METHODS OF FINDING DIFFUSION AND THERMAL CONDUCTIVITY COEFFICIENTS OF HEAT AND MASS TRANSFER

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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 package. 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.

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ЖЫЛУ ЖӘНЕ ЫЛҒАЛ ТАСЫМАЛЫНЫҢДИФФУЗИЯ ЖӘНЕ ЖЫЛУӨТКІЗГІШТІК КОЭФФИЦИЕНТТЕРІН ТАБУ ТӘСІЛДЕРІ

Бұл мақалада Лыков теңдеулер жүйесімен берілген топырақтағы жылу және ылғал тасымалының диффузиялық коэффициенті мен жылу өткізгіштік коэффициентін табу әдістері қарастырылады. Бастапқы-шектік тура есеп жәнеқолжетімді шекарада алынған қосымша шекаралық шарттар көмегімен түйіндес есеп құрастырылады. Топырақ ылғалдылығының диффузиялық коэффициенті және жылу өткізгіштік коэффициентін табудың итерациялық формулалары арнайы құрастырылған функционалды минимумға келтіре отырып және тура және қосымша есептерді шешу арқылы алынды. Тура және қосымша есеп Дюфарт-Франкель әдісімен шешілді. Коэффициенттік кері есепті шешу алгоритмі жасалып, Matlab бағдарламалық пакетінде программа жазылды. Итерациялық процестердің жинақтылығын тексеру үшін сандық есептеулер жүргізілді.
Түйін сөздер: кері есептер, жылу және ылғалтасымалы, түйіндес есеп, диффузия коэффициенті, жылуөткізгіштік коэффициенті.

Аннотация
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МЕТОДЫ НАХОЖДЕНИЯ КОЭФФИЦИЕНТОВ ДИФФУЗИИ И ТЕПЛОПРОВОДНОСТИ ТЕПЛОМАССОПЕРЕНОСА

Данная статья посвящена разработке методов нахождения коэффициента диффузии почвенной влаги и коэффициента теплопроводности почвы с использованием системы уравнений Лыкова для тепломассопереноса в почве. С помощью прямой начально-краевой задачи и дополнительных краевых условий на доступной границе строится сопряженная задача. Получены итерационные формулы нахождения коэффициента диффузии почвенной влаги и коэффициента теплопроводности путем минимизации специально построенного функционала

и решения прямой и сопряженной задачи. Прямая и сопряженная задача дискретизируется методом Дюфарта-Франкеля. Разработан алгоритм решения коэффициентно-обратной задачи и написана программа в пакете программ Matlab. Для проверки сходимости итерационных процессов проводятся численные расчеты.

Ключевые слова: обратные задачи, тепломассообмен, сопряженная задача, коэффициент диффузии, коэффициент теплопроводности.

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 interior air quality, heatingcomfort, along with energy efficiency in a building [1]. As a result, several models have been proposed by many scientists to forecast the influence of moisture on the energy performance of buildings. The main overview on this topic is given in the work [2]. From the physical point of view, the transport of air through porous construction medium has a decisive influence on the amount of moisture. Various studies emphasize these effects using experimental and numerical results [3] - [4]. A number of numerical models are studied in order to forecast the physical phenomena of conjugate transfer of heat, moisture and air through porous materials of building. Physical concepts of the study are based on conservation laws of mass for dry air, steam and liquid water, in addition to it on the conservation law of energy, which was described in detail in an early work of Lykov [5]. As a succession of the work, numerical models presented in later studies can be splitted into two major groups. The first group considers three evolutionary differential equations for calculating temperature, mass content, and air pressure in a porous medium. Papers [6] - [7] 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 [8]. The authors of this work specify the scheme that is based on a time-explicit finite element approach. The main drawback of these numerical models ison their computational costs. The implicit scheme requires costly sub-iterations at eachperiod of time to deal with severe nonlinearities of the problem. An explicit approachneeds very delicate time steps to satisfy the Courant-Friedrichs-Levy (CFL) stability conditions. And, 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 can be in the form of liquid, vapor and inert gas; at negative temperatures - in the form of ice, subcooled liquid, vapor and gas. Depending on the type of relation between moisture and body, the freezing temperature of liquid will vary within wide ranges. Therefore, there is always a certain amount of subcooled liquid in capillary-porous bodies at negative temperatures with different forms of moisture bonding [9, 10].

