



DEVELOPMENT OF METHODS FOR DETERMINING DIFFUSION AND THERMAL CONDUCTIVITY COEFFICIENTS BASED ON THE HEAT AND MASS TRANSFER EQUATION

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ABSTRACT

This manuscript is devoted to the development of methods for finding the diffusion coefficient of soil moisture and the thermal conductivity coefficient of soil by using the system of Lykov's equations for heat and mass transfer in the soil. The conjugate system of partial differential equations is constructed by using the direct initial-boundary value problem and additional boundary conditions on the accessible boundary of the region. Iterative formulas for finding the diffusion coefficient of soil moisture and the thermal conductivity coefficient are derived from the minimization of specially constructed functional and solution of direct and conjugate problems. The direct and conjugate problems are discretized by the Dufort-Frankel Difference scheme. An algorithm for solving the coefficient-inverse problem is developed and the program is designed in Matlab software. Numerical calculations are conducted in order to verify the convergence of iterative processes.

Keywords: inverse problems, heat and mass transfer, conjugate problem, diffusion coefficient, thermal conductivity coefficient.

List of symbols

k_q	thermal conductivity coefficient	$[W/(m \cdot K)]$
k_m	moisture conductivity coefficient	$[kg/(m \cdot s \cdot ^\circ M)]$
c_q	heat capacity	$[J/(kg \cdot K)]$
c_m	moisture capacity	$[kg(moisture)/(kg(dry\ body) \cdot ^\circ M)]$
ρ	dry body density	$[kg/m^3]$
ε	ratio of vapor diffusion coefficient to the coefficient of total moisture diffusion	
λ	heat of phase change	$[J/kg]$
δ	thermogradient coefficient	$[^\circ M/K]$
α_q	convective heat transfer coefficient	$[W/(m^2 \cdot K)]$
α_m	convective mass transfer coefficient	$[kg/(m^2 \cdot s \cdot ^\circ M)]$
H	thickness	$[m]$
T_0	initial temperature	$[K]$
T_a	air temperature	$[K]$
U_0	initial moisture potential	$[^\circ M]$
U_a	air moisture potential	$[^\circ M]$

1. INTRODUCTION

The number of new porous materials in construction keeps increasing. Therefore, we have chosen the transfer of moisture and heat in a porous medium. The object of research is porous materials, while the subject of

research is a system of nonlinear differential equations with partial derivatives. The moisture-conducting and heat-conducting characteristics of new materials are usually unknown. In this regard, the development of methods for finding material parameters becomes a relevant task. Therefore, we aim to develop approximate methods for finding the above parameters. The purpose of research is to generate new methods for calculating the moisture-conducting characteristics of material. The research methodology is the method of mathematical modeling.

Moisture is a key factor in the durability and performance of buildings. Excessive levels reduce structural quality, affect indoor air quality, thermal comfort, along with energy efficiency in a building [1]. As a consequence, a number of models have been proposed by many scientists to predict the impact of moisture on the energy performance of buildings. The main overview can be found in the work [2]. Among the physical phenomena, the transport of air through porous construction medium has a decisive influence on the amount of moisture. Various studies enhance these effects using both experimental and numerical results [3]-[5]. Several numerical models are studied in order to predict the physical phenomena of conjugate transfer of heat, air, and moisture through porous building materials. Their physical concepts are based on conservation laws of mass for dry air, steam and liquid water, as well as on the conservation law of energy, which was described in detail in an early work of Lykov [6]. As a succession of his work, numerical models proposed in later studies can be divided into two main groups. The first group considers three evolutionary differential equations for calculating temperature, mass content, and air pressure in a porous medium. Papers [7] - [9] propose a model that investigates transfer through hollow porous blocks. It is based on an implicit finite



difference numeric scheme. Just recently, commercial COMSOLTM software has been used to research a numerical model for this kind of physical problems [10]. The authors of this work specify the scheme that is based on a time-explicit finite element approach. The main disadvantage of these numerical models is their computational cost. The implicit approach requires costly sub-iterations at each time step to handle severe nonlinearities of the problem. An explicit scheme requires very delicate time steps to satisfy the so-called Courant-Friedrichs-Levy (CFL) stability conditions. Indeed, the characteristic time of air transfer is very short in comparison with time for heat and mass transfer.

