MATHEMATICAL MODELING OF SOLUTE TRANSPORT IN AERATION ZONE CONSIDERING INFILTRATION AND EVAPORATION

ABSTRACT

Mathematical model of solute transport in aeration zone is considered. Given model takes into consideration soil moisture content variation effecting to solute transport and sorption due to evaporation processes and recondensation of water vapor. Computational investigations of solute transport in aeration zone at rainfalls infiltration and moisture evaporation from soil surface have been done.

1. INTRODUCTION

Currently the decision on placing of the enterprise with harmful emissions or a waste burial is accepted taking into account the effect on environment. Generally the evaluation of this effect is determined as estimation of contaminant distribution from the polluting object and the possibility of contaminant penetration in groundwater in concentrations exceeding maximum allowable level is analyzed.

For this purpose special systems of mathematical modeling of water and solute transport in saturated and nonsaturated soils such as Earth Science Module from COMSOL Multiphysics (www.comsol.com), GMS (www.ems-i.com) and HYDRUS (www.hydrus2d.com) have been developed. Meanwhile, in the majority of these programs for calculation of water and solute transport in soil it is necessary to set the rate of infiltration as entrance parameter. As it is known the infiltration of water basically is defined by a rainfall, evaporation and hydraulic conductivity of soil. Therefore to define this parameter for concrete soil and specific weather conditions is rather inconvenient. Moreover, it should be stressed that all mentioned above modeling systems do not consider conditions of water evaporation from the soil surface and recondensation of water vapor and their effect to solute transport. At the same time these processes significantly influence on soil moisture content that result in moisture films thickness changing on which molecular diffusion of solute is carried out. Consequently, the higher moisture content, the higher solute flow.

Considering the above stated the purpose of the present work was to develop the mathematical model which allows calculating infiltration and water transport in soil using the meteorological data and taking into account evaporation and water vapor recondensation processes. All this will allow to predict contaminant transport more authentically.

2. MATHEMATICAL MODEL

2.1 Non-isothermal water transport

Let's take up capillary-porous medium containing water vapor and liquid. Meanwhile, it is supposed that skeleton of porous medium is a rigid solid water-insoluble and water non-reacting. Thus, thermal transport equations:

$$C_{\text{eff}} \frac{\partial T}{\partial t} = \nabla\left(\lambda_{\text{eff}} \nabla T\right) + r_{\text{ev}} I_{\text{liq}}, \qquad (1)$$

and equation of water vapor and liquid mass conservation are applicable:

$$\frac{\partial(\rho_\text{v}\theta_\text{v})}{\partial t} = \nabla(\rho_\text{v}\boldsymbol{\upsilon}_\text{v}) + I_\text{v}, \tag{2}$$

$$\frac{\partial(\rho_\text{liq}\theta_\text{liq})}{\partial t} = \nabla(\rho_\text{liq}\boldsymbol{\upsilon}_\text{liq}) - I_\text{liq}. \tag{3}$$

Summing up equations (2) and (3), and taking into account the principle of local thermodynamic balance mass exchange rates between phases I_v and I_liq could be calculated as:

$$I_\text{liq} = \frac{\partial(\rho_\text{liq}\theta_\text{e})}{\partial t},\ I_\text{v} = \frac{\partial(\rho_\text{v}\theta_\text{e})}{\partial t}. \tag{4}$$

As a result the following equation of non-isothermal moisture transfer is obtained:

$$\frac{\partial w}{\partial t} = \nabla(\rho_\text{v}\boldsymbol{\upsilon}_\text{v}) + \nabla(\rho_\text{liq}\boldsymbol{\upsilon}_\text{liq}). \tag{5}$$

Where $w = \rho_\text{v}\theta_\text{v} + \rho_\text{liq}\theta_\text{liq}$ – moisture content of capillary-porous medium demonstrates the ratio of water vapor and water mass to the porous medium volume.

It should be noted that equation system (2) and (3) is not closed. However, according to the theory of two-phase filtration for the vapor and water velocity calculation generalized Darsy's law could be used [1]:

$$\boldsymbol{\upsilon}_\text{v} = \frac{KK_\text{v}(\theta_\text{v})}{\eta_\text{v}} \nabla[P_\text{v}(w,T) - \rho_\text{v} gz], \tag{6}$$

$$\boldsymbol{\upsilon}_\text{liq} = \frac{KK_\text{liq}(\theta_\text{liq})}{\eta_\text{liq}} \nabla[P_\text{liq}(w,T) - \rho_\text{liq} gz]. \tag{7}$$

For the calculation relationship between moisture content, temperature and vapor pressure it is suggested to use moisture sorption (desorption) isotherms at different temperatures [2].