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 [11]. 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 [12, 13]. Kabanikhin S. I. et al [13] 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.

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 [5]:

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

$$\frac{\partial W}{\partial t} = \frac{\partial}{\partial x}\left(D_W \frac{\partial W}{\partial x} + D_\theta \frac{\partial \theta}{\partial x}\right), \tag{2}$$

where θ and W are functions that characterize the change in temperature and mass transfer potential, respectively, x is the thickness of the layer, t is the time, D_W is diffusion coefficient, D_θ is thermal diffusion coefficient, C_q is the heat capacity, ρ is the density, k_q is the thermal conductivity coefficient, ε is the ratio of vapor diffusion coefficient to the coefficient of total moisture diffusion, and $r = \lambda \rho C_m$, where λ is the heat of phase change, C_m is the moisture capacity.

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

$$k_q \frac{\partial \theta}{\partial x}\bigg|_{x=H} = -\alpha_q\left(\theta - \theta_a(t)\right)\big|_{x=H} - (1-\varepsilon)r\alpha_m'\left(W - W_a(t)\right)\big|_{x=H}, \tag{3}$$

$$\left(D_W \frac{\partial W}{\partial x} + D_\theta \frac{\partial \theta}{\partial x}\right)\bigg|_{x=H} = -\alpha_m'\left(W - W_a(t)\right)\big|_{x=H}, \tag{4}$$

where α_q is the convective heat transfer coefficient, θ_a is the air temperature, W_a is the air moisture potential, and $\alpha_m' = \dfrac{\alpha_m}{\rho C_m}$, where α_m is the convective mass transfer coefficient.

Boundary conditions at the lower boundary of the region are:

$$\frac{\partial \theta(x,t)}{\partial x}\bigg|_{x=0} = 0, \qquad \frac{\partial W(x,t)}{\partial x}\bigg|_{x=0} = 0. \tag{5}$$

The following initial conditions are set:

$$\theta(x,t)\big|_{t=0} = T_0, \qquad W(x,t)\big|_{t=0} = W_0, \tag{6}$$

where T_0 is the initial temperature, W_0 is the initial moisture potential.

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 find the distribution of heat and moisture, the thermal conductivity coefficient k_q and the diffusion coefficient D_W. 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:

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

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

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

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

$$\frac{\partial T(0,t^*)}{\partial x^*}\bigg|_{x^*=0} = 0, \qquad \frac{\partial U(0,t^*)}{\partial x^*}\bigg|_{x^*=0} = 0, \tag{11}$$

$$T(x^*, 0) = 1, \qquad U(x^*, 0) = 1, \tag{12}$$

where

$$t^* = \frac{t}{t_{\max}}, \ x^* = \frac{x}{H}, \ T = \frac{\theta}{T_0}, \ U = \frac{W}{W_0}, D_W^* = \frac{D_W}{D_{W0}},$$

$$F_{11} = \frac{k_{q0}t_{\max}}{C_q \rho H^2} \ , F_{12} = \frac{rW_0}{C_q \rho T_0}, \ F_{21} = \frac{D_{W0}\delta T_0 t_{\max}}{W_0 H^2} \ , \ F_{22} = \frac{D_{W0}t_{\max}}{H^2},$$

$$F_{oq1} = \frac{\alpha_q t_{\max}}{\rho C_q H} \ , \ F_{oq2} = \frac{\alpha_m \lambda W_0 t_{\max}}{\rho C_q T_0 H} \ , F_{om} = \frac{\alpha_m t_{\max}}{\rho C_m H} \ .$$

2.2 Construction of conjugate problem

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

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

where W_0 and T_0 are taken from the initial condition.

