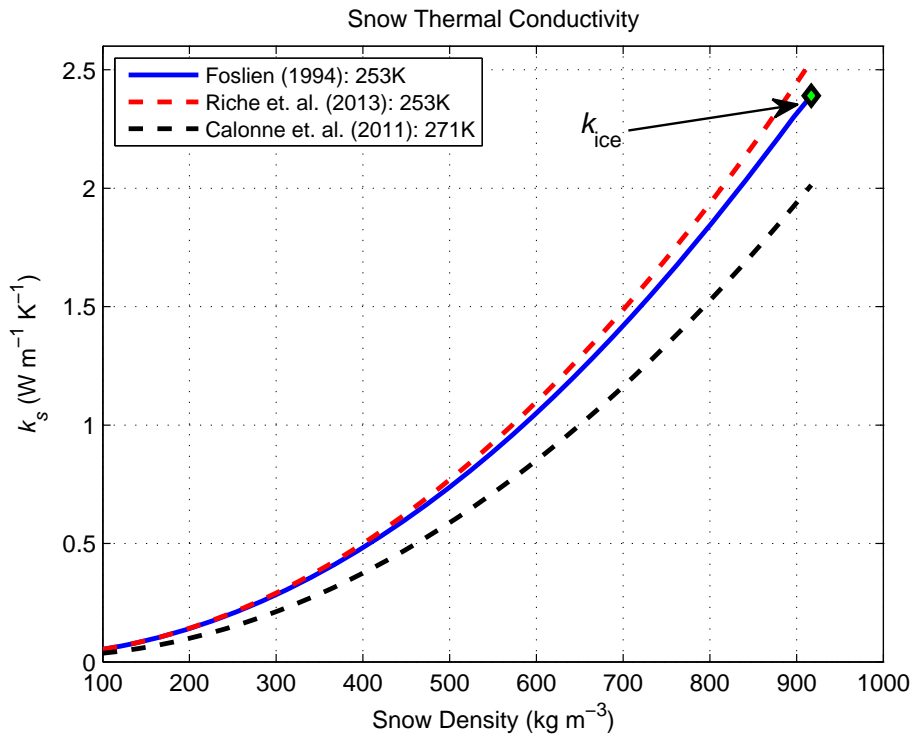
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Figure 4. Thermal conductivity analytical prediction of Foslien (1994) vs. finite element predictions of Calonne et al. (2011) and Riche (2013).

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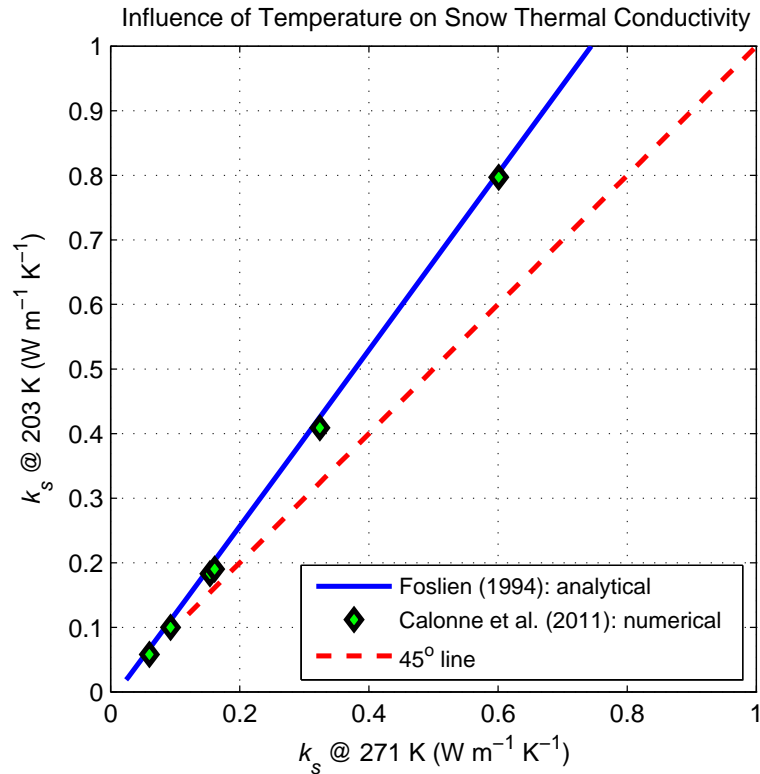


