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Analytical Methods for Estimating Thermal Conductivity of Multi-Component Natural Systems in Permafrost Areas

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1. Introduction

Frozen soils consist of soil solids, ice, unfrozen water, and gas (vapour). The solid particles vary in size and composition and may be composed of one or more minerals or of organic material. Based on particle size, soils are classified into soil types which vary between the many classification systems in use throughout the world. The classification which is most generally used in Russia is that of V.V. Okhotin (Sergeev, 1971), with the basic soil types being sand, sand-silt, silt-clay, and clay which are further subdivided into a large number of subtypes. Soils that have been subject to repeated cycles of freezing and thawing generally have higher silt contents.

The bound water is structurally and energetically heterogeneous. Water bonding to the mineral particles is provided predominantly by the active centres on the surface and the exchange cations. The most important active centres for water adsorption in the crystalline lattice of clay minerals are hydroxyl groups and coordinately unsaturated atoms of oxygen, silicon, aluminium and other elements.

In quantitative terms, it is an undeniable fact that the pore water freezes over a range of negative temperatures rather than at a single temperature, depending on soil moisture content and solute concentration. This is due to distortion of the bound water structure by the active centres on the particle surfaces and dissolved ions, resulting in a kinetic barrier which makes water crystallization difficult.

The phase composition of water (or solution) changes with temperature following the dynamic equilibrium state principle established by Tsytoich (1945) and experimentally confirmed by Nersesova (1953). This principle states that the amount of unfrozen water for a given soil type (non-saline) is a function of the temperature below 0°C and is virtually independent of the total soil moisture content. It is quantitatively described by the equation (Ivanov, 1962):

$$W_{uw} = W_0 + A' \left[\frac{1}{1 + a'|\Delta t| + b'\Delta t^2} - 1 \right], \quad (1)$$

where $\Delta t = t - t_f$; t_f is the initial freezing temperature of water; W_0 is the equilibrium moisture content at t_f ; and A' , a' and b' are the characteristic soil parameters. For a narrow range of freezing temperatures ($|\Delta t| \leq 10^\circ\text{C}$), Eq. (1) can be simplified by assuming $b' = 0$.

The thermodynamic instability of the phase composition of water in frozen soils causes their properties to be highly dynamic at subzero temperatures. The presence of unfrozen water below 0°C provides conditions for water migration during freezing. This results in the formation of cryostructures and cryotextures that, in turn, cause the anisotropy of soil thermal and other properties. All cryostructural types can be grouped into three broad classes: massive, layered, and reticulate (Everdingen, 2002).

Model calculations generally consider heat conduction in frozen soils. It is characterized by an effective value of the heat flux transferred by the solid particles and interstitial medium (ice, water and vapour) and through the contacts. It depends on multiple variables which reflect the origin and history of the soil, including moisture content, temperature, dry density, grain size distribution, mineralogical composition, salinity, structure, and texture.

A large number of theoretical models and methods were developed for estimating the thermal conductivity of various particulate materials. However, most of them do not address the structural transformations and their validity is limited to a narrow range of material's density. In permafrost investigations, it is essential that properties of snow, soils and rocks be studied in relation to the history of sediment formation through geologic time. Therefore, a universal theoretical model with changing particle shapes was proposed by the present author to describe the processes of rock formation, snow compaction and glacierization with account for diagenetic and post-diagenetic structural modifications, as well the processes of rock weathering and soil formation. A detailed description of the model was given in earlier publications (Gavril'ev, 1992, Gavriliev, 1996, Gavriliev, 1998). Since then, the model has been amended and improved. We therefore find it necessary to present a brief description of the geometric models and the final predictive equations.

2. Theoretical model accounting for structural transformations of sediments

2.1 Soils and sedimentary rocks

A model for estimating the thermal conductivity of soils and sedimentary rocks should take into account the changes in particle shape over the entire range of porosity from 0 to 1 in order to consider the entire cycle of sediment changes since its deposition. In developing such a model, it should be kept in mind that mineral rock particles undergo some kind of plastic deformation through geologic time, gradually filling the entire space. Particles bind together at the contacts ("the contact spot") and rigid crystal bindings develop between the particles.

Following the real picture of rock weathering and particle shape changes through diagenesis, the author has proposed a model, which presents the solid component in a cubic cell by three intersecting ellipsoids of revolution (Fig. 1) (Gavril'ev, 1992).

In this scheme, depending on the semi-axes ratio of the ellipsoids a/R , the porosity of the system varies from 0 to 1 and the particle attains a variety of shapes, such as cubical, faceted, spherical, worn, and cruciate. This logically represents the real changes in particle shape through the sedimentary history, i.e., the key requirement to the model - adequate representation of the real system - is met. In this scheme, the particles always maintain contacts with each other and the system remains stable and isotropic. The coordinate

number is constant and equal to 6; the relation between the thermal conductivity and porosity is realized by changing the particle shape at various size ratios of the ellipsoids of revolution. At $a/R \geq 1$, a contact spot appears automatically in the model, which represents rigid bonding between the particles that provides hard, monolithic rock structure (Gavriliiev, 1996).

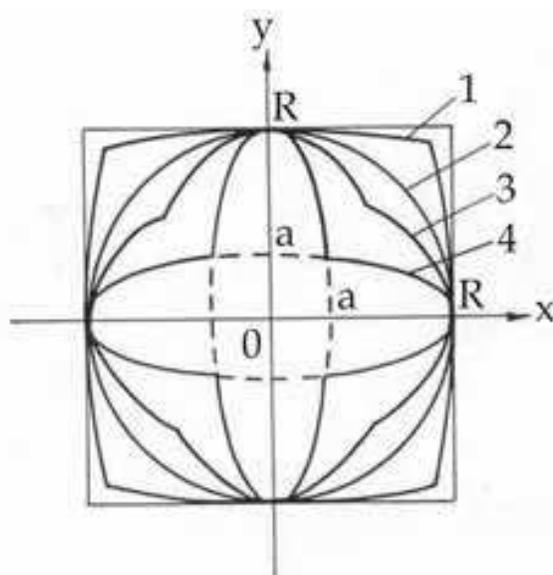


Fig. 1. Particle shapes in the soil thermal conductivity model at different semi-axes ratios of ellipsoids $\delta = a/R$: 1 - faceted ($\delta > 1$); 2 - spherical ($\delta = 1$); 3 - worn ($\delta < 1$); 4 - cruciate ($\delta < 1$)

All calculations are made in terms of the parameter $\delta = a/R$, which is a unique function of the porosity m_2 (dry density γ_s):

$$\lambda = \lambda_{\text{mod}} + \varphi_{\text{sc}} \quad (2)$$

where λ_{mod} is the resulting thermal conductivity of the model and φ_{sc} is the correction for heat transfer across the contact spot, $W/(m \cdot K)$:

$$\lambda_{\text{mod}} = \lambda_{\text{ad}} \left[1 + \left(\frac{1.3}{1 + 0.5\vartheta - 0.26\vartheta^2} - 1 \right) \sin \pi m_2 \right], \quad (3)$$

where $\vartheta = \lambda_2/\lambda_1$; $0 \leq \vartheta \leq 1$; λ_{ad} is the thermal conductivity of the system where the elementary cell is divided by adiabatic planes; the subscripts "1" and "2" refer to the particle and the fill (air, water and ice), respectively.

The thermal conductivity of the model, λ_{ad} , is given by the following equations: at $\delta \leq 1$

$$\frac{\lambda_{\text{ad}}}{\lambda_2} = 1 - \frac{\pi\delta}{2} - \delta^2 H + \delta \arcsin \delta / X + \frac{\pi}{\delta K_1} \left[(1 - \delta) \left(1 - \frac{1}{\delta K_1} \ln \left| \frac{1}{1 - \delta K_1} \right| \right) - (1 - \delta^4) \left(\frac{1}{X} + \frac{1}{\delta K_1} \ln \left| 1 - \frac{\delta K_1}{X} \right| \right) \right] \times \left[1 - \frac{4 \arcsin \delta / X - \pi \delta}{2\pi(1 - \delta)} \right], \quad (4)$$

at $\delta \geq 1$

$$\frac{\lambda_{ad}}{\lambda_2} = 1 - \frac{\pi}{4} - \delta^2 H + \frac{\pi}{2K_1} \left(\delta^2 - \frac{1}{\delta^2} \right) \times \left(\frac{1}{K_1} \ln \left| 1 - \frac{\delta K_1}{X} \right| + \frac{\delta}{X} \right) + \frac{\delta K_1}{X - \delta K_1} \left(\delta \arcsin 1/X - \frac{\pi}{4} \right), \quad (5)$$

where $\delta = a/R$; $X = \sqrt{1 + \delta^2}$; $H = \frac{\pi}{2K_1} \left(\frac{1}{K_1} \ln |1 - K_1| + 1 \right)$; $K_1 = 1 - \frac{\lambda_2}{\lambda_1}$.