The substance associated with the capillary-porous body in the region of positive temperatures ($t > 0^\circ\text{C}$) can be in the form of liquid, vapor and inert gas; at negative temperatures ($t < 0^\circ\text{C}$) - in the form of ice, subcooled liquid, vapor and gas [11]. Depending on the type of relation between moisture and body, the freezing temperature of liquid will vary within wide ranges [12 - 14]. Therefore, there is always a certain amount of subcooled liquid in capillary-porous bodies at negative temperatures with different forms of moisture bonding [15, 16].

The second specific feature of mass and heat transfer in capillary-porous bodies is the partial filling of pores and capillaries with moisture. That is, part of the capillaries is filled with liquid and ice, and the rest is filled with a vapor-gas mixture. The amount of moisture changes in the process of mass and heat transfer for both states [17]. Therefore, when deriving transfer equations, it is necessary to take into account the change in the concentration of moisture in capillaries of the body. Methods for solving inverse problems are studied in [18, 19]. Kabanikhin S. I. *et al* [19] investigated the mass transfer in liquid, which is governed by the equation with liquid diffusion coefficient depended on the concentration. Numerical algorithm for solving direct and inverse problems is presented. The works [20, 21] researches the method of numerical construction of curvilinear structured grids in doubly connected domains and the numerical simulation of convective flow of an unevenly heated fluid in a curvilinear coordinate system. Calculations were performed for various configurations of the cavity and temperature conditions at the boundary.

2. MATHEMATICAL MODEL

The mathematical model of interrelated heat and mass transfer in one-dimensional case is written in the form of system of Lykov's differential equations [6]:

$$C_q \rho \frac{\partial \theta}{\partial t} = \frac{\partial}{\partial x} \left(k_q \frac{\partial \theta}{\partial x} \right) + \varepsilon r \frac{\partial W}{\partial t}, \quad (1)$$

$$\frac{\partial W}{\partial t} = \frac{\partial}{\partial x} \left(D_w \frac{\partial W}{\partial x} + D_\theta \frac{\partial \theta}{\partial x} \right). \quad (2)$$

Here $\theta(x, t)$ and $W(x, t)$ are functions that characterize the change in temperature and mass transfer potential, x is the stretched coordinate over the layer thickness, t is the time, $r = \lambda \rho C_m$, D_w is diffusion coefficient and D_θ is thermal diffusion coefficient.

Boundary conditions of the third kind for possible real situations on the earth's surface are revealed as:

$$k_q \frac{\partial \theta}{\partial x} \Big|_{x=H} = -\alpha_q (\theta - \theta_a(t)) \Big|_{x=H} - (1 - \varepsilon) r \alpha'_m (W - W_a(t)) \Big|_{x=H}, \quad (3)$$

$$\left(D_w \frac{\partial W}{\partial x} + D_\theta \frac{\partial \theta}{\partial x} \right) \Big|_{x=H} = -\alpha'_m (W - W_a(t)) \Big|_{x=H}, \quad (4)$$

$$\text{where } \alpha'_m = \frac{\alpha_m}{\rho C_m}.$$

Boundary conditions at the lower boundary of the region $x = 0$ are:

$$\frac{\partial \theta(x, t)}{\partial x} \Big|_{x=0} = 0, \quad \frac{\partial W(x, t)}{\partial x} \Big|_{x=0} = 0. \quad (5)$$

At the initial moment of time, the following conditions are set:

$$\theta(x, t) \Big|_{t=0} = T_0, \quad W(x, t) \Big|_{t=0} = W_0. \quad (6)$$

In addition, measured values of temperature and moisture potential $T_g(t)$, $W_g(t)$ on the earth's surface are given. It is required to determine the distribution of heat and moisture, the diffusion coefficient D_w and the thermal conductivity coefficient k_q . The inverse problem is solved in the area $Q = (0, H) \times (0, t_{\max})$.

