

Development of Mathematical Model of Heat and Mass Transfer in Soil, with Provision for Gradients of Soil-Water and Soil-Salt Potentials. Part 1.

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Abstract

Frost heaving of soils has a significant influence on the stability of various buildings and constructions. It causes a rise of shallow foundation of buildings and pile of overhead pipeline, the destruction of roads and strong bends of underground pipelines on the short distance. This process is associated with the mass transfer of liquid water from thawed to frozen soil. The paper considers the problem of mathematical modeling of mass transfer in soils. The introduction of thermodynamic parameters - soil-salt potential is proved. This potential, like soil-water potential, is not constant. There is proof that the potential of all components of water-salt solution in soil may consist of the chemical potential and the potential of external volume forces, which are non-zero. The differential equation of the dynamics of pore solution was derived. This equation takes into account the gradients of potential of all components of solution, gradient of hydrostatic pressure, gravity and bulk frictional force. The paper also shown that the friction body force does not depend of type of drive force (external acceleration, the gradient of pressure or potential) at a first approximation and for small speed. Using this approach allows to describe the dynamics of the pore solution with only transmissibility coefficient.

Keywords: frost heaving, film diffusion, diffusion mass transfer, kinetic theory of liquids

INTRODUCTION

Forecasting the processes of mass transfer in heaving soil very important under the construction of buildings, pipelines and roads [5, 6, 10, 13, 14].

The frost heaving of soils is inseparably associated with the ability of freezing soils to suck significant amounts of water

from nearby thawed layers of soil. Crossing the frost boundary, the water freezes, expands and deforms the engineering structures.

The mathematical description of the driving forces of the movement of ground moisture is the big interest, because allow to predict the frost heaving. Today in the engineering practice is used a generalized thermodynamic approach, the founders of which are Buckingham, Richards, Collis George, Childs [12]. The basis of this approach is the union of different moving forces of soil moisture to a single generalized force - the gradient of soil-water potential. For example, I.L. Kalyuzhny and S.A. Lavrov recommend the following modifications of the Richards equation to describe the motion of water and salts [7]:

$$\frac{\partial W}{\partial t} = \nabla \cdot \left(\lambda_w \left(\frac{\partial \psi_w}{\partial W_l} \nabla W_l + \frac{\partial \psi_w}{\partial \Pi} \nabla \Pi \right) - \lambda_w \vec{e}_z \right), \quad (1)$$

$$\frac{\partial (W_l \omega_s)}{\partial t} = \nabla \cdot (D_{ws} \nabla \omega_s + \omega_s \vec{V}), \quad (2)$$

where W – total bulk water content, u.f.; W_l – total bulk liquid water content, u.f.; Π – porosity, u.f.; ψ_w – soil-water potential, J/kg; λ_w – moisture conduction coefficient, s; ω_s – total bulk salinity, u.f.; D_{ws} – diffusion coefficient, m/s²; \vec{V} – vector of convective moisture flow velocity, m/c; \vec{e}_z – unit vector along z-axis (vertical axis). Similar equations are proposed by Ershov, Globus [2, 11].

Soil-water potential ψ_w is the energy for isobaric-isothermal adding of mass unit in soil. It takes negative values, which indicates the positive binding energy of water molecules with the mineral surface of the soil system. Soil-water potential also has significantly changes when the water content of the soil also changes. In the interval of low water content, the potential is mainly due to polymolecular adsorption on the surface of mineral soil particles – it's adsorbed water. When

water content increases, the energy of adsorption of water rapidly decreases and is replaced by the energy of electrostatic interactions. Further increase of water content increase the part of energy connected with the negative pressure of the curvature of the interphase surface, that conform to the meniscus and pendular water. The hydrostatic pressure confirm the gravitational water and almost zero value of soil-water potential [3].

