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Modeling of the process of mass transfer by surface and groundwater flows during furrow irrigation of agricultural crops

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Abstract. The article presents the results of research on modeling the process of mass transfer by interacting ground and surface water flows, taking into account the migration of moisture in the humidification zone using the dimensionality analysis method, as when solving the problem of mass transfer by interacting ground and surface water flows in the humidification zone, associated with the determination of the mass transfer coefficient, the method of dimension analysis acquires special importance. Based on these considerations, stochastic differential equations of changes in the parameters of the infiltration flow in the humidification zone are derived and a one-dimensional hydraulic model of convective moisture transfer in hydromorphic media caused by irrigation of agricultural crops is obtained.
Key words: mass transfer, water-salt regime, hydraulic model, aeration zone, dispersed systems, groundwater, geohydrodynamicprocesses, hydromorphic medium.

1 Introduction

In land reclamation, many scientists and researchers have been engaged in modeling the water-salt regime of underground and surface waters [2,3,6,10,11,12], while these studies were carried out based on simplified models for individual components of the water flow. Models of mass transfer by interconnected flows of ground and surface water, as well as moisture in the humidification zone, taking into account mass transfer between various components of water runoff and the problems of managing changes in the state of the humidification zone have not been considered so far. This significantly limited the possibility of using joint runoff models in solving many applied tasks to assess the ecological and reclamation status of irrigated lands and the quality of ground and surface waters.

Deterministic models of geohydrodynamic processes study the general laws of substance transfer (mass, heat and momentum) based on traditional representations of continuum mechanics. For heterophase polydisperse media, where there are random (stochastic) processes, in particular, changes in the size of soil-soil particles, the specified

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description principle turns out to be somewhat incomplete. Changes in the size and shape of particles in hydromorphic media caused by phase (dissolution, evaporation, condensation, crystallization) transformations, hydrodynamic phenomena significantly deform the density function of particle size and time distribution, thereby having a significant impact on the phenomena of mass, heat and momentum transfer in heterogeneous systems.

2 Materials and methods

During the research, the methods adopted for field and field conditions, the theory of unsteady water filtration in soils and modeling the dynamics and direction of hydrological, hydrogeological and soil reclamation processes using modern technical means of observation and mathematical methods were used. Experimental studies of plant water consumption were carried out on a natural background and on a lysimeter based on generally accepted methods.

3 Results and Discussion

In practical applications of dispersed systems in hydromorphic media, solid particles, droplets and bubbles are characterized by polydispersity of the state, i.e. the particle sizes can vary from minimum to maximum values, although the average size is always used in mass heat transfer calculations. The shape of the particles that make up dispersed systems is generally not spherical, although the spherical shape is a special case or an idealization of an irregular shape. Strictly spherical in the absence of shape deformation are droplets and bubbles that take a spherical shape under the action of surface tension in the absence of external fields (gravitational, electric, etc.). Droplets and bubbles of small sizes also retain a spherical shape.

Depending on the nature of the problem to be solved, different average diameters and spectra in size and mass should be used. It is important to note that when analyzing and solving problems of heat and mass transfer in the soil-soil humidification zone, it is desirable to use the average diameter on the surface. The state of a polydisperse system is determined by the particle size distribution function or the evolution of the size and time distribution function. Usually, in processes accompanied by physical phenomena (droplet evaporation, condensation, agglomeration, coagulation, etc.), i.e. accompanied by a change in particle size, the most effective representation of information on the state of a polydisperse system is a characteristic change and evolution of the function and distribution over residence time. In this case, the nature and form of the distribution function changes over time, starting from the initial distribution and ending with the limit value. In the steady state, which corresponds to constant particle sizes, well-known equations are used for continuous particle distribution functions: normal and lognormal distributions, etc., each of which is characterized by its own parameters. The density of the normal and lognormal particle size distribution is widely used in applied problems for various fields, including mass and heat transfer problems, they are used to construct the distribution function of fine and highly dispersed particles and nanoparticles. It is important to note that these types of distribution functions are characteristic of the steady state or constancy of the size of a polydisperse system.