2.1 System of Equations in Dimensionless Variables

After converting the original system of differential equations (1) - (6) to the dimensionless form we obtain:

$$\frac{\partial T(x^*, t^*)}{\partial t^*} = k_q^* F_{11} \frac{\partial^2 T(x^*, t^*)}{\partial x^{*2}} + F_{12} \varepsilon \frac{\partial U(x^*, t^*)}{\partial t^*}, \quad (7)$$

$$\frac{\partial U(x^*, t^*)}{\partial t^*} = D_w^* F_{21} \frac{\partial^2 T(x^*, t^*)}{\partial x^{*2}} + D_w^* F_{22} \frac{\partial^2 U(x^*, t^*)}{\partial x^{*2}}, \quad (8)$$

$$k_q^* F_{11} \frac{\partial T(1, t^*)}{\partial x^*} = -F_{oq1} (T(1, t^*) - T_a(t^*)) - (1 - \varepsilon) F_{oq2} (U(1, t^*) - U_a(t^*)), \quad (9)$$

$$D_w^* F_{22} \frac{\partial U(1, t^*)}{\partial x^*} + D_w^* F_{21} \frac{\partial T(1, t^*)}{\partial x^*} = -F_{om} (U(1, t^*) - U_a(t^*)), \quad (10)$$



$$\left. \frac{\partial T(0, t^*)}{\partial x^*} \right|_{x^*=0} = 0, \quad \left. \frac{\partial U(0, t^*)}{\partial x^*} \right|_{x^*=0} = 0, \quad (11)$$

$$T(x^*, 0) = 1, \quad U(x^*, 0) = 1, \quad (12)$$

Where $F_{11} = \frac{k_q t_{max}}{C_q \rho H^2}$, $F_{12} = \frac{r W_0}{C_q \rho T_0}$, $t^* = \frac{t}{t_{max}}$,
 $x^* = \frac{x}{H}$, $T = \frac{\theta}{T_0}$, $U = \frac{W}{W_0}$, $F_{21} = \frac{D_{W0} \delta T_0 t_{max}}{W_0 H^2}$,
 $F_{22} = \frac{D_{W0} t_{max}}{H^2}$, $D_W^* = \frac{D_W}{D_{W0}}$, $F_{oq1} = \frac{\alpha_q t_{max}}{\rho C_q H}$,
 $F_{oq2} = \frac{\alpha_m \lambda W_0 t_{max}}{\rho C_q T_0 H}$, $F_{om} = \frac{\alpha_m t_{max}}{\rho C_m H}$.

In the discussion that follows, x^* , t^* , k_q^* and D_W^* will be denoted as x , t , k_q and D_W .

2.2 Construction of Conjugate Problem

The measured values of temperature and moisture in dimensionless form are written in the following form:

$$U_g^*(t) = \frac{W_g(t)}{W_0}, \quad T_g^*(t) = \frac{T_g(t)}{T_0},$$

where W_0 and T_0 are taken from the initial condition.

$$\frac{\partial \Delta T(x, t)}{\partial t} = k_q F_{11} \frac{\partial^2 \Delta T(x, t)}{\partial x^2} + \Delta k_q F_{11} \frac{\partial^2 \Delta T(x, t)}{\partial x^2} + \Delta k_q F_{11} \frac{\partial^2 T(x, t)}{\partial x^2} + F_{12} \varepsilon \frac{\partial \Delta U(x, t)}{\partial t}, \quad (14)$$

$$\begin{aligned} \frac{\partial \Delta U(x, t)}{\partial t} &= D_W F_{21} \frac{\partial^2 \Delta T(x, t)}{\partial x^2} + \Delta D_W F_{21} \frac{\partial^2 \Delta T(x, t)}{\partial x^2} + \Delta D_W F_{21} \frac{\partial^2 T(x, t)}{\partial x^2} + \\ &+ D_W F_{22} \frac{\partial^2 \Delta U(x, t)}{\partial x^2} + \Delta D_W F_{22} \frac{\partial^2 \Delta U(x, t)}{\partial x^2} + \Delta D_W F_{22} \frac{\partial^2 U(x, t)}{\partial x^2}, \end{aligned} \quad (15)$$

$$k_q F_{11} \frac{\partial \Delta T(1, t)}{\partial x} + \Delta k_q F_{11} \frac{\partial \Delta T(1, t)}{\partial x} + \Delta k_q F_{11} \frac{\partial T(1, t)}{\partial x} = -F_{oq1} \Delta T(1, t) - (1 - \varepsilon) F_{oq2} \Delta U(1, t), \quad (16)$$

$$\begin{aligned} D_W F_{21} \frac{\partial \Delta T(x, t)}{\partial x} + \Delta D_W F_{21} \frac{\partial \Delta T(x, t)}{\partial x} + \Delta D_W F_{21} \frac{\partial T(x, t)}{\partial x} + \\ + D_W F_{22} \frac{\partial \Delta U(x, t)}{\partial x} + \Delta D_W F_{22} \frac{\partial \Delta U(x, t)}{\partial x} + \Delta D_W F_{22} \frac{\partial U(x, t)}{\partial x} = -F_{om} \Delta U(1, t), \end{aligned} \quad (17)$$

