

PHYSICAL MODELS FOR DETERMINING CHANGES IN MICROSTRUCTURE OF SNOW DURING METAMORPHISM

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Abstract: Since the internal microstructure is important for determining the mechanical, thermal and physical properties of snow, a study was undertaken to develop a physical model that can predict changes in microstructure of snow due to metamorphism and mechanical loads. The microstructure was defined in terms of the 3-D coordination number, mean grain size, mean bond radius and mean neck length. For situations where temperature gradients were small, a mixture theory was used to calculate growth for grains and bonds. These calculated results were then compared with experimental data and found to adequately predict changes in these variables. In situations where temperature gradient effects dominate, a physical model was developed which calculated grain and bond growth rates. This model was found to give results that appear to be representative of what happens in snow under TG conditions. However, a lack of data to date has precluded a thorough evaluation. For mechanical effects, another physical model was developed to determine bond growth rates due to stresses applied to the snow. These models have been incorporated into the SNOWPACK program, which was developed by the Swiss Federal Institute for Snow and Avalanche Research as a tool for assisting avalanche hazard forecasters.

Keywords: snow, microstructure, metamorphism, sintering

1. Introduction

Snow cover metamorphism models are now in relatively common use for predicting changes in snow cover properties in response to changing weather and loading conditions (Brun et al., 1989, 1992; Jordan, 1991, Lehning et al., 1998). The model by Jordan, SNTHRM, was developed primarily to calculate temperatures within the snowpack and at the surface. It has been used within the American continent in conjunction with snowmelt hydrology. The model developed by the French (Brun et al., 1989) is called CROCUS and was developed as a tool to assist avalanche hazard forecasters. Finally, SNOWPACK was developed by the Swiss (Lehning et al., 1998) as a avalanche hazard forecasting tool.

Initially these models calculated heat and mass transport within the snowpack but did not determine how the internal structure and strength of the snow would change in response to weather. The French model initially was able to calculate temperature and density profiles and settling rates. Later empirical laws were incorporated into CROCUS to calculate the "dendricity" and the "sphericity" of the snow. Dendricity provides a measure of how much of the original dendritic structure of the new snow remains, while

sphericity measures the roundness of the grains. These laws were largely empirical, having been developed from an extensive set of laboratory data. The settling of the snowpack, as determined by the material viscosity, was calculated in terms of the temperature and snow density. The snow conductivity was also based on empirically derived relations using density as the single variable. Later versions of CROCUS also predicted changes in grain size and grain shape, but again this was based on empirical laws derived from substantial laboratory data bases.

SNOWPACK uses physical laws to model heat and mass transport within the snow pack. Automatic weather stations located at more than 45 points within the Swiss Alps provided the upper boundary conditions (temperature, wind speed solar radiation, new snow fall) for the program to calculate temperature profiles and settling rates. As with CROCUS, the original forms of SNOWPACK used empirical laws to calculate the viscosity and conductivity of the snow. The current form of SNOWPACK also calculates dendricity and sphericity with the same empirical laws used for CROCUS. SNOWPACK has also had added to it physically based laws that calculate conductivity (Adams and Sato, 1993; Brown et al., 1998), viscosity and changes in grain and bond size

In this paper we present the development of these theories. First the use of a mixture theory to calculate grain and bond growth rates is presented for cases where temperature gradients are small. Then, for large temperature gradients, a physical model is developed. Finally, a microstructure-based viscosity model is presented to demonstrate the importance of such a formulation for detailed modeling of density layering in snowpack.

2. Grain and Bond Growth Under Equitemperature Conditions

When the temperature gradient is small (normally less than $10\text{ }^{\circ}\text{C/m}$), the growth and decay of bonds and grains are determined by differences between equilibrium vapor pressures of the various ice surfaces within the snow. Small grains with highly convex surfaces will normally lose mass, since the vapor pressure over its surface is higher than the vapor pressure existing over the ice surface of a neck or large ice grain. Consequently vapor sublimates off the small grains and migrates to necks or large grains and condenses there. Over time, small grains continue to lose mass and large grains continue to grow. The necks connecting the grains also continue to grow. Temperature differences between these ice surfaces develop because such mass transfers between grains and necks also involve heat transfer. Such microscale temperature variations exist but cannot be easily measured and would not be evident with normal means of measuring snowpack temperatures.

