Thesis Proposal

Computational aspects of direct and inverse problems in permafrost geophysics

Dmitry J. Nicolsky

Abstract. One of the goals is to develop of a numerical model of differential frost heave dynamics, based on physically realistic assumptions. The frost heave model has a numerous set of input parameters. Some values of these parameters can not be measured directly in a laboratory. The way to obtain them is to solve inverse problems. The second part of the PhD dissertation is devoted to the study of the so-called non-sorted circles developed in the Arctic tundra.

1. Introduction

The research related to my Ph.D. thesis is focused on the development of a general thermo-mechanical model of soil freezing/thawing and its applications to certain areas of the subsurface science: engineering, subsurface hydrology, geocryology, and arctic biology and ecology. The area of possible applications of the model includes the simulation of frost heave and thaw settlement and diffusion of water or solutes in seasonally freezing and perennially frozen ground. The numerical implementation of the model realizes its predictive capabilities to simulate complex systems and to gain better understanding of interactions between physical and biological processes in the arctic ecosystems.

Currently, after a year of development, the model is based on thermo-mechanic equilibrium for a homogeneous fully saturated mixture of ice, water and soil particles. The elasticity laws govern the deformations of the mixture. These deformations are developed by forces due to the pore water migration towards the freezing zone and its consequent freezing. The finite element implementation of the model was used to calculate the temperature, moisture regime, and frost heave dynamics at one of our field research sites on the

North Slope of Alaska. Comparison between calculated and measured temperature and moisture dynamics show a very good agreement.

The current numerical implementation of the model is also capable to realistically predict a frost heave. We believe that the model could be very instrumental in studying the interaction between physical and biological processes in the arctic ecosystems. Therefore, one of the applications of this model will focus on cryoturbation processes in the Arctic tundra and on mechanisms that cause differential frost heave in the active layer. The project will be concerned with the modeling of non-sorted circles along the Arctic climatic gradient and with the reaction of these ecosystems to changes in climate, in the active layer, and in vegetation cover. The main question to be addressed is, "How can changes in surface conditions such as vegetation, snow cover, and climate affect the seasonal dynamics of water and heat fluxes within non-sorted circles in the Alaskan Arctic?"

2. Brief description of the general thermo-mechanical model of ground freezing

To describe the processes in the freezing soil, we use the theory of mixtures. The theory is aimed to represent the phenomena of heat transfer, diffusion of liquids and solutes and mechanical deformation of the ground.

Let us consider a mixture of m constituents occupying the region Ω_t in space at the time t. Let $\boldsymbol{x}_k$ be the coordinate vector of a particle of the k-th constituent. We mark all quantities related to the k-th constituent with subscript k. Denote by β_k the volume fraction defined as $\beta_k = \frac{dv_k}{dv}$, where dv_k is the volume element of the constituent of the mixture occupying the volume element dv. The volume fractions β_k $k = 1, \ldots, m$ depend of the coordinate vector $\boldsymbol{x}_k$ and satisfy the following constrain $\sum_k \beta_k(\boldsymbol{x}_k, t) = 1$, $\forall \boldsymbol{x}_k \in \Omega_t$.

Let ρ_k be the apparent mass density related to the intrinsic density $\bar{\rho}_k$ as $\rho_k(\boldsymbol{x}_k, t) = \beta_k(\boldsymbol{x}_k, t)\bar{\rho}_k$.