However, water is not the only mobile component of the soil system. The pore moisture has always dissolved mineral salts. The energy of molecular bonds of various substances with the mineral surface of the soil does not have to be the constant. In this case we can talk about the presence of new thermodynamic parameter of pore moisture: soil-salt potential ψ_s . We can also expect, that soil-salt potential is not the constant, like soil-water potential not the constant too.

Soil-salt potential also is the driving forces of salt movement as exemplified by zero of total differential of the total thermodynamic potential of each component in the case of thermodynamic equilibrium (similar to the soil-water potential) [9].

The equations (1, 2) not take into account the soil-salt gradients, like driving forces of salt movement. The concentration of soil-salt solution determine the temperature of freezing point and the temperature of frost heaving beginning. By this means the reliable prediction of frost heaving in saline soil is impossible without considering the soil-salt potential.

OBJECT AND PURPOSE

Purpose: to develop the mathematical model of heat and mass transfer in thawed, freezing and frozen soils, taking into account the gradients of the potentials in soil of all components of the pore solution, L.Onsager's reciprocal relations and another laws of linear nonequilibrium thermodynamics.

In first part of this paper authors set a problems:

- to investigate the nature of the soil-salt and soil-water potentials; Determine whether these potential are the driving force its movement;
- to establish the equations for the dynamics of the water-salt solution in soils, taking into account the gradients of the potentials of salt and water in soil in the isothermal case;
- to prove the independence of the volumetric frictional force from the type of driving forces (the gravitation, the hydrostatic pressure gradient, the gradients of soil-water or soil-salt potential) in the first approximation and low speeds.

RESEARCH METHOD

The development of the mathematical model of heat and mass transfer in soils, taking into account the gradients of the potentials in soil of all components of the pore solution, requires a preliminary analysis of the physical meaning of term "soil-water potential" or "soil-salt potential". Thus, firstly an analysis set up on the laws of equilibrium thermodynamics is carried out, that allow to get the necessary conclusions about experimental pressure and potential of salt and water. Comparison of the equations of equilibrium and dynamics in isothermal water-salt solution allow to establish a relationship between the driving forces and the volume friction force.

CONSIDERATION OF THE NATURE OF THE CAPILLARY-SORPTION POTENTIAL FROM THE STANDPOINT OF EQUILIBRIUM THERMODYNAMICS

To investigate the nature of soil-salt and soil-water potential, we write the total differential of the total thermodynamic potential of the i -component of the water-salt solution in the soil [9]:

$$d\Omega_i = d\Phi_i + dG_i = v_i^s dP - s_i dT + d\mu_i^c + d\psi_i + \vec{a} \cdot d\vec{r}, \quad (3)$$

where Ω_i – total thermodynamic potential of the i -th component of the water-salt solution in the soil, J/kg; Φ_i – potential of external volume forces of the i -th component, J/kg; G_i – chemical potential (Gibbs free energy) of the i -th component, J/kg; v_i^s – specific volume of the i -th component in the solution (the ratio of volume to mass of the i -th component in solution), m³/kg; P – pressure, Pa; s_i – entropy i -th component, J/(kg·K); T – temperature, K; μ_i^c – decreasing of the chemical potential of the i -th component in the free solution in comparison with the pure substance, due to a change of solution concentration, J/kg; ψ_i – decreasing of the potential of the i -th component in soil solution in comparison with free solution, J/kg; \vec{a} – external acceleration (gravitation for example), m/s²; \vec{r} – radius-vector, m.

Formally, this form of noting allow us to refer ψ_i to both potential: the external forces potential Φ_i and Gibbs free energy G_i . Many researchers, (Brushkov, Ershov, Globus) relate ψ_i to the Gibbs free energy [1, 2, 11]. Later we will show that this approach is not enough accurate.