Figure 5. The influence of temperature on thermal conductivity as predicted by the model of Foslien (1994) and Calonne et al. (2011) through finite element analysis.

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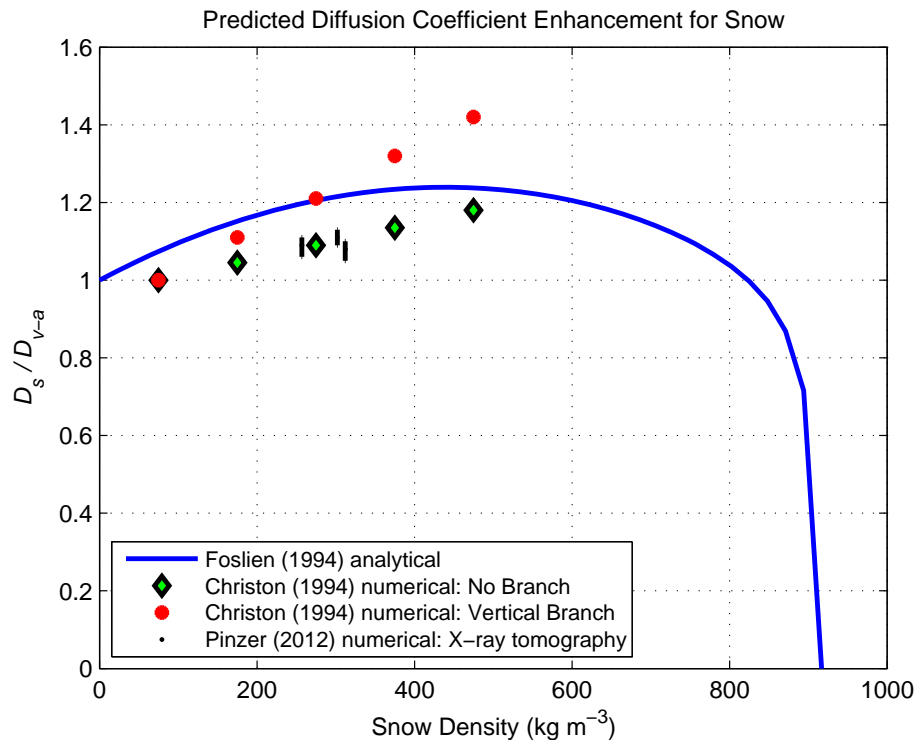


Figure 6. Effective diffusion coefficient enhancement for snow predicted by Foslien (1994) vs. finite element predictions of Christon (1990) and Pinzer (2012).