The correction factor φ_{sc} is given by

$$\varphi_{sc} = \frac{\pi \lambda_1 \delta^2}{2} \left[\frac{r_c^2}{2R^2 \delta^2} + \frac{9}{K_1} \left(1 - \sqrt{1 - \frac{r_c^2}{R^2 \delta^2}} \right) + \frac{9}{K_1^2} \ln \frac{1 - K_1}{1 - K_1 \sqrt{1 - \frac{r_c^2}{R^2 \delta^2}}} \right], \quad (6)$$

where r_c is the radius of the contact spot between the particles.

It is assumed in Eq. (6) that the spot contact between particles is formed of the same material as the particle by its flattening at high pressure or by its squeezing (solution and crystallization) due to selective growth of cement in sandstones (quartz cement grows on quartz particles and feldspar on feldspar particles). In a general case however, the contact spot may consist of a foreign material resulting, for example, from precipitation of salts from solution at the particle contacts. In this case, the correction factor φ_{sc} is given by

$$\varphi_{sc} = \frac{\pi a}{2R^2} \left[\frac{\lambda_3}{K_1^2} \ln \left| \frac{1 - K_1 \sqrt{1 - r_c^2/a}}{(1 - K_1)} \right| - \frac{\lambda_2}{K_2^2} \ln \left| \frac{1 - K_2 \sqrt{1 - r_c^2/a^2}}{(1 - K_2)} \right| + \left(\frac{\lambda_2}{K_2} - \frac{\lambda_3}{K_1} \right) \left(1 - \sqrt{1 - r_c^2/a^2} \right) \right], \quad (7)$$

where $K_2 = 1 - \lambda_3/\lambda_1$; λ_1 , λ_2 and λ_3 are the thermal conductivities of the solid, medium and contact spot (contact cement), respectively.

The relative size of the contact spot is expressed in terms of the system's porosity as:

$$\frac{r_c}{R} = 1.69 \sqrt{1 - 3 \sqrt{\frac{\pi}{6(1 - m_2)}}}. \quad (8)$$

The soil porosity m_2 or the volume fraction of the mineral particle m_1 is a unique function of the parameter δ and is given by the following equations:

at $\delta \leq 1$

$$m_1 = \frac{\pi \delta^2}{6} \left[1 - \frac{1 - \delta^2}{\delta} + \frac{1 - \delta}{X} \left(\frac{1 + \delta}{\delta} - \frac{1}{X^2} + 3 \right) \right], \quad (9)$$

at $\delta \geq 1$

$$m_1 = \frac{\pi \delta^2}{6} \left(1 - \frac{\delta^2 - 1}{\delta X} \right) + \frac{\delta (1 + 2\delta^2)}{16X^2} \left(\frac{1}{X} + \frac{1}{\sqrt{2 + \delta^2}} \right) \times \left(4\delta \arcsin \frac{1}{\delta X} - \pi \right). \quad (10)$$

The increase in the volume fraction of the solids due to the contact spot is expressed by

$$m_{sc} = \frac{\pi}{4} \left[\frac{r_c^2}{R^2} - 2 \left(\delta^2 - \frac{r_c^2}{R^2} \right) \left(1 - \sqrt{1 - \frac{r_c^2}{R^2 \delta^2}} \right) \right]. \quad (11)$$

The dry density of the soil is

$$\gamma_d = (m_1 + m_{sc}) \rho_s, \quad (12)$$

where ρ_s is the solids unit weight.

The above equations can be used to calculate the thermal conductivity of soils and sedimentary rocks in the saturated frozen and unfrozen states, as well as in the air-dry state in relation to the porosity m_2 and the thermal conductivity λ_1 of the solid particles (a two-component system). The predictions obtained are presented as nomograms in Fig. 2. It should be noted that in this case, the porosity m_2 refers to the entire volume fraction of the soil or rock which is completely filled either with ice, water, or air. This porosity is related to the volume fraction m_s and dry density γ_s by

$$m_2 = 1 - m_s = 1 - m_1 - m_{sc} = 1 - \gamma_s / \rho_s. \quad (13)$$

The model assumes that the material consists of mineral particles of the same composition. However, naturally occurring soils always contain particles of various compositions and they can be treated in modelling as multi-component heterogeneous systems with a statistical particle distribution.

In computations based on the universal model, the average thermal conductivity of soil solid particles may be used, which is approximately estimated in terms of the thermal conductivity and volume fraction of constituent minerals according to the equation (Gavriliiev, 1989):

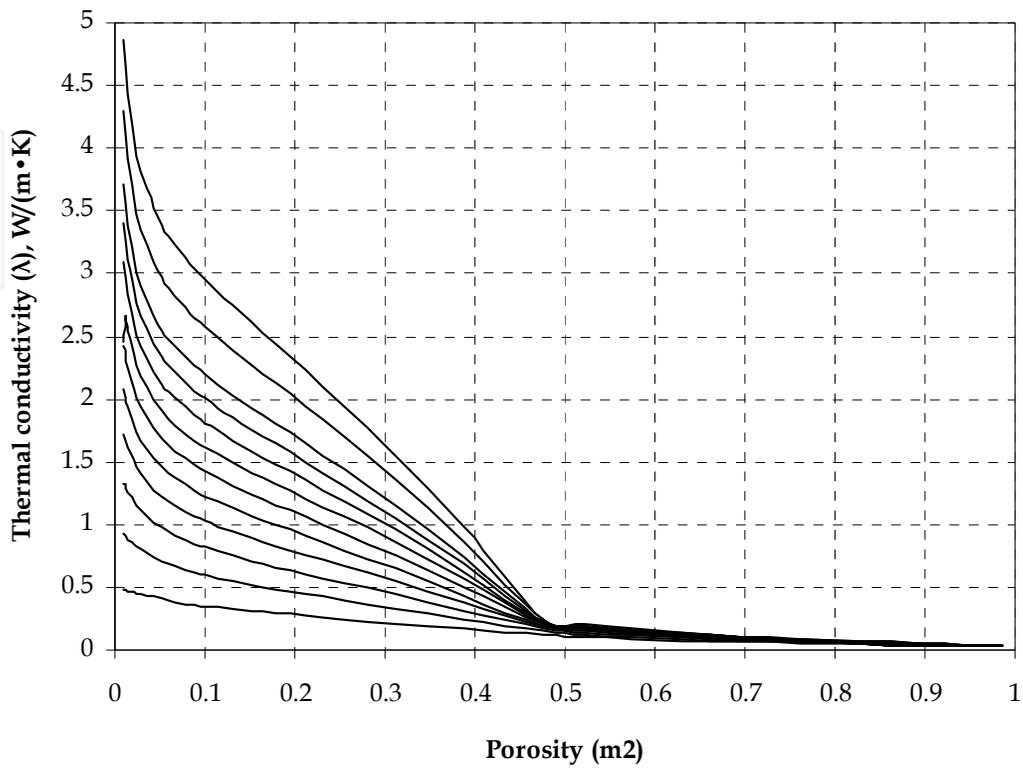
$$\bar{\lambda}_1 = 0.5 \left[\sum_{j=1}^n \lambda_j m_j + \frac{1}{\sum_{j=1}^n \frac{m_j}{\lambda_j}} \right], \quad (14)$$

where λ_j and m_j are the thermal conductivity and volume fraction of the j -th mineral of the soil, respectively. This equation can also be used for calculating the thermal conductivity of rocks characterized by the plane contacts between mineral aggregates.

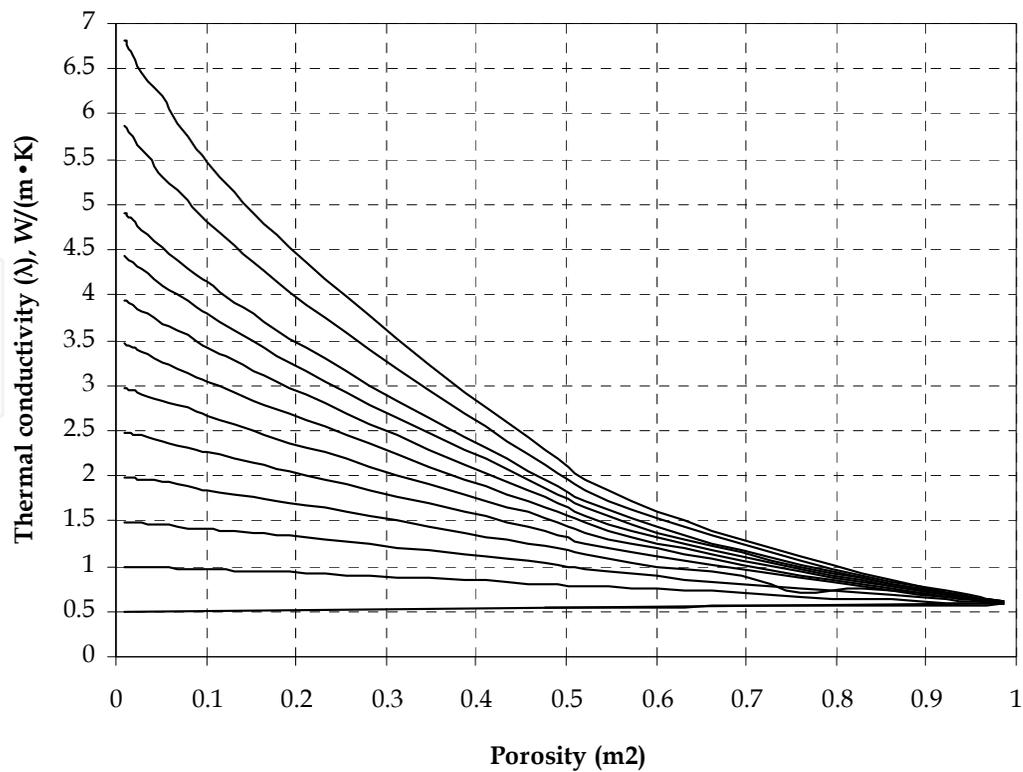
2.2 Snow

In snowpack, the structural changes of ice crystals occur continuously throughout the winter. The thermodynamic processes in snowpack result in a multi-branch openwork structure of

contacting ice crystals with shapes that continuously change throughout the period of snow existence.