Stochastic differential equations of changes in the parameters of the infiltration flow in the humidification zone during furrow irrigation of agricultural crops. When modeling the process of mass transfer by interacting currents of ground and surface waters, taking into account the migration of moisture in the humidification zone, we use the method of dimensional analysis.

The main method of similarity theory is the analysis of the dimensions of the physical quantities characterizing the state of the process under study, and the parameters that determine this state. The dimension of a physical quantity is understood as the expression of the relationship between it by the physical quantities underlying the system of units. The basis of dimension analysis is the requirement that the basic equations expressing the relationship between variables and process parameters should be valid for any choice of units of measurement of the quantities included in them. It follows from this requirement that all the terms of each equation must have the same dimensions. When solving the problem of mass transfer by interacting currents of ground and surface waters, taking into account the migration of moisture in the humidification zone associated with the determination of the mass transfer coefficient, the method of dimensional analysis acquires special importance. Usually, the dimension is written symbolically in the form of a formula in which it is customary to denote the symbol of the unit of length *L*, the unit of mass *M*, the unit of time *T* and the unit of temperature *θ*. Table 1 below shows the main variables and their corresponding dimensions.

Table 1. Variables and their dimensions

	Variable Dimension	**Symbols**	**Dimensions**
Main	Mass Length Time Temperature	m l t T	$[M]$ $[L]$ $[T]$ $[\theta]$
Mechanical	Speed Boost Density Dynamic viscosity Force	V g ρ η F	$[LT^{-1}]$ $[LT^{-2}]$ $[ML^{-3}]$ $[ML^{-1}T^{-1}]$
Thermal	Thermal Conductivity Heat capacity Heat transfer coefficient	λ c α	$[MLT^{-2}\theta^{-1}]$ $[LT^{-2}\theta^{-1}]$ $[MT^{-3}\theta^{-1}]$
Diffusion	Concentration Diffusion coefficient Mass transfer coefficient	C D B	$[ML^{-3}]$ $[LT^{-2}]$ $[LT^{-1}]$

Similarly, the coefficients of thermal conductivity, heat transfer and heat capacity can be expressed

$$\lambda = 1\frac{vt}{m\,^0C} = \frac{kgm}{sec\,^0C}, \quad \alpha = 1\frac{vt}{m^2\,^0C} = \frac{kg}{sec\,^0C}, \quad C_p = 1\frac{kal}{kg\,^0C} = \frac{m^2}{sec\,^0C}$$

The main content of dimension theory is the n-theorem, which is formulated as follows. Let there be some functional dependence between different quantities $f(X_1, X_2, \ldots X_n)=0$. Let the maximum number of these dimensional quantities with independent dimensions be *m*. Then the initial relationship between dimensional quantities expressing a certain physical law can be represented as a relation between *(n–m)* dimensionless quantities, each of which has the form of a power-law monomial. The number of basic units of measurement by which all these variables are measured is

$$\Delta P = ML^{-1}T^{-2} = H/м^2 = кг/c^2м, \; V = LT^{-1} = м^2/c, \; \rho = ML^{-3} = H/м^3 =,$$
$$v = L^2T^{-1} = m^2/s \; .$$

So, let's assume that some parameter of the mass transfer process N is related to other parameters of the process N,A,B,C,D by dependence

$$N = f(A,B,C,D) = kA^a B^b C^c D^d \quad (1)$$

Here k, f, c, d -are unknown coefficients determined on the basis of experimental studies. Suppose that the process parameters N,A,B,C,D depend on the physical properties of the infiltration flow (viscosity, density, velocity, temperature), which in the symbols of dimension will be represented as

$$N = L^{a_0}T^{m_0}\theta^{k_0}M^{n_0};\ A = L^{a_1}T^{m_1}\theta^{k_1}M^{n_1};\ B = L^{a_2}T^{m_2}\theta^{k_2}M^{n_2};\ C = L^{a_3}T^{m_3}\theta^{k_3}M^{n_3};$$
$$D = L^{a_4}T^{m_4}\theta^{k_4}M^{n_4}$$