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

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

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

$$T(x,t;n) = T_n(x,t), U(x,t;n) = U_n(x,t),$$
$$T(x,t;n+1) = T_{n+1}(x,t), U(x,t;n+1) = U_{n+1}(x,t).$$

Hence for functions

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

the following equalities are derived:

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

$$\frac{\partial \Delta U(x,t)}{\partial t} = D_W F_{21} \frac{\partial^2 \Delta T(x,t)}{\partial x^2} + \Delta D_W F_{21} \frac{\partial^2 \Delta T(x,t)}{\partial x^2} + \Delta D_W F_{21} \frac{\partial^2 T(x,t)}{\partial x^2} +$$
$$+ D_W F_{22} \frac{\partial^2 \Delta U(x,t)}{\partial x^2} + \Delta D_W F_{22} \frac{\partial^2 \Delta U(x,t)}{\partial x^2} + \Delta D_W F_{22} \frac{\partial^2 U(x,t)}{\partial x^2}, \tag{15}$$

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

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

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

$$\Delta T(x,0) = 0, \qquad \Delta U(x,0) = 0. \tag{19}$$

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:

$$\left(\Delta T, \psi\right)\Big|_{t=0}^{t=1} - \left(\Delta T, \frac{\partial \psi}{\partial t}\right) = \left(k_q F_{11} \frac{\partial \Delta T}{\partial x} + \Delta k_q F_{11} \frac{\partial \Delta T}{\partial x} + \Delta k_q F_{11} \frac{\partial T}{\partial x}, \psi\right)\Big|_{x=0}^{x=1} -$$

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

We introduce the following notations:

$$\left(f, g\right) = \int\limits_0^1 dt \int\limits_0^1 f(x,t)g(x,t)dx,$$

$$\left(f, g\right)\Big|_{x=1} = \int\limits_0^1 f(1,t)g(1,t)dt,$$

$$\left(f, g\right)\Big|_{t=1} = \int\limits_0^1 f(x,1)g(x,1)dx.$$

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

$$-\left(\Delta T, \frac{\partial \psi}{\partial t}\right) = -\left(\Delta T, F_{oq1}\psi\right)\Big|_{x=1} - \left(\Delta U, (1-\varepsilon)F_{oq2}\psi\right)\Big|_{x=1} - \left(\Delta T, k_q F_{11} \frac{\partial \psi}{\partial x}\right)\Big|_{x=1} -$$

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

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:

$$\left(\Delta U, \eta\right)\Big|_{t=0}^{t=1} - \left(\Delta U, \frac{\partial \eta}{\partial t}\right) = -\left(\Delta U, F_{om}\eta\right)\Big|_{x=1} - \left(D_W F_{22} \frac{\partial \Delta U}{\partial x} + \Delta D_W F_{22} \frac{\partial \Delta U}{\partial x} + \Delta D_W F_{22} \frac{\partial U}{\partial x} + \right.$$

$$\left. + D_W F_{21} \frac{\partial \Delta T}{\partial x} + \Delta D_W F_{21} \frac{\partial \Delta T}{\partial x} + \Delta D_W F_{21} \frac{\partial T}{\partial x}, \frac{\partial \eta}{\partial x}\right). \tag{22}$$

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

$$\left(\Delta T, \frac{\partial \psi}{\partial t}\right) - \left(\Delta T, F_{oq1}\psi\right)\Big|_{x=1} - \left(\Delta U, (1-\varepsilon)F_{oq2}\psi\right)\Big|_{x=1} - \left(\Delta T, k_q F_{11} \frac{\partial \psi}{\partial x}\right)\Big|_{x=1} + \left(\Delta T, k_q F_{11} \frac{\partial^2 \psi}{\partial x^2}\right) -$$

$$-\left(\Delta k_q F_{11} \frac{\partial T_{n+1}}{\partial x}, \frac{\partial \psi}{\partial x}\right) - \left(\Delta U, \varepsilon F_{12} \frac{\partial \psi}{\partial t}\right) + \left(\Delta U, \frac{\partial \eta}{\partial t}\right) - \left(\Delta U, F_{om}\eta\right)\Big|_{x=1} -$$

$$-\left(\Delta U, D_W F_{22} \frac{\partial \eta}{\partial x}\right)\Big|_{x=1} - \left(\Delta T, D_W F_{21} \frac{\partial \eta}{\partial x}\right)\Big|_{x=1} - \left(\Delta D_W F_{22} \frac{\partial U_{n+1}}{\partial x}, \frac{\partial \eta}{\partial x}\right) -$$

$$-\left(\Delta D_W F_{21} \frac{\partial T_{n+1}}{\partial x}, \frac{\partial \eta}{\partial x}\right) + \left(\Delta U, D_W F_{22} \frac{\partial^2 \eta}{\partial x^2}\right) + \left(\Delta T, D_W F_{21} \frac{\partial^2 \eta}{\partial x^2}\right). \tag{24}$$