In order to calculate changes in grain and bond size under equitemperature conditions, a mixture theory (Brown et al., 2000) was utilized. This formulation used the principles of conservation of mass, momentum and energy as well as the second law to characterize the interchange of mass and energy between necks and grains. The details of this formulation are too involved and lengthy to present here, so the reader is referred to Brown et al (2000) for a detailed discussion of the theory.

For this particular application of the mixture theory, the snow was assumed to consist of an air phase, a vapor phase, a distribution of twenty grains sizes and a distribution of twenty bond sizes. This mixture therefore consisted of 42 constituents. Each constituent had its own mass density, local velocity, temperature, stress, strain energy, entropy, and Helmholtz free energy

Each ice constituent (there are forty of them in this application) exchanges mass with the pore vapor which serves to transfer the mass

between the other constituents. In this application the direct interchange of mass between ice constituents by means of surface diffusion or grain boundary diffusion was neglected. Recent work by Colbeck (1997, 1998) indicates that grain boundary diffusion may be a significant part of the sintering process. If so, the theory given here would have to be modified to include this additional process.

The theoretical results were compared with experimental data. The bond size and grain size were determined with a quantitative stereology software package developed at Montana State University (Edens and Brown, 1994, 2000). The calculated and measured results were then used to develop a set of equations that would be used by the SNOWPACK program to predict bond and grain growth under conditions of low temperature gradients.

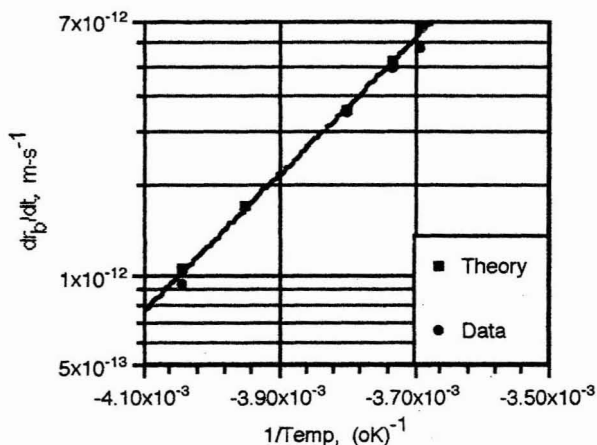


Figure 1. Comparison of theoretical and experimental bond growth rates

Figure 1 shows predicted bond growth rates as a function of temperature while figure 2 compares theory with data for grain growth. The data was obtained in experiments on very fine-grained manufactured snow with an initial mean grain size of approximately $50\text{ }\mu\text{m}$ (Edens and Brown, 1994).

The results of the mixture theory show the appropriate trends for grain growth and bond growth rates as functions of temperature. The one disturbing result is the poor correlation for grain growth rate at the coldest temperature of $244\text{ }^{\circ}\text{K}$ ($-20\text{ }^{\circ}\text{F}$) in figure 2.

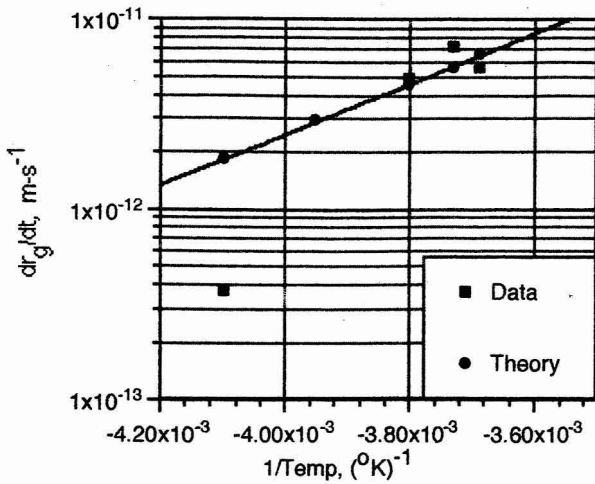


Figure 2. Comparison of theoretical and experimental grain growth rates

As another measure of the ability of the theory to model ET metamorphism, consider the changes in grain size distribution over a 30-day period. The results show how the distribution of grain size changes during the period in which the snow was held at a constant temperature with no temperature gradients applied to the material. The data is for the same samples used in figures 1 and 2. Shown in figure 3 is the grains size distributions at times of 0, 14, and 30 days. The vertical scale in figure 3 gives the fraction of grains for each grain size depicted on the horizontal scale. The grain size distribution was set equal to the measured distribution at time $t = 0$ days. As can be seen, there does exist a divergence between the theory and experimentally measured results, but the trends toward larger grain distribution is modeled by the theory.