Sorption isotherm is experimentally obtained relation between equilibrium volumetric moisture content and relative humidity: $\theta_\text{e} = f(\varphi, T)$ [3]. At that, for the modeling of non-isothermal moisture transfer the data of sorption isotherms at different temperatures is need(Fig. 1), and it could be approximated by the following function:

$$\theta_\text{e} = (p_1 + p_2\varphi^{p_3})(p_4 + p_5 T). \tag{8}$$

Relative humidity and water vapor pressure are bounded with one another by the expression:

$$\varphi = \frac{P_\text{v}}{P_\text{sat}}. \tag{9}$$

At that the relationship of saturated vapor pressure and the temperature is described by a simple mathematic equation [4]:

$$P_\text{sat} = 10^5 \left(\frac{T}{373}\right)^{15}. \tag{10}$$

Using sorption isotherm (8), expressions (8)–(10), considering that water density is much higher than vapor density and as a result $w \approx \rho_\text{liq}\theta_\text{liq}$, functional dependence that specify the relationship between moisture content, temperature and vapor pressure $P_\text{v} = f(w,T)$ and inverse relation $w_e = F(P_\text{v}, T)$ are obtained.

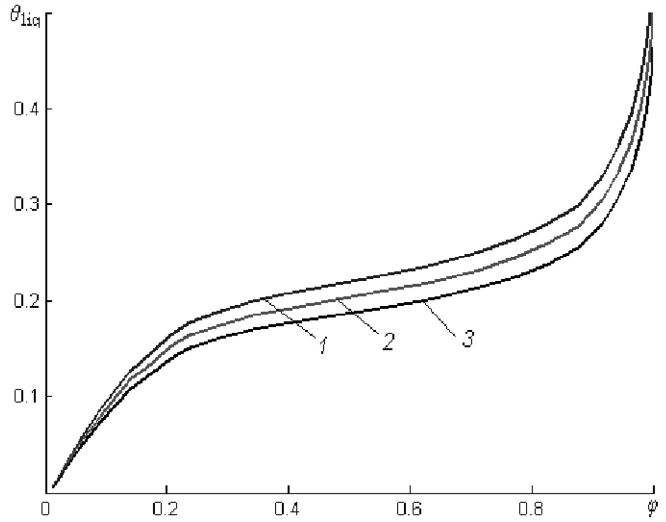


Figure 1. Soil moisture sorption isotherms at different temperatures: *1* – *T* = 275 K; *2* – 295; *3* – 315

As far as liquid pressure is much higher than water vapor pressure using Kelvin equation the relationship between moisture content, temperature and liquid pressure is received:

$$P_{\text{liq}}(w,T) \approx \frac{RT\rho_{\text{liq}}}{M} \ln \frac{P_{\text{v}}(w,T)}{P_{\text{sat}}}. \tag{11}$$

Obtained relationship (11) reflects physical-chemical features of liquid, structural specific features of porous medium and it is required while solving moisture transfer equations (5) as a relationship between temperature, moisture content and liquid pressure.

Latent heat of water-vapor phase transformations in the equation of heat conduction (1) is estimated through Clapeyron-Clausius equation taking into consideration dependence on moisture content, temperature and vapor pressure [2]:

$$r_{\text{ev}} = r_0 - \frac{RT^2}{M}\left(\frac{\partial \ln P_{\text{v}}(w,T)}{\partial T}\right), \tag{12}$$

where the last component determines the contribution of sorption heat.

So, considering all mentioned above we receive the following equation system of non-isothermal moisture transfer:

$$C_{\text{eff}} \frac{\partial T}{\partial t} = \nabla(\lambda_{\text{eff}} \nabla T) + \left(r_0 - \frac{RT^2}{M}\left[\frac{\partial \ln P_{\text{v}}(w,T)}{\partial T}\right]\right)\frac{\partial w_e}{\partial t}, \tag{13}$$

$$\frac{\partial w}{\partial t} = \rho_{\text{liq}} \frac{KK_{\text{liq}}(\theta_{\text{liq}})}{\eta_{\text{liq}}} \nabla\left[P_{\text{liq}}(w,T) - \rho_{\text{liq}} g x\right] + \rho_{\text{v}} \frac{KK_{\text{v}}(\theta_{\text{v}})}{\eta_{\text{v}}} \nabla\left[P_{\text{v}}(w,T) - \rho_{\text{v}} g z\right]. \tag{14}$$

Obtained system of equations (13), (14) with closure equations (8)–(11), that bind vapor and liquid pressure with moisture content and temperature, allows to calculate the dynamics of moisture field and liquid flow rate in capillary-porous medium at non-isothermal conditions. Obtained values of moisture content and liquid flow rate could be used for estimation of convective diffusion of solute in aeration zone. Having formulated proper boundary conditions to the obtained system of equations (will be discussed below) we could estimate the effect of rainfall infiltration and evaporation intensity from the soil surface to solute transport in it.