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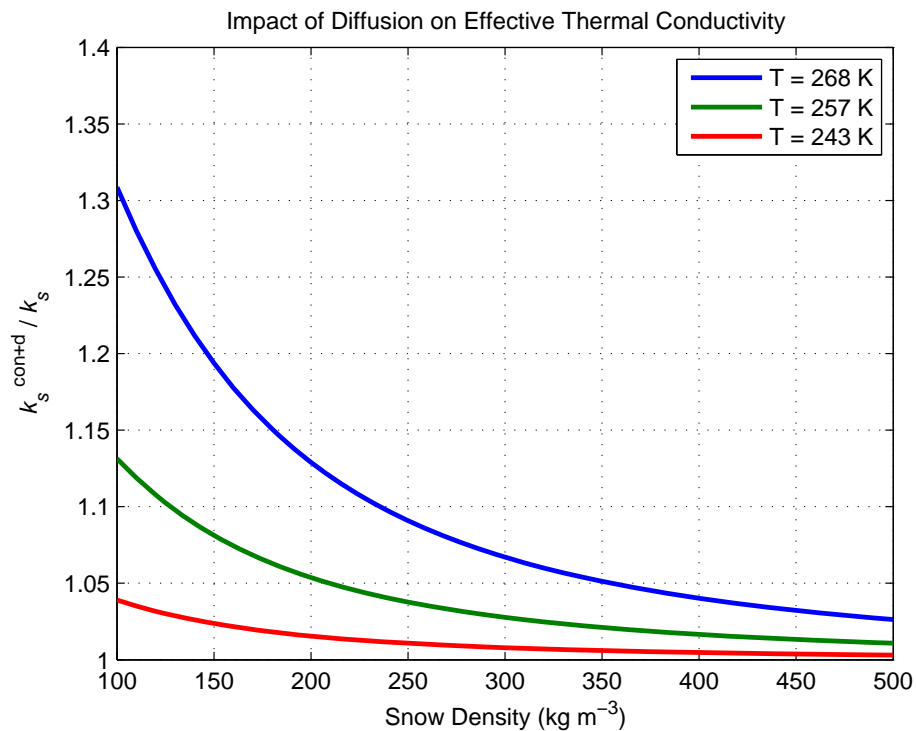


Figure 7. Effective thermal conductivity enhancement due to diffusion predicted by Foslien (1994).

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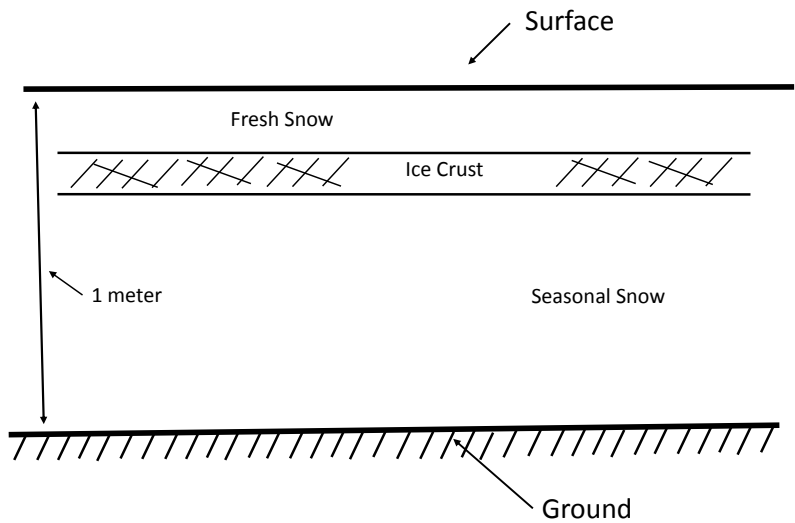


Figure 8. Snow cover characteristics for the macroscale heat and mass transfer numerical studies.

