

Development of a Mathematical Model of the Diffusion-Filtration Mass Transfer in a Porous Plastically Deformable Medium

Sergey A. Pulnikov*, Evgeniy V. Markov, Yuri S. Sysoev and Natalia V. Kazakova

*Industrial University of Tyumen,
38, Volodarskogo, Tyumen 625000, Russian Federation.*

Abstract

Frost heaving of the ground is a significant problem in the operation of main pipelines with a negative product temperature. Thermal interaction between the ground and the pipeline forms the area with negative temperature. It attracts moisture from the surrounding thawed ground. Crossing the front of freezing, the moisture that is outside the adsorption layer of tightly bound water freezes forming clusters of ice schlieren. Unlike seasonal processes of frost heaving, a continuous technogenic impact contributes to the increased growth of ice schlieren, which, increasing in volume, deform the pipeline. Existing mathematical models of frost heaving forecast are based on a phenomenological approach. As the main driving force for moving the moisture a capillary sorption capacity gradient is used, which can be a function of humidity, porosity, and at a temperature below the freezing point of the pore solution, a function of temperature. This approach allows a satisfactory description of the mass transfer processes in binary ground solutions. However, it does not allow taking into account the mass transfer in ground associated with diffusion in multicomponent solutions. Changing the salt concentration leads to a shift in the temperature of the water freezing start, which affects the value of frost heaving. Therefore, the authors have set and solved the problem of developing a mathematical model of mass transfer, which allows taking into account the diffusion mass transfer caused by the inhomogeneity of the energy states of molecules of ground moisture, non-uniform temperature fields, concentrations and total water content. Applying methods of the kinetic theory of liquids it has been shown that the amount of diffusion flows of aqueous saline solution components in the ground is not equal to zero, which indicates the presence of the diffusion mass transfer. The equations of mass transfer are supplemented by closing equations of the deformation theory of elasticity, enabling determination of the pore moisture pressure.

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

INTRODUCTION

Frost heaving of the ground is a significant problem in the operation of main pipelines with a negative product temperature [1, 2]. A continuous man-made impact contributes to the increased growth of ice schlieren, which, increasing in volume, deform the pipeline [3, 4]. Heaving develops

especially intensively under the pipelines that are capable of maintaining the temperature of the ground around $-1 \dots -4 \text{ }^\circ\text{C}$, due to the high permeability of the ground at these temperatures [5, 6].

Prediction of pore water movement processes, the value of vertical deformation and frost heaving pressure today is complicated by the lack of a unified physical model of permeability and diffusion processes in the thawed, freezing and frozen ground. Despite a considerable number of hypotheses about the nature of the forces that cause the movement of water, many of them do not have a sufficient quantitative basis upon which to perform calculations [7]. In this regard, a phenomenological area was actively developing dedicated to the establishment of quantitative relationships between empirical laws.

In the world of ground hydrophysics to simulate the dynamics of pore water various modifications of Richards differential equation are most commonly used [7, 8, 9]. In these equations the phenomenological approach is used. As the main driving force of moisture migration, capillary-sorption potential gradient is selected which may be a function of moisture, porosity and, at a temperature below freezing point of the pore solution, a function of temperature. Integration of Richards equation allows you to calculate the density of the flow of water and salts in the thawed, freezing and frozen ground, and determine the mass of segregation ice formation. This approach allows a satisfactory description of the mass transfer processes in binary ground solutions and with free upper boundary. However, for the polymineral ground loaded by surface forces, it is necessary to take into account a possible increase in the ground water pressure, which can counterbalance the influx of moisture in the heaving zone and a decrease in the freezing temperature of the ground solution when salinity changes.

The authors have set the task to develop a model in which the phenomena of mass transfer of water and salts both in the thawed and freezing and frozen ground occur under the influence of body and surface forces, as well as by diffusion.

METHODS

It is known that in the ground homogeneous in its physico-mechanical properties at constant external pressure and temperature water moves from an area with high humidity to a low-humidity area. This mass transfer is caused by two main

mechanisms: filtering and diffusion. Diffusion, in this case usually referred to as film diffusion, occurs in films of the water-salt solution adsorbed on the surface of the mineral particles of the ground system.