2.2 Solute transport in aeration zone

For mathematical description of solute transport in porous media, the equation of convective diffusion is commonly used [1, 5]. In case of considering of sorption linear kinetics the following system of equations could be used for modeling of absorbed solute through pore space of capillary-porous medium containing liquid [2]:

$$\theta_{\mathrm{liq}}\frac{\partial C}{\partial t}+C\frac{\partial\theta_{\mathrm{liq}}}{\partial t}+\rho_{\mathrm{b}}\frac{\partial a}{\partial t}=\nabla\left(\theta_{\mathrm{liq}}\mathbf{D}\nabla C-\mathbf{u}C\right)+F,$$

$$\rho_{\mathrm{b}}\frac{\partial a}{\partial t}=\beta\left(C-\frac{a}{K_{\mathrm{d}}}\right). \tag{15}$$

Rate of substance transport **u** by liquid depends on liquid velocity in capillary-porous medium $\boldsymbol{\upsilon}_{\mathrm{liq}}$ according to equation [1] of Darsy's law:

$$\mathbf{u}=\frac{\boldsymbol{\upsilon}_{\mathrm{liq}}}{\theta_{\mathrm{liq}}}, \tag{16}$$

As it is evident from (15) moisture content is vividly included in the equation of convective diffusion. Physical sense of the effect of porous medium moisture content to solute transport is the following: variation of moisture content leads to variation of thickness of moisture film through which molecular diffusion is conducted. Thus, the higher moisture content – the higher substance flow (substance flow is amounts of substance passing through the unit of area in the unit of time) and vice versa. It should be noted that soil moisture content could vary not only at the cost of liquid transport under the effect of moisture gradient, but also at the cost of vapor recondensation and thermo-capillary flows. That is why for modeling of solute transport in aeration zone, equation of convective diffusion should be supplemented by above presented equations of non-isothermal moisture transfer, which based on medium hydrological features and climatic factors allow to estimate dynamics of moisture fields and liquid velocity in the medium.

3. COMPUTATIONAL INVESTIGATION OF SOLUTE TRANSPORT IN AERATION ZONE AT INFILTRATION AND EVAPORATION

Using worked out mathematical model let's conduct computational investigation of *solubles* transport in aeration zone. Supposing that in the initial moment of time solution of insorbate is contained in soil layer of 0–0.1 m. Let's examine two cases of vertical transport of this substance. In the first case rainfall rate on the soil surface is H = 5·10^{-7} m/s. Initial volumetric liquid water content at that is θ_{liq0} = 0.15 m^3/m^3, and the temperature at soil surface is T_{top} = 293 K and T_{bot} = 273 K 1.5 m depth. In the second case evaporation occurs, at that air relative humidity at soil surface is φ_{env} = 35 % and initial distributions of water content and temperature are the same as in the first case.

At that equation of non-isothermal moister transfer is solved with the following boundary conditions. In case of rainfalls at z = 0 for equation of moisture transport (14) on the boundary the following condition is written:

$$\rho_{\mathrm{liq}}\frac{KK_{\mathrm{liq}}(\theta_{\mathrm{liq}})}{\eta_{\mathrm{liq}}}\nabla\left[P_{\mathrm{liq}}(w,T)-\rho_{\mathrm{liq}}gz\right]+\rho_{\mathrm{v}}\frac{KK_{\mathrm{v}}(\theta_{\mathrm{v}})}{\eta_{\mathrm{v}}}\nabla\left[P_{\mathrm{v}}(w,T)-\rho_{\mathrm{v}}gz\right]=H\,. \tag{17}$$

It should be noted that when volumetric liquid water content of soil upper layer is close to saturated state, relative humidity in the pores is tended to unity. So, according to closure equation (11) liquid pressure is tended to zero. That is why the amount of absorbed rainfalls will be determined not by the rainfalls rate H, but by moisture filtration rate in a lower soil layer.