Then equation (1) can be written as

$$L^{a_0}T^{m_0}\theta^{k_0}M^{n_0} = k(L^{a_1}T^{m_1}\theta^{k_1}M^{n_1})(L^{a_2}T^{m_2}\theta^{k_2}M^{n_2})(L^{a_3}T^{m_3}\theta^{k_3}M^{n_3})(L^{a_4}T^{m_4}\theta^{k_4}M^{n_4})^d \quad (2)$$

Comparing the degrees at the same dimensions, we get

$$a_0 = a\alpha_1 + b\alpha_2 + c\alpha_3 + d\alpha_4$$
$$m_0 = am_1 + bm_2 + cm_3 + dm_4;\ k_0 = ak_1 + bk_2 + ck_3 + dk_4;$$
$$n_0 = an_1 + bn_2 + cn_3 + dn_4$$

In this equation, the number of unknown coefficients (k,a,b,c,d) is greater than the number of equations, and the values of the coefficients (α_i,m_i,k_i,n_i) are known according to the dimension of the corresponding parameters. To solve this system of equations with respect to a,b,c,d and taking *(n-m)*(*n*- is the number of unknown coefficients, *m* is the number of equations) the coefficients are key, we express the remaining coefficients through these.To solve equation (2), it is necessary to determine the mass transfer coefficient. Using the dimensionality method, we define an empirical expression for the mass transfer coefficient $\beta[LT^{-1}]$, assuming that the latter is a function of the characteristic body size $r[L]$, with a flow rate $V[LT^{-1}]$, a flow density $\rho[ML^{-3}]$ viscosity $\eta[MT^{-1}L^{-1}]$ and a coefficient diffusion of $D[L^2T^{-1}]$.

Let 's define the mass transfer coefficient in the form

$$\beta_L = kr^aV^b\rho^c\eta^dD^c$$

Substituting the dimension values, we get

$$LT^{-1} = kL^a(LT^{-1})^b(ML^{-3})^c(MT^{-1}L^{-1})^d(L^2T^{-1})^e$$

Comparing the degrees for the corresponding dimensions, we obtain

$$L: 1 = a + b - 3c - d + 2e\ T: -1 = -b - d - e;\ M: 0 = c + d \quad (3)$$

In this equation, the number of unknown coefficients is n=5, and the number of equations is m=3. The number of key parameters is n-m=2. We will take b,d as the key parameters and express the remaining coefficients through these coefficients. From the last equation (3) we have $c=-d$, from the second equation- $e=1-b-d$. Then from the first equation we get $a=b-1$. Given these values, we Given these values, we can write

$$\beta_L = kr^{b-1}V^b\rho^{-d}\eta^dD^{1-b-d}$$

Let 's write this equation in the form

$$\frac{\beta_L r}{D} = k\frac{r^b V^b \eta^d}{D^b \rho^d D^d}$$

$$Sh = \frac{\beta_L r}{D}, Pe = \frac{Vr}{D}, Sc = \frac{\eta}{\rho D}$$

By entering the criteria and, the equation for calculating the mass transfer coefficient is presented as

$$Sh = kPe^b Se^d$$

Pe=ReSc, then we can write

$$Sh = kPe^b Sc^{b+d}$$

Coefficients (*k*, *b*, *d*) for any mass transfer process can be determined using experimental data.

Now, using the dimensionality method, we define an empirical formula for calculating the heat transfer coefficient $a = \frac{vt}{m^2K} = \frac{\kappa g}{sek^3K} = [MT^{-3}\theta^{-1}]$, depending on the body size $r[L]$, the flow velocity $V[LT^{-1}]$, the density of the medium $\rho[ML^{-3}]$, the viscosity of the medium $\eta[MT^{-1}L]^{-}$ the thermal conductivity of the medium and the heat capacity of the flow $\lambda[LMT^{-3}\theta^{-1}]$, i.e.