From the standpoint of the kinetic theory of liquids developed by Frenkel, the transition of the molecule from one equilibrium position to another can be regarded as a sequence of two events: "evaporation" from the original position of equilibrium into the intermediate one followed by "condensation" to the new position of equilibrium. In this case, the average travel speed of a molecule can be regarded as the distance between two equilibrium positions (equal to the free path in the liquid), divided by the residence time of the molecule in equilibrium[10]:

$$u = \frac{\delta}{\tau} e^{-\left(\frac{EM}{RT}\right)}, \quad (1)$$

where u – the average speed of the molecule movement in an arbitrary direction, m/s;

δ – the free path of the molecule of a liquid between the two positions of temporal equilibrium, m; τ – the average residence time of the molecule near the temporal position, s; E – the potential barrier per 1 kg of substance, J/kg; k – the Boltzmann constant, J/K; T – the temperature, K; M – the molar mass, kg/mol; $R=8.31$ – the universal gas constant, J/(mol·K).

Given the fundamental differences between the liquid and gas, we assume that the path length δ does not submit to the law of Clausius, and has approximately the same value[10]. We derive an equation for the diffusion flux based on the Frenkel's theory for the i -th component of the water-salt solution. Let us make three planes in the bulk solution: $x = x_0, x = x_0 + \delta_i, x = x_0 - \delta_i$. If the mean free path of the molecule of the i -th component is equal to δ_i , then the plane $x = x_0$ can be crossed by only those molecules that are within $x = x_0 \pm \delta_i$. Because molecules can move in 6 different directions (forward-backward, up-down, left-right), the mass of the fluid that crosses the plane $x = x_0$ from bottom to top equals:

$$\Delta m_{du} = \frac{1}{6} (\rho_i^r |_{x_0 - \delta_i/2}) \Delta x \Delta y \Delta z, \quad (2)$$

where $\rho_i^r |_{x_0 - \delta_i/2}$ – the partial density of the i -th component of the water-salt solution taken in the center of the cell, kg/m³. Then the density of the mass flow passing through the plane $x = x_0$ from bottom to top per unit time is:

$$g_{du} = \frac{\Delta m_{du}}{\Delta y \Delta z \Delta t} = \frac{\rho_i^r |_{x_0 - \delta_i/2}}{6} \frac{\Delta x}{\tau |_{x_0 - \delta_i/2}}. \quad (3)$$

But, $\Delta x = \delta_i$, so considering (1) we have:

$$g_{du} = \frac{(u_i \rho_i^r) |_{x_0 - \delta_i/2}}{6}. \quad (4)$$

We have a similar formula for the flow coming from the top down:

$$g_{ud} = \frac{(u_i \rho_i^r) |_{x_0 + \delta_i/2}}{6}. \quad (5)$$

If we assume that the mass flow density varies little with distance, we can decompose it into a Taylor series leaving only the first summands:

$$g_{du} = \frac{(u_i \rho_i^r) |_{x_0 - \delta_i/2}}{6} = \frac{1}{6} (u_i \rho_i^r) |_{x_0} - \frac{1}{6} \frac{\partial (u_i \rho_i^r)}{\partial x} \Big|_{x_0} \frac{\delta_i}{2}, \quad (6)$$

$$g_{ud} = \frac{(u_i \rho_i^r) |_{x_0 + \delta_i/2}}{6} = \frac{1}{6} (u_i \rho_i^r) |_{x_0} + \frac{1}{6} \frac{\partial (u_i \rho_i^r)}{\partial x} \Big|_{x_0} \frac{\delta_i}{2}. \quad (7)$$

Then, for the resulting mass flow density of the i -th component going in the direction of the axis x :

$$g_{i,x}^n = g_{du} - g_{ud} = -\frac{\delta_i}{6} \frac{\partial (u_i \rho_i^r)}{\partial x}. \quad (8)$$

Generalizing the equation (8), we write it in a vector form taking into account(1):

$$\vec{g}_i^r = -\frac{\delta_i^2}{6\tau_i} \vec{\nabla} (\rho_i^r e^{-\left(\frac{E_i M_i}{RT}\right)}), \quad (9)$$

where \vec{g}_i^r – a purely diffusional mass flow density of the i -th component as a relation of the mass flow rate to the surface area occupied by the solution, kg/(s·m²).