At z = 1.5 m for equation of moisture transfer boundary condition is written the following way:

$$\rho_{\text{liq}}\frac{KK_{\text{liq}}(\theta_{\text{liq}})}{\eta_{\text{liq}}}\nabla\left[P_{\text{liq}}(w,T)-\rho_{\text{liq}}gz\right]+\rho_{\text{v}}\frac{KK_{\text{v}}(\theta_{\text{v}})}{\eta_{\text{v}}}\nabla\left[P_{\text{v}}(w,T)-\rho_{\text{v}}gz\right]=0\,. \qquad (18)$$

In case of moisture evaporation from the soil surface at z = 0 for equation of moisture transfer (14) the value of water content on the boundary is set as $w_{z=0}$, which is calculated from sorption isotherm at temperature equal to T_{top} and vapor pressure:

$$P_{\text{v}\,z=0}=\varphi_{\text{env}}P_{\text{sat}}(T_{top}), \qquad (19)$$

At z = 1.5 m for the equations of non-isothermal moister transfer the same boundary conditions are set as in case of rainfalls.

Analytical solution of above presented system of equations is impossible, so for mathematic modeling we should use numerical computing (finite-element method, finite difference method, etc.) [6]. For solution of considered problem obtained system of equations was solved using finite-element method in Galerkin statement (projection method) through computer program implemented by the authors in MATLAB. At that, at discretization by time the Crank-Nicholson differencing scheme (central difference scheme) was used [6], and solution of non-linear system of algebraic equation was done through Newton-Raphson method [7].

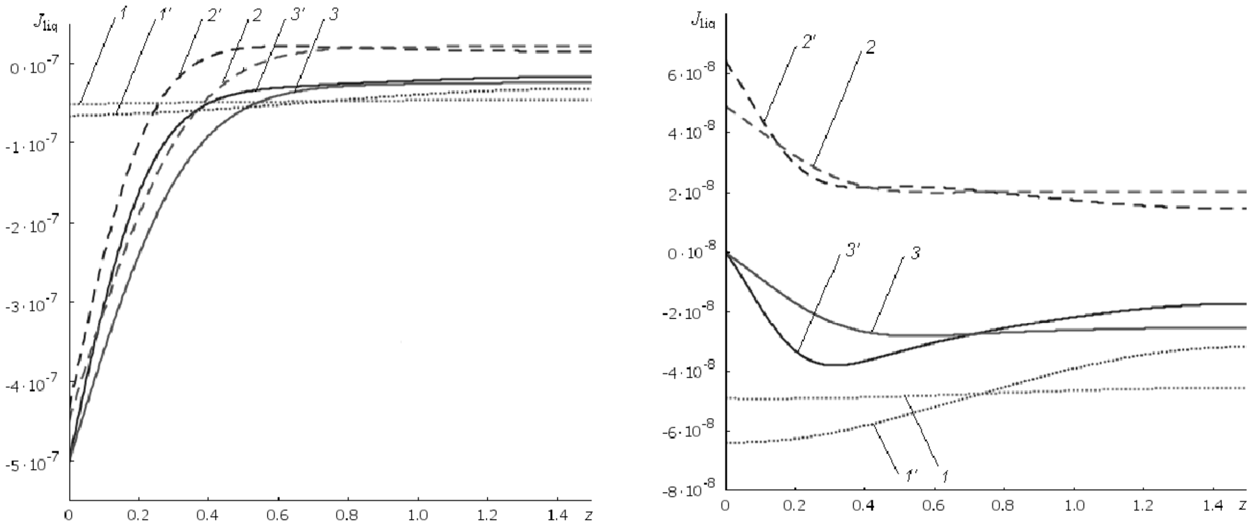
Using considered mathematical model of non-isothermal moisture transfer there was calculated the alteration of moisture fields and liquid flow in soil (Fig. 2). Hydrological and thermal-physical features of soil used for calculations are presented in Table 1. The other values specifying the process of sorbless solute transport were set the following way: bulk density of the soil ρ_{b} = 1200 кг/м^3; molecular diffusion coefficient D_{m} = $4\cdot10^{-8}$ м^2/c; soil parameters specifying hydrodynamic dispersion: α_x = 0.005 m and τ = 0.75.