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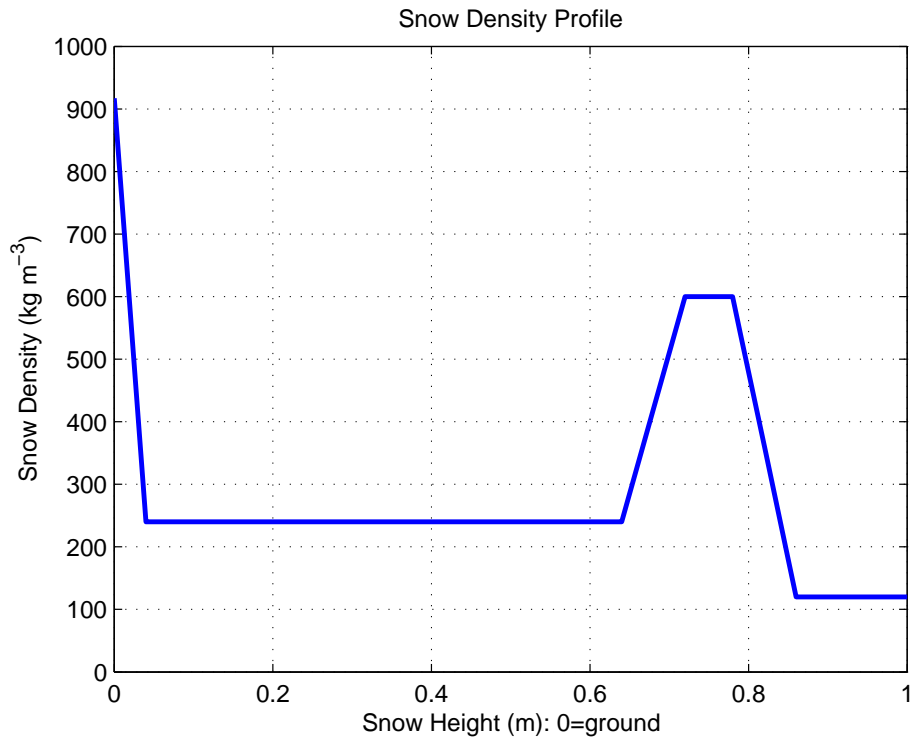


Figure 9. Snow density profile for the numerical studies.

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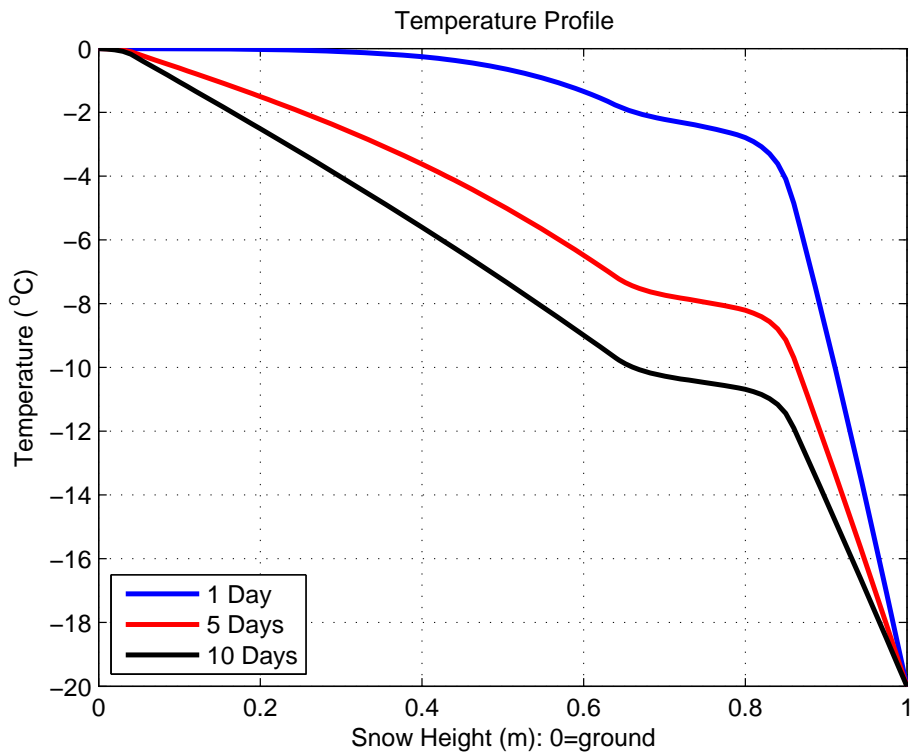


Figure 10. Snowpack temperature profile at 1, 5, and 10 days, respectively.

