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MATHEMATICAL MODELLING OF PRESSURE INDUCED FREEZING POINT DEPRESSION WITHIN SOILS EXHIBITING STRONG CAPILLARY PRESSURE EFFECT

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Abstract. Many geotechnical applications are affected by the melting and formation of ice in soils. Current state of practice involves incorporating the presence of ice within hydrological models for unsaturated soils using the so-called generalised Clapeyron equation [1]. This represents a modification of the conventional Clapeyron equation by allowing for the pressure in ice and liquid to be different at an ice-liquid interface. Such an idea has come about due to the effects of surface tension, which become important within the pores of porous materials such as soil and rock. However, a common assumption when using the generalised Clapeyron equation is that the ice pressure remains constant [2], which leads to unrealistic behaviour in the presence of significant pore-water pressure changes. Here we develop a new mathematical modelling framework to explore the impact of pressure induced freezing point depression within soils exhibiting strong capillary pressure effect. We solve the coupled mass and energy conservation problem using method of lines (e.g., [3]) with pressure and enthalpy as the primary dependent variables. Strong non-linear coupling develops through the chemical potential equation accounting for coexistence of ice and water in the presence of surface tension [5]. We present a sensitivity analysis showing how freezing point depression evolves within a porous block subject to temperature surface boundary cooling and varied capillary pressures.

Key words: Ice; Clapeyron equation; Porous media; Enthalpy; Surface tension; Method of lines

1 Problem description

In this work we develop the necessary equations for studying pressure induced freezing point depression in porous materials with capillary pressure effects. We construct the coupled mass and energy conservation problem that takes into account the heat conduction in the heterogeneous (partly frozen) porous material together with the latent heat of fusion, which is deposited at the freezing boundary layer. It is assumed that there is no convection as it is prevented by the low permeability of the material considered, which greatly simplifies the problem. The solid grains that comprise the porous material are assumed to be in thermal equilibrium with the water and ice contained within the pore-space. We also assume that in the same volume, there is always the same mass of solid grains.

Let us consider a horizontal porous column of length, L [L], with fully saturated pores, which are initially set at a uniform temperature, T_I [Θ], and pressure, p_I [ML⁻¹T⁻²], respectively (see Fig. 1). One of the boundaries is then treated as adiabatic whilst the other boundary is fixed at temperature, T_0 [Θ]. The boundary temperature is chosen to be less than the freezing-point temperature associated with the initial conditions. The coefficients of isothermal compressibility, α_T [M⁻¹LT²], and isobaric thermal expansivity, β_P [Θ^{-1}], are assumed to be constant, and the relationship between the freezing point temperature, $T_c(p)$ [Θ], and pressure, p, is determined through a chemical potential equation accounting for the coexistence of ice and water in the presence of a surface tension. The ice is considered to be compressible and subjected to thermal expansion. The total mass of water component does not change over time due to there being zero permeability and no evaporation.



Figure 1: Schematic diagram of conceptual model.

The heat conduction problem takes the following form

$$\frac{\partial U}{\partial t} = \frac{\partial}{\partial x} \left(\kappa \frac{\partial T}{\partial x} \right), \quad T(x,0) = T_I(x), \quad T(x=L,t) = T_0, \quad -\kappa \frac{\partial T}{\partial x} \Big|_{x=0,t} = 0.$$
(1)

where x [L] is distance, T $[\Theta]$ is temperature, U [ML⁻¹T⁻²] is internal energy density and κ [MLT⁻³ Θ^{-1}] is thermal conductivity.

Let G_m [ML⁻³] be the mass of water per unit volume of porous material found from

$$G_w = \phi [S_w \rho_w + (1 - S_w) \rho_i], \qquad (2)$$

where ϕ [–] is the porosity, S_w [–] is the saturation degree of water, ρ_w [ML⁻³] is the mass density of liquid water and ρ_i [ML⁻³] is the mass density of ice.