(a)



(b)

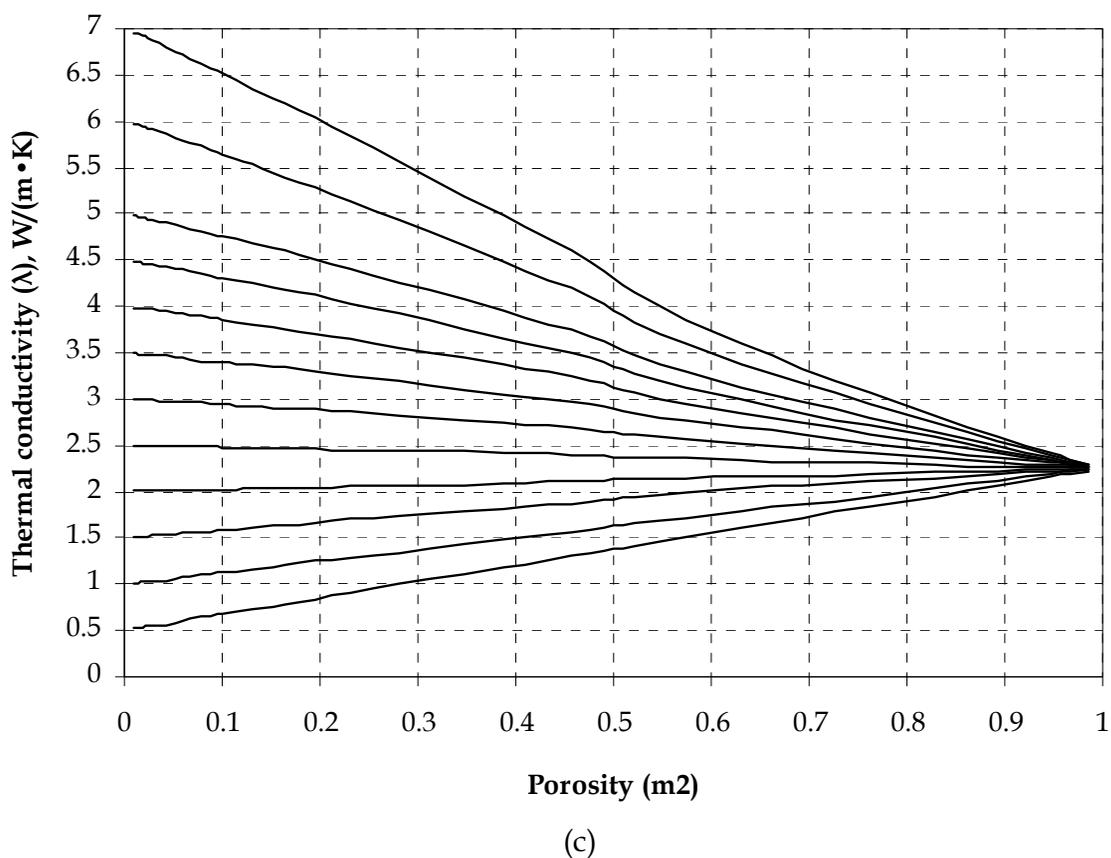


Fig. 2. Nomograms for calculating the thermal conductivity of soils and rocks in dry (a), saturated unfrozen (b) and frozen (c) states in terms of total porosity m_2 and solids thermal conductivity λ_1 (W/(m·K)): 1 - 0.5; 2 - 1.0; 3 - 1.5; 4 - 2.0; 5 - 2.5; 6 - 3.0; 7 - 3.5; 8 - 4.0; 9 - 4.5; 10 - 5.0; 11 - 6.0; 12 - 7.0

These changes in snow structure through the whole cycle from deposition to glacier formation can be fairly well represented by the same model shown in Fig. 1 (Gavrilyev, 1996a). But the calculations should take into account the heat convection by vapour diffusion due to a temperature gradient in the snow. This can be done by substituting in Eqs. (3) - (6) the effective thermal conductivity of air in snow for its thermal conductivity (λ_a) which is given by

$$\lambda_{ae} = \lambda_a + \frac{LD_s e_0}{R_v T^2} \left(\frac{L}{R_v T} - 1 \right) \times \exp \left[\frac{L(T - T_0)}{R_v T_0 T} \right], \quad (15)$$

where $e_0 = 6.1 \cdot 10^2$ Pa is the saturation vapour pressure at 0°C ($T_0 = 273$ K); $R_v = 4.6 \cdot 10^2$ J/(kg·K) is the gas constant of water vapour; T is the absolute temperature, K; L is the latent heat of ice sublimation; D_s is the diffusion coefficient of water vapour in snow; and λ_a is the thermal conductivity of calm air.

The thermal conductivity of air in relation to temperature may be calculated by an equation given by Vargaftik (1963):

$$\lambda_a = \lambda_a^0 \left(\frac{T}{T_0} \right)^{0.82}, \quad (16)$$

where $\lambda_a^0 = 0.0244 \text{ W}/(\text{m}\cdot\text{K})$ is the thermal conductivity of air at temperature T_0 . It is convenient for practical calculations to express the radius of a contact spot directly in terms of the parameter $\delta = a/R$, although this relationship is indirectly reflected in Eq. (8) in terms of porosity. The following correlations have been derived (Gavriliiev, 1998):
at $a/R \leq 1$

$$\frac{r_c}{R} = 0.25 \left(\frac{a}{R} \right)^{2.5}, \quad (17)$$

at $a/R \geq 1$

$$\frac{r_c}{R} = 1.25 - \exp \left[-0.6 \left(\frac{a}{R} - 1 \right) \right]. \quad (18)$$

Fig. 3 presents a nomogram which can be used to find the thermal conductivity of snow from its temperature and porosity. This nomogram has been developed based on the above theoretical model which takes into account the heat transfer by thermal diffusion of water vapour. In the computations, the diffusion coefficient of water vapour in snow, D_s , is taken to be $0.66 \text{ cm}^2/\text{s}$, which is the average of the experimental values reported in the literature ranging from $0.40 \text{ cm}^2/\text{s}$ (Sulakvelidze & Okudzhava, 1959) to $0.90 \text{ cm}^2/\text{s}$ (Pavlov, 1962).

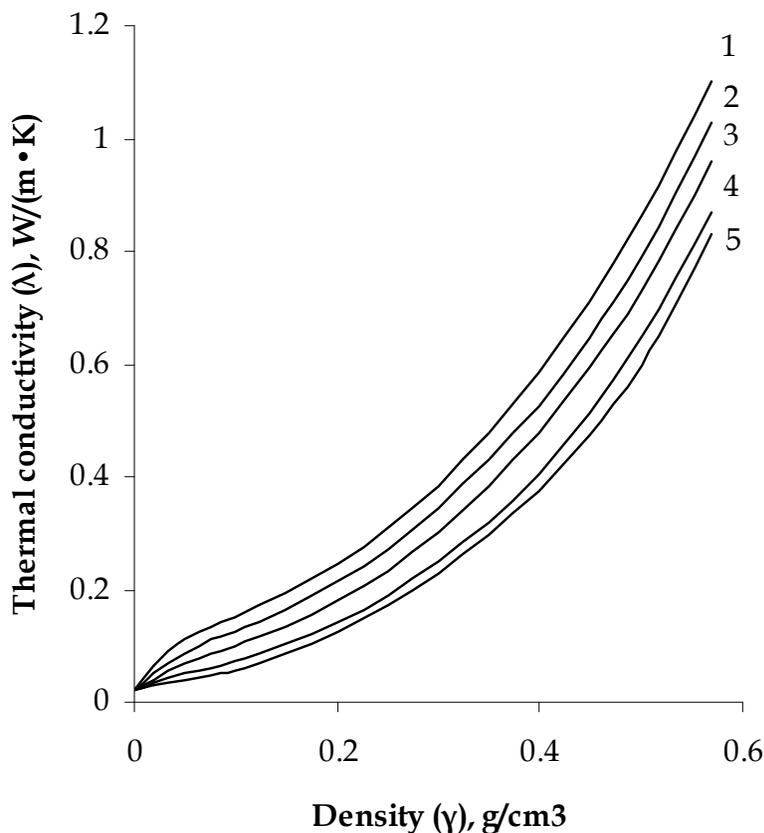


Fig. 3. Nomogram for the calculation of thermal conductivity of snowcover from its density and temperature, °C: (1) -0; (2) -5; (3) -10; (4) -20; (5) -30

3. Effects of coarse inclusions and the layered and reticulate cryostructures on thermal conductivity of frozen soils

For the thermal conductivity of media containing spherical and cubic inclusions with no contacts (or with point contacts), Maxwell (1873) (for a sphere) and Odelevsky (1951) (for a cube) developed a similar equation of the type:

$$\lambda = \lambda_2 \left[1 + \frac{(\lambda_1 - \lambda_2) m_1}{\lambda_2 + 0.33 (1 - m_1) (\lambda_1 - \lambda_2)} \right], \quad (19)$$

where (as before) the subscripts "1" and "2" refer to the inclusions (particles) and the medium, respectively. For the cubical particle shape, Eq. (19) is formally valid across the range of inclusion contents: $0 \leq m_1 \leq 1$.