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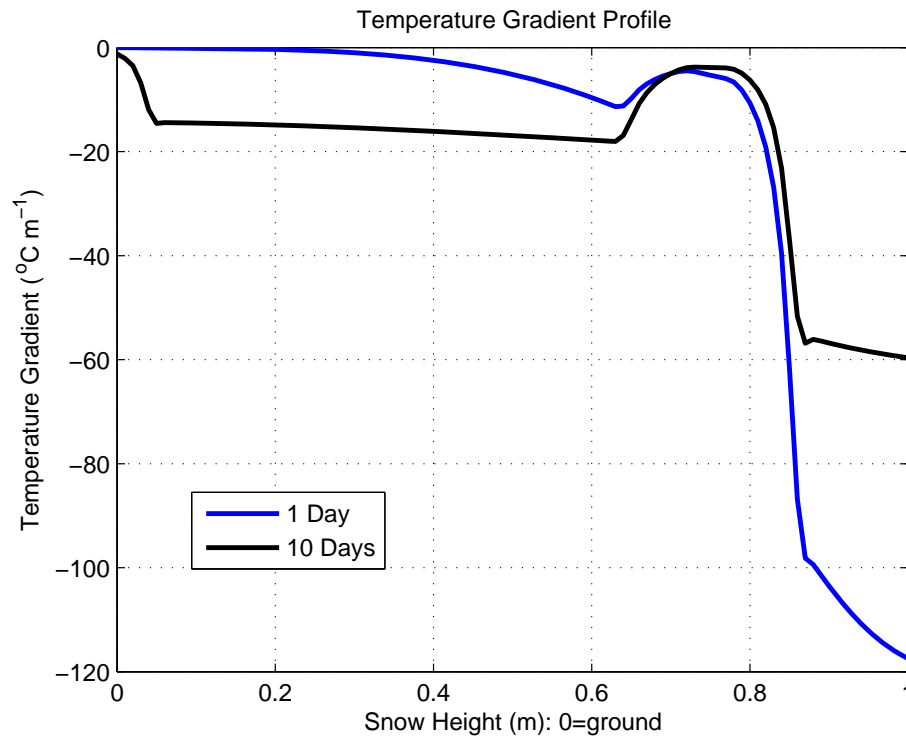
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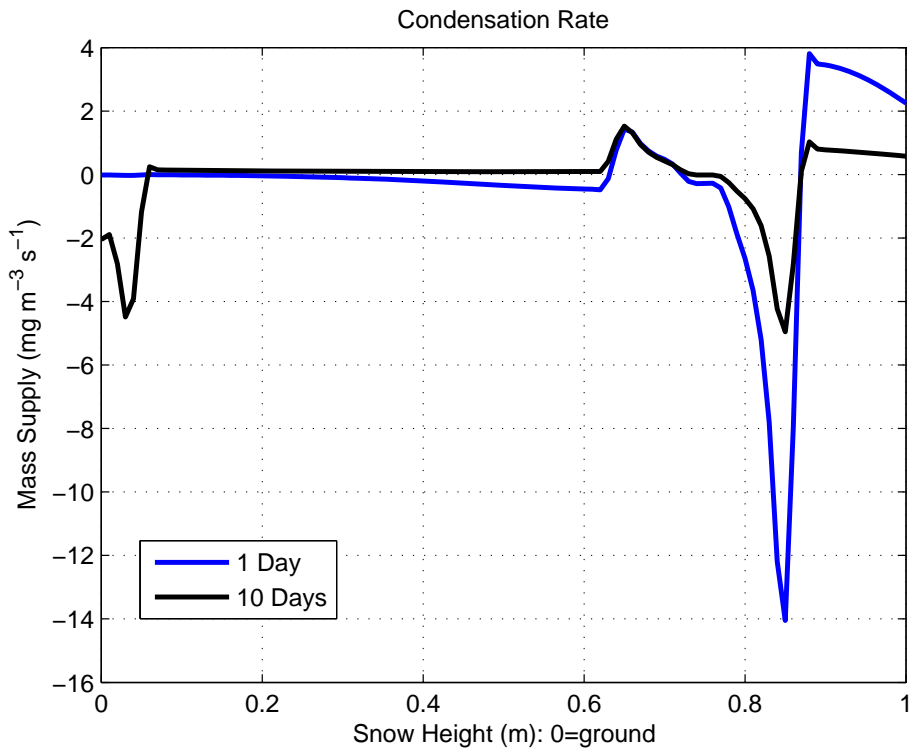