$$\left. \frac{\partial \Delta T(0, t)}{\partial x} \right|_{x=0} = 0, \quad \left. \frac{\partial \Delta U(0, t)}{\partial x} \right|_{x=0} = 0, \quad (18)$$

$$\Delta T(x, 0) = 0, \quad \Delta U(x, 0) = 0. \quad (19)$$

Using the system (7) - (12), it is required to determine $T(x, t)$, $U(x, t)$, D_W , k_q .

From this point on, $U_g^*(t)$ and $T_g^*(t)$ will be denoted as $U_g(t)$ and $T_g(t)$.

The problem is solved by an iterative method. Firstly, the initial approximations $D_W(n)$ and $k_q(n)$, when $n = 0$, are given and the next approximations are determined from the monotony of the functional

$$J(D_W, k_q) = \int_0^1 (T(1, t) - T_g(t))^2 dt + \int_0^1 (U(1, t) - U_g(t))^2 dt. \quad (13)$$

The corresponding solutions of the problem (7) - (12) for $D_W(n)$, $k_q(n)$ and $D_W(n+1)$, $k_q(n+1)$ are denoted as

$$\begin{aligned} T(x, t; n) &= T_n(x, t), \quad U(x, t; n) = U_n(x, t), \\ T(x, t; n+1) &= T_{n+1}(x, t), \quad U(x, t; n+1) = U_{n+1}(x, t). \end{aligned}$$

Hence for functions

$$\begin{aligned} \Delta T(x, t) &= T_{n+1}(x, t) - T_n(x, t), \\ \Delta U(x, t) &= U_{n+1}(x, t) - U_n(x, t), \end{aligned}$$

the following equalities are derived:

Multiply (14) by an arbitrary function $\psi(x, t)$ and integrate over the entire domain $Q = (0,1) \times (0,1)$.



After a single integration by parts over x and t , the next equality is obtained:

$$\begin{aligned}
 (\Delta T, \psi)_{t=0}^{t=1} - \left(\Delta T, \frac{\partial \psi}{\partial t} \right) &= \left(k_q F_{11} \frac{\partial \Delta T}{\partial x} + \Delta k_q F_{11} \frac{\partial \Delta T}{\partial x} + \Delta k_q F_{11} \frac{\partial T}{\partial x}, \psi \right)_{x=0}^{x=1} - \\
 - \left(k_q F_{11} \frac{\partial \Delta T}{\partial x} + \Delta k_q F_{11} \frac{\partial \Delta T}{\partial x} + \Delta k_q F_{11} \frac{\partial T}{\partial x}, \frac{\partial \psi}{\partial x} \right) &+ (\varepsilon F_{12} \Delta U, \psi)_{t=0}^{t=1} - \left(\varepsilon F_{12} \Delta U, \frac{\partial \psi}{\partial t} \right). \tag{20}
 \end{aligned}$$

We introduce the following notations:

$$(f, g) = \int_0^1 dt \int_0^1 f(x, t) g(x, t) dx,$$

$$(f, g)_{x=1} = \int_0^1 f(1, t) g(1, t) dt,$$

$$(f, g)_{t=1} = \int_0^1 f(x, 1) g(x, 1) dx.$$

Assume that $\psi(x, 1) = 0$, $\frac{\partial \psi(0, t)}{\partial x} = 0$.

Taking into account the initial-boundary conditions (12), (11), (9) and (18), we apply differentiation by parts over the variable x to the fourth term of the right-hand side of equality (20) and deduce that,

$$\begin{aligned}
 - \left(\Delta T, \frac{\partial \psi}{\partial t} \right) &= - (\Delta T, F_{oq1} \psi)_{x=1} - (\Delta U, (1 - \varepsilon) F_{oq2} \psi)_{x=1} - \left(\Delta T, k_q F_{11} \frac{\partial \psi}{\partial x} \right)_{x=1} - \\
 - \left(\Delta k_q F_{11} \frac{\partial T_{n+1}}{\partial x}, \frac{\partial \psi}{\partial x} \right) &+ \left(\Delta T, k_q F_{11} \frac{\partial^2 \psi}{\partial x^2} \right) - \left(\varepsilon F_{12} \Delta U, \frac{\partial \psi}{\partial t} \right). \tag{21}
 \end{aligned}$$