The distributions of grain and bond size were measured with the stereology package developed at Montana State University (Edens and Brown, 1994, 2000). As indicated earlier, these experiments were conducted on very fine-grained snow with predominantly spherical particles. This was done so that measurable results could be obtained in a relatively short period of 30 days. Metamorphism proceeds much more quickly with fine-grained particles than with large-grained snow.

While not shown, results similar to figure 3 were obtained for the bond size distributions. The mixture theory was able to calculate the bond size distribution changing in a fashion similar to what was measured.

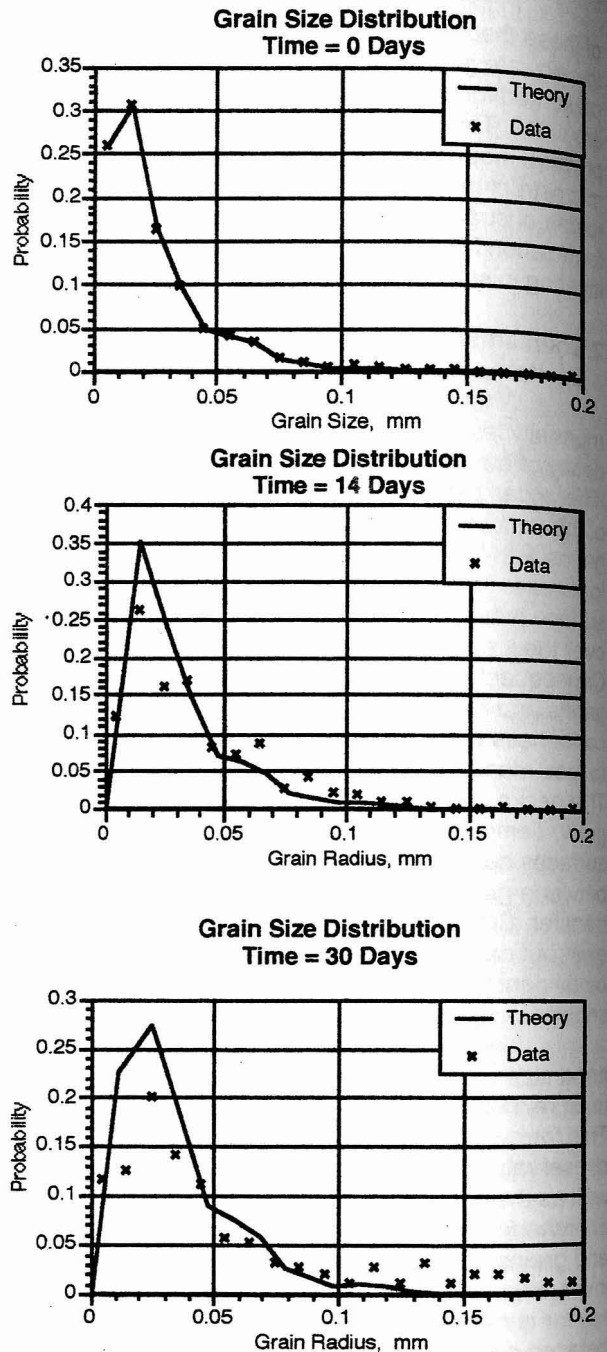


Figure 3. A comparison of theory with data for determining grain size distribution change with time,

With the above results, equations defining grain and bond growth rates in terms of grain size, bond size, density and temperature were generated and then implemented in the SNOWPACK program. For grain growth, the relation is:

$$\dot{r}_g(\theta, t) = S_{ph} \left(A_1 + \frac{A_2}{r_g} \right) e^{A_3(\sqrt{\theta_R - \theta})} \quad (1)$$

In the above, $\theta_R = 273 \text{ }^\circ\text{K}$, $A_1 = 5.860 \times 10^{-12} \text{ m/s}$, $A_2 = 9.403 \times 10^{-17} \text{ m}^2/\text{s}$, and $A_3 = 2.900 \times 10^{-3} \text{ }^\circ\text{K}$. The term S_{ph} is the sphericity of the snow. This term was developed earlier by Brun et al. (1992) to define the degree of roundness of the snow grains. S_{ph} ranges from 0.0 for fully faceted snow to 1.0 for fully rounded granular snow. Under ET conditions, this factor limits the rate of grain growth due to faceting. Faceted surfaces on a grain inhibit grain growth, because these surfaces are stable with low equilibrium vapor pressures. The lack of curved surfaces then limits the rate at which grains will grow.