The advantage of Eq. (19) is its simplicity. In some cases, Eq. (19) is applicable to permafrost problems, for example, for estimating the thermal conductivity of soils with a cryostructure or of soils containing gravel- or cobble-size inclusions. However, at large differences between the λ_1 and λ_2 values, such as in air-dry soils, the degree of roundness of gravel and cobble inclusions may affect the accuracy of calculations.

For a more general formulation of the problem, an ellipsoidal particle shape may be considered in Eq. (19), since with the change in the ratio of semi-axes the particles transform into other figures, such as a sphere, plate, or cylinder. Eq. (19) may be presented in the following generalized form (Gavriliiev, 1986):

$$\lambda = \lambda_2 \left[1 + \frac{(\lambda_1 - \lambda_2) m_1}{\lambda_2 + K_f (1 - m_1) (\lambda_1 - \lambda_2)} \right], \quad (20)$$

where K_f is the shape factor of particles or inclusions.

In Eq. (20), the inclusion shape factor, K_f , is

$$K_f = abcC(0), \quad (21)$$

where a , b , and c are the semi-axes of the ellipsoids ($a > b > c$); and $C(0)$ is the integral of the form (Ovchinnikov, 1971)

$$C(0) = \frac{2}{a^3} \left[\frac{\sqrt{1 - p^2 \sin^2 \psi} \operatorname{tg} \psi - E(\psi, p)}{1 - p^2} \right]. \quad (22)$$

$E(\psi, p)$ is the elliptic integral of the second kind, $\psi = \arcsin \sqrt{1 - c^2/a^2}$ - is the amplitude and $p = \sqrt{(1 - b^2/a^2)/(1 - c^2/a^2)}$ - is the modulus of the integral.

The elliptic integral $E(\psi, p)$ is tabulated, and the shape factor of inclusions can be readily found from the ratio of the particle dimensions a , b , and c . For practical purposes, calculations can be limited to the more simple case of ellipsoids of revolution. Then, the integral $C(0)$ is expressed in terms of elementary functions (Carslaw & Jaeger, 1959). Let us consider two examples.

1. The particles have a shape of an oblate ellipsoid of revolution ($a = b > c$). Then, along the semi-axes we have

$$K_{fc} = \frac{1}{\beta} \left(1 - \frac{c}{a\beta} \arcsin \sqrt{\beta} \right), \quad (23)$$

$$K_{fa} = K_{fb} = \frac{c}{2a\beta} \left(\frac{c}{\sqrt{\beta}} \arcsin \sqrt{\beta} - \frac{c}{a} \right), \quad (24)$$

where $\beta = 1 - c^2/a^2$.

2. The inclusions have a shape of a prolate ellipsoid of revolution ($b = c < a$)

$$K_{fc} = K_{fb} = \frac{1}{2\beta} \left(1 - \frac{c^2}{2a^2\beta} \ln \frac{1 + \sqrt{\beta}}{1 - \sqrt{\beta}} \right), \quad (25)$$

$$K_{fa} = \frac{c^2}{a^2\beta} \left(\frac{1}{2\sqrt{\beta}} \ln \frac{1 + \sqrt{\beta}}{1 - \sqrt{\beta}} \right). \quad (26)$$

Fig. 4 shows graphically the shape factors K_f for oblate and prolate ellipsoids of revolution calculated with Eqs. (23) - (26) in relation to the ratio of the ellipse's semi-minor (c) and semi-major (a) axes at different directions. In the case of a layered cryostructure ($c/a = 0$), we have $K_f = 1$ (curve 1) for the ice-soil layers oriented across the flow, and $K_f = 0$ (curve 1') for the orientation along the flow. In the case of cylindrical inclusions ($c/a = 1$), it follows that perpendicular to the heat flow $K_f = 1/2$ (curve 2') and parallel to the flow $K_f = 0$ (curve 2).

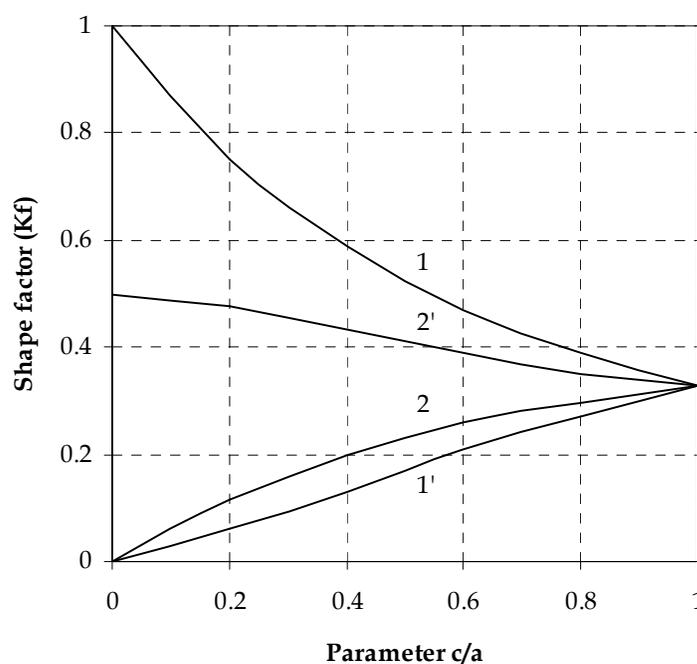


Fig. 4. Shape factor K_f of soil particles in the form of oblate (1 and 1') and prolate (2 and 2') ellipsoids of revolution versus parameter c/a for different directions: 1 and 2 - along the axis of revolution; 1' and 2' - perpendicular to the axis of revolution

As an example, we will consider frozen soils with cryostructures in more detail below. Soils with a layered cryostructure exhibit the highest anisotropy of thermophysical properties. In thermal terms, it makes sense to identify the following categories of layered cryostructure: vertical layered, cross layered, and horizontal layered. These cryostructural categories are equivalent to the three main directions of the heat-flow vector relative to the orientation of ice layers: perpendicular, parallel, and intermediate (Fig. 5 a-c).

Soils with a reticulate cryostructure are also anisotropic. The degree of anisotropy depends on the geometry of a reticulate ice network and the direction of the heat-flow vector (Fig. 5 d).

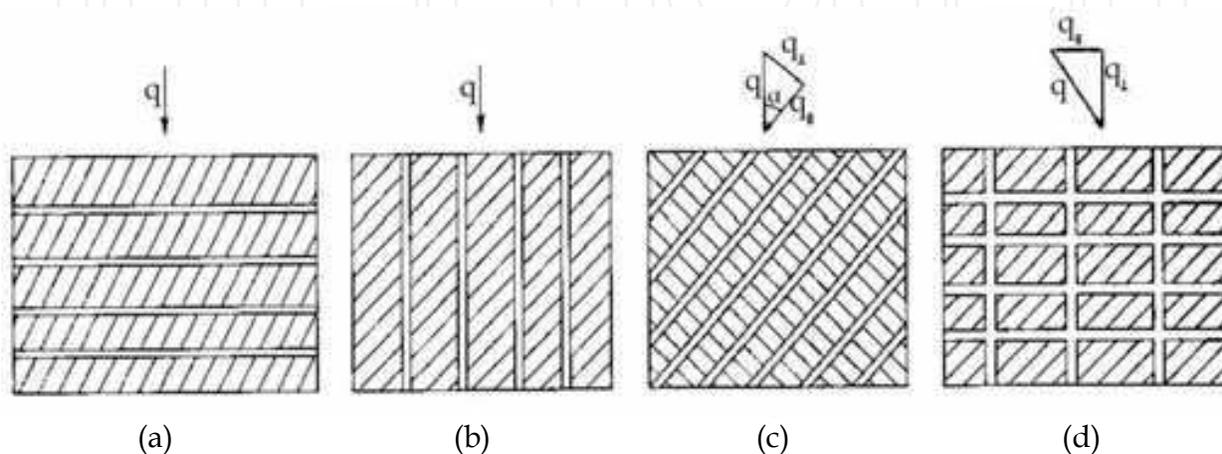


Fig. 5. Schematic representation of frozen soils with layered and reticulate cryostructures at different directions of heat-flow vector. Layered cryostructure for normal (a), parallel (b) and intermediate (c) directions of heat-flow vector relative ice orientation; d - reticulate cryostructure; q - heat-flow vector