From (9) we can see that purely diffusion flows of salt and water, generally speaking, may vary. Excessive accumulation of a substance per unit volume must be compensated by the convective (mass) flow of matter as a whole \vec{g}_{conv} .

We derive an expression for the convective flow of matter \vec{g}_{conv} . To do this, we select a parallelepiped in the solution with sides $\Delta x \Delta y \Delta z$. We assume that the volume of the parallelepiped is so small that within it the true density of the water-salt solution ρ_{sol}^r , and partial densities of all components ρ_i^r change insignificantly. In this case, we can assume that the values ρ_{sol}^r and ρ_i^r within the volume $\Delta x \Delta y \Delta z$ are constant and equal to their values at the center of the parallelepiped. We write down the standard laws of conservation of matter for each component and for the mixture as a whole:

$$\frac{\partial \rho_i^r}{\partial t} = -\nabla \cdot (\vec{g}_i^r + \omega_i \vec{g}_{conv}); \quad (10)$$

$$\rho_{sol}^r = \sum_{i=1}^m \rho_i^r; \quad (11)$$

$$\frac{\partial \rho_{sol}^r}{\partial t} = -\nabla \cdot (\sum_{i=1}^m \vec{g}_i^r + \vec{g}_{conv}), \quad (12)$$

where \vec{g}_{conv} – the convective flow of matter as a whole, kg/(s·m²); ρ_{sol}^r – the true density of the solution, kg/m³; ω_i – the mass fraction of the i -th component in the solution, unit fraction.

However, equations (11) and (12) are not merely the sum of equations (10) for all components. The true density of the mixture ρ_{sol}^r at constant pressure (which corresponds to the normal concentration diffusion) is a known function of the

concentration (m-1) of a mixture of components (determined experimentally) $\rho_{sol}^r = f(\omega_1, \dots, \omega_i, \dots, \omega_{m-1})$:

$$\frac{\partial \rho_{sol}^r}{\partial t} = \sum_{i=1}^{m-1} \frac{\partial \rho_{sol}^r}{\partial \omega_i} \frac{\partial \omega_i}{\partial t}. \quad (13)$$

The true density dependence of the water-salt solution (13) can be transformed, considering that the concentration ω_i is partial density divided by the true density of the solution:

$$\frac{\partial \rho_{sol}^r}{\partial t} = \sum_{i=1}^{m-1} \left(\frac{\partial \rho_{sol}^r}{\partial \omega_i} \right) \left(\frac{\partial \rho_i^r}{\partial t} \frac{\rho_{sol}^r}{(\rho_{sol}^r)^2} - \frac{\partial \rho_{sol}^r}{\partial t} \frac{\rho_i^r}{(\rho_{sol}^r)^2} \right). \quad (14)$$

Rearranging the summands in equation (14), we obtain:

$$\frac{\partial \rho_{sol}^r}{\partial t} = \frac{\sum_{i=1}^{m-1} \left(\frac{\partial \rho_{sol}^r}{\partial \omega_i} \right) \left(\frac{\partial \rho_i^r}{\partial t} \right)}{\left(\rho_{sol}^r + \sum_{i=1}^{m-1} \left(\frac{\partial \rho_{sol}^r}{\partial \omega_i} \omega_i \right) \right)}. \quad (15)$$

Now we can substitute (15) into equation (12):

$$\frac{\sum_{i=1}^{m-1} \left(\frac{\partial \rho_{sol}^r}{\partial \omega_i} \right) \left(\frac{\partial \rho_i^r}{\partial t} \right)}{\left(\rho_{sol}^r + \sum_{i=1}^{m-1} \left(\frac{\partial \rho_{sol}^r}{\partial \omega_i} \omega_i \right) \right)} = -\nabla \cdot \left(\sum_{i=1}^m \vec{g}_i^r + \vec{g}_{conv} \right). \quad (16)$$

After substituting (10) into (31) we obtain the differential equation relating the convective flow with the rest:

$$-\frac{\sum_{i=1}^{m-1} \left(\frac{\partial \rho_{sol}^r}{\partial \omega_i} \right) \left(\nabla \cdot (\vec{g}_i^r + \omega_i \vec{g}_{conv}) \right)}{\left(\rho_{sol}^r + \sum_{i=1}^{m-1} \left(\frac{\partial \rho_{sol}^r}{\partial \omega_i} \omega_i \right) \right)} = -\nabla \cdot \left(\sum_{i=1}^m \vec{g}_i^r + \vec{g}_{conv} \right) \quad (17)$$