At any point in Ω, we consider the actions on the part of the constituent k occupying Ω and calculate the rates of growth of mass c_k, linear momentum $\boldsymbol{m}_k$ and energy e_k. It is shown in [**1, 2**] that

$$c_k = \frac{\partial \rho_k}{\partial t} + \nabla \cdot \rho_k \frac{d\boldsymbol{x}_k}{dt} \tag{1}$$

$$\boldsymbol{m}_k = c_k \frac{d\boldsymbol{x}_k}{dt} + \rho_k \frac{d^2\boldsymbol{x}_k}{dt^2} - \nabla \cdot \boldsymbol{T}_k - \rho_k f_k \tag{2}$$

$$e_k = \boldsymbol{m}_k \cdot \frac{d\boldsymbol{x}_k}{dt} + c_k(\epsilon_k - \frac{1}{2}\frac{d\boldsymbol{x}_k}{dt} \cdot \frac{d\boldsymbol{x}_k}{dt}) + \rho_k \frac{d\epsilon_k}{dt} - \boldsymbol{T}_k : \nabla \frac{d\boldsymbol{x}_k}{dt} - \nabla \cdot \boldsymbol{h}_k - \rho_k r_k \tag{3}$$

where $\boldsymbol{T}_k, \epsilon_k, f_k, \boldsymbol{h}_k$ and r_k stand for the stress tensor, specific energy, body force, heat flux and body heating, respectively. We impose the following constrains

$$\sum_k c_k = 0, \quad \sum_k \boldsymbol{m}_k = 0, \quad \sum_k e_k = 0,$$

which are derived from the conservation principle of the mass, linear momentum and energy for the whole mixture. The internal dissipation in the mixture is introduced by considering the specific entropy s_k. While the entropy of each constituent may change, the entropy of the whole mixture cannot decrease. We regard this statement as expressing the content of Clausius' postulate:

$$\Phi \equiv T \sum_k \eta_k \geq 0, \quad \eta_k = c_k s_k + \rho_k \frac{ds_k}{dt} - \nabla \cdot (\frac{\boldsymbol{h}_k}{T}) - \frac{\rho_k r_k}{T},$$

where η_k is the growth of entropy and T is the common temperature for the whole mixture. The so-called dissipation function $\Phi = \Phi(T, \boldsymbol{h}_i, c_i^+, \beta_i, \nabla \boldsymbol{x}_k, \nabla \boldsymbol{x}'_k)$ and the set of the specific free energies $\psi_k \equiv \epsilon_k - T s_k$, $k = 1, \ldots, m$ define physical processes in the mixture. The specific free energy ψ_k is given by

$$\psi_k = \tilde{\psi}_k(T, \beta_i, \nabla \boldsymbol{x}_k, \boldsymbol{T}_k) + \frac{T}{\bar{\rho}_k} I(\beta_1, \ldots, \beta_m),$$

where function I has the following properties: $I(\beta_1, \ldots, \beta_m) = 0$ if $\sum_k \beta_k = 1$ and $\beta_k \geq 0$; or $+\infty$ otherwise. An appropriate choice of the specific free energy for each constituent (ice, liquid water and soil particles) and the dissipation function sets up the realistic model of soil freezing. More details can be found in [**3**].

3. Modelling of the non-sorted circles.

Non-sorted circles are defined as circular patterned ground features without a border of stones, usually with barren or sparsely vegetated central area 0.5 to 3.0 m in diameter. Figure 1, left shows that the soil profile beneath the non-sorted circle and its complement area (inter-circle) differ markedly. The non-sorter circles occur on Turbic Cryosols, i.e. mineral soils that have permafrost within 2.0 m of the surface and show marked evidence of cryoturbation laterally within the active layer, as indicated by disrupted mix of broken horizons, or displaced material, or a combination of both. Turbic Cryosols generally have an organic-rich mineral horizon (Ah) and (Bmy) horizon, in the sequel, referred as the vegetation cover. Underneath the