An expression similar to Equation (1) was also found for the bond growth:

$$\dot{r}_b = A_o \left[e^{-\frac{B_1}{r_n}} - e^{-\frac{B_1}{r_g}} \right] e^{B_2 \left(\frac{1}{T_R} - \frac{1}{T} \right)} \quad (2)$$

where $A_o = 1.46 \times 10^{-3} \text{ m/s}$, $B_1 = 1.885 \times 10^{-9} \text{ m}$, and $B_2 = 4.669 \times 10^3 \text{ }^\circ\text{K}$.

3. Changes in Grain and Bond Size During Temperature Gradient Metamorphism

When temperature gradients exceed approximately $10 \text{ }^\circ\text{K/m}$, vapor pressure gradients associated with the temperature gradient dominate the flux of vapor to and from ice surfaces. To determine this effect, the ice matrix was modeled as an assembly of ice grains, necks and pore spaces. A cubic arrangement was used (figure 4) to model the physics of this process.

In this figure the temperatures at the various points are denoted by θ_i , $i = 1, \dots, 8$. The heat fluxes through the various parts of the ice and pore regions are denoted by q_i , $i = 1, \dots, 7$. The mean temperature gradient over the region is:

$$TG_{mean} = \frac{\theta_8 - \theta_1}{8r_g + 2L + h} \quad (3)$$

All fluxes q_1, \dots, q_7 were set equal, and then these fluxes were equated to the heat flux in the snow,

$$q_s = -k_s A \cdot TG_{mean} \quad (4)$$

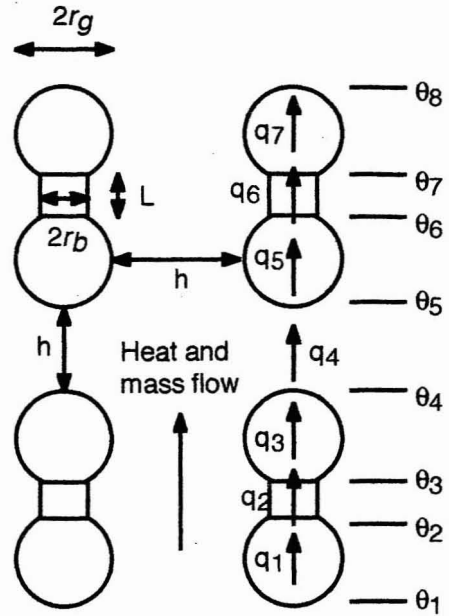


Figure 4. Schematic of model for calculating growth rates under TG conditions.

The temperatures $\theta_2, \dots, \theta_7$ were found in terms of θ_1 and θ_8 . In the above, k_s is the effective thermal conductivity of snow. This snow conductivity was obtained from the relations developed by Adams and Sato (1993) and Brown et al. (1998). With this information, the temperature gradients in the grains, necks and pores were calculated and found to have the forms:

$$\begin{aligned} TG_{microbond} &= \frac{k_s A}{k_i A_b} TG_{mean} \\ TG_{micropore} &= \frac{k_s A}{k_a A_b} TG_{mean} \\ TG_{micrograin} &= \frac{k_s A}{k_i A_g} TG_{mean} \end{aligned} \quad (5)$$

In the above k_i and k_a are respectively the conductivity of ice and air. Once the temperature gradients across the necks, grains and pores were found, the rates of deposition/sublimation at the necks and grains were determined. This was done by using Fick's law of diffusion to determine the mass transfer along the neck and grain. The bond radius was found to be:

$$\dot{r}_b = \frac{DPL}{R^2 \theta^3} TG_{microbond} \left(\frac{r_g^2}{r_b L} - \frac{r_b}{2L} \right) \quad (6)$$

Satyawali (1994) used a similar approach to find the grain growth rate to be:

$$\dot{r}_g = 1.65D \left(\frac{h + 2r_g + L}{r_b} \right) T G_{mean} \frac{1}{\rho} \frac{d\rho}{d\theta} \quad (7)$$

D is the diffusion coefficient of water vapor in air, and ρ is the vapor density. It should be mentioned that, since both the grain size and bond size change with time, the temperature gradients given in Equation (5) also changes with time. This in turn will affect how quickly the bonds and grains change size. Figure 5 illustrates the bond growth rates for snow with an initial density of about 250 kg/m³. For this example, the temperature gradient is -30 °C/m, and growth rates are shown for two different temperatures. The growth rate is very high until the bond is well established and begins to conduct more of the heat. After that the growth rate drops off.