Now, we multiply (15) by an arbitrary function $\eta(x, t)$ and integrate over x from 0 to 1, and over t from 0

to 1. After a single integration by parts over x and t , the following equality is constructed:

$$\begin{aligned}
 (\Delta U, \eta)_{t=0}^{t=1} - \left(\Delta U, \frac{\partial \eta}{\partial t} \right) &= - (\Delta U, F_{om} \eta)_{x=1} - \left(D_w F_{22} \frac{\partial \Delta U}{\partial x} + \Delta D_w F_{22} \frac{\partial \Delta U}{\partial x} + \Delta D_w F_{22} \frac{\partial U}{\partial x} + \right. \\
 + D_w F_{21} \frac{\partial \Delta T}{\partial x} &+ \Delta D_w F_{21} \frac{\partial \Delta T}{\partial x} + \Delta D_w F_{21} \frac{\partial T}{\partial x}, \frac{\partial \eta}{\partial x} \left. \right). \tag{22}
 \end{aligned}$$

Suppose that $\eta(x, 1) = 0$, $\frac{\partial \eta(0, t)}{\partial x} = 0$

formula of integration by parts to the second and fifth term of the right-hand side of equality (22) we obtain

.Considering (12), (11), (10) and (19), and applying the

$$\begin{aligned}
 - \left(\Delta U, \frac{\partial \eta}{\partial t} \right) &= - (\Delta U, F_{om} \eta)_{x=1} - \left(D_w F_{22} \Delta U, \frac{\partial \eta}{\partial x} \right)_{x=1} - \left(D_w F_{21} \Delta T, \frac{\partial \eta}{\partial x} \right)_{x=1} - \\
 - \left(\Delta D_w F_{22} \frac{\partial U_{n+1}}{\partial x}, \frac{\partial \eta}{\partial x} \right) &- \left(\Delta D_w F_{21} \frac{\partial T_{n+1}}{\partial x}, \frac{\partial \eta}{\partial x} \right) + \left(\Delta U, D_w F_{22} \frac{\partial^2 \eta}{\partial x^2} \right) + \left(\Delta T, D_w F_{21} \frac{\partial^2 \eta}{\partial x^2} \right). \tag{23}
 \end{aligned}$$

By putting together equations (21), (22), and collecting similar terms, we derive that,

$$\begin{aligned}
 \left(\Delta T, \frac{\partial \psi}{\partial t} \right) - (\Delta T, F_{oq1} \psi)_{x=1} &- (\Delta U, (1 - \varepsilon) F_{oq2} \psi)_{x=1} - \left(\Delta T, k_q F_{11} \frac{\partial \psi}{\partial x} \right)_{x=1} + \left(\Delta T, k_q F_{11} \frac{\partial^2 \psi}{\partial x^2} \right) - \\
 - \left(\Delta k_q F_{11} \frac{\partial T_{n+1}}{\partial x}, \frac{\partial \psi}{\partial x} \right) &- \left(\Delta U, \varepsilon F_{12} \frac{\partial \psi}{\partial t} \right) + \left(\Delta U, \frac{\partial \eta}{\partial t} \right) - (\Delta U, F_{om} \eta)_{x=1} -
 \end{aligned}$$



$$\begin{aligned}
 & - \left(\Delta U, D_w F_{22} \frac{\partial \eta}{\partial x} \right) \Big|_{x=1} - \left(\Delta T, D_w F_{21} \frac{\partial \eta}{\partial x} \right) \Big|_{x=1} - \left(\Delta D_w F_{22} \frac{\partial U_{n+1}}{\partial x}, \frac{\partial \eta}{\partial x} \right) - \\
 & - \left(\Delta D_w F_{21} \frac{\partial T_{n+1}}{\partial x}, \frac{\partial \eta}{\partial x} \right) + \left(\Delta U, D_w F_{22} \frac{\partial^2 \eta}{\partial x^2} \right) + \left(\Delta T, D_w F_{21} \frac{\partial^2 \eta}{\partial x^2} \right). \tag{24}
 \end{aligned}$$