From the results of modeling (Fig. 2) it is evident that liquid flow in soil $J_{\text{liq}}=\rho_{\text{liq}}\upsilon_{\text{liq}}$ is specified by uneven distribution of moisture and temperature through soil profile. In case of rainfalls, humidity of soil surface layer is increased and water flow is directed from surface deep into the soil (Fig. 2, *a*, curve *2*). Meanwhile, the temperature on the surface is 10 K higher than the temperature at a depth of 1.5 m, it means that capillary sorption pressure at soil surface will be higher as compared to the depth (considering sign) and moisture will move from the point with higher temperature to the point with lower temperature. It specifies thermo-capillary liquid flow (Fig. 2, *a*, curve *1*). It should be noted that in case of rainfalls thermo-capillary flow contributes insignificantly to resulting liquid flow (Fig. 2, *a*, curve *3*), that is why distributions of substance through soil profile estimated using the model considering non-isothermal moisture transfer is actually equal to the outcomes obtained without taking into account the temperature effect to moisture redistribution (Fig. 3, *a*).

TABLE 1 Values of parameters in the equations of non-isothermal moisture transfer

Soil properties	**Parameter values**
Porosity	m = 0.4 м^3/м^3
Volumetric heat capacity	$C_{\text{eff}}=\left(1.92\cdot10^{6}(1-m)+4.18\cdot10^{6}\theta_{\text{liq}}\right)$
Thermal conductivity	$\lambda_{\text{eff}}=0.925+1.68\theta_{\text{liq}}+0.643\exp\left(-\left[\theta_{\text{liq}}\right]^{4}\right)$
Intrinsic permeability	K = $1.61\cdot10^{-12}$
Relative liquid permeability	$K_{\text{liq}}=\left(\dfrac{\theta_{\text{liq}}}{m}\right)^{10.7}$
Relative vapor permeability	$K_{\text{v}}=\left(1-\dfrac{\theta_{\text{liq}}}{m}\right)^{10.7}$

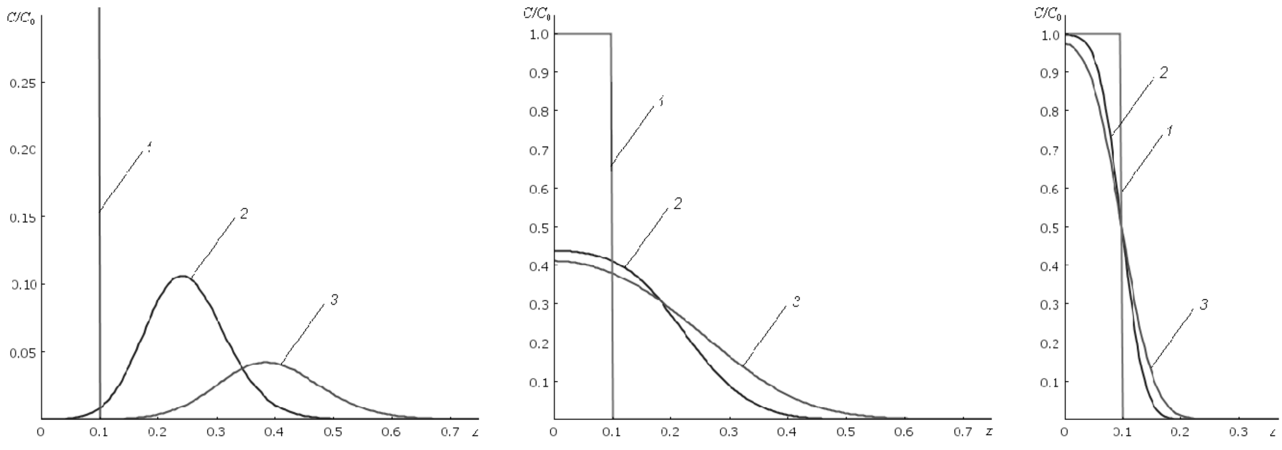
Dependence of vapor pressure from the water content and temperature	$P_v = P_{sat}(T)\exp\left[\frac{M}{R\rho_{liq}}\left(2.1-\frac{1601}{T}\right)\left(\frac{m}{\theta_{liq}}\right)^{3.85}\right]$
Dependence of liquid pressure from the water content and temperature	$P_{liq} = (2.1T-1601)\left(\frac{m}{\theta_{liq}}\right)^{3.85}$



a) *b*)

Fig. 2. Distribution of liquid flow through soil profile for different time moments: *1* and *1'* – liquid flow specified by temperature gradient 10 and 5 days after, correspondingly, *2* and *2'* – liquid flow specified by moisture gradient 10 and 5 days after, correspondingly, *3* and *3'* – resulting liquid flow 10 and 5 days after, correspondingly; *a*) in case of rainfalls, *b*) in case of evaporation