Given the consistency of the density of the mixture and partial densities of the components, within the selected volume $dx dy dz$, the following equation can be written under the sign of divergence:

$$\frac{\sum_{i=1}^{m-1} \left(\frac{\partial \rho_{sol}^r}{\partial \omega_i} \right) (\vec{g}_i^r + \omega_i \vec{g}_{conv})}{\left(\rho_{sol}^r + \sum_{i=1}^{m-1} \left(\frac{\partial \rho_{sol}^r}{\partial \omega_i} \omega_i \right) \right)} = \left(\sum_{i=1}^m \vec{g}_i^r + \vec{g}_{conv} \right). \quad (18)$$

After simplifying (18), we obtain an expression for the convective flow:

$$\vec{g}_{conv} = - \left(\sum_{i=1}^m \vec{g}_i^r \right) \left(1 + \sum_{i=1}^{m-1} \left(\frac{\partial \rho_{sol}^r}{\partial \omega_i} \frac{\omega_i}{\rho_{sol}^r} \right) \right) + \sum_{i=1}^{m-1} \left(\frac{\partial \rho_{sol}^r}{\partial \omega_i} \frac{\vec{g}_i^r}{\rho_{sol}^r} \right). \quad (19)$$

If we put in equation (34) that $\frac{\partial \rho_{sol}^r}{\partial \omega_i} = 0$ (no dependence of the solution content on the concentration of the i -th component, which corresponds to the constant density of the water-salt solution), we come to the standard equation for the convective

flow, which is simply the sum of flows of all the components of the mixture [11]:

$$\vec{g}_{conv} = - \left(\sum_{i=1}^m \vec{g}_i^r \right). \quad (20)$$

Knowing the value of the convective mass flow, we can write the expression for the diffusion flow, considering the removal of the convective mass flow:

$$\vec{g}_{di}^r = \vec{g}_i^r + \omega_i \vec{g}_{conv}, \quad (21)$$

where \vec{g}_{di}^r – the diffusion-convective flow of the i -th component $\text{kg}/(\text{s}\cdot\text{m}^2)$;

It is important to note that equation (21) is only suitable for diffusion in the bulk solution (without primer). To bring the equation (21) to the mass flow through the surface area of the ground it is necessary to sum \vec{g}_{di}^r by the area occupied by the solution S_{sol} and then divide by the ground area S_{gr} near the point:

$$\theta = \frac{V_{sol}^r}{V_{gr}} = \frac{\rho_{sol}^{gr}}{\rho_{sol}^r} = \frac{S_{sol}}{S_{gr}}, \quad (22)$$

where V_{sol}^r – the true volume of the unfrozen water-salt solution, m^3 ; V_{gr} – the ground volume, m^3 ; θ – the volume fraction of the unfrozen water-salt solution in the ground.

$$\vec{g}_{dw}^{rp} = K_b \theta \vec{g}_{di}^r, \quad (23)$$

where K_b – the diffusion inhibition factor in porous media; \vec{g}_{dw}^{rp} – the diffusion-convective flow of the i -th component of the area through the ground surface, $\text{kg}/(\text{s}\cdot\text{m}^2)$;

We write the expression for the filtration flow of the i -th component given the pressure gradient and all the mass forces for the stationary case:

$$\vec{g}_{fi}^{rp} = -\lambda_p \omega_i \rho_{bc}^{rp} \left(\sum_{i=1}^m \omega_i \vec{\nabla} \psi_i + \vec{\nabla} P \right), \quad (24)$$

where λ_p – the hydraulic conductivity coefficient by Kolumin [12], s.

RESULTS

So now we can write the equation of mass transfer, in which summands are clearly structurally isolated, connected with the mass transfer of the substance due to various mechanisms:

$$\frac{\partial \rho_i^{gr}}{\partial t} = -\nabla \cdot \left(\vec{g}_{di}^{gr} + \vec{g}_{fi}^{gr} \right) + Q_i, \quad (25)$$

where the diffusion-convective flow corresponds to \vec{g}_{di}^{rp} , and filtration – to the flow \vec{g}_{fi}^{rp} ; Q_i – the volume source of the i -th component associated with the freezing and supersaturation of the solution, $\text{kg}/(\text{s}\cdot\text{m}^3)$.

