Mass transfer processes in a heterogeneous medium occurring in the aeration zone during infiltration of surface waters

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Abstract. The article discusses issues related to the creation of mathematical models that are used to solve various problems arising in the hydrological and hydrogeological cycles. The analysis of the mathematical correctness of the solved problems, which correspond to the initial boundary conditions, is given. When studying the phenomena associated with the exchange of mass between surface and groundwater flows, it becomes necessary to study several issues in order to hydraulically substantiate the models being developed and their numerical implementation. This circumstance is of great importance when creating a picture of the interacting processes of runoff and water infiltration.

1 Introduction

Numerous studies of scientists have been devoted to the modeling of water and salt regimes of surface and groundwater in land reclamation [1-3]. Basically, this problem was solved using simple models that took into account certain components of the considered elements of the water regime. The mass transfer by surface and ground waters, as well as the dynamics of humidity in the aeration zone, which take into account the mass transfer by various components of the water flow and the management of these interrelated processes, are currently insufficiently studied. This circumstance largely limited the use of hydraulic models that take into account the effect of surface and groundwater runoff in solving applied problems. This prevented the correct assessment of the ecological and reclamation status of irrigated lands and the quality of water supplied for irrigation.

In the process of studying issues related to mass transfer between surface and groundwater, there is often a need to study several problems related to the creation of hydraulic models and their numerical implementation in field experiments. This circumstance contributes to the creation of the principles of unification of mathematical models that correspond to various directions of the hydrological cycle. In this case, the development of numerical methods and available calculation algorithms, initial and boundary conditions for non-standard systems of equations that could take into account various features of this process acquires a special place [4-11].

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2 Materials and methods

During the research, we used standard methods adopted for field experiments, the theory of unsteady water filtration and a methodology for modeling the dynamics of humidity changes in the aeration zone, as well as in hydrological, hydrogeological and reclamation processes using modern technical means of observation and mathematical methods.

3 Results

The basis of infiltration processes is mass transfer, i.e. irreversible mass transfer within one phase or from one phase to another. The mass transfer process is carried out as a result of chaotic motion of medium molecules (molecular diffusion), as a result of macroscopic motion of the medium (convective transport), and in turbulent flows as a result of chaotic motion of pulsating vortices of various sizes. Mass transfer includes: a) mass transfer, where the transfer of substances is carried out from the interphase boundary into the volume of the flow; b) mass transfer, where mass transfer from one phase to another is carried out through the interface of phases; c) mass conduction, where mass transfer is carried out into the volume of a porous body [1-4]. Just as heat transfer occurs only when there is a deviation from the equilibrium state, i.e. when there is a temperature difference between the heat carriers, so the transition of a substance from one phase to another occurs in the absence of equilibrium between the phases. Accordingly, when deviating from the equilibrium state, a substance transitions from a phase in which its content is higher than equilibrium to a phase where the content of this substance is lower than equilibrium. The speed of movement of a substance depends on the degree of its deviation, which can be expressed as a concentration difference - the concentration of a substance in one phase and the equilibrium concentration of this substance on it, as well as the interfacial surface of the contemplation of phases. This concentration difference is the driving force of the mass exchange process. Thus, the speed of movement of matter from one phase to another can be defined as a unit of transition time between one phase and another.

$$M = KF\Delta c \tag{1}$$

Where M - is the number of substances transferred from one phase to another, is the mass transfer coefficient, F - is the contact surface of the phases; $\Delta c=(c^*-c)$ - is the mass transfer force; c^*-is the equilibrium concentration of the substance.

It is important to note that if the concentration of a substance in a given phase is higher than the equilibrium concentration, then the substance will move from this phase to another. There are two main types of mass transfer: a) mass transfer between a liquid and a gas or between two immiscible liquids (rectification, absorption, liquid extraction, separation of emulsions, mass transfer in dispersed systems, etc.); b) mass transfer between a solid and a liquid, gas or steam (adsorption, catalytic processes, drying, humidification, etc.). Three substances are involved in most mass transfer processes: a) the distributing substance constituting the first phase; b) the distributing substance that makes up the second phase; c) the distributed substance that passes from one phase to another. In all solved problems of mass transfer, it is necessary to determine mainly two parameters: a) concentration distribution in the interfacial layer; b) calculation and estimation of the amount of transferred substance from one phase to another; c) calculation of the mass transfer coefficient. The latter problem, for the most part, taking into account hydrodynamic and thermal factors, is presented in the form of criterion equations. Among the main dimensionless criteria used in mass transfer calculations, it is important to note the following:

- Reynolds number, expressing a measure of the ratio of inertia forces and viscosity $\mathrm{Re} = VL / \nu$.
- The Prandtl diffusion number or Schmidt number, which characterizes a measure of the ratio of the viscous and concentration properties of the flow.
- The Nusselt diffusion number or the Sherwood number, which characterizes a dimensionless amount of transferred mass.
- The Peclet diffusion number, which expresses the ratio of the amount of mass transferred by convection to the amount of mass transferred by diffusion. e) the Fourier number or homochromity number, which characterizes the change in time of the rate of transfer of matter with unsteady mass transfer.
- The Weber number, which characterizes the measure of the ratio of the inertia forces of surface tension, here V -is the flow velocity, L -is the characteristic size, m, D -is the diffusion coefficient, β- is the mass transfer coefficient, ν- is the viscosity, σ- is the surface tension coefficient.

For the conditions of dispersed systems, mass transfer between phases can be expressed in various ways [4-6]. At the same time, in this medium, the mass is transferred from the solid state to the liquid state (dissolution of solid particles, separation of the substance from the solid phase with a liquid solvent by extraction). In addition, the reverse process may occur, accompanied by a transition from the liquid phase to the solid phase (solid particles crystallization from solution, solid particle deposition processes. There is also a third case when mass transfer occurs from one to another liquid phase or from the gas to the liquid phase, as well as from the liquid to the gas phase.