$$a = kr^a V^b \rho^c \eta^d \lambda^e C_p^f \quad (4)$$

Given the dimensions of the corresponding quantities, we can write. Comparing degrees of the same size, we get

$$MT^{-3}\theta^{-1} = kL^a (LT^{-1})^b (ML^{-3})^c (MT^{-1}L^{-1})^d (MLT^{-3}\theta^{-1})^e (L^2T^{-2}\theta^{-1})^f$$

$$L: 0 = a + b - 3c + d + e + 2f$$

$$T: -3 = -b - d - 3e - 2f;\ M: 1 = c + d + e;\ \theta: -1 = -e - f$$

In this system, there are n-6 unknown coefficients and *m*=4 equations. Taking *c* and *f* as the key coefficients, we express the remaining coefficients through them. From the last equation we have *e=1-f*, from the third equation *d=f-c*, from the second equation *-b=c*, then from the first equation we have *a=c-1*. Substituting these coefficient values into the above equation and grouping the corresponding variables, we obtain

$$\frac{ar}{\lambda} = k\left(\frac{rV\rho}{\eta}\right)^c \left(\frac{\eta C_p}{\lambda}\right)^f$$

$$Nu = \frac{ar}{\lambda}, Re = \frac{rV\rho}{\eta} = \frac{rV}{v}, \mathrm{Pr} = \frac{\eta C_p}{\lambda}$$

$$Nu = K(Re)^c (\mathrm{Pr})^f$$

In this expression, the coefficients *k*, *c*, *f* are determined based on the experimental values of the measured quantities. From the modeling condition, it becomes necessary to determine the coefficient of resistance of solid particles. In this case, the resistance force of solid particles $F[MLT^{-2}]$ depends on: particle diameter $a[L]$, flow velocity $V[LT^{-1}]$, density $\rho[ML^{-3}]$ and dynamic viscosity $\eta[ML^{-1}T^{-1}]$. The general expression for the resistance force can be written as

$$F_D = kd_p^a V^b \rho^c \eta^d$$

Moving on to the dimensional values, we get Comparing the same degrees, we have

$$MLT^{-2} = kL^{a}(LT^{-1})^{b}(ML^{-3})^{c}(ML^{-1}T^{-1})$$
$$L:1 = a + b - 3c - d$$
$$T:-2 = -b - d$$
$$M:1 = c + d$$

Taking the coefficient d as the key, we express the remaining coefficients as $a = 2 - d$, $b = 2 - d$, $c = 1 - d$.

Then we can write

$$F_D = kd_p^{2-d}V^{2-d}\rho^{1-d}\eta^{d}$$

$$Re_d = \frac{Va\rho}{\eta}$$

$$F_D = kd_p^{2}V^{2}Re_d^{-d}$$

$$F_D = C_d S\frac{\rho V^2}{2}$$

By entering a dimensionless number, we get $S = \frac{\pi d_p^2}{4}$

Expressing the resistance force as , we finally get $C_D = \frac{24}{\mathrm{Re}_d}$,

$$C_D = \frac{8}{\pi}\left(\frac{F_D}{d_p^2V^2}\right) = \frac{8K}{\pi\,\mathrm{Re}_d^{-d}} = A\,\mathrm{Re}_d^{-d} = f(\mathrm{Re}_d)$$

where A *i*s some experimentally determined coefficient. As noted above, for small values of Re <<1, the value of A=24 and d=1,d=1, i.e. similarly, we determine the resistance force for a particle in a non-Newtonian fluid by putting $F=f(\rho,d,k,d,V)$, k- is the consistency coefficient-the exponent. In addition to the above, we have the following dimensions: k=[$ML^{-1}T^{n-2}$], n=[$M^{0}L^{0}T^{0}$]. Similarly to the above calculations, for the resistance force or resistance coefficient, we obtain

$$C_D = \frac{F_d}{\rho V^2 d_p^2} = f\left(\frac{\rho V^{2-n}d_p^{n}}{k}, n\right) = f(\mathrm{Re}_d, n)$$

The theory of similarity and dimensions is a strong tool in the analysis of transfer processes if it is not possible to obtain analytical solutions of differential equations with boundary conditions. However, it should be noted that when analyzing dimensions, it is important to choose the right parameters on which the transfer coefficients depend.