Functions $\psi(x, t)$ and $\eta(x, t)$ are selected in such a way that the following equality is valid:

$$\frac{\partial \psi}{\partial t} + \frac{\partial}{\partial x} \left(k_q F_{11} \frac{\partial \psi}{\partial x} \right) + \frac{\partial}{\partial x} \left(D_w F_{21} \frac{\partial \eta}{\partial x} \right) = 0, \tag{25}$$

$$\frac{\partial \eta}{\partial t} + \frac{\partial}{\partial x} \left(D_w F_{22} \frac{\partial \eta}{\partial x} \right) - \varepsilon F_{12} \frac{\partial \psi}{\partial t} = 0. \tag{26}$$

And we set the following boundary conditions for functions $\psi(x, t)$ and $\eta(x, t)$:

$$- \left(F_{oq1} \psi + k_q F_{11} \frac{\partial \psi}{\partial x} + D_w F_{21} \frac{\partial \eta}{\partial x} \right) \Big|_{x=1} = 2(T(1, t) - T_g(t)), \tag{27}$$

$$\begin{aligned}
 & 2(T(1, t) - T_g(t), \Delta T) + 2(U(1, t) - U_g(t), \Delta U) = - \left(\Delta D_w F_{22} \frac{\partial U_{n+1}}{\partial x}, \frac{\partial \eta}{\partial x} \right) - \left(\Delta D_w F_{21} \frac{\partial T_{n+1}}{\partial x}, \frac{\partial \eta}{\partial x} \right) - \\
 & - \left(\Delta k_q F_{11} \frac{\partial T_{n+1}}{\partial x}, \frac{\partial \psi}{\partial x} \right). \tag{31}
 \end{aligned}$$

$$\begin{aligned}
 & J(D_w(n+1), k_q(n+1)) - J(D_w(n), k_q(n)) = 2 \int_0^1 (T(1, t) - T_g(t)) \Delta T(1, t) dt + 2 \int_0^1 (U(1, t) - U_g(t)) \Delta U(1, t) dt + \\
 & + \int_0^1 (\Delta T(1, t))^2 dt + \int_0^1 \Delta(U(1, t))^2 dt.
 \end{aligned}$$

Taking into account (31), we derive the equality:

$$\begin{aligned}
 & J(D_w(n+1), k_q(n+1)) - J(D_w(n), k_q(n)) = \int_0^1 (\Delta T(1, t))^2 dt + \int_0^1 \Delta(U(1, t))^2 dt - \\
 & - F_{22} \left(\Delta D_w \frac{\partial \Delta U_n}{\partial x}, \frac{\partial \eta}{\partial x} \right) - F_{21} \left(\Delta D_w \frac{\partial \Delta T_n}{\partial x}, \frac{\partial \eta}{\partial x} \right) - F_{11} \left(\Delta k_q \frac{\partial \Delta T_n}{\partial x}, \frac{\partial \psi}{\partial x} \right) - \\
 & - \left(F_{22} \left(\Delta D_w \frac{\partial U_n}{\partial x}, \frac{\partial \eta}{\partial x} \right) - F_{21} \left(\Delta D_w \frac{\partial T_n}{\partial x}, \frac{\partial \eta}{\partial x} \right) - F_{11} \left(\Delta k_q \frac{\partial T_n}{\partial x}, \frac{\partial \psi}{\partial x} \right) \right).
 \end{aligned}$$

The first five terms on the right-hand side of equality are the second-order infinitesimal. Therefore, the sign of the left-hand side is determined by the sign of the last three terms standing on the right-hand side of the equal sign. We aim for the monotonical decrease of functional from iteration to iteration, hence,

$$- \left((1 - \varepsilon) F_{oq2} \psi + F_{om} \eta + D_w F_{22} \frac{\partial \eta}{\partial x} \right) \Big|_{x=1} = 2(U(1, t) - U_g(t)) \tag{28}$$

$$\frac{\partial \psi(0, t)}{\partial x} = 0, \quad \frac{\partial \eta(0, t)}{\partial x} = 0, \tag{29}$$

At $t = 1$ the following conditions are set:

$$\psi(x, 1) = 0, \quad \eta(x, 1) = 0. \tag{30}$$

System (25) - (30) is called the conjugate problem of the system (7) - (12).