In equations (24, 25) the value of the pressure gradient remains to be determined. It can be found by solving the problem of the stress-strain state of the ground. First step is to select the ground model.

The essential difference of frozen ground from thawed is that ice increases the ground resistance to deformation and fracture in the first moments of load application. However, in case of prolonged exposure to the same loads the layered ice structure promotes damped or undamped creep. The main proof - the same order of long-term strength characteristics of thawed and frozen ground (grip and angle of internal friction). The time of deformation relaxation in the ground is measured in hours, and the growth time of ice schlieren - in days. Therefore, we can assume that the ground immediately takes the new equilibrium position when the mass content of ice changes. And each new equilibrium position corresponds to deformation with prolonged exposure to loads.

Therefore, it is possible to use ground models not taking into account strain development in time, but taking into account the non-linear nature of the soil deformation. The deformation theory of elasticity corresponds to this requirement. Since equations (45) already take into account the presence of the pore pressure gradient, ground characteristics must conform to the consolidated undrained laboratory tests.

Relative deformation is calculated using the following formulas:

$$\varepsilon_j = \frac{(\sigma_{jj} - \sigma_{av})}{2G} + \frac{\sigma_{av}}{3K} + \frac{1}{3} \left(\sum_{i=1}^m \left(\frac{\rho_i^{gr}}{\rho_i^r} \right) + \frac{\rho_{ice}^{gr}}{\rho_{ice}^r} - \frac{e}{e+1} \right), \quad (26)$$

where ε_j - the relative deformation along the j axis, unit fraction; σ_{jj} - the normal stress along the j axis, Pa; σ_{av} - the first invariant of the stress tensor, Pa; G - the shear modulus, Pa; K - the bulk modulus, Pa; e - the porosity as the ratio of the pore volume to the solids volume, unit fraction; ρ_i^{gr} - the content of the i -th component per unit volume of soil, kg/m³; ρ_{ice}^{gr} - the ice content per unit volume of soil, kg/m³; ρ_{ice}^r - the true density of ice, kg/m³.

The bulk modulus of elasticity of water saturated soils can be assumed to be constant and calculated by the deformation characteristics of pure components, and of non-water saturated - taken with a compression test curve and assume that a reduction in the ground volume occurs due to the displacement of vapor-air mixture. The shear modulus is calculated according to the formula recommended by Z.G. Ter-Martirosyan [13]:

$$G = G_0(1 - \eta), \quad (27)$$

$$\eta = \frac{\sigma_1 - \sigma_3}{(\sigma_1 + \sigma_3)\sin(\varphi) + 2c \cdot \cos(\varphi)}, \quad (28)$$

where G_0 - the shear modulus in the initial section of the shear test curve, Pa; η - the degree of approximation of the current state of tension to the limit; σ_1, σ_3 - the largest and smallest principal stress, Pa; φ - the angle of internal friction, rad; c - the grip, Pa.

Equations (26-28) are substituted into the equilibrium equations of the classical theory of elasticity.

DISCUSSION

Let us analyze the equation (25). This equation contains the diffusion-convective flow of the i -th substance \vec{g}_{di}^{gr} . However, the sum of flows is not equal to zero based on the formulas (19 - 21). Consequently, there is mass transfer. Usually, in the literature, the diffusion flow of the i -th component is called a flow the sum of which for all components is zero. In view of the abovementioned let us transform the expression for \vec{g}_{di}^{gr} :

$$\vec{g}_{di}^{gr} = \vec{j}_i^{gr} + \omega_i \vec{j}_{conv}^{gr}, \quad (29)$$

where \vec{j}_{conv}^{gr} - the mass flow associated with the diffusion, kg/(s·m²); \vec{j}_i^{gr} - the diffusion flow of the i -th component, кг/(с·m²).