When deriving equation (2), it is assumed that the stochastic process under consideration obeys the nonlinear equation

$$\frac{da(t)}{dt} = f(a(t),t) + G\zeta(t) \tag{5}$$

With normal white noise, zero expectation and a given covariance matrix (delta function). It should be noted that the function expresses the rate of change in particle sizes depending on the ongoing processes of mass transfer and heat exchange.

$$M[\zeta(t)]=0$$
$$Cov[\zeta(t)\zeta(\tau)]=B\delta(t-\tau)\delta(t-\tau) \qquad (6)$$
$$f(a(t),t)$$

If $f(a(t),t)$, then it characterizes the growth of particle sizes in the processes of infiltration, condensation, etc. If $f(a(t),t)>0$, $f(a(t),t)<0$, then it characterizes the change in particle size in processes such as infiltration, evaporation, etc. If the function is nonlinear, then great difficulties arise in the analytical solution of equation (1). An important condition for using the distribution function is the normalization condition $\int_0^\tau P(a)da=1$.. The solution of stochastic equations differs significantly from the solution of ordinary differential equations.

The solution of ordinary differential equations is reduced to the determination of unknown functions at an arbitrary time according to the given initial conditions [5,7,8,9,13,14]. The solution of a stochastic differential equation is associated with determining the distribution of the values of the desired functions at an arbitrary time. The analytical solution (1) is allowed only for special cases and in general presents great difficulties related to the structure of the function and the nature of the initial distribution. However, in some cases, there is a possibility of an approximate solution of (1) by reducing the latter to a system of ordinary differential equations. In particular, if we linearize the function in the neighborhood of some mean

$$f(a(t),t)\approx f(\mu_a(t),t)+\frac{\partial f(\mu_a(t),t)}{\partial \mu_a(t)}(a(t)-\mu_a(t)) \qquad (6a)$$

assuming that the nature and type of the distribution density function remains constant throughout the entire period of its evolution, then the system of differential equations, in particular, for the normal distribution, which allows us to determine the change in the elements of variance and mean б $\sigma^2(a)$, will be represented as

$$\mu_a(a)$$
$$\frac{d\mu_a(a)}{dt}=f(\mu_a(t),t) \qquad (7)$$
$$\frac{d\sigma_n^2}{dt}=\frac{\partial f(\mu_a(t),t)}{\partial \mu_a}\sigma_n^2+\sigma_n^2\frac{\partial f^T(\mu_a(t),t)}{\partial \mu_a}+G(\mu_a(t),t)BG^T(\mu_a(t),t)$$

with the specified initial value $(\mu_a(0)=\mu_{a0},\sigma_n^2(0)=\sigma_{n0}^2$. Solutions (1) provide a condition for the constancy of the distribution function over the entire period of evolution, except for the maximum and average values.

Let's assume that the distribution function does not change its character over the entire period of evolution and obeys the normal law

$$P(a,t)=\frac{1}{\sigma_n\sqrt{2\pi}}\exp\left[\frac{(a-\mu_a)^2}{2\sigma_n^2}\right] \qquad (6\ а)$$

and the change in the coordinate is described by a linear equation

$$d(a)=-Aa+\zeta(t) \qquad (6\ в)$$

This equation describes the change in the size of capillaries, where the particle size decreases monotonically over time to a minimum value.

It is required to determine the laws of variation of variance and mean and to construct the evolution of the distribution function.

Then we get the equation in the form

$$\frac{\partial P(a)}{\partial t} = \frac{\partial}{\partial a}\left(\frac{da}{dt}P(a)\right) + \frac{B\partial^2 P(a)}{2\partial a^2} \quad \text{(7 b)}$$

Having determined the derivatives included in this equation from (6 a) and substituting them into equation (7 b) after separating the variables for variance and mean, we obtain $a_s = \mu_a$

$$\frac{d\sigma_a^2}{dt} = -2A\sigma_a^2 + B\,,\ \sigma_a^2(t)\Big|_{t=0} = \sigma_{a0}^2$$

$$\frac{d\mu_a}{dt} = -A\mu_a\,,\ \mu_a(t)\Big|_{t=0} = \mu_{a0}$$

The solution of this system of equations with initial values gives $\sigma_a^2 = \sigma_{a0}^2$

$$\mu_a = \mu_{a0}\exp(-At) + \frac{B}{2A}\left[1-\exp(-2At)\right] \quad (8)$$

Thus, substituting these values for the variance of the mean in (6 a), we determine the value of the distribution function at any given time.