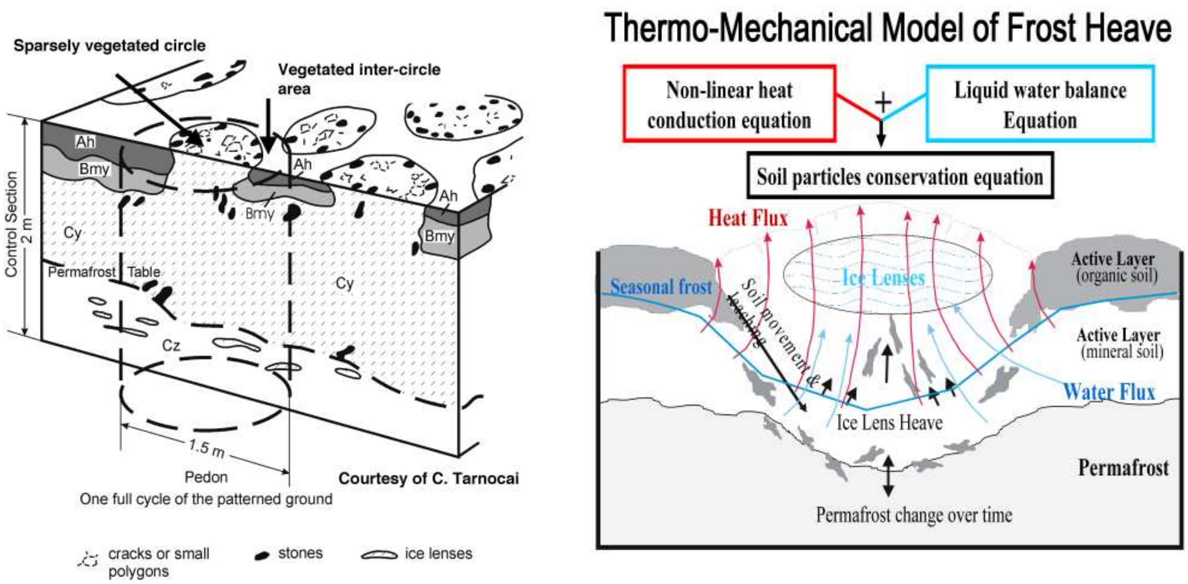

Figure 1: Schematic description of physical processes in the non-sorted circles.

Soil horizons and layers:

A-Mineral horizon forms at or near the surface in the zone of leaching or eluviation of materials in solution or suspension, or of maximum in situ accumulation of organic matter or both.

B-Mineral horizon is characterized by enrichment in organic matter, sesquioxides, or clay; or by the development of soil structure; or by a change of color denoting hydrolysis, reduction, or oxidation.

C-Mineral horizon is comparatively unaffected by the pedogenic processes operating in A and B horizons.

h-A horizon enriched with organic matter

m-A horizon slightly altered by hydrolysis, oxidation, or solution, or all three to give a change in color or structure, or both.

y-A horizon affected by cryoturbation as manifested by disrupted and broken horizons, incorporation of materials from other horizons, and mechanical sorting in at least half of the cross section of the pedon.

z-A frozen layer.

vegetation cover the mineral horizon (Cy/Cz) is located. This horizon is comparatively unaffected by the pedogenic processes operating in A and B horizons. Ah and Bmy horizons are less than 0.1 m thick.

The major hypothesis and assumptions regarding to the non-sorted circles that we are using in our research are:

- The vegetation and organic layers have thermo-rheological properties that are different from ones corresponding to the layer of mineral soil lying underneath the vegetation cover. However, the mineral soil inside the circle is equivalent to the mineral soil inside the inter-circle.
- To model the non-sorted circle dynamics, we hypothesize that the soil is always fully saturated, i.e. there is enough liquid water to supply the processes that cause frost heave. This hypothesis

is modeled by prescribing the constant water pressure on the outer boundary of the non-sorted circles.

- Water freezing and mechanical deformation produces ice lenses and micro cracks in the near-surface portion of the mineral soil that is seasonally thawed. Therefore, it is reasonable to assume that rheological properties of the mineral soil are distinct above and below the depth of the active layer thickness. This hypothesis is modelled by assuming that the soil in the permafrost has higher values of the Young's modulus, or the stiffness coefficient.
- Among the other assumptions are the isotropy of the material, the small strains, the piecewise linear elasticity of the skeleton. Also we assume that the flow of ice with respect to the skeleton is negligible, the phase change that occurs between water and ice is reversible, the kinetic energy terms and terms due to deformations in the expression of the balance of energy can be neglected.