To better understand the question of the belonging ψ_i , we consider a concrete example. Consider the case the soil with constant temperature ($dT = 0$), constant water content and without salt. Then put it to a vertical column ($\vec{a} = \vec{g}$). As the result, the water in the soil is redistributed: lower layers of soil has more water than top layer. If the water content is everywhere lower than the maximum water content (no gravitational water), then the pressure gauge indication will be zero ($dP = 0$). Then equation (3) can be simplified:

$$d\Omega_i = d\mu_i^c + d\psi_i + \vec{g} \cdot d\vec{r} = 0, \quad (4)$$

where \vec{g} – acceleration vector of free fall on the Earth's surface, m/s².

Potential ψ_i is submitted like sum of chemical potential ψ_i^{ch} and potential of external volume forces ψ_i^{evf} :

$$\psi_i = \psi_i^{ch} + \psi_i^{evf} \quad (5)$$

where ψ_i^{ch} – part of ψ_i , belong to chemical potential, J/kg; ψ_i^{evf} – part of ψ_i belong to potential of external volume forces, J/kg.

The further problem is to clarify the belonging of each component of formula (5). To do this, we multiply equation (4) by the mass concentration of the i -th component (ω_i) and sum over all components.

$$\sum_{i=1}^m (\omega_i d\mu_i^c + \omega_i d\psi_i^{ch} + \omega_i d\psi_i^{evf}) + \vec{g} \cdot d\vec{r} = 0, \quad (6)$$

Equation (6) allow to determine the possible interval of variation of ψ_i^{ch} and ψ_i^{evf} .

Statement

Potential ψ_i of i -th component of solution in soil consist of two kind of potential: chemical potential (ψ_i^{ch}) and potential of external volume forces (ψ_i^{evf}), with potential of external volume forces (ψ_i^{evf}) can not be zero.

Proof

Firstly, it will be shown that the ψ_i can not related only to the chemical potential (Gibbs free energy). Then it will be proved that the ψ_i must be partially or completely related to the potential of external mass forces.

We construct the proof of the first part of the statement from the converse. Suppose that potential of external mass forces (ψ_i^{evf}) always zero. Then $\psi_i = \psi_i^{ch}$, that allow to write Gibbs–Duhem equation for solution in soil:

$$\sum_{i=1}^m (\omega_i d\mu_i^c + \omega_i d\psi_i^{ch}) = 0. \quad (7)$$

The chemical potential μ_i^c describe the decreasing of the chemical potential of the i -th component in the free solution in comparison with the pure substance without interaction with soil. This feature allow to write next Gibbs–Duhem equation for free solution:

$$\sum_{i=1}^m (\omega_i d\mu_i^c) = 0. \quad (8)$$

By this means, equation (8) allow to simplify equation (7):

$$\sum_{i=1}^m (\omega_i d\psi_i^{ch}) = 0. \quad (9)$$

Using (6, 8, 9) get the next result:

$$\vec{g} \cdot d\vec{r} = 0. \quad (10)$$

Equation (10) indicates that equilibrium is possible only if the angle between the vectors \vec{r} and \vec{g} is 90 degrees. The soil must be decomposed into an infinitely thin layer over a surface perpendicular to the vector \vec{g} . However, equilibrium is also possible with any finite thickness. Consequently, $\psi_i^{evf} \neq 0$ and potential ψ_i can not belong to the chemical potential ψ_i^{ch} only. The first part of the statement is proved.

Now prove the second part of the statement. We consider the case when $\psi_i^{evf} \neq 0$ and $\psi_i^{ch} \neq 0$. Using equations (6), (8), (9) again we obtain:

$$\sum_{i=1}^m \omega_i d\psi_i^{evf} + \vec{g} \cdot d\vec{r} = 0. \quad (11)$$

From the axiom of existence of equilibrium of the water-salt solution in the vertical column and equation (11), we can conclude that the potential ψ_i can consist of both potential: the chemical potential (ψ_i^{ch}) and the potential of external volume forces (ψ_i^{evf}), with potential of external volume forces (ψ_i^{evf}) is not zero. The statement is proved.