However, in case of moisture evaporation from the soil surface just opposite situation is observed. Due to evaporation water content of soil upper layer is decreased. It stimulates liquid flow from lower layers to soil surface (Fig. 2, *b*, curve *2*). Meanwhile, uneven distribution of temperature stimulates thermo-capillary flow of moisture (Fig. 2, *b*, curve *1*) from upper soil layer to the depth. As it is evident from the modeling results (Fig. 2, *б*), in case of moisture evaporation from the soil surface thermo-capillary flow of moisture contributes significantly to resulting moisture flow in soil.



a) *b*) *c*)

Fig. 3. Results of modeling of solute transport in soil: *1* – initial distribution, *2* – distribution 5 days after, *3* – distribution 10 days after; *a*) in case of rainfalls, *b*) in case of evaporation taking into account non-isothermal moisture transfer, *c*) in case of evaporation without taking into account non-isothermal moisture transfer

It should be noted that in the models of substance transport in soil presented in [1, 5] when estimating liquid flow, equations of convective diffusion do not take into account moisture flow caused by temperature gradient and recondensation of water vapor (for case of moisture evaporation from the soil surface in these models liquid flow in the equation of convective diffusion will be equal to zero). However, as it is evident from above presented results of modeling (Fig. 3, *b* and 3, *c*), it could cause significant errors. It is important that in real natural conditions along with rainfall infiltration processes moisture evaporation from soil surface and thermo-capillary moister transfer always occur. All this unambiguously evidences that while modeling the process of soluble transport in soil, water content and liquid flow in the equation of convective diffusion should be estimated considering non-isothermal moisture transfer.

4. CONCLUSION

A mathematical model of solute transport in aeration zone considering non-isothermal moisture transfer is proposed. It is based on the equations of convective diffusion, sorption kinetics, two-phase filtration, moisture sorption isotherms and thermodynamic laws.

Presented computational investigations have demonstrated that in order to get more reliable results of soluble transport forecast in aeration zone, mathematical model should take into consideration moisture transfer processes dealing not only with the gradients of moisture and temperature but also with water vapor recondensation and moisture flow tending to surface due to evaporation.

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NOMENCLATURE

a – solute concentration that sorbed to solid particles, kg/kg; C – solute concentration in the liquid, kg/m^3; C_{eff} – effective volumetric heat capacity of soil, J/(m^3·K); $\mathbf{D}$ – hydrodynamic dispersion tensor, m^2/s; F – denotes a solute source and sink, kg/(m^3·s); g – gravitational acceleration, m/s^2; H – rainfall rate, m/s; I_{liq} – phase change water flux, kg/(m^3·s); I_{v} – phase change vapour flux, kg/(m^3·s); K – intrinsic permeability of the porous medium, m^2; K_{d} – distribution coefficient, m^3/kg; K_{liq} – relative liquid permeability; K_{v} – relative vapour permeability; M – molar mass of water, kg/mole; m – total porosity of soil, m^3/m^3; P_{liq} – liquid pressure, Pa; P_{sat} – saturation vapor pressure, Pa; P_{v} – vapour pressure, Pa; p_1, p_2, p_3, p_4 and p_5 – empirical coefficients in equation of sorption isotherm; R – absolute gas constant, J/(mole·K); $\boldsymbol{\upsilon}_{\mathrm{liq}}$ – vector of liquid velocities, (м/с); υ_{v} – vector of water vapour velocities, (m/s); r_0 – heat of evaporation, J/kg; r_{ev} – specific heat of water adsorbed, J/kg; T – temperature, K; t – time, s; $\mathbf{u}$ – vector of solute velocities, m/s; w – water content, kg/m^3; z – coordinate in vertical direction; β – sorbtion rate, 1/s; η_{liq} – liquid dynamic viscosity, Pa·s; η_{v} – vapour dynamic viscosity, Pa·s; θ_{e} – equilibrium liquid volume fraction, m^3/m^3; θ_{liq} – volumetric liquid water content, m^3/m^3; θ_{sat} – saturated volume fraction, m^3/m^3; θ_{v} – volumetric water vapour content, m^3/m^3; λ_{eff} – effective heat conductivity, W/(m·K); ρ_{b} – bulk density of the soil, kg/m^3; ρ_{liq} – liquid density, kg/m^3; ρ_{v} – vapour density, kg/m^3; φ – relative humidity.