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MODELING OF MOVING BOUNDARIES AND INTERFACES IN REAL WATER SYSTEMS

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A mathematical model of a conjugate description of aqueous media with moving phase interfaces of different types is presented.

The urgent problem of creation of reliable evolution models of various environmental situations, in particular, in real water systems, raises problems of conjugate description of nonhomogeneous multiphase systems with moving continuous (extended) or disperse interfaces. If the first type of phase interface requires, for adequate description, allowance for local dynamic and heat and mass transfer processes in conjugate phases (including the transition phase proper), then in modeling the dynamics of disperse phase interfaces the problem of coordination of local and integral (ensemble) effects arises. The latter can be taken into account by introduction of the corresponding probability (thermodynamically equilibrium) or calculational distribution functions into mathematical models of real physical systems. This approach seems to be quite substantiated.

Systems of conservation equations for individual phases form the basis of the complex model of real aqueous systems presented in this work. These systems are solved numerically simultaneously with equations describing processes of interphase transfer and the dynamics of phase interfaces, including the processes of coagulation and decomposition, surface waves, capillary effects and wetting of a solid surface by a liquid.

In general form the systems of conservation equations for each phase considered have the form [1-3]

$$\frac{\partial \rho W_i}{\partial x_i} = 0 ; \tag{1}$$

$$\frac{\partial W_i}{\partial t} + W_j \frac{\partial W_i}{\partial x_j} = -\frac{1}{\rho}\frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j}\left(\nu \frac{\partial W_i}{\partial x_j} - \overline{W_i' W_j'}\right) ; \tag{2}$$

$$\frac{\partial T}{\partial t} + W_j \frac{\partial T}{\partial x_j} = \frac{\partial}{\partial x_j}\left(a_{\text{eff}} \frac{\partial T}{\partial x_j}\right) , \tag{3}$$

where in the k-ε approximation the second-order models are

$$-\overline{W_i' W_j'} = \nu_{\text{eff}}\left(\frac{\partial W_i}{\partial x_j} + \frac{\partial W_j}{\partial x_i}\right) - \frac{2}{3}\delta_{ij} K ; \tag{4}$$

$$\frac{\partial K}{\partial t} + W_j \frac{\partial K}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\frac{\nu_{\text{eff}}}{\sigma_k}\right)\frac{\partial K}{\partial x_j} + \nu_t \left(\frac{\partial \overline{W}_i}{\partial x_j}\right)^2 - \varepsilon ; \tag{5}$$

$$\frac{\partial \varepsilon}{\partial t} + W_j \frac{\partial \varepsilon}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\frac{\nu_{\text{eff}}}{\sigma_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_j} + C_{\varepsilon 1}\frac{\varepsilon}{K}\nu_t \left(\frac{\partial \overline{W}_i}{\partial x_j}\right)^2 - C_{\varepsilon 2}\frac{\varepsilon^2}{K} ; \tag{6}$$

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$$\nu_{\text{eff}} = \nu_{\text{lam}} + \nu_t ; \quad \nu_t = F_\mu C_\mu \frac{K^2}{\varepsilon} ;$$

$$\sigma_k = 1.0 ; \quad \sigma_\varepsilon = 1.3 ; \quad C_\mu = 0.09 ; \quad C_{\varepsilon_1} = 1.44 ;$$

$$F_\mu = \exp(-2.51/(1 + 0.02\text{Re}_t)) ; \quad \text{Re}_t = \frac{K^2}{\nu\varepsilon} ;$$

$$C_{\varepsilon_2} = 2(1 - 0.3\exp(-\text{Re}_t^2)) ; \quad a_{\text{eff}} = \frac{\nu_{\text{lam}}}{\text{Pr}_{\text{lam}}} + \frac{\nu_t}{\text{Pr}_t} ; \quad \text{Pr}_t \simeq 1 ; \tag{7}$$

$$\Delta P = \sigma \left(\pm \frac{1}{R_1} \pm \frac{1}{R_2} \right) ; \tag{8}$$

$$\Delta\sigma = \sigma_{g\,\text{liq}} (\cos\theta - \cos\theta) ; \tag{9}$$

a is the thermal diffusivity; K is the turbulent kinetic energy; P is the pressure; R is the curvature radius; t is the time; W is the velocity; x is the coordinate; Pr is the Prandtl number; ε is the rate of dissipation of turbulent kinetic energy; σ is the coefficient of surface tension; ν is the coefficient of kinematic viscosity; ρ is the density; θ is the wetting angle at the place of contact of three phases. Subscripts: i, j are the coordinates along the axes x_i, x_j; eff is the effective value; lam, t are laminar and turbulent regimes; 0 is the equilibrium value; g, liq are gas, liquid.