It is important to note that the presence of polydispersity of particles involved in mass transfer processes imposes additional conditions on the solution of transfer problems. This is primarily due to the time evolution of the particle size distribution function, the determination of the average volume, the average interfacial surface and the average particle size. In addition, the presence of polydisperse systems requires the need to take into account complex phenomena when calculating the distribution function and the time variable of the interfacial surface. This circumstance causes a change in the surface boundary conditions and the concentration of particles per unit volume, thereby affecting the dissipative processes.

The conditions of phase contact in mass transfer processes are diverse, which is determined by the purpose of the main process. Thus, in the infiltration processes, pore air and moisture are in direct contact, which contributes to the transfer of less components from steam to liquid. In adsorption processes, the gas mixture is separated as a result of selective sorption of one of the components on the surface of the solid adsorbent.

4 Discussion

The traditional approach to solving mass transfer problems is reduced to the study of convective transport equations, in which the velocity components are determined from the hydrodynamic problem under consideration. In many cases, chemical and phase transformations occur in streams and their kinetic features (the speed of the process) are affected by convective mass transfer. At the same time, the presence of phase transformations in the flow (evaporation, condensation) can significantly change the hydrodynamic velocity fields, as a result of the appearance of various convective flows (due to changes in surface tension, temperature and pressure differences) and changes in the properties of the medium-the density and viscosity of the current medium, which depend on the composition of the phases. The proposed task is very complex and defies theoretical analysis and solution. When considering mass transfer problems, it is assumed that hydrodynamics affects mass transfer, and diffusion flows have little effect on the flow. At the same time, such an approach to the study of mass transfer problems is effective, taking into account complex hydrodynamic conditions, both in laminar and turbulent flow [11-18].

Mass transfer by convection and diffusion. Mass transfer between the two phases (binary systems) is carried out by diffusion and convective means, although it is important to note the influence of the effects of thermodiffusion, barodiffusion and a number of other transfers associated with hydrodynamic flow. At the same time, an important role in the transfer of mass is played by the hydrodynamic flow, which determines the nature of diffusion and convective transfers of matter. In heterogeneous processes, mass transfer is carried out in an interphase layer formed between different phases. If physical and chemical transformations occur in the soil moisture or in the volume of the interfacial layer, then the distribution of concentration in coordinate and time depends on the rate of these transformations.

Thus, mass transfer caused by a change in concentration is carried out in two ways:

- Convective, due to macroscopic motion of the medium. In this case, the composition of each moving volume does not change, but at each point in space, the concentration of the component located in this place of the liquid will change.
- By diffusion, which results in a change in the concentration of the substance of the mixture by molecular and turbulent transfer.

Equalizing the concentration by directly changing the composition of the liquid is called diffusion. Diffusion is an irreversible process (dissipative system) and is one of the sources of energy dissipation in a heterogeneous mixture. Characteristic of the diffusion process, the diffusion coefficient determines the diffusion flow in the presence of a concentration gradient. The diffusion flow caused by the temperature and pressure gradient is determined, respectively, by the coefficient of thermodiffusion and bar diffusion.

The rate of transition of a substance from one phase to another is proportional to the degree of deviation from equilibrium, which can be expressed as the difference in concentrations of the working concentration of a substance in one of the phases of the equilibrium concentration of a given substance in it. This concentration difference $\Delta C=C-C^*$ is the driving force of the mass transfer process. The amount of transferred substance from one phase to another per unit of time is proportional to the concentration difference at the interface of the phases and in the volume of the flow.

The driving force of the process. The driving force of the transfer of a component from one phase to another is expressed in terms of the difference in the chemical potentials of this component in the interacting phases. However, in practice, the driving force of mass transfer is usually expressed in terms of a concentration gradient, which greatly simplifies the relationship between the speed of the process and the composition of the moving flows. At the same time, the driving force of the process is the main factor determining the amount of transferred substance from one phase to another. In general, the value of the driving force changes with the change of concentrations in the flow. For practical calculations, it is convenient to use the average driving force.

Convective mass transfer. Convective mass transfer is the most common, but also a complex type of transfer, and therefore, there are great difficulties in determining the mass transfer coefficients β.

When the process of convective mass transfer is considered by the fluid flow, two directions of motion of matter are distinguished, where the first direction coincides with the gravitational direction from top to bottom, and the second is perpendicular to the mass transfer flow. In this case, the main amount of convective mass transfer is carried out by the first longitudinal direction of the flow, and diffusion transfer occurs in the transverse direction. The transition of a substance from a solid phase to a liquid occurs mainly during transverse diffusion mass transfer. Thus, the concentration of the transported mass is leveled by turbulent mixing along the cross section. In this case, a much larger amount of mass occurs compared to the molecular diffusion of D_T, but the particle cannot reach the wall, since a thin laminar boundary layer is formed near it, where the transfer is carried out mainly by molecular diffusion.

Therefore, within the viscous boundary layer, the equation $j =- DgradC$ includes the molecular diffusion coefficient D. The mass transfer coefficient in complex processes is determined using a series of simplified theoretical models of substance transfer.

5 Conclusion

- The regularity of mass transfer by interacting currents of ground and surface waters has been developed, taking into account the migration of moisture in the humidification zone and the general conditions of coupling of ground and surface waters.
- The criterion of the marginal transition in the parameters of the interface of groundwater and infiltration waters is established.
- A stochastic model of the process of changing the parameters of the infiltration flow-the filtration rate and pressure of a heterogeneous mixture in the humidification zone during furrow irrigation of agricultural crops has been developed.

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