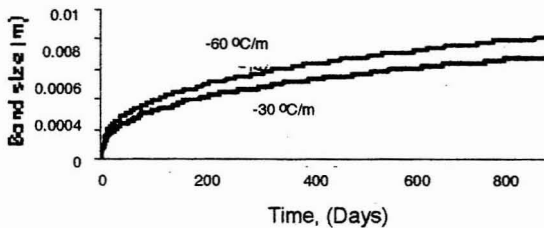


Figure 5. Bond growth at different temperatures.

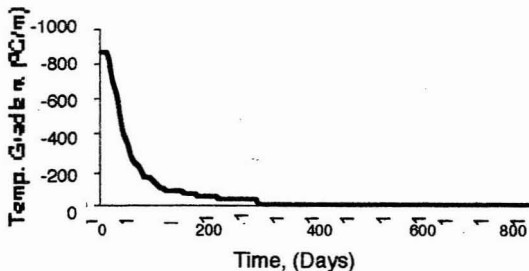


Figure 6. Variation of temperature gradient in bond with time.

Figure 6 shows the variation of the temperature gradient in the neck, $Tg_{microbond}$. As can be seen, the gradient in the neck is initially very high since the conductivity of the neck is low due to its small radius. As the neck radius increases, the gradient needed to conduct the heat decreases.

5. Snow Viscosity and its relation to Microstructure

To illustrate the importance of microstructure in the description of material properties, we express snow compactive viscosity in terms of neck length, grain size, bond size and coordination number. It is noted that this formulation is a one dimensional one and does not describe the effect of anisotropy on properties.

The ability of the material to settle and densify can be determined by the material viscosity, η , which is related to the pressure p_s and the strain rate $d\epsilon/dt$ by the relationship:

$$\dot{\epsilon} = -\frac{p_s}{\eta} \quad (8)$$

Therefore, low values of viscosity will result with large rates of settlement while large viscosities will yield low settlement rates. Since the necks are the regions of maximum stress, most of the deformation takes place there. The ice grains themselves experience some deformation when the snow is under load, but the large majority of the snow deformation is due to the intergranular motion of the grains that accompanies the deformation of the necks. The stresses in the necks may be more than 100 times larger than the stresses in the grains, depending grain size, bond size, neck length, etc.. The necks may be directly compressed under pressure, but they can also deform in shear. The result is that under compressive loads, the ice grains move closer to each other, the pores occupy a smaller portion of the snow volume, and the density increases.

The calculation of viscosity is broken into two parts: a nonlinear range and a linear range. This is determined by the properties of ice itself. At low stresses, less than 400 kPa, ice exhibits a nearly linear behavior. Following the approach of Mahajan and Brown (1993) the viscosity in the nonlinear range was found to be:

$$\eta^{-1} = \left[\frac{3l}{r_g + l} \right] \dot{\epsilon}_{p1}(\theta_o) e^{\left[\frac{\theta}{R} \left(\frac{1}{\theta_R} - \frac{1}{\theta} \right) \right]} \left(\frac{4A}{N_3 \phi_s \sigma_{ni}} \right)^3 \left(\frac{r_g}{r_b} \right)^6 p_s^2 \quad (9)$$

The above relation is valid whenever the snow stress is large enough to produce a nonlinear behavior in the neck. When the stresses drop below a certain level, the stress behavior becomes linear, and the snow viscosity becomes:

$$\eta = \frac{N_3 \phi_s}{4} \left(\frac{r_b}{r_g} \right)^2 \frac{l + r_g}{l} \eta_0 \quad (10)$$

Figure 8 shows the results of the above equations. A snow stress of 500 Pa is applied to snow with different bond/grain ratios and densities.