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 $\eta(x,t)$:

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

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

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

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

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

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)

$$2(T(1,t) - T_g(t), \Delta T) + 2(U(1,t) - U_g(t), \Delta U) = -\left(\Delta D_W F_{22}\frac{\partial U_{n+1}}{\partial x}, \frac{\partial \eta}{\partial x}\right) - \left(\Delta D_W F_{21}\frac{\partial T_{n+1}}{\partial x}, \frac{\partial \eta}{\partial x}\right) -$$

$$-\left(\Delta k_q F_{11}\frac{\partial T_{n+1}}{\partial x}, \frac{\partial \psi}{\partial x}\right). \tag{31}$$

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

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

$$+ \int_0^1 (\Delta T(1,t))^2 dt + \int_0^1 \Delta(U(1,t))^2 dt.$$

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

$$J(D_W(n+1), k_q(n+1)) - J(D_W(n), k_q(n)) = \int_0^1 (\Delta T(1,t))^2 dt + \int_0^1 \Delta(U(1,t))^2 dt -$$

$$- F_{22}\left(\Delta D_W \frac{\partial \Delta U_n}{\partial x}, \frac{\partial \eta}{\partial x}\right) - F_{21}\left(\Delta D_W \frac{\partial \Delta T_n}{\partial x}, \frac{\partial \eta}{\partial x}\right) - F_{11}\left(\Delta k_q \frac{\partial \Delta T_n}{\partial x}, \frac{\partial \psi}{\partial x}\right) -$$

$$- \left(F_{22}\left(\Delta D_W \frac{\partial U_n}{\partial x}, \frac{\partial \eta}{\partial x}\right) - F_{21}\left(\Delta D_W \frac{\partial T_n}{\partial x}, \frac{\partial \eta}{\partial x}\right) - F_{11}\left(\Delta k_q \frac{\partial T_n}{\partial x}, \frac{\partial \psi}{\partial x}\right)\right).$$

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,

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

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

where $\beta_1(n) = \dfrac{\overline{\beta_1}}{(1+n)^{\mu_1}}$, $\beta_2(n) = \dfrac{\overline{\beta_2}}{(1+n)^{\mu_2}}$; $\mu_1, \mu_2 > 1$ are descent parameters.

3 Numericalresults

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 [14].

At $t = 0$, the material is considered with uniform fields, with a temperature $T_0 = 10^0 C$ and initial moisture potential $U_0 = 86\%$. The boundary conditions are represented by air temperature $T_a = 20^0 C$ and air moisture potential $U_a = 4^0 M$. 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%.
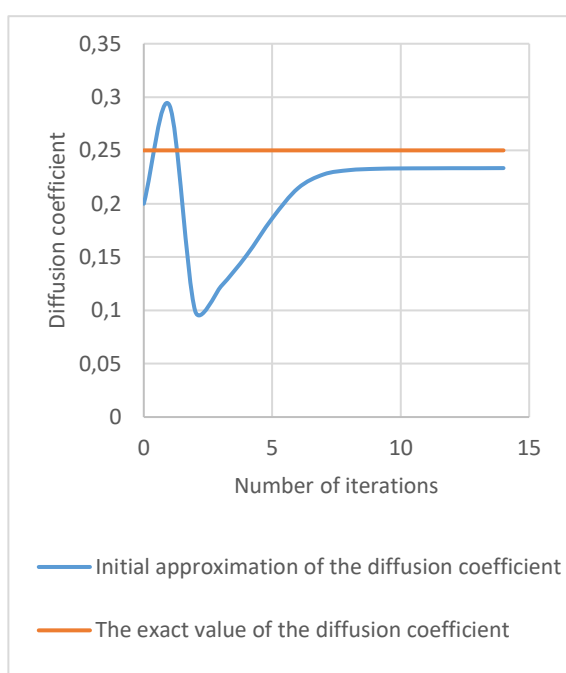