Based on the above assumption we can formulate expressions for the specific free energies

$$\Psi_i = -C_i T ln(\frac{T}{T_0}) + \frac{1}{\bar{\rho}_i} W_i + \frac{T}{\bar{\rho}_i} I(\beta_i, \beta_w, \beta_s) \tag{4}$$

$$\Psi_s = -C_s T ln(\frac{T}{T_0}) + \frac{1}{\bar{\rho}_s} W_s + \frac{T}{\bar{\rho}_s} I(\beta_i, \beta_w, \beta_s) \tag{5}$$

$$\Psi_w = -C_w T ln(\frac{T}{T_0}) - [(C_i - C_w)T_0 + L]\frac{T - T_0}{T_0} + \frac{LT}{T_0} f(\beta_i, \beta_w, \beta_s) + \frac{T}{\bar{\rho}_s} I(\beta_i, \beta_w, \beta_s) \tag{6}$$

for ice, skeleton and liquid water, respectively. In the above, C_k is the specific heat capacity, T_0 is the temperature of fusion, L is the latent heat of fusion, W_k is the strain energy function and f is the so-called the adsorption function of the skeleton. The form of function f is verified by experiments [**4**]. A sketch of processes occurring inside the non-sorted circles are shown on figure 1, right.

In order to apply the model, numerous geophysical, thermal and hydraulic properties of the soils are required. The required soil properties include the following: density, thermal conductivity (frozen and unfrozen), heat capacity (frozen and unfrozen), water content, and porosity. We also specify the hydraulic conductivity and freezing temperature of the soils as a function of unfrozen water content. Standard techniques are available to determine these properties and parameters.

The initial and boundary conditions can be derived from field measurements. The instrumentation at our field sites allows monitoring of soil temperatures, soil moisture, frost heave, and cryoturbation activity.

4. Results up to date

For one non-sorted circle temperature and moisture distributions were measured at the Franklin Bluffs site over the period of one year. The value of the maximum frost heave was also estimated at the same site. The maximum frost heave equals to the maximum displacement of the ground surface relative to its position by the end of summer when the active layer depth is maximal. For this specific circle, soil properties were evaluated and used to simulate freezing of the non-sorted circle. As the result, the calculated temperature and moisture at certain depths were compared to the measured ones and are shown in Figure 2. The calculated value of the maximal frost heave is within the uncertainty of measurements. This example gives us assurance that the physical model represents the reality objectively and our developed numerical model can be used to investigate the process of frost heave and the development of non-sorted circles.

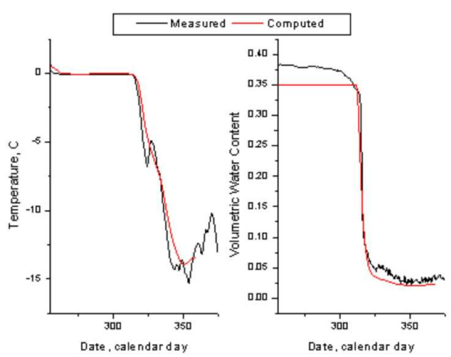

Figure 2: Measured and calculated temperature and volumetric water content in the center of the circle at the depth of 0.35cm.

One of the questions that we will explore in our research is "How can changes in surface conditions such as vegetation, snow cover and climate affect the seasonal dynamics of water and heat within non-sorted circles?" We have to note that the modelling of the non-sorted circles as a whole is complicated, since processes interact with each other and produce a non-linear behavior of the entire system. Therefore, to obtain the answer to this posted question, we have to understand how each process influence the dynamics of the system as a whole. We plan to apply a sensitivity analysis where we will investigate this by changing crucial parameters that characterize the certain process one by one and observe changes in the model's output.