Figure 12. Snowpack condensation rates at 1 and 10 days, respectively. Positive values indicate condensation while negative values indicate sublimation.

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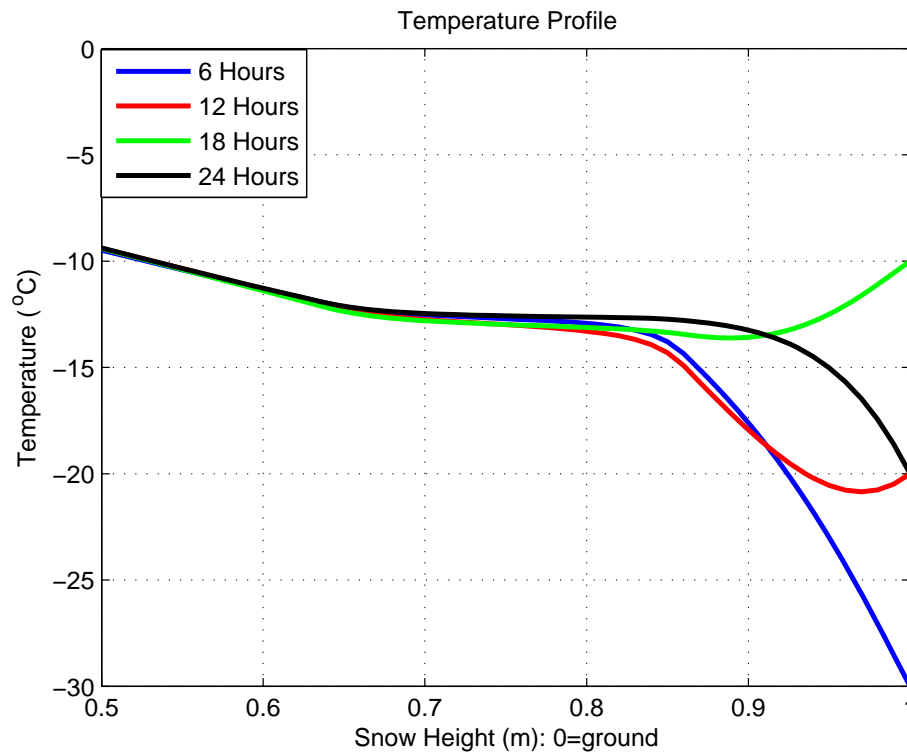


Figure 13. Snowpack temperatures over a 24 h period with time dependent surface boundary conditions given by Eq. (79).