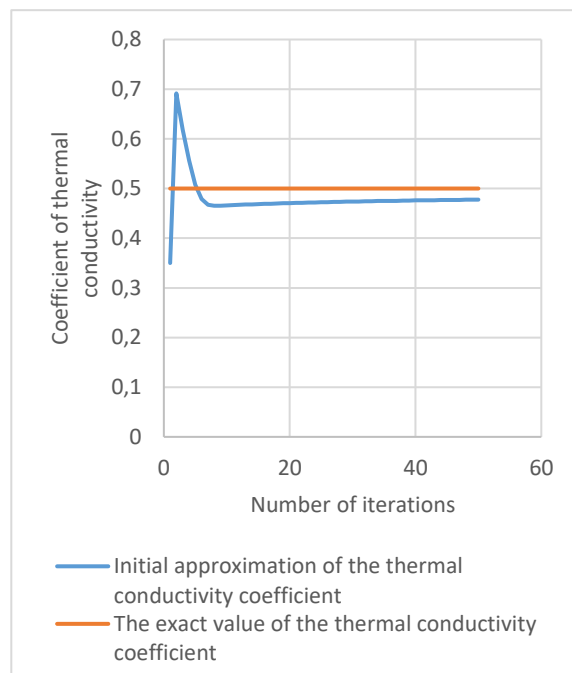*Figure 1. Diffusion coefficient with an initial approximation deviated by 20%*

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 $\Delta x = 10^{-2}$, $\Delta t = 10^{-3}$.
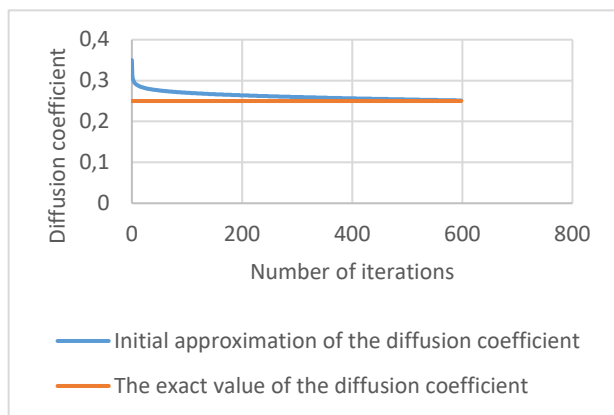
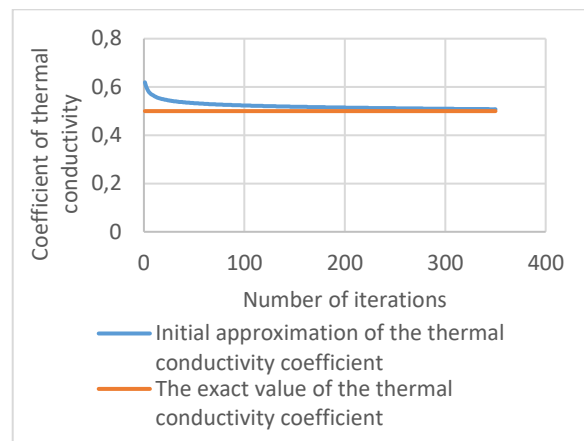*Figure 3. Diffusion coefficient with an initial approximation deviated by 35%*

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

4 Conclusions

In this paper, we consider the inverse problem of heat and mass transfer in the soil, which is described by the system of partial differential equations. The following results are obtained:

- a conjugate problem is derived from the direct initial-boundary heat and mass transferproblem;

-iterative formulas for calculating the thermal conductivity and diffusion coefficients are derived based on the functional minimization;

-direct and conjugate difference problems are constructed using the DuFort–Frankel scheme;

-an algorithm is developed for obtaining the unknown parameters of 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.

For solving the system (1) - (2) it was used the Dufort-Frankel scheme, which is described in detailin [15]. And this work demonstrates that the Dufort-Frankel scheme is unconditionally stable. However, our numerical calculations show that the solution of the coefficient inverse problem of finding diffusion and thermal conductivity coefficients by Dufort-Frankel scheme gives conditional stability at $\Delta t \leq 10^{-3}$.

5 Acknowledgements

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