As an example, Figure 3 shows several graphs of the maximal frost heave (the result of computations), corresponding to the sets of input parameters, where all elements but B were the same. The constant B parameterizes the unfrozen water content in the freezing soil as the function of temperature, shown in figure

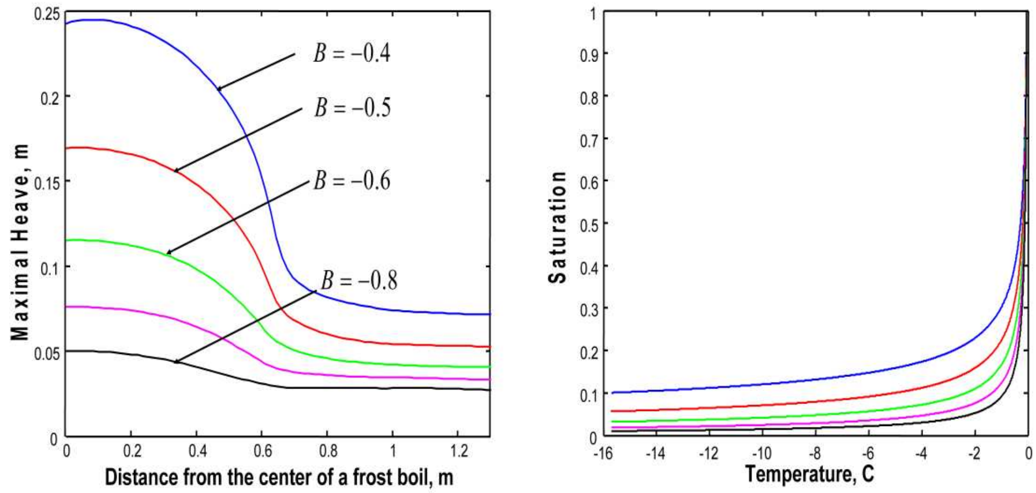

Figure 3: Higher values of B correspond to higher amount of liquid water in partially frozen pores, and more significant body forces caused by the so-called "cryogenic suction".

.

3, right. The lower values of B correspond to soil that have more fine texture such as silt and clay. The bigger values relate to sand or organic matter. In the above calculations the different values of constant B corresponded to the different textures of soil inside the circle. The modeled situations correspond to observed facts that the finer the soil texture inside the circle the bigger values of the frost heave.

5. Improvements of the non-sorted circle model

As major improvements to the existing model we plan:

1. to include the thaw settlement of frozen ground in the model. This would allow us to model the non-sorted circle during the entire year and observe its evolution in time. The self-organization between vegetation cover and deferential frost heave might be considered,
2. to model insulating effects of the snow cover explicitly, by introducing an additional layer of a variable thickness above the ground,
3. to include the diffusion of solutes in the frozen ground that can be modeled by introducing other constituents in the mixture, and by modifying the dissipation function to include the irreversible mixing of constituents,

4. to introduce in the model a more realistic thermo-rheological parameterization of the soil component by modifying the strain energy W_k in (4)-(6), modification of the dissipation function Φ to describe hysteresis during the process of the water freezing.

References

[1] C. Truesdell. *Rational Thermodynamics*. Modern applied mathematics. McGraw-Hill, 1969.

[2] G. D.C Kuiken. *Thermodynamics of irreversible processes, Applications to Diffusion and Rheology*. Willey tutorial series in Theoretical chemistry. Willey, 1994.

[3] J. Hartikainen M. Mikkola. Mathematical model of soil frezzing and its numerical application. *Int. J. Numer. Meth. in Engng*, 52:543–557, 2001. DOI: 10.1002/nme.300.

[4] M. Mikkola M. Fremond. Thermomechanical modelling of frezing soil. *In Ground Freezing 91, Proceedings of the 6th International Symposium on Ground Freezing*, pages 17–24, 1991. Yu X, Wang C (eds), Balkema: Rotterdam, 1991.

Geophysical Institute, University of Alaska Fairbanks, PO Box 757320, Fairbanks, AK 99775

E-mail address: ftdjn@uaf.edu