To allow for thermal convection, the term accounting for gravitation is written in the Boussinesq approximation

$$(\rho g) \to \bar{\rho}(1 - \beta(T - \bar{T})) , \tag{10}$$

where β is the coefficient of thermal expansion.

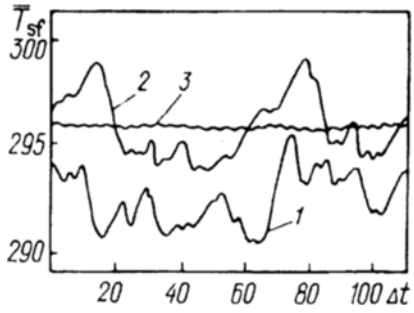
This model, as applied to the description of different physical systems with moving phase interfaces, was realized numerically by the method of splitting over individual processes [4], which makes it possible to allow more completely for the physical representations of the individual processes under consideration that are included in the mathematical model. The method of marking was used to follow the dynamics of the phase interface [5]; here the curvature radii and the wetting angle were determined from an analysis of marker values in the nearest cells.

It should be noted that without substantiated simplifications it is rather difficult and in some problems ineffective to use systems of conservation equations of the type (1)-(10) simultaneously with a complete set of initial and boundary conditions to describe real aqueous systems. Each real situation requires preliminary analysis of symmetry conditions and the ratio of macro- and microprocesses in the regions adjacent to a phase interface.

Thus, in modeling processes of transfer through the surface of reservoirs-coolers (RC) we solved the problem of conjugate description of a quasistationary convective-diffusive layer and a nonstationary gas–liquid skin-layer with possible intensification by bubbling [6-9]. In this case the assumptions of cylindrical symmetry and a laminar character for microflows in the computational regions were introduced. Moreover, in addition to the conditions of conjugation and Marangoni instability on the phase interface the total heat flux associated with both convective and radiative components and the phase transition (evaporation) was taken into account. We determined the latter within the framework of a diffusion layer in the form

$$q_{\text{ev}} = \frac{\text{Nu}}{l^*} D^{\tilde{}} \rho_{\text{mx}} \kappa \ln \left\{ \frac{(m_{\text{mx}}(1 - C^{\tilde{}}))_\infty}{(m_{\text{mx}}(1 - C^{\tilde{}}))_{\text{sf}}} \right\} , \tag{11}$$

where $(m_{\text{mx}})_{\text{sf},\infty}$ is the molecular mass of the vapor–gas mixture on the phase interface and at a distance from it; $C^{\tilde{}}$ is the vapor concentration; κ is the latent heat of evaporation; $D^{\tilde{}}$ is the coefficient of vapor diffusion; l^* is a characteristic dimension.



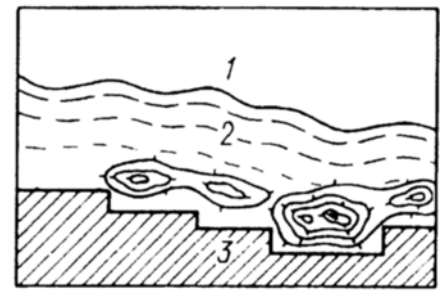


Fig. 1. Averaged temperatures of an RC surface: 1) without disturbances; 2) "weak" bubbling; 3) "strong" bubbling. T_{sf}, K; Δt, sec.

Fig. 2. Change in the concentrations of impurity substances in the near-bottom region of a transport flow: 1) outer air medium; 2) transport flow; 3) underlying ground.

The legitimacy of this approach is established by the agreement between the results of numerical simulation, laboratory experiments, and natural observation. In fact, in a near-surface skin-layer, zones of local supercooling are formed that are characterized by substantial nonstationarity. Figure 1, where temperature profiles averaged over the phase interface are presented for regimes of RC operation with and without intensification by bubbling, can serve as the illustration of this process.

On the other hand, in modeling running water systems [10, 11] that contain impurities that are soluble and insoluble in water, it becomes important to allow for turbulent characteristics of the transport flow, the shape of the phase interface at the "transport flow–solid bottom" boundary and local processes of transfer in the near-bottom region. Here, the mathematical model (1)-(10) is considered in full volume and, besides, is supplemented by the concentration equation for an admixture phase of the form

$$\frac{\partial C_i}{\partial t} + W_{ji}\frac{\partial C_i}{\partial x_j} = \frac{\partial}{\partial x_j}\left(D_i\frac{\partial C_i}{\partial x_j}\right) + J_i, \tag{12}$$

where W_{ji} is the velocity of particles obtained from the solution of equations of motion of particles having different dimensions; J_i is the mass source; C_i is the concentration of particles.

