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Non-equilibrium crystallization in freezing porous media: Numerical solution

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ABSTRACT

The boundary value problem which arises during heat and moisture transfer in freezing fine-grained porous media under phase transition conditions is solved. It is assumed that the phase transition process occurs with finite rate of the water crystallization. So, the non-instantaneous kinetics is considered. Since the problem is significantly nonlinear the numerical method for the solution is applied. For the approximation of the system of differential equations the implicit two-level finite-difference scheme with central differences for space coordinate and one-side differences for time is used. The finite-difference system of equations is solved by "double sweep method." It was shown the stability of "double sweep method" and solvability of the problem. Based on the correlation analysis, the dimensionless form for the diffusion coefficient as a function of moisture is obtained and used for the modeling. It is shown that the results for the characteristic distributions — temperature and total moisture, obtained in numerical solution, are in a good agreement with experimental investigations. The effect of the main criteria for the considered process — Lewis and Stefan numbers on the temperature, moisture, ice content and total moisture distributions is discussed. Especial attention was paid on the formation of the kinetic zone and its transformation in the course of non-equilibrium freezing. It was shown that the kinetic zone has a width of about 20–40% of the overall dimension of the system. Therefore the simulation of the phase transition zone as an infinitely thin front in freezing process, which is an approach incorporated in most theoretical models, is not suitable for the non-equilibrium water crystallization processes in fine-grained soils, and thereby conforms the validity of the kinetic approach.

1. Introduction

The peculiarities of the cryogenic structure of fine-grained soils depend greatly upon the conditions of freezing. The formation of ice layers creates a water concentration gradient which is the driving force behind the moisture diffusion process and causes moisture and temperature profiles redistribution in both the frozen and unfrozen regions (Bronfenbrener, 2012; Ershov, 1979a; Hoekstra, 1966; Konrad and Morgenstern, 1980). Since the moisture diffusion coefficients in the frozen zone are significantly smaller than those in the unfrozen part of the soil, most theoretical models neglect the effect of mass transfer in the frozen regions in such systems and consider a classical scheme — frozen and unfrozen zone with jump conditions at the front.

Nevertheless the formation of ice layers observed in experimental investigations is the direct result of water migration in fine-grained soils at the temperatures below the phase transition temperature. It is also necessary to note that during the freezing process, the increase in frozen soil volume is not only due to the different densities of water and ice, but also mainly to a water migration process (from the unfrozen zone towards the freezing front), which promotes to ice lenses formation, and, as a consequence, to the uplifting of the ground surface. This phenomenon is known as "frost heave" and it is a result of the strongly coupled heat and mass transfer process. As shown in experimental investigations (Bittelli et al., 2004; Bronfenbrener and Korin, 2002; Danielian et al., 1983; Ershov, 1979a, b; Michalowski and Zhu, 2006), the equilibrium unfrozen water content in the frozen zone is essentially a nonlinear function. Nevertheless, in many studies it is assumed that the moisture distribution in the frozen zone is uniform.

From the theoretical and experimental studies on the freezing processes (Danielian and Yanitcky, 1983; Danielian et al., 1983; Ershov, 1979a,b; Feldman, 1988; Konrad and Morgenstern, 1980; Takeda and Nakano, 1990; Nakano, 1990, 1992; Talamucci, 2003), it is also known that the front of macroscopic ice formation lags significantly behind the boundary of incipient freezing. These experimental results may be attributed to the existence of the freezing zone. In the study based on the quasi-steady approach (Bronfenbrener and Korin, 1999) the criterion for freezing zone formation was derived as a function of soil properties and freezing conditions. This criterion, a priori, enables the correct choice of the problem's solution, i.e. whether to consider the phase change interface as a boundary that divides the soil region into frozen and unfrozen zones — two-zone model, or to consider the phase front by allowing the presence of a freezing zone — three-zone model. As

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was shown in the above-mentioned work, the freezing zone is formed in fine-grained soils. A similar result was obtained from the analysis of the experimental investigations (Danielian et al., 1983; Ershov, 1979a; Takeda and Nakano, 1990).

Attention should be paid to one of the important aspects of this problem. The number of models dealing with phase transition relaxation in fine-grained soils is almost absent. Nevertheless, the relaxation terms in the system of equations allow for the introduction into the model of the crystallization rate function, producing results describing ice distribution. In reference to this matter we point to two works. In the study carried out by Yanitcky (1988) the solution was obtained for a specimen that is found under frozen condition — one-zone model. The same problem in stationary statement was solved on the basis of a two-zone (frozen and unfrozen) model (Yanitcky, 1990). But in this solution the moisture in the frozen zone (equilibrium unfrozen water content) was assumed to be constant for linear temperature distribution. In our opinion, this assumption does not reflect the unfrozen water content as a function of the temperature.

In addition the relaxation model allows taking into account the non-instantaneous kinetics, i.e. to consider the finite rate of crystallization. It is known that the non-equilibrium phase transitions of moisture in the soil are relaxed in nature (Devies and Lamp, 1956; Ershov, 1979b; Furukawa and Shimada, 1993; Lifshitc and Pitaevsky, 1979). Actually, if frozen soil is brought to some temperature $T_*<T_{*0}$, where T_{*0} is the initial temperature of phase transition, then the transition of the "soil–water–ice" system to the state of thermodynamic equilibrium may take a certain amount of time. In such transition the soil moisture reaches the equilibrium unfrozen water content $W_*=W_{\mathrm{eq}}(T_*)$ for that particular temperature.