The second side of the question about the nature of soil-water and soil-salt potentials is related to how it is measured in the laboratory. To do this, we consider pure water in soil and introduce the notion: "true soil-water potential". This is the potential, which creates a mineral surface of the soil. And just "soil-water potential" – is the potential that can be directly measured in laboratory conditions (desiccator, tensometric or column method) and takes into account disjoining pressure.

It is known that pore moisture sandwiched between mineral particles under high pressure (since the most soils are hydrophilic), which is called disjoining pressure [4]. At the same time, outside the interaction with the soil system, there is also some hydrostatic pressure. We rewrite the equation for the total differential of the total thermodynamic potential (3) and separate the hydrostatic P and disjoining P_{disj} pressure:

$$d\Omega_i = v_i^s dP_{disj} + v_i^s dP - s_i dT + d\mu_i^c + d\hat{\psi}_i + \vec{a} \cdot d\vec{r}, \quad (12)$$

where P_{disj} – disjoining pressure of pore moisture, sandwiched between mineral particles, Pa; P – hydrostatic pressure of volume phase в объемной фазе (outside the influence of the soil system), Pa; $\hat{\psi}_i$ – true soil-water potential of water, J/kg, i – belong to water in (12-15).

The functional relationship between decreasing of potential of pore water in comparison with pure water and water content is measured in laboratory (for example in desiccator) [2]:

$$d\Omega_i = v_i^s dP_{disj} + v_i^s dP + d\mu_i^c + d\hat{\psi}_i + \vec{a} \cdot d\vec{r} = \frac{RT}{M_i} d(\ln(\varphi_i)) = f(W_i), \quad (13)$$

where φ – equilibrium relative humidity of air above ground at a given temperature and given soil water content, u.f.; R – universal gas constant, J/(mole·K); M_i – molar mass of water, kg/mole.

This equation has two unknown variables: dP_{disj} and $d\hat{\psi}_i$. Direct measurement of the disjoining pressure distribution P_{disj} in the soil system is extremely problematic, because it strongly depends on the geometry of the pore space. Direct measurement of $\hat{\psi}_i$ has similar difficulties. Consequently, the separate determination of the variables dP_{disj} and $d\hat{\psi}_i$ in practical applications seems unreasonable. But, the union of these variables into one potential ψ_i allow to get important conclusion:

$$v_i^c dP + d\mu_i^c + d\psi_i + \vec{a} \cdot d\vec{r} = \frac{RT}{M_i} d(\ln(\varphi)) = f(W_i), \quad (14)$$

$$d\psi_i = d\hat{\psi}_i + v_i^c dP_{disj}. \quad (15)$$

If $dP = 0$, $d\mu_i^c = 0$, $\vec{a} \cdot d\vec{r} = 0$, then the functional $f(W_i) = d\psi_i$ is exactly soil-water potential, which is measured in laboratory (for example in desiccator).

By this means, we showed that the soil-water potential ψ_i , which is measured in desiccator, is the sum of true soil-water potential $\hat{\psi}_i$ and potential of disjoining pressure $v_i^c dP_{disj}$. In this case the pressure in the equation (3) is always hydrostatic pressure P , because disjoining pressure P_{disj} was included in the soil-water potential ψ_i (15). This approach avoids the problems associated with determining the distribution of the disjoining pressure in the complex geometry of the pore space.