The mechanism by which cryostructures develop in sediment is not as yet clearly understood, but the underlying effect is known to be the movement of water to the freezing front. Growing ice lenses dissect the homogeneous (massive) frozen soil into bands or blocks, i.e., the soil elements in the cryostructure are approximately similar in composition and thermal properties. In the reticulate structure, ice is the matrix material and the enclosed soil blocks are commonly rectangular in shape. For estimating the thermal conductivity of soils containing a cryostructure, Ivanov & Gavriliev (1965) considered series and parallel heat flows separately for the layered cryostructure and in combination for the reticulate cryostructure. In the latter case, difficulty arose in practice with how to account for the thickness of ice layers separately along and across the heat flow. A more simple way of taking into account the cryostructure in frozen soils can be found from the theory of generalized conductivity of media containing foreign inclusions. For generality, let us consider the inclusions of ellipsoidal shape, because any type of cryostructure can be obtained by changing the ratio of ellipsoid's semi-axes. For ellipsoids of revolution, for example, the layered cryostructure is obtained by flattening the ellipsoids: $c/a \rightarrow 0$ (c and a are the semi-minor and semi-major axes of the ellipsoid, respectively), when they change into plane layers. In the case of prolate ellipsoids of revolution with radius c , at $c/a \rightarrow 0$ the soil inclusions in the cryostructure become cylindrical. Any other values of the c/a ratio give reticulate cryostructures with one or other degree of elongation or flattening of the soil inclusions. At $c/a = 1$ the inclusions attain a spherical shape (an analogue of a cubic shape).

Let us consider the cryostructure as an ice matrix with soil inclusions in the form of ellipsoids. We assume in the general case that the soil inclusions are non-uniform in composition. Then, for the effective thermal conductivity of frozen soil, $\lambda_{\perp, \parallel, +}$ we can use the equation derived earlier by the author (Gavrilyev, 1996b) for very coarse soils with particles of different mineralogical compositions

$$\lambda_{\perp, \parallel, +} = \lambda_i \left(1 + \frac{1}{B - K_f} \right), \quad (27)$$

where

$$B = 1 / \sum_{j=1}^n \frac{(\lambda_j - \lambda_i) m_j}{(\lambda_j - \lambda_i) / K_f + \lambda_i}; \quad (28)$$

K_f is the shape factor of soil inclusions or layers; λ_i is the thermal conductivity of the ice matrix; λ_j and m_j are the thermal conductivity and the volumetric content of the j -th soil inclusion.

The volume fraction of ice, m_i , is

$$m_i = 1 - \sum_{j=1}^n m_j. \quad (29)$$

It is assumed in Eqs. (27) - (29) that the soil inclusions have a massive structure and are fully saturated (see Section 3 for permafrost soils with a massive cryostructure).

When the ice lenses occur in the soil at angle α to the direction of heat flow, the thermal conductivity of the frozen soil mass is given by

$$\lambda_{\alpha} = \sqrt{\lambda_{\perp}^2 \sin^2 \alpha + \lambda_{\parallel}^2 \cos^2 \alpha}, \quad (30)$$

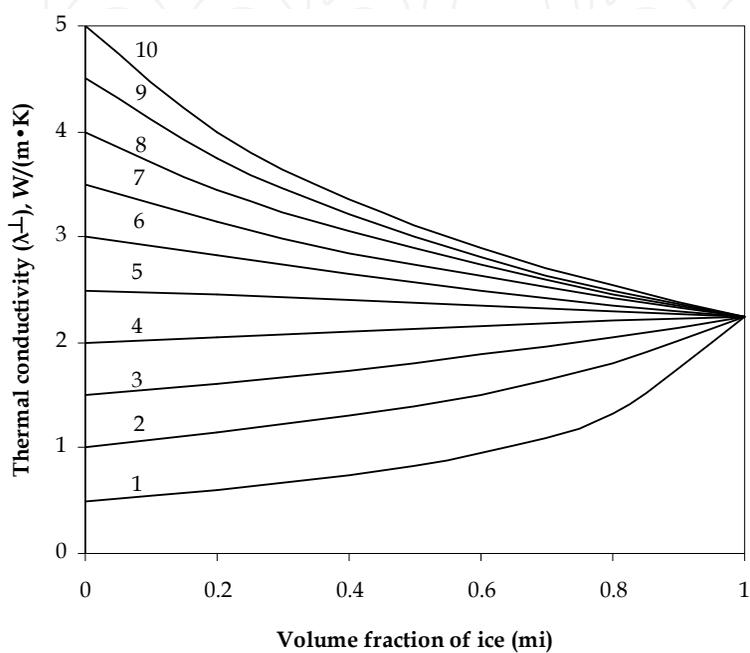
where λ_{\perp} and λ_{\parallel} are the thermal conductivities of the soil with a layered cryostructure, defined by Eq. (27) at corresponding K_f values, for the ice-soil layers perpendicular and parallel to heat flow direction.

The change of rectangular soil inclusions for ellipsoidal ones does not detract from the accuracy of calculations, as it is known from the theoretical predictions of thermal parameters that in the case of inclusions dispersed in a medium, the shape of inclusions has no significant effect on the final calculation results. In case of the uniform composition of frozen soil inclusions, Eq. (27) simplifies to Eq. (20).

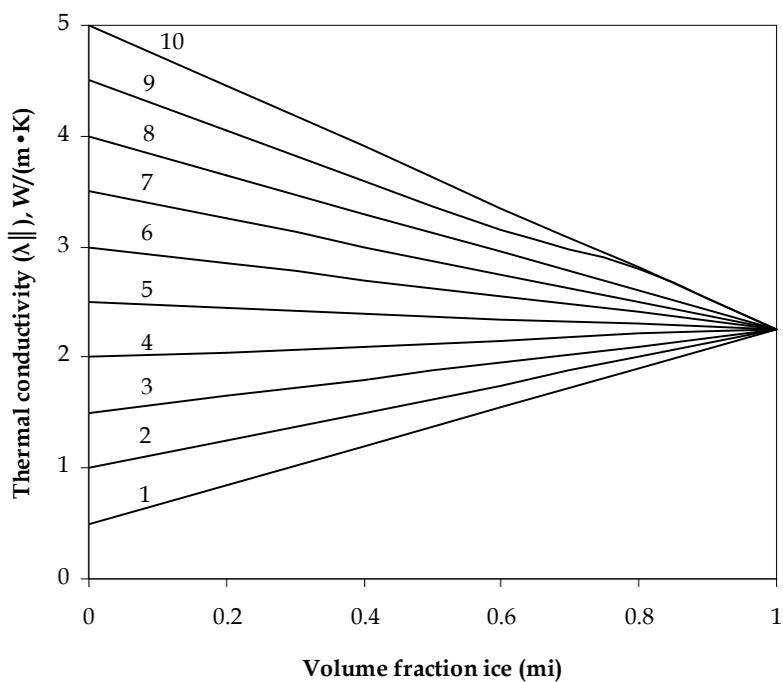
Computations of the thermal conductivity of frozen soils with layered and reticulate cryostructures were performed for the ice layers parallel, perpendicular and at 45° angle to the heat flow vector, and for spherical or cubical ($c/a = 1$ and $K_f = 0.33$) soil inclusions in the reticulate cryostructure. The thermal conductivity of the soil containing a cryostructure depends on the size (volume fraction) and orientation of the ice and soil layers relative heat flow direction, as well as the thermal conductivity of these layers.

In the cryostructures, the intermediate layers or inclusions are made of a macroscopically isotropic (massive structure) frozen mass of mineral or organic soils which can vary in

thermal conductivity from 0.5 to 5.0 W/(m•K). It is assumed that the soils comprising the intermediate layers and inclusions are perennially frozen; their thermal properties in relation to natural moisture content have been fairly well studied (Gavriliiev, 1989, 1998; Gavriliiev & Eliseev, 1970). It is known, for example, that the thermal conductivity of peat in its naturally frozen state is independent of moisture content and is approximately equal to 1.27 W/(m•K). The thermal conductivity of perennially frozen soils in relation to natural moisture content will be discussed in the next section.