As results of numerical investigations showed, the presence of secondary flows can change substantially the concentration profiles in the transport flow and result in "dynamic" localization of impurities inside near-bottom macrovortices (Fig. 2).

The processes of suspension and sedimentation of solids are also a determining factor of mass transfer in the near-bottom region. The mechanism of the transition of particles to a movable state has a rather complex probability character and is caused by a number of mutually dependent processes. In this paper, the Einstein probability relations form the basis for the procedure of calculation of mass transfer in the near-bottom region. In this case the equilibrium value of the particle flow in the near-bottom region is determined by the equation

$$q_s' = q_s - q_{sus} = \frac{q_s^*(C_{bot} - C_{fl})}{1 - \varepsilon}, \tag{13}$$

where q_{sus} and q_s are the particle flows in suspension and sedimentation; C_{bot} and C_{fl} are the concentrations of particles on the bottom and in the flow; ε is the bottom porosity; q_s^* is the coefficient of generalized surface conductivity of the particles, which characterizes the stability of bottom deposits.

The adequacy of these presentations to really observed physical processes is ullustrated by Fig. 3, where the transformation of the portion of a bottom relief caused by the mobility of bottom deposits is presented.

The description of local simultaneous interactions of all three phases (liquid, gas, and solid) should be referred to a special class of model problems arising in considering aqueous media with moving phase interfaces [12]. In precisely these cases such characteristics of liquid media as wetting and surface tension manifest themselves

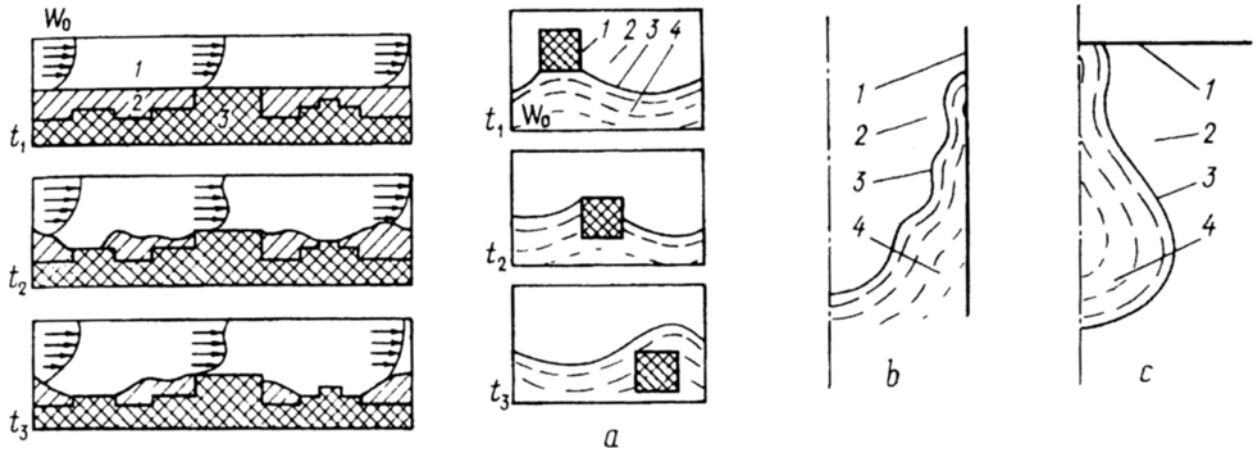


Fig. 3. Transformation of a portion of the bottom relief in a transport flow: 1) transport flow; 2) near-bottom pumps; 3) motionless underlying ground.

Fig. 4. Modeling of three-phase interactions in a transport flow: a) transfer of a solid impurity through the surface of the transport flow; b) liquid permeability in the porous structure of the bottom; c) transfer of liquid to underground horizons: 1) solid surface, 2) gaseous medium, 3) gas–liquid interface, 4) aqueous medium.

appreciably. Figure 4, where typical model situations of the interaction of media of different phase compositions are presented, can serve as an illustration of the efficiency of the application of a complex model of aqueous media (with the corresponding boundary and initial conditions) to a number of model situations associated with transfer of an impurity substance by a transport flow.

By and large, as results of numerical experiments and their comparison with laboratory and natural observations showed, the suggested complex model is characterized by universality, validity sufficient for the given class of problems, and the possibility of numerical implementation on personal computers. The latter, it seems to us, is especially important for its practical use.

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