THE EQUATION OF THE DYNAMICS OF WATER-SALT SOLUTION IN SOILS

To establish the relationship between the gradient of the soil-water and soil-salt potentials and the velocity of movement of the water-salt solution in the soil, we analyze the equation of the dynamics of pore solution. Usually, the equation of the dynamics of pore solution in an isothermal soil is wrote in the form of Newton's second law:

$$\rho_{sol}^{mc} \frac{d\vec{w}_{sol}^{tr}}{dt} = -n\nabla P + \sum_{i=1}^m \rho_i^{mc} \vec{F}_i + \rho_{sol}^{mc} (\vec{a} + \vec{F}_{fr}), \quad (16)$$

where F_i – specific force, acting to the i -th solution component, H/kr; ρ_i^{mc} – mass content of i -th solution component in soil, like the ratio of i -th component mass to volume of soil, kg/m³; \vec{w}_{sol}^{tr} – vector of true velocity of water-salt solution in soil, m/s; ρ_{sol}^{mc} – solution content, like the ratio of soil-water solution mass to volume of soil, kg/ m; n – the ratio of volume of solution to volume of soil, u.f.; \vec{F}_{fr} – bulk frictional force, N/kg.

However, the equilibrium equation (11) allow to find the bulk frictional force:

$$\vec{F}_i = -\nabla\psi_i^{evf}. \quad (17)$$

We substitute equation (5) and (17) into (16), additionally use (9) and get the equation of the dynamics of water-salt solution

in soils:

$$\rho_{sol}^{mc} \frac{d\vec{w}_{sol}^{tr}}{dt} = -n\nabla P + \sum_{i=1}^m (-\rho_i^{mc} \nabla\psi_i) + \rho_{sol}^{mc} (\vec{a} + \vec{F}_{fr}). \quad (18)$$

The last transformations indicate that there is no necessity to determine ψ_i^{evf} and ψ_i^{ch} separately, that is very important advantage in practical applications of equation (18).

Let now the water-salt solution is at rest, then the equation of the dynamics of pore solution (18) in the isothermal case is simplified, and we obtain the equilibrium equation:

$$-n\nabla P + \sum_{i=1}^m (-\rho_i^{mc} \nabla\psi_i) + \rho_{sol}^{mc} \vec{a} = 0. \quad (19)$$

Now we take equation (3), multiply by ρ_i^{mc} and sum over all components. Using equation (8), we find that it completely coincides with equation (19). Thus, the equation of dynamics (19) has turned into the equation of thermodynamic equilibrium. It shows that the bulk frictional force in the last term of equation (18) at least in the first approximation and at low velocity does not depend on the nature of the driving forces of the water-salt solution. Consequently, in the first approximation, it is sufficient to know only transmissibility coefficient to describe the dynamics of pore solution. This coefficient enters into the bulk frictional force:

$$\vec{F}_{fr} = -\frac{\vec{w}^f g}{\lambda_p} = -\frac{n\vec{w}^{tr} g}{\lambda_p}, \quad (20)$$

где λ_p – transmissibility coefficient, m/s [8].

The formula (20) shows that the driving forces of all components of water-salt solution are the gradient of the hydrostatic pressure ∇P , external acceleration and the gradient of the soil-water and soil-salt potentials of all components of water-salt solution $\nabla\psi_i$.

CONCLUSION

When analysis of the nature of the soil-water and soil-salt potentials of the water-salt solution in the soil has shown that:

- the soil-water and soil salt potentials can consist of two potentials: the chemical potential (Gibbs free energy) and the potential of external volume forces, besides the potential of external volume forces is not zero;
- the pressure in the equation of thermodynamic equilibrium take in only hydrostatic pressure. The disjoining pressure is already included in the soil-water potential;
- gradient of the capillary-sorption potential ψ_i is the driving force of the movement of pore solution;
- the bulk frictional force resulting from water-salt solution moves in soils in the first approximation and at low velocity, does not depend on type of driving forces (external acceleration, the pressure gradient or the gradients of the soil-water and soil-salt potentials). Consequently, in the first approximation, it is sufficient to know only transmissibility

coefficient to describe the dynamics of pore solution.

The equation of the dynamics of pore solution (18), which describes the convective motion of a water-salt solution, taking into account the gradients of the soil-water and soil-salt potentials of all components, is derived. This equation will be used in the second part of this paper in the deriving of the equations of heat and mass transfer.

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