One of important subjects of the problem is the determination of the time required for transition of the system to the equilibrium state. This time can vary from minutes for sandy soils, to hours for fine-grained soils (clay, silt and loamy soils). In experimental investigations (Bittelli et al., 2004; Bronfenbrener and Korin, 2002; Ershov, 1979b) the study of the water crystallization process was carried out. The relaxation time and also the equilibrium unfrozen water content as a function of temperature were obtained. Thus, the non-instantaneous crystallization process has its own characteristic time-scale. In the present study we consider the simplest (first order) law of crystallization kinetics in linear form (see for instance Danielian and Yanitcky, 1983; Atkins, 1990; Keusch, 2003). For this kinetics the water crystallization rate is directly proportional to the difference between the prevailing and equilibrium moisture. The theoretical calculation results obtained in these works show a good agreement with experimental investigations. It should be also noted that the consideration of non-instantaneous kinetics enables to eliminate the discontinuation at the frozen front, which is formulate in analytical models. Moreover, the concept "frozen front" as such disappears.

In this paper we present numerical solution and results for the freezing process in fine-grained porous medium, in particular in soils. According to the theory of crystal growth we assume a first-order model for kinetics of non-equilibrium phase transitions. The crystallization is assumed to take place in the kinetic zone, which is defined as a range within which supercooling occurs. In this way the application of the numerical methods makes it possible to eliminate the discontinuation at the phase front which it is used for obtaining analytical solution, and thereby to solve the problem in a general statement. Contrary to analytical approaches, as is shown in this study, both the moisture diffusion in all spectrum of the temperatures and non-instantaneous kinetics which is taken into account, lead to results, as reflected in the experimental studies (see for example Ershov, 1979a; Perfect and Williams, 1980; Danielian et al., 1983, etc.) We focus our attention on the description of the theoretical model and validation against experimental results from the literature as well as on the theoretical results relating to the effect of Lewis and Stefan numbers on redistribution of the temperature and moisture profiles and, as a consequence, on the ice content and total moisture. The special attention is paid on the formation and transformation of the kinetic zone against time and in dependence on the criteria of the problem.

According to the subject of the study this paper is organized as follows. In next section we describe 1-D boundary value problem which is based on the heat and mass transfer process in finite region of the soil. The mathematical formulation of the problem and system of equations in physical coordinate system and in dimensionless variables are also presented in this section. In Section 4, based on the correlation analysis we obtained the dimensionless form for the approximation of the experimental data, which is the best form for the modeling of the diffusion coefficient. It is shown that the functional dependence in dimensionless variables $\bar{D}(\omega)$ is in good agreement with experimental distribution. The obtained function was used in the numerical model presented. The central point of the Section 5 is the numerical modeling of freezing process in soil on the basis of the non-instantaneous kinetic model. This approach gives a possibility to describe the real process more closely, to solve the problem in general statement and, thereby, to reflect the main regularities of the phenomenon. In this respect, the stability of the finite-difference scheme and convergence of the iteration process are analyzed. The appropriate estimations and criteria for the stability and convergence are obtained. In Section 7 we give and discuss results of calculations: temperature and moisture distributions as well as the ice content and total moisture. The effect of main criteria — Stefan and Lewis, which are characterized the phase transition and moisture migration, on the freezing process is analyzed. The special attention is paid on the formation of the kinetic zone and its transformation in time and in dependence from the criteria Stefan and Lewis. In the end of the paper the conclusions resulting from this study are summarized.

2. Statement of the problem

A schematic description of the system model is given in Fig. 2.1.

We consider a transient 1-D problem relating to homogeneous water saturation fine-grained soil in the range of $0 \le x \le S$. Initially the system is at the uniform temperature T_0 and has the water content W_0 (mass of water per unit mass of skeleton). At the time $t>0$ the left side of the domain (at $x=0$) obeys the step function T_b which is lower than T_{*0} defined as the initial temperature of phase transition, corresponding to the moisture W_0. Freezing of the soil begins from $x=0$ and propagates in x direction. The coordinate x_* is coordinate of the phase transition beginning at which temperature $T=T_{*0}$. The diffusion coefficient in the unfrozen and kinetic zone is

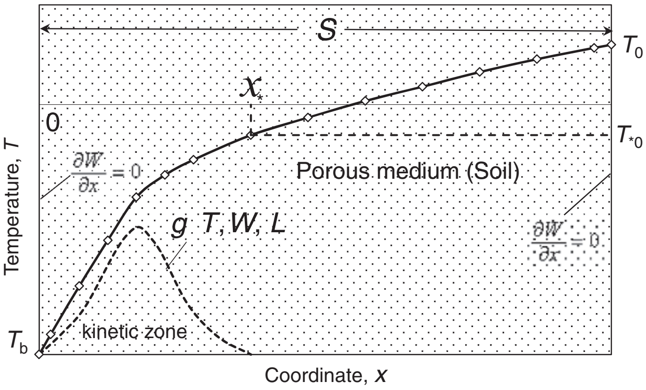

Fig. 2.1. Schematic description of model system.