(a)



(b)

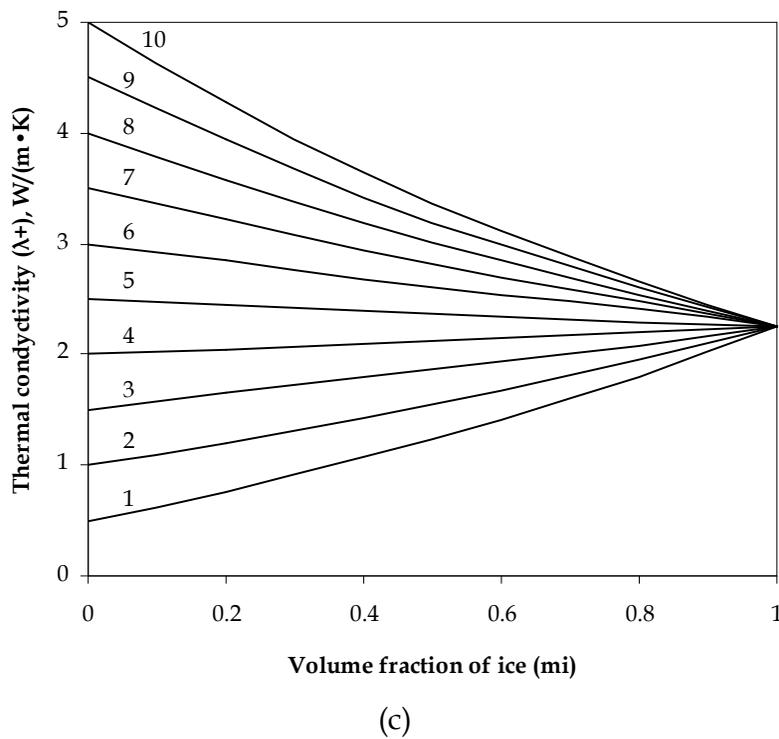


Fig. 6. Thermal conductivities λ_{\perp} (a), λ_{\parallel} (b) and λ_{+} (c) of frozen soils with a cryostructure as a function of volume fraction of ice layers (m_i) for various thermal conductivities of intermediate layers or inclusions comprised of frozen organic and mineral soils (λ_{fi} , $W/(m \cdot K)$). λ_{fi} values: 1-0.5; 2-1.0; 3-1.5; 4-2.0; 5-2.5; 6-3.0; 7-3.5; 8-4.0; 9-4.5; 10-5.0

Based on the calculated thermal conductivity values for the frozen soils with layered and reticulate cryostructures as a function of the volume fraction of ice layers m_i at different thermal conductivities of intermediate layers λ_{fi} (here the subscript “fl” refers to frozen soil), nomograms were developed shown in Fig. 6. For the layered cryostructure, the volume fraction of ice layers m_i is equal to their relative thickness l_i .

At the same values of m_i and λ_{fi} , the thermal conductivity of frozen soils is highest for a layered cryostructure with the soil and ice layers parallel to heat flow and lowest for that with the heat flow direction normal to the ice and soil layers. The soils containing reticulate and layered cryostructures with the ice and soil layers at 45° to heat flow direction have intermediate thermal conductivity values.

4. Permafrost soils with a massive cryostructure

In engineering practice, thermal properties of a given soil type are usually examined in relation to moisture content and dry density. For permafrost soils, there is a unique relationship between these parameters, because naturally occurring soils are near saturation and the air porosity comprises only 2-3% of the total soil volume. The density of frozen soil is then given by Votyakov’s equation (1975):

$$\gamma_f = \frac{2.4(1+W)}{2.7W+0.9}, \quad (31)$$

where W is the gravimetric moisture content of the frozen soil expressed as a fraction.

It is sufficient for analysis of the thermal behaviour of permafrost to only consider one of these parameters. Natural moisture content is preferably chosen, since it is easily measured even in the field.

The total moisture content of frozen soils, especially fine-grained soils, varies over a wide range due to moisture migration. For frozen alluvial deposits in Yakutia, for example, the typical values range from 0.07 to 0.30 for sands and from 0.20 to 0.60 for sand-silts and silt-clays (Votyakov, 1975). Correspondingly, the thermal conductivity of soils may exhibit considerable variation.

Fig. 7 shows the experimental results for thermal conductivity, λ , of frozen Yakutian alluvial soils in the wide range of saturation moisture contents W_{sat} . It should be noted that full saturation was assumed in the experiments as a model of the natural state of permafrost soils. As is seen, the dependence of λ on W_{sat} differs between coarse- and fine-grained soils. With increasing W_{sat} , the thermal conductivity of the frozen sand at the point of full saturation decreases, while that of the silt-clay increases tending to the thermal conductivity of ice. The sand-silts are intermediate between these two soil types.

The observed differences in λ (W_{sat}) can be explained by the differences in the unfrozen water content and in the mineralogical composition of the soils. In the fine soils, the unfrozen water content is quite high (about 0.1) at the measurement temperatures (about -10°C). At low moisture contents, silt-clay can thus be considered as an unfrozen soil. The effect of ice inclusions on overall heat conduction increases with increasing water content, resulting in higher soil thermal conductivity. At high moisture contents, the thermal conductivity of the silt-clay tends to that of ice. In the sands, the unfrozen water content is low and the mineral particles are in direct contact with ice. As the mineral particles have a higher thermal conductivity than ice, the thermal conductivity of the sand decreases with increasing water (ice) content. The same is true for the unfrozen soils. The effect of the unfrozen water film coating the mineral particles is less in the sand-silt compared to the silt-clay. The thermal conductivity of the "mineral particle + unfrozen water" system is likely to have the same values as for ice. The frozen saturated sand-silt has therefore a nearly constant thermal conductivity over the entire range of saturation moisture contents. The mineralogical composition has also an effect, resulting in an increase in the thermal conductivity of solids from finer to coarser soils.

The above features of permafrost thermal conductivity can be estimated based on the analytical theory of thermal conductivity of composite materials. The possible structural models of soil follow from the mechanism of water binding by mineral particles. Soil particles possess excess surface energy which depends on their size and mineral composition. When water enters the ground, it interacts with the mineral particles under the influence of molecular forces and surrounds them in concentric layers until the excess of surface energy is removed. The particles interact through the bound water layer, forming a stable system with dispersed particles. The remaining part of the soil pores is filled with free water. As the soil temperature decreases, primarily near 0°C , the free water begins to freeze. Then more of the bound water freezes with a further decrease in temperature. The strongly bound water remains unfrozen down to about -20°C . When frozen, the system of dispersed particles is cemented by ice, becoming even more stable. Hence, the thermal conductivity of fine-grained permafrost soils at different subzero temperatures can be estimated considering a three-component shell system (mineral particle + unfrozen water + ice) as shown in Fig. 8. Mineral particles in this scheme are assumed to be spherical in shape.

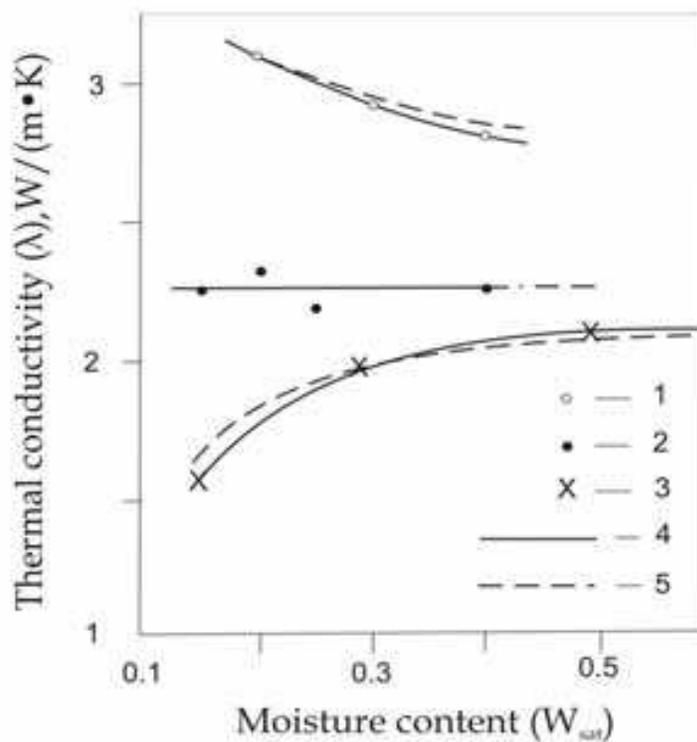


Fig. 7. Thermal conductivity vs. saturation moisture content for alluvial sediments in frozen state: 1 - sand; 2 - sand-silt; 3 - silt-clay; 4 - experimental curves; 5 - predicted curves

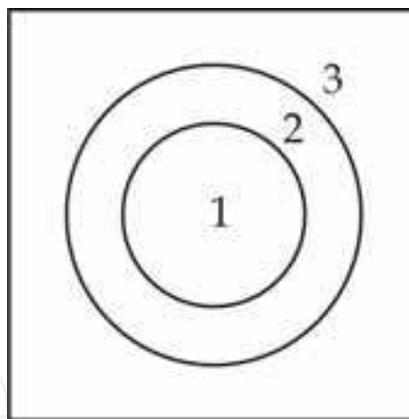


Fig. 8. Three-component shell medium: 1 - soil mineral particle; 2 - unfrozen water; 3 - ice

The effective conductivity λ of such a shell system can be predicted using the Maxwell method based on the solution of Laplace's equation for a medium with a constant temperature gradient at a distance from the spherical particle with a shell. The equation has the form (Belskaya, 1981)

$$\frac{\lambda - \lambda_i}{\lambda - 2\lambda_i} = \frac{\sigma \left[\lambda_{uw} - \lambda_i - \frac{\varepsilon(\lambda_{uw} - \lambda_s)(2\lambda_{uw} + \lambda_i)}{2\lambda_{uw} + \lambda_s} \right]}{2\lambda_i + \lambda_{uw} + \frac{2\varepsilon(\lambda_{uw} - \lambda_s)(\lambda_i - \lambda_{uw})}{2\lambda_{uw} + \lambda_s}}, \quad (32)$$

where $\varepsilon = \frac{4\pi R_s^3}{3} / \frac{4\pi R_{uw+s}^3}{3}$ is the volume fraction of the mineral soil solids in the two-component system consisting of mineral solids and unfrozen water; σ is the volume fraction of the mineral solids and unfrozen water in the soil; the subscripts "s", "i" and "uw" refer to the mineral solids, ice and unfrozen water, respectively.