By taking the full differential of G_w and choosing the pressure and enthalpy density, H [ML⁻¹T⁻²], as the primary dependent variables ($G_w = G_w(H, p)$), we get

$$dG_w = \frac{\partial G_w}{\partial H} dH + \frac{\partial G_w}{\partial p} dp.$$
(3)

Differentiating G_w from Eq. (2) with respect to p and H gives

$$\frac{\partial G_w}{\partial p} = G_w \frac{(1-\phi)}{\phi} \alpha_r + \phi [S_w \rho_w \alpha_w + (1-S_w)\rho_i \alpha_i] + \phi (\rho_w - \rho_i) \frac{\partial S_w}{\partial p}, \tag{4}$$

and

$$\frac{\partial G_w}{\partial H} = -\left\{G_w \frac{(1-\phi)}{\phi}\beta_r + \phi [S_w \rho_w \beta_w + (1-S_w)\rho_i \beta_i]\right\} \frac{\partial T}{\partial H} + \phi (\rho_w - \rho_i) \frac{\partial S_w}{\partial H}.$$
(5)

The evolution of G_w in time can be obtained by considering the time-derivative form of Eq. (3)

$$\frac{\partial G_w}{\partial t} = \frac{\partial G_w}{\partial H} \frac{\partial H}{\partial t} + \frac{\partial G_w}{\partial p} \frac{\partial p}{\partial t}.$$
(6)

Note that because of the absence of any convection (due to the zero permeability assumption), the mass is conserved, i.e. $\partial G_w/\partial t = 0$.

The constructed coupled mass and energy conservation problem is solved using the *method of lines*. For the numerical solution, we use one of the ordinary differential equations solvers available in MATLAB — ode15s — a variable-step, variable-order solver based on the numerical differentiation formulas of orders 1 to 5 [4].

The strong non-linear coupling develops through the chemical potential equation accounting for the coexistence of ice and water in the presence of surface tension:

$$\frac{dp}{dT_c} = \frac{L_f}{T_c(\bar{v}_w - \bar{v}_i)} + \frac{\bar{v}_i}{\bar{v}_w - \bar{v}_i} \frac{dp_c}{dT_c},\tag{7}$$

where $L_f [L^2 T^{-2}]$ is the latent heat of fusion, $p_c [ML^{-1}T^{-2}]$ is the capillary pressure, $\bar{v}_w [L^3 M^{-1}]$ is the specific volume of liquid water and $\bar{v}_i [L^3 M^{-1}]$ is the specific volume of ice.

2 Numerical results

In the following simulation cases we compared the curves of freezing point temperature, $T_c(x,t)$, and water degree of saturation, $S_w(x,t)$, obtained with (p_c = some constant) and without (p_c = 0) the influence of capillary pressure.

Figs. 2 and 3 compare results, at different times for when the capillary pressure is zero and $p_c = 5$ MPa (lower magnitudes showed negligible effect). Increasing the capillary pressure leads to the soil freezing at a lower temperature (see Fig. 2). The water saturation distribution during the freezing period (see Fig. 3) becomes higher when capillary pressure is introduced because of the capillary forces that prevent liquid water from freezing.

Figs. 4 and 5 shows how the response of our model, after one day, is affected by a wider variation in capillary pressure, from 1450 Pa (almost no influence) to 10 MPa (strong influence). The influence of capillary pressure, in this context, is found to be negligible for values < 1 MPa. The freezing point temperature in Fig. 4 is lowered by the high capillary pressure due to the surface tension effects as expected. Fig. 5 shows that the slope of the water saturation curve (for region where $S_w < 1$) looks similar for all values of capillary pressure, and this effect needs to be studied further.

3 Conclusions

Our preliminary results demonstrate important aspects concerning the effect of water freezing on the temperature of porous material. A series of numerical experiments regarding the capillarity effect was conducted to demonstrate how freezing point depression and water saturation evolve within a porous block subject to temperature surface boundary cooling and varied capillary pressures. The proposed study intends to form a basis for the development of a liquid water–vapour–heat transfer model in unsaturated freezing soils to help better understand porous materials processes taking place in climate change–induced hydrological and ecological changes to frozen regions.



Figure 2: Plots of freezing point temperature for various times and p_c values as indicated in the legend.



Figure 4: Plots of freezing point temperature after 1 day with various p_c values as indicated in the legend.



Figure 3: Plots of water saturation for various times and p_c values as indicated in the legend.



Figure 5: Plots of water saturation after 1 day with various p_c values as indicated in the legend.

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