By introducing the following assumptions: a) the nature of the distribution function is constant; b) the number of particles per unit volume is equal to $\mu_{a0} = 2$; $N\int_0^a P(a)da$; c) the stochastic diffusion coefficient is equivalent to the diffusion coefficients of fine particles. Integrating (7b) in the range from 0 to *r*, we obtain an expression representing the equation of convective mass transfer.

$$\frac{\partial N}{\partial t} = D\left(\frac{\partial^2 N}{\partial r^2} + \frac{2\partial N}{r\partial r}\right) + \omega(r,t| \quad (9)$$

Mass transfer in three directions is found as the product of the solution of the equation for convective transport in the vertical direction by a certain function [12]:

$$N(x,y,z,t) = \frac{\exp(-\frac{y}{2})}{\sqrt{2x}}\theta(t,z) \quad \text{(9 a)}$$

We will determine the desired function from the moisture transfer equation

$$\frac{\partial\theta}{\partial t} + \frac{\partial u\theta}{\partial z} = \kappa\frac{\partial^2\theta}{\partial z^2} \quad (10)$$

Now we will conduct hydraulic modeling of convective moisture transfer in hydromorphic media caused by changes in the groundwater level. We proceed from the fact that moisture changes in hydromorphic media are related to the magnitude and are determined by the difference in filtration rates, and moisture transfer associated with the magnitude is the difference in moisture. In this regard, to describe the hydraulic parameters of moisture transfer in the soil space, we use the criterion of similarity to the Heat [1,4].

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We introduce dimensionless parameters $z = l\bar{z}$, $t = \frac{l^2}{\nu}\tau$, where l, ν -are characteristic dimensional values (characteristic length, which determines the average path of moisture and kinematic viscosity, respectively). Further, let's assume that the relationship between humidity and suction height is linear, and the moisture transfer coefficient is averaged by humidity. To determine the flow structure in the convective transfer of moisture in hydromorphic media, we use the criterion of similarity to the Furnace, then equation (10) will take the form:

$$\frac{\nu}{l^2}\frac{\partial\theta}{\partial\tau} + \frac{u}{l}\frac{\partial\theta}{\partial\bar{z}} = \frac{\kappa}{l^2}\frac{\partial^2\theta}{\partial\bar{z}^2} \tag{11}$$

Multiplying both parts of the equation by $\frac{l}{u}$, and taking into account $\mathrm{Re} = \frac{ul}{\nu}$ - the Reynolds number and $Pe = \frac{ul}{\kappa}$ - the Peclet number, we get:

$$\frac{1}{\mathrm{Re}}\frac{\partial\theta}{\partial\tau} + \frac{\partial\theta}{\partial\bar{z}} = \frac{1}{Pe}\frac{\partial^2\theta}{\partial\bar{z}^2} \tag{12}$$

Multiplying both parts of equation (12) by Pe, we get

$$\mathrm{Pr}_T\frac{\partial\theta}{\partial\tau} + Pe\frac{\partial\theta}{\partial\bar{z}} = \frac{\partial^2\theta}{\partial\bar{z}^2} \tag{13}$$

where is the Prandtl diffusion number.

4 Conclusions

Stochastic differential equations for changing the parameters of the infiltration flow in the humidification zone during furrow irrigation of agricultural crops have been developed.When studying the process of convective transport, the Prandtl similarity criterion is essential. The Prandtl diffusion number characterizes the relationship between the velocity field and the concentration field. In this regard, the Prandtl similarity criterion was used to describe the specific features of the convective moisture transfer process in hydromorphic media. Thus, a one-dimensional hydraulic model (13) of convective moisture transfer in hydromorphic media caused by irrigation of agricultural crops is obtained.

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