Parameters ε and ν in Eq. (32) can be expressed in terms of the volume fractions of soil solids m_s and unfrozen water m_{uw}

$$\varepsilon = \frac{m_s}{m_s + m_{uw}} \text{ and } \sigma = m_s + m_{uw}$$

Considering the relation of m_s and m_{uw} to the saturation moisture content W_{sat} and unfrozen water content m_{uw}

$$m_s = \frac{\rho_s}{1 + W_{sat}\rho_s} \text{ and } m_{uw} = \frac{\rho_s W_{uw}}{1 + W_{sat}\rho_s},$$

(ρ_s is the solids density), we finally obtain the following expression for the thermal conductivity λ of a saturated frozen soil (Gavriliiev, 1989):

$$\lambda = \lambda_i \frac{N + 2M}{N - M}, \tag{33}$$

where

$$N = (1 + W_{sat}\rho_s) \left[2\lambda_i + \lambda_{uw} + \frac{2}{1 + W_{uw}\rho_s} \cdot \frac{(\lambda_{uw} - \lambda_s)(\lambda_i - \lambda_{uw})}{2\lambda_{uw} + \lambda_s} \right], \tag{34}$$

$$M = (1 + W_{uw}\rho_s)(\lambda_{uw} - \lambda_i) - \frac{(\lambda_{uw} - \lambda_s)(2\lambda_{uw} + \lambda_i)}{2\lambda_{uw} + \lambda_s}. \tag{35}$$

In Eqs. (33) - (35), all limiting conditions are satisfied. At $W_{sat} \rightarrow \infty$, $\lambda = \lambda_i$. If $W_{sat} = 0$ and $W_{uw} = 0$, then $\lambda = \lambda_s$. When $W_{uw} = 0$, the well-known Maxwell-Odolevsky equation for a two-component medium is obtained, which can be expressed in terms of moisture content as

$$\lambda = \lambda_i \frac{(1 + W_{sat}\rho_s)(2\lambda_i + \lambda_s) + 2(\lambda_s - \lambda_i)}{(1 + W_{sat}\rho_s)(2\lambda_i + \lambda_s) - (\lambda_s - \lambda_i)}. \tag{36}$$

Eq. (36) is also applicable to unfrozen soils, if the thermal conductivity of water λ_w is used instead of λ_i .

The presence of entrapped air reduces the thermal conductivity of frozen soils, and this can be expressed as:

$$\lambda = \frac{2\lambda(1 + W\rho_s)}{2 + \rho_s(3W_{sat} - W)}, \tag{37}$$

where W is the actual moisture content of the soil which should vary in the range

$$W \geq \left(1 - \frac{0.4}{\rho_{\text{moi}}} \right) W_{\text{sat}} - \frac{0.4}{\rho_s}, \quad (38)$$

where ρ_{moi} is the parameter dependent on the soil condition which has a value of 1 above 0°C and 0.92 below 0°C.

The relation (38) may be particularly useful for estimating the thermal conductivity of the thawed soils where any excess water escapes on thawing (if the thawing layer is not underlain by frozen soil) and only part of the moisture is retained due to surface tension.

For actual computations, the values for thermal conductivity of soil constituents should be specified in Eqs. (34) and (35). For pure ice at $t = 0^\circ\text{C}$ $\lambda = 2.25 \text{ W}/(\text{m}\cdot\text{K})$. The thermal conductivity of unfrozen water can be taken approximately equal to that of free, i.e., $\lambda = 0.58 \text{ W}/(\text{m}\cdot\text{K})$, since all anomalies in the properties of bound water are related to its strongly adsorbed portion which is insignificant in amount. The thermal conductivity of mineral soil solids depends on the mineral composition of particles and may be approximately estimated by Eq. (14).

The distribution of minerals in soils is influenced by sedimentary conditions which vary widely in nature. The amount of minerals in a soil can be estimated approximately based on the relationship between particle mineralogy and size distribution. The three particle sizes used for soil classification are clay (< 0.002 mm), silt (0.002-0.05 mm), and sand (0.05-2.0 mm). In practice, it is assumed that the content of clay minerals, such as kaolinite, is equal to the amount of clay-sized particles and 50% of silt-sized particles (Kokshenov, 1957). The remainder of the soil consists predominantly of quartz and feldspar, and their relative proportions vary widely depending on the soil origin. If no appropriate data are available, the ratio of quartz to feldspar may be taken as 0.6:0.4 (Kokshenov, 1957).

In computations, the following values for λ_j may be used [$\text{W}/(\text{m}\cdot\text{K})$]: 6-7 for quartz, 1.9 for feldspars, and 1.2 for kaolinite.

The distribution of particle sizes in a soil strongly depends on sedimentation conditions. If no granulometric data are available, the values given in Table 1 may be used for approximate estimations.

| Soil type | Particle size | | |
|-----------|---------------|------|------|
| | Clay | Silt | Sand |
| Sand | 0.02 | 0.10 | 0.88 |
| Sand-silt | 0.06 | 0.30 | 0.64 |
| Silt-clay | 0.20 | 0.37 | 0.43 |

Table 1. Relative proportions of particles sizes in soils

Comparison of the predicted and experimental data (see Fig. 7) shows that Eqs. (33) - (35) provide satisfactory results. The following values were used in the computations: for λ_s [$\text{W}/(\text{m}\cdot\text{K})$]: 3.50 for sand, 2.70 for sand-silt, 2.30 for silt-clay; for W_{uw} : 0 for sand, 0.03 for sand-silt and 0.10 for silt-clay.

5. Effect of organic matter on soil thermal conductivity

The unconsolidated soil layer on the immediate surface of the earth is enriched with organic remains in the form of humus due to the effects of vegetation, animals (mainly

microorganisms), climate, and human activity. The presence of organic matter has a strong effect on the soil thermal properties.

Humic substances of the soil are specific high-molecular compounds. They play a significant role in creating the soil structure (Tsyganov, 1958). The organic substances exist in the form of very fine particles smaller than 0.2μ referred to as colloids. Colloids have a very large specific surface area that provides strong bonding of water in soil and the presence of large amounts of unfrozen water at temperatures below freezing. Colloidal particles occur as sols and gels. Sols are smaller particles which can aggregate into gels by coagulation. When bound with water, organic particles form colloidal micelles having a core of an electrically neutral mineral particle surrounded by ionic layers of adsorbed molecules of colloid aggregate matter (hydrates: SiO_2 , Al_2O_3 , MnO_2 , etc.) and electrolyte (water). At temperatures below 0°C , the diffuse layer of water freezes, while the bound water remains unfrozen.

At the present stage of research, the problem of organic content effect on the thermal conductivity of soils can only be approached using analytical methods, since there are virtually no experimental data available.

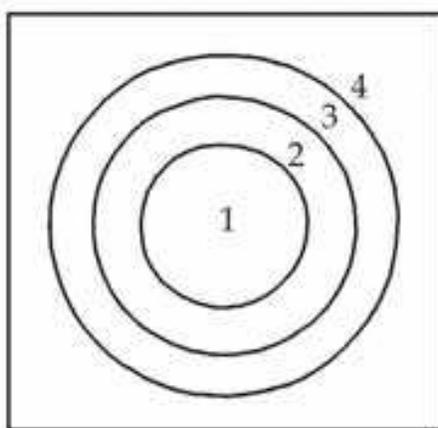


Fig. 9. Schematic representation of the saturated frozen organic soil: 1 - mineral particle; 2 - colloid aggregate; 3 - unfrozen water; 4 - ice

Let us consider the saturated soils. Based on the above consideration, the saturated soil containing organic matter can be represented as a four-component shell system within a cubic cell (Fig. 9) consisting of a mineral particle (1), organic matter (humus) (2), unfrozen water (3), and ice (4). The thermal conductivity of this system (frozen organic soil) calculated with the successive use of Maxwell's method is described by the equation (Gavrilyev, 2001)

$$\lambda_f = \lambda_4 \left[1 + \frac{3Z(1 - m_i)}{3\lambda_i + Zm_i} \right], \quad (39)$$

where

$$Z = \lambda_{uw} \frac{2\lambda_{uw} m_{uw} D + \lambda_{org} Q [3(1 - m_i) - 2m_{uw}]}{\lambda_{uw} D [3(1 - m_i) - m_{uw}] + \lambda_{org} m_{uw} Q} - \lambda_i, \quad (40)$$

$$D = \lambda_s m_{org} + \lambda_{org} (3m_s + m_{org}), \quad (41)$$

$$Q = 2\lambda_{\text{org}}m_{\text{org}} + \lambda_s(3m_s + m_{\text{org}}), \quad (42)$$