2.3 Iterative Formula for Calculating Coefficients

After construction of conjugate problem, the following integral equality is derived from the equality (24)

Subtracting values of the functional of two different iterations from the formula (13), we deduce that,

$$D_w(n+1) = D_w(n) + \beta_1(n) \left(F_{22} \left(\frac{\partial U_n}{\partial x}, \frac{\partial \eta}{\partial x} \right) + F_{21} \left(\frac{\partial T_n}{\partial x}, \frac{\partial \eta}{\partial x} \right) \right),$$

$$k_q(n+1) = k_q(n) + \beta_2(n) F_{11} \left(\frac{\partial T_n}{\partial x}, \frac{\partial \psi}{\partial x} \right).$$

where

$$\beta_1(n) = \frac{\bar{\beta}_1}{(1+n)^{\mu_1}}, \quad \beta_2(n) = \frac{\bar{\beta}_2}{(1+n)^{\mu_2}}; \quad \mu_1, \mu_2 > 1 \text{ are}$$

descent parameters.

3. NUMERICAL RESULTS

The computational experiment was carried out by the Matlab software package. In order to verify feasibility of the method, the following experimentally determined thermophysical soil characteristics are taken from [22]:



thermal conductivity coefficient, $k_q = 0.65 \text{ W}/(\text{m} \cdot \text{K})$;
 moisture conductivity coefficient,
 $k_m = 2.2 \times 10^{-8} \text{ kg}/(\text{m} \cdot \text{s} \cdot ^\circ \text{M})$;
 heat capacity, $c_q = 2500 \text{ J}/(\text{kg} \cdot \text{K})$;
 moisture capacity,
 $c_m = 0.01 \text{ kg}(\text{moisture})/(\text{kg}(\text{dry body}) \cdot ^\circ \text{M})$;
 dry body density, $\rho = 370 \text{ kg}/\text{m}^3$;
 ratio of vapor diffusion coefficient to the coefficient of
 total moisture diffusion, $\varepsilon = 0.3$;
 heat of phase change, $\lambda = 2.5 \times 10^6 \text{ J}/\text{kg}$;
 thermogradient coefficient, $\delta = 2.0 \text{ }^\circ \text{M}/\text{K}$;
 convective heat transfer coefficient,
 $\alpha_q = 22.5 \text{ W}/(\text{m}^2 \cdot \text{K})$;
 convective mass transfer coefficient,
 $\alpha_m = 2.5 \times 10^{-6} \text{ kg}/(\text{m}^2 \cdot \text{s} \cdot ^\circ \text{M})$.

At $t = 0$, the material is considered with uniform fields, with a temperature $T_0 = 10^\circ \text{C}$ and initial moisture potential $U_0 = 86^\circ \text{M}$. The boundary conditions are represented by air temperature $T_a = 20^\circ \text{C}$ and air moisture potential $U_a = 4^\circ \text{M}$. The computational experiment is carried out for soil with a depth of 1 m, within 24 hours.

Dimensionless numerical values are obtained by using formulas from chapter 2. The numerical solution is calculated by DuFort–Frankel different scheme with spatial discretization parameter $\Delta x = 10^{-2}$ and time discretization parameter $\Delta t = 10^{-3}$.

Figures 1 and 2 show the numerical results obtained at $\Delta x = 10^{-2}$, $\Delta t = 10^{-3}$ with initial approximations of the iterative method, diffusion and thermal conductivity coefficients of which deviate from the exact value by 20%.

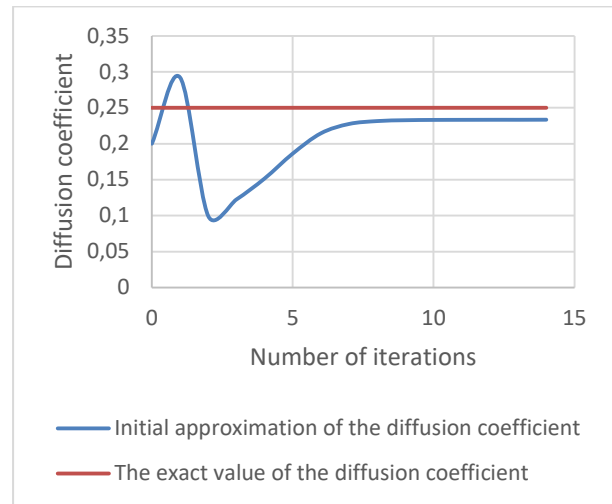


Figure-1. Diffusion coefficient with an initial approximation deviated by 20%.