Writing equation (29) for each component we obtain m of equations and $m+1$ of unknowns: $\vec{j}_1^{gr}, \dots, \vec{j}_i^{gr}, \dots, \vec{j}_m^{gr}, \vec{j}_{conv}^{gr}$. Adding here the equation:

$$\sum_{i=1}^m \vec{j}_i^{gr} = 1, \sum_{i=1}^m \omega_i = 1, \quad (30)$$

We obtain the following equation for the diffusion flows:

$$\vec{j}_{conv}^{gr} = \sum_{i=1}^m \vec{g}_{di}^{gr} \quad (31)$$

$$\vec{j}_i^{gr} = \vec{g}_{di}^{gr} - \omega_i \sum_{i=1}^m \vec{g}_{di}^{gr} \quad (32)$$

Thus, it is shown that diffusion not only generates the transfer of the substance, but also the mass transfer in the ground, which also affects the magnitude of the relative ground deformation (26).

CONCLUSION

Using the approach based on the kinetic theory of liquids, a mathematical model for mass transfer in the soil medium was developed that explicitly determines the contribution of various mechanisms. Within the mathematical model expressions were obtained:

- for the diffusion flow of the i -th component of the solution, taking into account the heterogeneity of the energy states of molecules, the heterogeneity of temperature fields, concentrations and total moisture content;
- for the convective flow of the solution as a whole, associated with the diffusion of its components.

The possibility of applying the deformation plasticity theory to determine the pressure in the pore solution was substantiated.

REFERENCES

- [1] Gorkovenko A.I. Fundamentals of the theory for calculating the spatial position of an underground pipeline under the influence of seasonal processes: dissertation for D.Sc. -Tyumen, 2006. -305 p.
- [2] Ivanov I.A. et al. Geotechnical problems of pipeline transport: tutorial / I.A. Ivanov, S.Ya. Kushnir, S.A. Pulnikov. Tyumen: TyumGNGU, 2011. 208 p.
- [3] Lazarev S.A., Pulnikov S.A., Sysoev Yu.S. Diagnosing extended spatially deformed sections of pipelines in the technical state and integrity control system of PJSC "Gazprom" // Territory Neftegaz. 2016. № 4. pp. 106-115.
- [4] Mihailov P.Yu. Dynamics of heat and mass transfer processes and the heat and power interaction of freeze-through soils with underground pipelines: dissertation for D.Sc. – Tyumen, 2012. -175 p.
- [5] Karnauhov M.Yu., Lazarev S.A., Pulnikov S.A., Sysoev Yu.S. The study of the formation of the operating position of extended sections of MG Urengoy - Chelyabinsk in the complex hydrogeological conditions // Gas Industry. 2015. № S (724). pp. 53-58.
- [6] Pulnikov S.A. Interaction of underground pipelines with frozen soil: tutorial / S. A. Pulnikov, Yu. S. Sysoev, E. V. Markov. - Tyumen: IUT, 2016. - 86 p.
- [7] Kalyuzhniy I.L., Lavrov S.A. Hydrophysical processes in the catchment area: Experimental studies and modeling: monograph. – SPb : Nestor-Istoriya, 2012. – 616 p.
- [8] Terleev V.V., Mirschel W., Badenko V.L., Guseva I.Yu., Gurin P.D. Physical and statistical interpretation of the parameters of the function of the soil water-holding capacity // Physics, biophysics and ecology of soil. 2012. № 4(8). pp. 1-8.
- [9] Fundamentals of Geocryology. P. 1: Physical and chemical bases of Geocryology / Ed. by E. D. Ershov. – M.: Publ.house MSU, 1995. – 368 p.
- [10] Frenkel Ja.I. Kinetic Theory of Liquids. Publ.house "Nauka", Leningr. otd., L., 1975, 592 p.
- [11] Kikoin A.K., Kikoin I.K. Molecular physics. – M.: Nauka, 1976. — 480 p.
- [12] Kolunin V.S. Modelling of heat and mass transfer processes in the permafrost with a movable component of ice: dissertation for D.Sc. – Tyumen, 2011. -262 p.
- [13] Mechanics of soils, bases and foundations: tutorial for construction students / S. B. Uhov, V.V. Semenov, V. V. Znamenskiy et al; ed. by S. B. Uhov. – 3rd ed., corr. – M.: Vyssh.shk, 2004. – 556 p.