λ and m are the thermal conductivity and volume fractions of the components, respectively. In the saturated unfrozen organic soil, the ice content m_i is zero, and from Eq. (39) we obtain the following equation for the thermal conductivity λ_t

$$\lambda_t = \lambda_{\text{uw}} \frac{2\lambda_{\text{uw}}m_{\text{uw}}D + \lambda_{\text{org}}Q(3 - 2m_{\text{uw}})}{\lambda_{\text{uw}}D(3 - m_{\text{uw}}) + \lambda_{\text{org}}m_{\text{uw}}Q}. \quad (43)$$

The volume fractions of the components of the organic soil in the saturated state, m_s , m_{org} , m_{uw} and m_i , can be found using the following equations:

$$m_s = \frac{1}{1 + W_{\text{sat}}^0 \rho_s}, \quad (44)$$

$$m_{\text{org}} = \frac{n_{\text{org}}\rho_s m_s}{\rho_{\text{org}}(1 - n_{\text{org}})}, \quad (45)$$

$$m_{\text{uw}} = W_{\text{uw}}\gamma_d, \quad (46)$$

$$m_i = (W_{\text{sat}} - W_{\text{uw}})\gamma_d, \quad (47)$$

$$\gamma_d = \rho_s m_s + \rho_{\text{org}} m_{\text{org}}, \quad (48)$$

$$m_s + m_{\text{org}} + m_{\text{uw}} + m_i = 1, \quad (49)$$

where $n_{\text{org}} = P_{\text{org}}/(P_s + P_{\text{org}})$ is the relative weight of organic matter; P_s and P_{org} are the weights of the soil mineral particles and organic matter in the dry state; ρ is the unit weight of the components; W_{sat}^0 is the saturation moisture content of the soil containing no organic matter (fraction).

The saturation moisture content of the organic soil W_{sat} is related to that of the soil containing no organics W_{sat}^0 by the relationship:

$$W_{\text{sat}} = W_{\text{sat}}^0(1 - n_{\text{org}}) - \frac{n_{\text{org}}\rho_{\text{uw}}}{\rho_{\text{org}}}. \quad (50)$$

For the saturated organic soil, the following relationship is valid:

$$\gamma_d = \frac{\rho'_s}{1 + W_{\text{sat}}\rho'_s}, \quad (51)$$

where $\rho'_s = (\rho_s m_s + \rho_{\text{org}} m_{\text{org}}) / (m_s + m_{\text{org}})$ is the unit weight of the organic soil.

In computations of the thermal conductivity of organic soils using Eqs. (39) - (43), the following λ values (W/(m•K)) can be taken for components: $\lambda_{\text{org}}=0.26$ (Farouki 1986), $\lambda_{\text{uw}}=0.58$ and $\lambda_i=2.25$. The value of λ_s is a function of the soil type of the C horizon and can be estimated from the mineral composition of the particles by Eq. (14).

The λ_j values of minerals are available in reference books (Birch, 1942; Clark, 1966; Kobranova, 1962; Missenard, 1965; Smyslov et al., 1979). The unit weight of organic matter (ρ_{org}) by analogy with peat (Gavriliiev & Eliseev, 1970) can be taken as $1.48 \cdot 10^3 \text{ kg/m}^3$.

Fig. 10 shows the relationship between the thermal conductivity of a silt-clay [$\lambda_s=2.50 \text{ W/(m}\cdot\text{K)}$] and the saturation moisture content at different organic contents. It is seen that reduction in the soil thermal conductivity due to the presence of organic matter is strongest at low humus contents ($n_{\text{org}} < 0.1$).

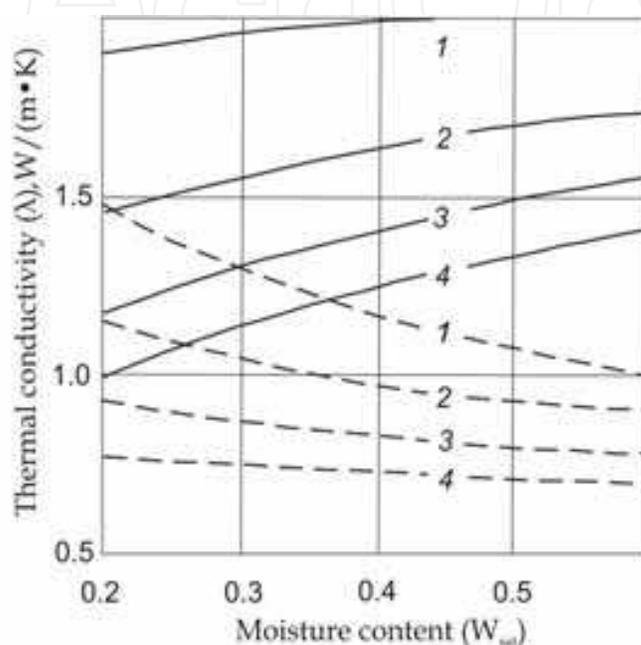


Fig. 10. Thermal conductivity of saturated silt-clay in frozen (solid lines) and thawed (dashed lines) states vs saturation moisture content W_{sat} at different organic contents n_{org} (unit fraction): 1 - 0; 2 - 0.1; 3 - 0.2; 4 - 0.3

We note in conclusion that Eq. (39) can lead to Eq. (33) for permafrost with no second component ($m_{\text{org}}=0$).

6. Summary

Frozen soils are complex multi-component and multi-phase systems consisting of mineral and organic particles, ice, unfrozen water, and gas (vapour). The specific conditions of sedimentation and subsequent diagenesis in permafrost environments result in sediments of permafrost-type with a very complex composition, structure and statistical particle distribution.

A deep understanding of the thermal properties of frozen soils can only be gained through an integral combination of experimental and analytical methods. Experimental methods have limitations in quantitative terms. Having obtained some basic information with experimental techniques, further in-depth study can be made using analytical methods. The development of theoretical approach is needed to understand heat transfer processes and to analyze experimental data on thermal properties of soils and rocks from a common point of view.

Considering the history of sediment formation over a geologic time, a universal model with changing particle shapes is proposed which describes the processes of rock formation from sediments, snow compaction and glacierization with account for diagenetic and post-diagenetic structural modifications, as well the processes of rock weathering and soil formation.

Based on the Maxwell's model with dispersed particles in the main medium, methods of estimating the thermal conductivity are given for:

1. Soils containing coarse inclusions and frozen soils of layered or reticulate cryostructure with account for variation in composition (a two-component system: coarse inclusions + fine fill, layers of frozen soil and ice for a case of layered cryostructure, and soil inclusions in the ice matrix for a case of reticulate cryostructure);
2. Permafrost with a massive cryostructure (a three-component spherical shell system: mineral particle + unfrozen water + ice);
3. Organic soils (a four-component spherical shell system: mineral particle + humus + unfrozen water + ice).

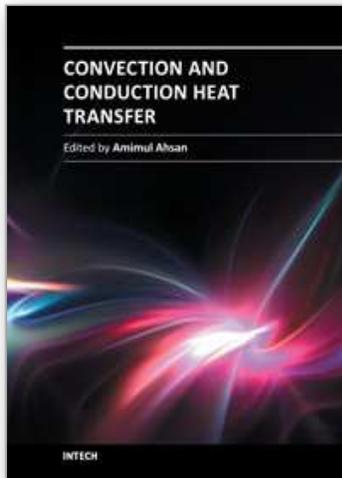
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The convection and conduction heat transfer, thermal conductivity, and phase transformations are significant issues in a design of wide range of industrial processes and devices. This book includes 18 advanced and revised contributions, and it covers mainly (1) heat convection, (2) heat conduction, and (3) heat transfer analysis. The first section introduces mixed convection studies on inclined channels, double diffusive coupling, and on lid driven trapezoidal cavity, forced natural convection through a roof, convection on non-isothermal jet oscillations, unsteady pulsed flow, and hydromagnetic flow with thermal radiation. The second section covers heat conduction in capillary porous bodies and in structures made of functionally graded materials, integral transforms for heat conduction problems, non-linear radiative-conductive heat transfer, thermal conductivity of gas diffusion layers and multi-component natural systems, thermal behavior of the ink, primer and paint, heating in biothermal systems, and RBF finite difference approach in heat conduction. The third section includes heat transfer analysis of reinforced concrete beam, modeling of heat transfer and phase transformations, boundary conditions-surface heat flux and temperature, simulation of phase change materials, and finite element methods of factorial design. The advanced idea and information described here will be fruitful for the readers to find a sustainable solution in an industrialized society.

How to reference

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