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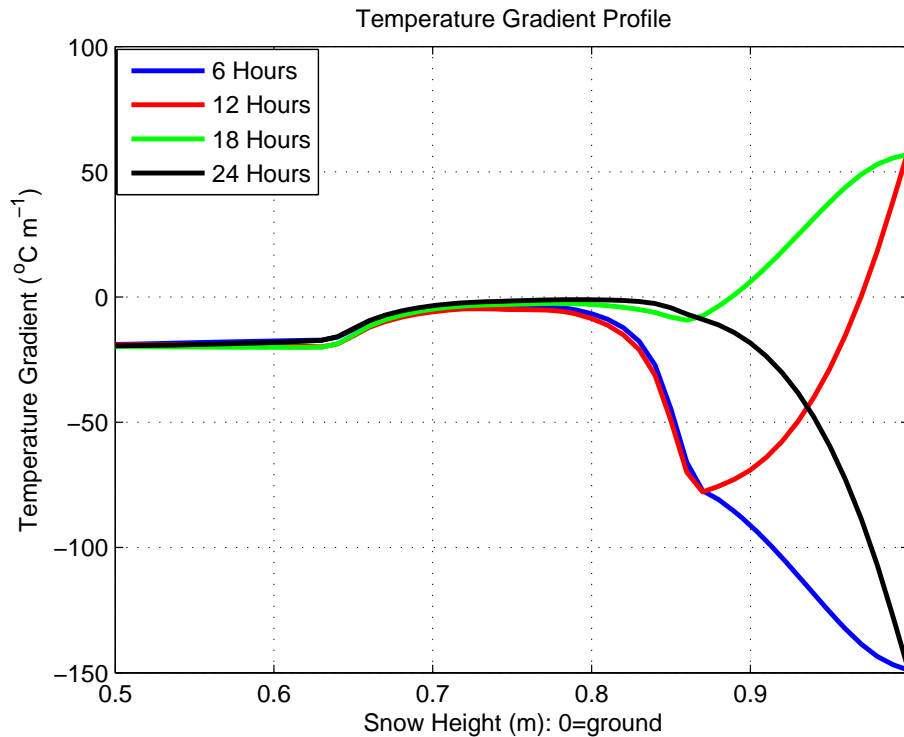


Figure 14. Snowpack temperature gradients over a 24 h period with time dependent surface boundary conditions given by Eq. (79).

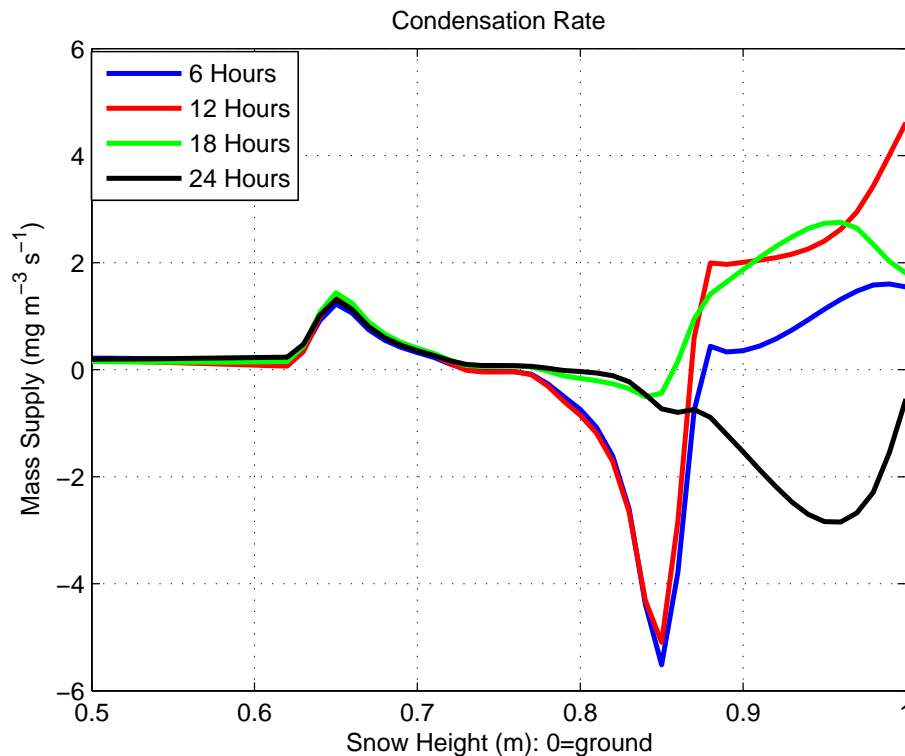
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Figure 15. Snowpack condensation rates over a 24 h period based on the diurnal boundary condition of Eq. (79). Positive values indicate condensation while negative values indicate sublimation.

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