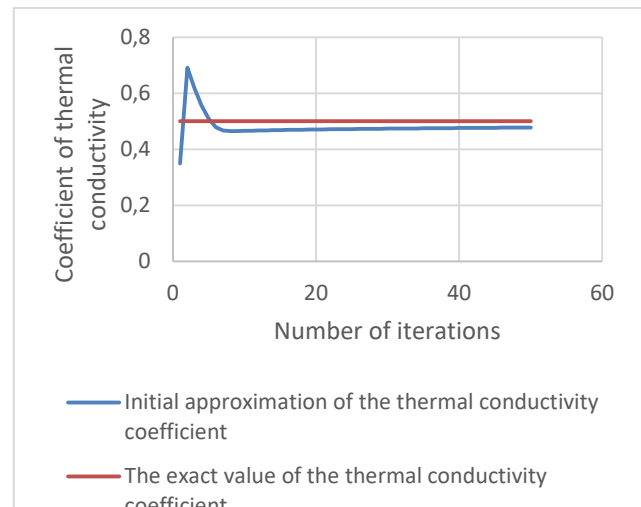


Figure-2. Thermal conductivity coefficient with an initial approximation deviated by 20%.

Figures 3 and 4 show the results of calculating diffusion and thermal conductivity coefficients with initial approximations deviated from the exact value by 35% at $\Delta x = 10^{-2}$, $\Delta t = 10^{-3}$.

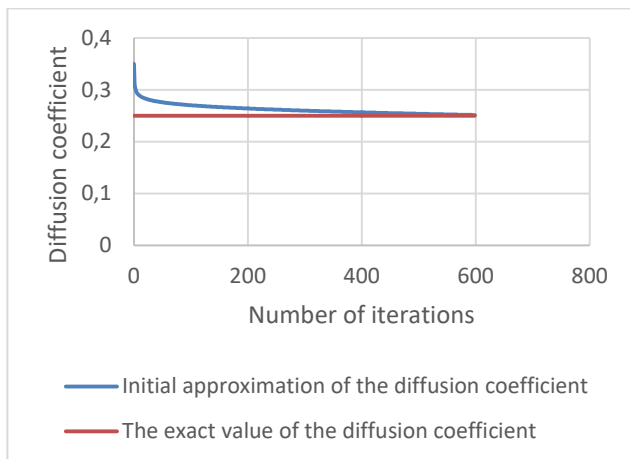


Figure-3. Diffusion coefficient with an initial approximation deviated by 35%.

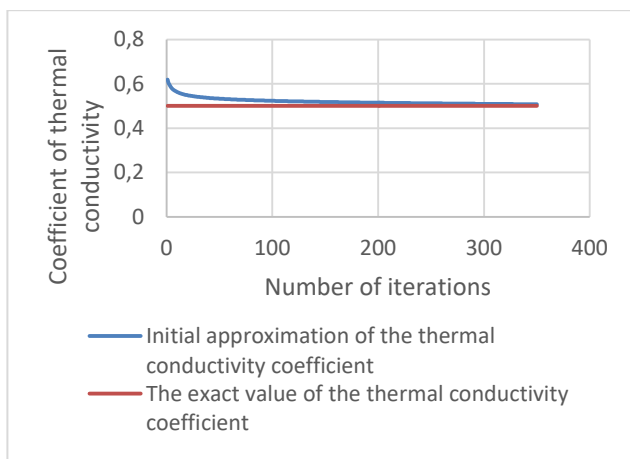


Figure-4. Thermal conductivity coefficient with an initial approximation deviated by 35%.

4. CONCLUSIONS AND DISCUSSIONS

In this paper, we consider the inverse problem for a system of partial differential equations, which describes the transfer of moisture and heat in the soil. The following results are obtained:

- a conjugate problem is derived from the direct initial-boundary value problem of heat and moisture transfer;
- iterative formulas for calculating the thermal conductivity and diffusion coefficients are derived based on the minimization of functional;
- direct and conjugate difference problems are constructed using the DuFort-Frankel scheme;
- an algorithm is developed for solving the inverse problem and the program is designed in the Matlab software package;
- numerical calculations have been carried out in order to prove the convergence of iterative processes.

It should be noted that the Dufort-Frankel scheme is used to solve the system (1) - (2) in [23]. And this work demonstrates that the Dufort-Frankel scheme is unconditionally stable. However, our numerical

calculations show that the solution of the inverse problem of finding diffusion and thermal conductivity coefficients by Dufort-Frankel scheme gives conditional stability at $\Delta t \leq 10^{-3}$.

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