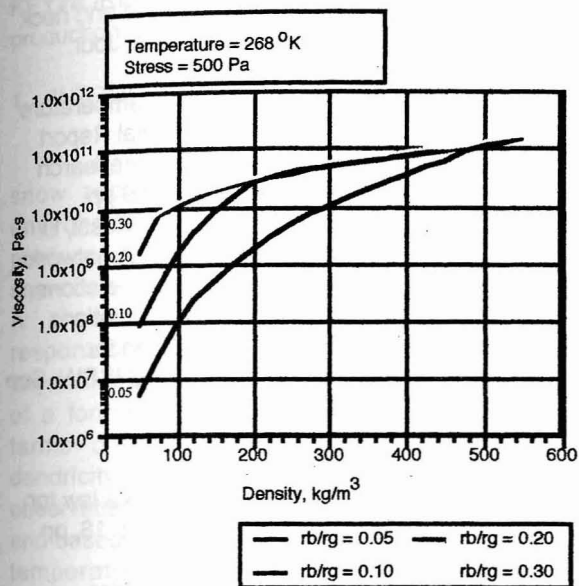


Figure 8. Calculated values of snow viscosity for a range of densities and bond/grain ratios.

In this figure the more well-bonded snow reaches the linear stage at lower densities than does the poorly bonded snow. For instance, snow with a bond/grain ratio of 0.3 is linear over the full range of densities, whereas the snow with a bond/grain ratio of 0.05 does not reach linearity until a density of 550 kg/m³ is reached.

6. Application to SNOWPACK Program

The formulations presented in the preceding section have been implemented in the SNOWPACK program to enable the program to calculate the grain size and bond size distributions over the full depth of the snowpack. This is a particularly important feature of the SNOWPACK program, since it uses physical models to determine grain and bond growth patterns. Values

of r_g and r_b are needed for the calculation of compactive viscosity and effective conductivity, since the program uses microstructural models for these two parameters. Consequently, such programs cannot reproduce the complicated density patterns that can evolve in natural snowpack. This is because, since the viscosity is strictly density dependent in such models, the snowpack will tend to evolve toward a uniformly varying density profile. However, with the ability to determine viscosity in terms of coordination number, bond radius and grain size, a more detailed and potentially more accurate density profile can be obtained. For instance, a layer with good intergranular bonding would not densify nearly as quickly as one with a similar density but with poor bonding, and measurable variations in the density profile would evolve. Figure 7 shows the density profile that SNOWPACK predicts for a typical snowpack in Davos Switzerland.

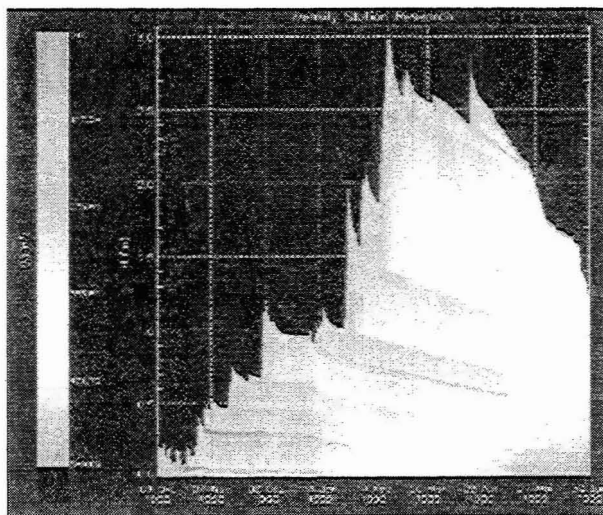


Figure 7. Density layering in mountain snowpack .

The horizontal scale gives the time, ranging from early October until early June. The vertical scale gives the snow depth and vertical location of all layers. The density is indicated by the color scale. As can be seen, a substantial amount of density layering results, and this layering can not be produced by assuming the compactive viscosity depended solely on density and temperature. Differences in bond/grain radius ratio will serve to provide longer lasting and more substantial variations in density with respect to depth.

7. Conclusions

In this paper we have presented the formulations that are used to calculate changes in bond radius and grain radius of snow on the ground. A mixture theory was used to characterize bond growth rates and grain growth rates when temperature gradients were less than 10 °C/m, while a physical model was used for higher temperature gradients. Neither of these formulations has been rigorously validated by experimental data, largely because the data does not exist. The mixture theory results was compared to some existing data and found to work quite well. However, more testing and validation is needed to provide a basis for improving these models.

Future research should be directed at developing an all-encompassing theory that will work continuously for temperature gradients ranging from 0 °C/m to higher than 100 °C/m. The mixture theory discussed here has the capability of providing such a model, but the physical model used for high temperature gradients also should work just as well, provided a more realistic geometric representation of the grain and pore space is utilized.

7. Acknowledgements

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